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# Asymptotic Spectral Analysis and Tunnelling for a class of Difference Operators

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# Contents

# CHAPTER 1

# Introduction

The central topic of this thesis is the investigation of a rather general class of families of difference operators $H_\varepsilon$, parameterized by a small parameter $\varepsilon$, $\varepsilon > 0$. They act on $\ell^2((\varepsilon\mathbb{Z})^d)$, the square summable functions on the lattice $(\varepsilon\mathbb{Z})^d$.

We are going to analyze the asymptotic behavior as $\varepsilon \to 0$ of the spectra and the eigenfunctions of these operators.

Inspired by the paper of Helffer and Sjöstrand [**33**], we give sharp estimates for interactions between different "wells" (minima) of the potential energy, in particular for the discrete tunnelling effect.

While the continuous case has been exhaustively explored (see for example Helffer-Sjöstrand [**33**], [**34**], [**35**], [**36**]), there exist very few results in the discrete setting (see Helffer-Sjöstrand [**37**], [**38**], [**39**] for the one dimensional Harper equation) and none, known to the author, in the generality presented here.

For a multiple well potential energy, the interaction between different wells is analyzed by comparing the eigenvalues of local operators at the wells with the eigenvalues of the original operator. Eigenvalues of the direct sum of the local operators, which are degenerate, correspond to eigenvalues of the original operator $H_\varepsilon$, which are exponentially close to each other. Thus we can say that the coupling of the wells induces a splitting of degenerate eigenvalues.

Furthermore, taking the matrix-representation of $H_\varepsilon$ with respect to the basis of eigenfunctions of the decoupled operators located at the wells, the non-diagonal terms describe the interaction and thus the tunnelling between these wells.

## 1.1. Definition of the Operator Class

We are going to analyze a discrete Hamilton operator $H_\varepsilon$, acting on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, the space of square summable functions on the $d$-dimensional $\varepsilon$-scaled lattice $(\varepsilon\mathbb{Z})^d$. The lattice parameter $\varepsilon > 0$ takes the role of a small parameter, analogously to the Planck constant in Schrödinger operators in the semi-classical setting. Thus we always assume that $\varepsilon$ is small and construct expansions with respect to $\varepsilon$ in the limit $\varepsilon \to 0$.

The operator $H_\varepsilon$ is given by

$$H_\varepsilon = (T_\varepsilon + V_\varepsilon) \qquad \text{where} \tag{1.1}$$
$$T_\varepsilon = \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\tau_\gamma$$

and $V_\varepsilon$ is a multiplication operator. The operator $\tau_\gamma$ denotes a translation, i.e. for $x, \gamma \in (\varepsilon\mathbb{Z})^d$

$$\tau_\gamma u(x) = u(x+\gamma)\ .$$

As a function of the lattice point $x$, $a_\gamma$ is assumed to be slowly varying, i.e., $a_\gamma$ together with all its derivatives should be bounded uniformly with respect to $\gamma$. The summand $a_0\tau_0$, which is in fact a multiplication operator, is chosen such that $T_\varepsilon$ can be interpreted as generalized kinetic energy in the sense of Definition 2.4 (in particular it has to be positive).

The kinetic energy of the usual Schrödinger operator is given by $-\hbar^2\Delta$, where the Planck constant $\hbar$ plays the role of the small parameter and is in our setting replaced by the lattice parameter $\varepsilon$. In contrast to this, the discrete kinetic energy $T_\varepsilon$ is not a differential operator of second order (not even polynomial as can be seen by the symbol given in (1.2)). Furthermore, it is of course not local, since the value of $T_\varepsilon u(x)$ depends not only on a neighborhood of $x$, but on all lattice points $x+\gamma$ with $a_\gamma(x) \neq 0$. In addition it is allowed to depend explicitly on the configuration space coordinates $x$ (this is also the case for the usual Schrödinger operator on a manifold, where the Laplace operator depends via the metric on $x$). A simple example for $T_\varepsilon$ is given by the discrete Laplace operator, i.e., for $a_0 = 2d$, $a_\gamma = -1$ for $\gamma = \pm\varepsilon e_i$ and $a_\gamma = 0$ otherwise.

The potential energy $V_\varepsilon$, which is a multiplication operator, is assumed to be the restriction to the lattice $(\varepsilon\mathbb{Z})^d$ of a function $\widehat{V}_\varepsilon \in \mathscr{C}^\infty\left(\mathbb{R}^d\right)$.

We assume that $\widehat{V}_\varepsilon$ can for any $N \in \mathbb{N}$ be written as asymptotic series

$$\widehat{V}_\varepsilon = V_0 + \sum_{k=1}^{N} \varepsilon^k V_k + R_N \ ,$$

where $R_N$ is of order $\varepsilon^{N+1}$ uniformly in any compact set and $V_k, k = 0, 1, \dots, N$ is independent of $\varepsilon$. In addition we assume that there exsists a constant $c > 0$ such that $V_\varepsilon \geq c > 0$ for all $\varepsilon \in ]0, \varepsilon_0]$ and that the leading term $V_0$ takes its minimal value only at a finite number of points – the potential wells – and these critical points are non-degenerate (for details see Hypothesis 3.1).

Near these wells of $V_0$, the potential can therefore be approximated by the potential of an harmonic oscillator.

We define an $\varepsilon$-dependent Fourier transform $\mathscr{F}_\varepsilon$, which is adapted to the discrete setting and maps lattice functions on $2\pi$-periodic functions and vice versa (2.3) by means of a Fourier series. This allows us to introduce in Appendix B a symbolic calculus and to derive microlocal estimates. The symbol $t$ associated to the kinetic energy $T_\varepsilon$ and the symbol $h$ associated to the Hamilton operator $H_\varepsilon$, respectively, are then given by

$$t(x,\xi) = \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x) e^{-\frac{i}{\varepsilon}\gamma\xi} \ , \quad h(x,\xi) = t(x,\xi) + V_\varepsilon(x)\, , \qquad x \in \mathbb{R}^d,\, \xi \in \mathbb{T}^d\, , \tag{1.2}$$

where $\mathbb{T}^d$ denotes the $d$-dimensional $2\pi$-torus. For any $x$, the coefficients $a_\gamma$ are the Fourier coefficients of the periodic function $\xi \mapsto t(x,\xi)$. It is shown that the regularity of $t$ is strongly related to the decay of $a_\gamma$ with respect to $\gamma$ (Lemmata A.1, A.2 and A.3). In the several parts of this work, the regularity we have to assume for $t$ is different, but by Hypothesis 2.7, the coefficients $a_\gamma$ are assumed to decrease at least polynomially. From Section 3 on, the $a_\gamma$ decay even exponentially (Hypothesis 3.1) with respect to $\gamma$, thus the amplitude of translations to distant points becomes exponentially small. Although the kinetic energy is non-local, $T_\varepsilon$ can by this property of $a_\gamma$ be viewed as weakly local.

One important tool in the various parts of this work lies in the approximation of $T_\varepsilon$ by the kinetic energy of a usual Schrödinger operator. With respect to the usual symbolic calculus and quantization procedure on $\mathbb{R}^d$ including the Planck constant $h$ as small parameter, which is introduced for example in Dimassi-Sjöstrand [**16**] and Robert [**50**], the symbol of $-\hbar^2\Delta$ is given by $\xi^2$. Localization of $t$ in phase space at a microlocal minimum $x = x_j$ and $\xi = 0$ thus leads to the assumption that the expansion of $t$ with respect to $\xi$ at a point $(x_j, 0)$ starts with a quadratic term in $\xi$ (Definition 2.4), which gives some further conditions for the coefficients $a_\gamma$ (Remark 2.5(d)).

We can summarize the assumptions on the Hamilton operator $H_\varepsilon$ by saying that it should be a translation operator with underlying potential, such that the leading order term in $\varepsilon$ for $x$ near a potential well and $\xi$ small is equal to an harmonic oscillator.

## 1.2. General Strategy and Main Results

The interaction between neighboring potential wells leads by means of the tunnelling effect to the fact that the eigenvalues and eigenfunctions are different from those of an operator with decoupled wells, which is realized by the direct sum of "Dirichlet-operators" situated at the several wells. Since the interaction is small, it can be treated as a perturbation of the decoupled system.

Thus the idea is to approximate the eigenfunctions of the original Hamilton operator $H_\varepsilon$ with respect to a fixed spectral interval by the eigenfunctions of the several Dirichlet operators situated at the different wells and to give a representation of $H_\varepsilon$ with respect to a basis of Dirichlet-eigenfunctions. The non-diagonal part of this matrix-representation can be interpreted as a current, describing the tunnelling between the different wells.

In a second step, these Dirichlet eigenfunctions are approximated by WKB-expansions at the wells using the eigenfunctions of the associated harmonic oscillators. This allows us to compute explicit expansions for the elements of the interaction matrix and to obtain sharp estimates for the leading order term.

We start the analysis of the spectrum and the eigenfunctions of discrete Hamilton operators in Chapter 2 by a stability result for the low lying spectrum. It is shown in Theorem 2.10 that the first $n$ eigenvalues of $H_\varepsilon$ are in the "continuum limit" $\varepsilon \to 0$ equal to the first $n$ eigenvalues of the direct sum of harmonic oscillators on $\mathbb{R}^d$ located at the several wells. Our proof is close to analogous estimates by Simon [**55**] (see also [**15**]) for Schrödinger operators. The main difficulty is the step from a discrete operator $H_\varepsilon$ on $\ell^2((\varepsilon\mathbb{Z})^d)$ to the associated operator $\widehat{H}$ on $\mathscr{L}^2(\mathbb{R}^d)$. A more technical difficulty is the fact that contrary to the situation discussed by Simon in [**55**], the kinetic energy term $T_\varepsilon$ is allowed to depend on the lattice point. The fact that $t$ is a function of $x$ and $\xi$ forces us to use microlocal estimates and thus to build up a full symbolic calculus, which is adapted to the discrete setting, allowing us to give a discrete version of the Calderon-Vaillancourt Theorem and of the Persson Theorem, which are essential for the proof of Theorem 2.10.

The quite rough result of Chapter 2 leads to the conjecture that the eigenfunctions associated to the first eigenvalues are localized in a small neighborhood of the union of the different wells. Therefore we restrict the system in Chapter 3 to a neighborhood of one well. Motivated by the wish to find approximate eigenfunctions, which decrease exponentially fast, we assume that the symbol $t$ of the kinetic energy has an analytic continuation to the complex plane with respect to $\xi$. Then by use of WKB-methods and conjugation with a suitable exponential weight (dilation), we construct asymptotic expansions with respect to $\varepsilon$ and $x$ for the quasi-modes and for the eigenvalues of $H_\varepsilon$. The quasi-modes decay exponentially fast with a real-valued rate function $\varphi$ solving the generalized eikonal equation

$$t(x, i\nabla\varphi(x)) + V_0(x) = 0 \tag{1.3}$$

near the well. One of the main difficulties in this chapter is that the symbol $t$ of the kinetic energy is periodic with respect to the momentum variable $\xi$.

In order to find a rate function describing the exponential behavior of the eigenfunctions away from the critical points, i.e., an extension of $\varphi$ outside of the neighborhood of the well, we introduce a Finsler distance $d$ on $\mathbb{R}^d$ in Chapter 4. Similar to the Jacobi metric (or the Agmon metric respectively) for Schrödinger operators, this distance function is adapted to the Hamilton operator in the sense that the base integral curves of the Hamiltonian vector field are geodesics with respect to the metric associated to $d$. Additional assumptions for $t$ are made in this chapter in order to ensure that the function $\tilde{h}_0(x,\xi) := -t(x, i\xi) - V_0(x)$, obtained by rotating the leading order term of $h$ in the complex plane, is a hyper-regular Hamilton function in the sense of Abraham-Marsden [**2**].

The distance function is derived by a variational process, inspired by the Maupertuis principle in classical mechanics. More specifically, we define for fixed energy $E$ the length of a path $\gamma$ in $\mathbb{R}^d$ as an integral over the canonical pairing $\xi \cdot \dot{\gamma}$. The momentum $\xi$ is chosen as the Legendre transform of $\dot{\gamma}$ multiplied with a scaling factor, such that $h(\gamma(t), \xi(t)) = E$ for all $t$, i.e., we force the path to lie within an energy shell. The distance between two points is then defined as the infimum of the length of all paths between them.

The fact that the adapted metric for a Schrödinger operator is euclidian, is strongly related to the property of the kinetic energy to be of second order in the momentum variable $\xi$. The symbol of the kinetic energy in our setting depends exponentially of $\xi$ (see (1.2)). One of the main results of this chapter is to show that it is nevertheless possible to define an adapted metric and that this metric turns out to be Finslerian (thus the metric tensor depends not only on the base point on the manifold, but also on the tangent vector, i.e., the velocity).

The aim of Chapter 5 is to show that the Finsler distance to a fixed well of the potential energy is actually the correct rate function to describe the exponential decay of the eigenfunctions of $H_\varepsilon$ in the neighborhood of this well. In Theorem 5.6 and 5.4 we give estimates for the $\ell^2$-norm of the eigenfunctions of a Dirichlet operator at a single well. In particular we show that the $\ell^2$-norm of these eigenfunctions multiplied with $e^{-\frac{d(x,x_j)}{\varepsilon}}$ is at most of order $\varepsilon^{-N_0}$ for some $N_0 \in \mathbb{N}$.

In Chapter 6 we return to the original setting of several wells and investigate the interaction between them. In order to analyze the eigenspace of $H_\varepsilon$ with respect to a given spectral interval $I_\varepsilon$, we proceed by methods similar to those used in semi-classical analysis.

Let $S_0$ denote the (Finsler) distance between the two closest wells. We start by showing in Theorem 6.9 that up to an error of order $e^{-\frac{S_0}{\varepsilon}}$, the eigenspace of $H_\varepsilon$ with respect to $I_\varepsilon$ can be approximated by the direct sum of the eigenspaces of Dirichlet operators near the various wells.

Then we refine the analysis of the error term by splitting off a part of quadratic order. We show in Theorem 6.13 that the Hamilton operator $H_\varepsilon$ restricted to the eigenspace with respect to the spectral interval $I_\varepsilon$ can, with respect to the basis of Dirichlet eigenfunctions, be written as the sum of a diagonal matrix, an interaction matrix given by the off-diagonal terms, which is of order $e^{-\frac{S_0}{\varepsilon}}$ and error terms of order $e^{-\frac{2S_0}{\varepsilon}}$. The interaction terms describe the tunnelling and can in first order be interpreted as a current between the wells.

In Theorem 6.33 we estimate the difference between the Dirichlet eigenfunctions and the approximate ones constructed in Chapter 3, where the phase function is replaced by the Finsler distance $d$. In the interaction matrix we then replace the (unknown) Dirichlet eigenfunctions by the approximate ones, which could be computed up to arbitrary high order in $\varepsilon$. This allows us to give in Proposition 6.35 and Theorem 6.37 expansions of the elements of the interaction matrix with respect to $\varepsilon$ and to derive in a particular setting in Theorem 6.38 refined estimates for the order of its magnitude.

## 1.3. Classification and Motivation

In quantum physics, the effect of tunnelling between two wells separated by a potential barrier is a well-known quantum phenomenon related to the description of the quantum state as a wave packet.

Although numerous experimental and technical applications of the tunnelling effect have been performed a long time ago, sharp theoretical results concerning the eigenvalues and eigenstates of the multi-well Schrödinger operator where not obtained until the 80's. In 1980, the one-dimensional double well potential was analyzed by Harrell [**27**] with WKB-methods. Subsequently there were approaches given by Combes-Duclos-Seiler [**13**] using the Krein-formula to analyze the difference of the spectra of the original operator with a Dirichlet version and in the case of more dimensions by Simon ([**55**],[**56**]) using large deviations. The finest results where obtained approximately at the same time by Helffer-Sjöstrand ([**33**],[**34**],[**35**],[**36**],[**29**]), where the interaction between several potential wells of a Schrödinger operator are analyzed in the semi-classical limit by use of WKB-expansions and pseudo-differential operators. The methods and the main approach of this thesis are in the spirit of the semi-classical analysis of Schrödinger operators used in these papers. It is already mentioned there that parts of the analysis remain valid in the case of a general pseudo-differential operator. Nevertheless, the strong relation between quasi-modes and the weighted norm estimates is not valid for differential operators of higher order, since the construction of the Finsler distance is missing.

On the other hand, the results obtained in this thesis can be seen as generalization and refinement of the analysis of the tunnelling effect of probabilistic operators on a lattice by means of probabilistic methods (see Bovier-Eckhoff-Gayrard-Klein [**11**]). In this paper, the special structure of probabilistic operators, described in (1.4), which we do not presume here, is a main ingredient of the analysis.

A treatment of statistical problems with semi-classical techniques is done by Helffer [**31**], using the Witten Laplacian or the analysis of transfer operators.

Nevertheless, little is done in the context of this thesis, i.e. of discrete Schrödinger operators on a lattice, and nothing with the present amount of generality.

From the methodological point of view, the main part of this thesis is inspired by the paper [**33**] by J. Sjöstrand and B. Helffer on Schrödinger operators with multiple well potential in the semi-classical limit (see also [**29**]). Although the operators we analyze are discrete in the sense that the kinetic part acts on a scaled lattice as translation operator, our assumptions are made in such a way that from a microlocal point of view, the multiple well Schrödinger operators analyzed in the papers mentioned above turn out to be the first order terms of our discrete operators with respect to micro-localization at the phase space minima $(x_j, 0)$. It should be mentioned that the symbols associated to lattice operators are defined by use of a Fourier series, which can be seen as Fourier transform relating the square summable lattice functions $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with the $2\pi$-periodic functions $\mathscr{L}\left(\mathbb{T}^d\right)$, where $\mathbb{T}^d$ denotes the $d$-dimensional torus. A different approach to pseudo-differential calculus on the torus is given in [**21**].

Therefore the interpretation of $H_\varepsilon$ as first order terms of Schrödinger operators with adapted potential still needs a transfer between the different kinds of symbols.

Based on these ideas, the first step of this thesis consists in tracing back $H_\varepsilon$ to a harmonic oscillator. This point is inspired by the theorem on the quasi-classical limit of the eigenvalues of a Schrödinger operator proven by B. Simon in [**55**] (see also [**15**]).

The method of constructing asymptotic solutions to the eigenvalue problem of a one-well Dirichlet version of $H_\varepsilon$ is inspired by a paper of Klein and Schwarz [**45**], where the FBI-transformation is avoided.

The following estimate on the decay properties of Dirichlet eigenfunctions are done in the spirit of the Agmon estimates for Schrödinger operators described in Agmon [**3**]. The Agmon distance, determining the rate of decay for Schrödinger eigenfunctions, must in our setting be replaced by a distance associated to a more general Finsler metric.

An overview on Finsler manifolds and metrics is given in Bao-Chern-Shen [**6**], Rund [**54**] and Abate-Patrizio [**1**], some applications are described in Asanov [**5**]. In the context of rate functions, a Finsler metric is introduced by Tintarev [**59**] to analyze short time asymptotics of the fundamental solutions of parabolic equations for a differential operator $A$ of even order $m > 2$ with real smooth coefficients. The principal symbol $a(x,\xi)$ of $A$ is assumed to be uniform elliptic, strongly convex with respect to $\xi$ and $\nabla_\xi a(x,\xi) \neq 0$ for all $\xi \in \mathbb{C}^d \setminus \{0\}$. For such an operator, the Finsler distance can be defined by $g(x,v) = m^{\frac{1}{m}}(\xi \cdot v)^{\frac{m-1}{m}}$, where $\xi$ denotes the Legendre transform of $v$. Then the Finsler distance is defined via variation of integration over this function along pathes between two points. Thus for $m = 2$ this Finsler distance is equal to the usual Agmon distance for Schrödinger operators. Again in the setting of higher order parabolic equations and heat kernels, Barbatis [**10**], [**9**], gives an equivalent definition of a Finsler metric. Under similar assumptions on the operator he introduces the set of Lipschitz-functions $\phi$, solving the equation $a(x, \nabla\phi(x)) \leq 1$ almost everywhere. Then the Finsler distance between two points $x$ and $y$ is defined to be the supremum over all such functions $\phi$ of the difference $\phi(x) - \phi(y)$. To the author´s knowledge, more general cases are not analyzed in the literature by use of a Finsler distance.

The last part of this work, dedicated to the interaction between several wells, is strongly influenced by the papers [**33**] of Helffer and Sjöstrand, concerning a Schrödinger operator which has a potential with a finite number of wells.

In the most general case, the translation operator analyzed in this work is localized only by means of the exponential decaying factor $a_\gamma$, thus translations to any point of the lattice are in principle allowed. In the Schrödinger case, the interaction matrix describing the tunnelling between two wells depends only on a hypersurface lying between these wells. Due to the non-locality, this is not the case for the translation operator in our discrete setting. Nevertheless in first order the values of the interaction matrix are determined by a small neighborhood of such a hypersurface and it can be interpreted as a physical current, since it is given by the derivative of the kinetic energy (compare Harrell [**27**] and Helffer-Sjöstrand [**33**]).

There are several fields in which the results of this work are applicable.

One motivation lies in problems connected with the theory of Markov chains. Given $\varepsilon > 0$, the relation between a Markov chain on $(\varepsilon\mathbb{Z})^d$ and a self adjoint operator on $\ell^2((\varepsilon\mathbb{Z})^d)$ is as follows. Defining a strictly positive probability measure $\mu$ on the $d$-dimensional lattice, we can consider a Markov chain determined by a probability matrix $P = (p_{xy})$, where $p_{xy}$ denotes the transition probability from the state $x$ to $y \in (\varepsilon\mathbb{Z})^d$. If the detailed balance condition holds, i.e. if $\mu_x p_{xy} = \mu_y p_{yx}$, the matrix $P$ induces a self adjoint diffusion operator on $\ell^2((\varepsilon\mathbb{Z})^d;\mu)$, the space of square summable functions with respect to the measure $\mu$, via

$$(1-P)u(x) = u(x) - \sum_{y\in(\varepsilon\mathbb{Z})^d} p_{xy}u(y)\ .$$

By conjugation with $\mu^{1/2}$, this yields a self adjoint Hamilton operator $H_\varepsilon := \mu^{\frac{1}{2}}(1-P)\mu^{-\frac{1}{2}}$ on $\ell^2((\varepsilon\mathbb{Z})^d)$ of the form (1.1), where $V_\varepsilon$ is assumed to be

$$V_\varepsilon(x) = \mu^{-1/2}(x)\left(T_\varepsilon\mu^{1/2}\right)(x)\ . \tag{1.4}$$

Thus the probabilistic operators generated by Markov chains or diffusion processes are examples for the kind of operators considered in this thesis. In particular the associated symbol $\tilde{h}_0$ is a hyper-regular Hamilton function on the cotangent bundle. But contrary to the quite general class of operators considered in this thesis, they obey the strong additional structure (1.4).

The theory of Markov chains can be applied in several fields of science.

A simple model for a statistical system with discrete scaled state space is the following. Consider a chain $s$ of particles with spin, more precisely $N$ undistinguishable particles in a fixed order, each of them being in one of two possible states $+1$ or $-1$ (“ spin up or down ”).

The probability for a particle to be, for example, in the state $+1$ depends on the state of the other particles and on the state of the environment, for example an external magnetic field. To the different states of the full chain $s$ we can associate macroscopic variables. An easy example is the magnetization $m$ defined as

$$m(s) = \frac{1}{N}\sum_{i=1}^{N} s_i\ ,$$

where $s_i$ denotes the state of the particle at position $i$, i.e., $s_i \in \{1,-1\}$. The minimal change of $m$, induced by one “spin flip”, i.e., the change of the state of one chain element, is scaled by $\varepsilon := \frac{1}{N}$. It is thus evident, that the space of the possible values of $d$ macroscopic variables can be modelled by the $\varepsilon$-scaled lattice $(\varepsilon\mathbb{Z})^d$ or a bounded subdomain.

There is a huge number of publications dealing with spin chains.

Further possible applications lie in the field of population dynamics, describing evolution processes as reproduction, selection and mutation (see Baake-Baake-Wagner [**8**], Baake-Baake-Bovier-Klein [**7**]).

## 1.4. Structure of this work

**1.4.1. Chapter 2.** As already mentioned, Chapter 2 is mainly concerned with the fact, that the spectrum of the discrete operator $H_\varepsilon$ on $\ell^2((\varepsilon\mathbb{Z})^d)$ is in the limit $\varepsilon \to 0$ asymptotically given by the spectrum of an adapted harmonic oscillator on $\mathscr{L}^2(\mathbb{R}^d)$. This can be considered as a generalized stability of the spectrum of the harmonic oscillator under a perturbation, since the perturbed and the unperturbed operator act on different spaces.

Chapter 2 starts with the setting and some basic definitions and notations, introducing the periodic kinetic energy function, inner product and Fourier transform on $\ell^2((\varepsilon\mathbb{Z})^d)$, which are used throughout the work. Furthermore the main assumptions for the Hamilton operator $H_\varepsilon$ are described in Hypothesis 2.7, postulating that near a phase space minimum $x = x_j$ and $\xi = 0$, the zero order term in $\varepsilon$ should behave like an adapted (slightly generalized) harmonic oscillator $H_0$.

Theorem 2.10 then states that for fixed $n \in \mathbb{N}$, the operator $H_\varepsilon$ has at least $n$ eigenvalues and the $n$-th eigenvalue of $H_\varepsilon$ is in the limit $\varepsilon \to 0$ equal to the $n$-th eigenvalue of $H_0$.

The proof splits into the two basic inequalities. For the first, we show that the expectation value of $H_0$ and $H_\varepsilon$ with respect to the eigenfunctions of $H_0$ and their restriction to the lattice, respectively, are equal modulo $O(\varepsilon^{\frac{6}{5}})$. Since $H_\varepsilon$ and $H_0$ are not acting on the same space, we have to perform the transfer between the different scalar products. In order to use the Rayleigh-Ritz-principle to get the first $n$ eigenvalues, we employ an analogue of Persson´s Theorem for the discrete setting with translation operator, which is proven in Section B.5 via the microlocal calculus introduced in Appendix B.

To prove the other inequality, it is necessary to introduce in Appendix B a symbolic calculus adapted to the discrete setting. In particular, we introduce a product of symbols which is related to the composition of the associated operators, give an expansion for this product and proof an analogue of the Calderon-Vaillancourt Theorem ([**12**]). Then the idea is to simultaneously localize $H_\varepsilon$ in $\varepsilon^{\frac{2}{5}}$-scaled neighborhoods of the phase space minima $(x_j, 0)$. The difference of the original and the localized operator can be estimated by determining the symbol class of the double commutator (in the sense of symbolic multiplication) of $t$ with the scaled cut-off functions. This allows us to reduce the operator not only to the zero order term in $\varepsilon$, but also to the first term in the Taylor expansions at these points, denoted by $H_j$. By the assumptions on $H_\varepsilon$, this is unitarily equivalent to a slightly generalized harmonic oscillator.

**1.4.2. Chapter 3.** The third chapter concerns the construction of formal asymptotic solutions of the Schrödinger problem for the "Dirichlet" version of $H_\varepsilon$ in a neighborhood $\Omega$ of one well $x_0$, i.e. for the operator $H_\varepsilon^\Omega := \mathbf{1}_\Omega\, H_\varepsilon\, \mathbf{1}_\Omega$. Here $\mathbf{1}_\Omega$ denotes the characteristic function on $\Omega$. The result of Chapter 2 suggests that the leading order term of the Dirichlet eigenfunctions behaves like the eigenfunctions of the appropriate harmonic oscillator, i.e. like Hermite polynomials in $\frac{x}{\sqrt{\varepsilon}}$, multiplied with an exponentially decreasing term. The rate of decrease is determined by a solution $\varphi$ of a generalized eikonal equation adapted to $H_\varepsilon$, which is given by

$$t(x, i\nabla\varphi(x)) + V_0(x) = 0\ . \tag{1.5}$$

The existence of $\varphi$ in a neighborhood of one well follows from the Stable Manifold Theorem. In addition to Hypothesis 2.7 in Chapter 2, we have to assume in Hypothesis 3.1 that the symbol $t$ of the kinetic energy is periodic, even and smooth in $\xi$. The main aim of this chapter is the construction of formal WKB-expansions for the eigenfunctions of the operator $\widehat{H}_\varepsilon$ on $\mathscr{L}^2(\mathbb{R}^d)$, where $\widehat{H}_\varepsilon u(x)$ is, for any $u \in \mathscr{L}^2(\mathbb{R}^d)$, given by the right hand side of (1.1). To this end, we define a dilation of $\widehat{H}_\varepsilon$ by means of the unitary transform $U_\varepsilon : \mathscr{L}^2(\mathbb{R}^d, dx) \to \mathscr{L}^2\left(\mathbb{R}^d, e^{-2\frac{\varphi(\sqrt{\varepsilon}y)}{\varepsilon}}dy\right)$ defined by $(U_\varepsilon(\varphi)f)(y) = \varepsilon^{\frac{d}{4}} e^{\frac{\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} f(\sqrt{\varepsilon}y)$. This means that we conjugate $H_\varepsilon$ with the expected exponential decrease factor $e^{-\frac{\varphi}{\varepsilon}}$ to take away the exponential behavior and pass to the variable $y = \frac{x}{\sqrt{\varepsilon}}$. Formal expansions with respect to $y$ allow us to treat eigenvalues, which are degenerate in the harmonic approximation.

The first step is the translation of the spectral problem for $H_\varepsilon$ into an algebraic problem for the formal Taylor expansion of $\widehat{G}_\varepsilon = \frac{1}{\varepsilon}U_\varepsilon(\varphi)H_\varepsilon U_\varepsilon^{-1}(\varphi)$, acting as symmetric operator on a space of formal power series in $y$. Given an eigenvalue $E_0$ of the harmonic part $G_0$, we define the associated spectral projection $\Pi$ of $G$ as contour integral of the residue $(G - E_0)^{-1}$ around $E_0$. Then on the range of $\Pi$ the spectral problem of $G$ is reduced to the diagonalization of a hermitian matrix over a field of Laurent series, leading by use of Hermite polynomials to formal asymptotic expansions for the eigenvalues and eigenfunctions. By a double Borel-procedure with respect both to $x$ and $\varepsilon$, we finally get approximate eigenfunctions and eigenvalues for $H_\varepsilon$, i.e., solutions of the spectral problem to arbitrary high polynomial order in $\varepsilon$ and $x$.

**1.4.3. Chapter 4.** In order to analyze the behavior of the Dirichlet eigenfunctions away from the wells, or more specifically their rate of decrease (which is done in Chapter 5), we have to find a notion of distance adapted to $H_\varepsilon$. This distance takes the role of the Agmon metric in the case of Schrödinger operators. This is done in Chapter 4.

In the first section of Chapter 4, we give general definitions and properties of a Finsler manifold and a Finsler metric. Furthermore some properties of Finsler distances are described. The aim of Section 4.2 is to construct a Finsler distance which is adapted to a hyper-regular Hamilton function $h$ on $\mathbb{R}^{2d}$ in the sense that its minimizing geodesics are the integral curves of the associated hamiltonian vector field $X_h$. Thus it describes the distance between two points under consideration of the energetic landscape determined by $h$ (Proposition 4.15). This is done by assigning a length to each $\mathscr{C}^2$-curve as curve integral over a slightly adapted version of the canonical pairing between moments and velocities. To ensure that the curve integral is independent of the parametrization of the curve, it is necessary to replace the original elements of the tangent bundle by their projection onto the energy shell for a fixed energy $E$. The distance between two points is then derived by a variational process as the infimum of the curve length taken over all $\mathscr{C}^2$-curves joining them.

In Section 4.3, it is shown (Proposition 4.18) that geodesics with respect to this Finsler metric are base integral curves of the associated hamiltonian vector field and vice versa. Since the phase space curve is fixed on the energy shell, this corresponds to the variational process leading to the Maupertuis principle in classical mechanics.

In Section 4.4, we apply the general constructions to the symbol $h_0$ of the zero order term of $H_\varepsilon$. We start with the additional assumptions that $a_\gamma \geq 0$ for $\gamma = 0$ and $a_\gamma \leq 0$ for $\gamma \neq 0$. Furthermore, we assume $\operatorname{span}\{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, a_\gamma < 0\} = \mathbb{R}^d$ and $\|a_\gamma e^{\frac{C|\gamma|}{\varepsilon}}\|_{\ell^2} \leq C$ uniformly in $x$.

Then the kinetic energy $t(x, -i\xi)$ is hyper-convex with respect to $\xi$, i.e., the second derivative is bounded from below by a positive constant, and thus hyper-regular (Proposition 4.12 and 4.22). This allows us to apply the results of the preceding sections to $h_0$ and thus to define a distance function $d$ adapted to $H_\varepsilon$. Then we show that the distance function $d^j(x) = d(x, x_j)$ to a fixed potential well $x_j$ satisfies the eikonal equation (1.5) in a neighborhood of this well and the eikonal inequality (4.80) everywhere.

**1.4.4. Chapter 5.** In Chapter 5 we prove weighted estimates for the $\ell^2$-norm of the eigenfunctions of a Dirichlet Hamiltonian $H_\varepsilon^{M_j}$, where $M_j$ is a neighborhood of the well $x_j$, which includes no other wells of $V_0$. We show, that the Finsler distance to a fixed well is the correct rate function, describing the exponential decrease of the Dirichlet eigenfunctions of this well. More precisely we show in Theorem 5.6, that if $v_j$ denotes an eigenfunction of the Dirichlet operator $H_\varepsilon^{M_j}$, then there exists a number $M_0 \in \mathbb{N}$ such that

$$\|e^{\frac{d^j}{\varepsilon}} v_j\|_{\ell^2(M_j)} = O\left(\varepsilon^{-M_0}\right) \ .$$

**1.4.5. Chapter 6.** Chapter 6 is concerned with the interaction between different wells of the potential energy. To be able to use the results for Dirichlet operators with one well derived in the preceding chapters, we consider Dirichlet operators on bounded regions $M_j$, each including exactly one well. We denote by $S_0$ the minimal Finsler distance between two wells. Then we show in Theorem 6.9, that for a fixed spectral interval the distance $\vec{\text{dist}}(E, F)$ between the direct sum of the Dirichlet eigenspaces $E$ and the exact eigenspace $F$ is for any $S < S_0$ of order $e^{-\frac{S}{\varepsilon}}$ (the non-symmetric distance between two Hilbert spaces is defined by $\vec{\text{dist}}(E, F) = \|\Pi_E - \Pi_E\Pi_F\|$, where $\Pi_E$ denotes the orthogonal projection on $E$). From this estimate it follows that the difference between associated eigenvalues is of the same order. In the next step we analyze the error term in more detail for $H_\varepsilon$ restricted to $F$, which is with respect to an appropriate orthonormal basis a finite symmetric matrix. We show in Theorem 6.13 that modulo a term of order $e^{-\frac{2S}{\varepsilon}}$, it is equal to a diagonal matrix with the Dirichlet eigenvalues on the diagonal plus the off-diagonal interaction matrix, which can be interpreted as a physical current, leading to the tunnelling between different wells. As an example we consider the case where the Dirichlet operators at two wells have exactly one eigenvalue in the chosen spectral interval.

In Section 6.4, we analyze the spectrum at a single well. At first it is shown that modulo $e^{-\frac{2S}{\varepsilon}}$, the spectrum is independent of the choice of $M_j$. Then we define the spectrum of the well as the collection of the spectra with respect to the different choices of $M_j$. If $r_j$ denotes the "sphere of influence" of the well $x_j$ with respect to a given eigenvalue $\lambda$ of $H_\varepsilon$, we show that the distance between the spectrum of $x_j$ and $\lambda$ is of order $e^{-\frac{2(r_j-\delta)}{\varepsilon}}$ for any $\delta > 0$.

In Section 6.5 we compare the exact Dirichlet eigenfunctions at the wells with the approximate eigenfunctions constructed in Chapter 3. It is shown in Theorem 6.33 that in $\ell^2$-norm the difference between a Dirichlet eigenfunction at a fixed well and the associated asymptotic expansion multiplied with the exponential weight $e^{\frac{d}{\varepsilon}}$ is of arbitrary high polynomial order in $\varepsilon$. This allows us to use the approximating eigenfunctions instead of the exact ones to compute the interaction matrix (Proposition 6.35). In the setting of only two wells, we give an expansion of the interaction matrix in terms of the Hermite polynomials used to construct the WKB-expansions for the Dirichlet operator (Theorem 6.37) and to derive an estimate for the leading order term.

**1.4.6. Appendix.** The appendix splits into part A and B. Appendix A includes some technical details, remarks and some basics as the notion of valuation. In Appendix B, an adapted version of the microlocal calculus is introduced and the necessary results are proven. After defining classes of $\varepsilon$-dependent pseudo-differential operators, the method of stationary phase is used to introduce the product in the symbolic calculus and to show that it reflects the composition of operators. This gives rise to some norm estimates for operators by use of estimates on the associated symbols via an adapted version of the Calderon-Vaillancourt Theorem. The proof follows the one given by Hwang [**28**] in the continuous setting. Furthermore a version of the Persson Theorem in the discrete setting is proven by use of the microlocal calculus. A crucial point is that a multiplication operator on the lattice with compact support is compact.

### 1.5. Open Questions related to this work

We want to mention briefly some fields to which one could proceed.

One point could be to investigate how far it is possible to follow the subsequent papers of Helffer and Sjöstrand ([**34**], [**35**], [**36**]). In particular, tunnelling through non-resonant wells is an interesting and difficult subject, which is relevant even in the case of simple probabilistic operators. It can be seen in the example of a discrete Schrödinger operator described in Section 2.3, that some of the minima of $V_0$ become saddle points (and thus non-resonant) by means of the first order term of the potential energy with respect to $\varepsilon$.

Furthermore one might try to find the leading order term of the interaction matrix analyzed in Section 6.6 in more general situations and in a more explicit form.

An interesting and direct application could be the transfer of the concept of Finsler functions constructed in this thesis to a broader class of differential operators, for example to elliptic operators of higher order. Furthermore we could compare these generalizations of our Finsler distance to the Finsler distance defined by Tintarev and Barbatis for higher order differential operators and analyze if these concepts lead to equivalent results.

Another interesting point is the applicability of the results obtained in this work to the theory of transfer operators and Witten-Laplace-operators in the context of statistical mechanics as discussed for example in Helffer [**31**].

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CHAPTER 2

# Stability of the spectrum

## 2.1. Notations and Preliminaries

**2.1.1. Norm, Scalar product and Fourier transform.** For $\varepsilon > 0$, we consider $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, the space of square summable functions on the $\varepsilon$-scaled lattice, with scalar product

$$\langle u\,,\,v\rangle_{\ell^2} := \sum_{x\in(\varepsilon\mathbb{Z})^d} \bar{u}(x)v(x), \qquad u,v\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)\ . \tag{2.1}$$

Denoting the $d$-dimensional $2\pi$-torus by $\mathbb{T}^d := \mathbb{R}^d/(2\pi)\mathbb{Z}^d$, we introduce the scalar product

$$\langle f\,,\,g\rangle_{\mathbb{T}} := \int_{[-\pi,\pi]^d} \bar{f}(\xi)g(\xi)\,d\xi, \qquad f,g\in\mathscr{L}^2(\mathbb{T}^d)\,, \tag{2.2}$$

where $\mathscr{L}^2(\mathbb{T}^d)$ denotes the space of square integrable functions on $\mathbb{T}^d$. We denote the associated norms by $\|\,.\,\|_{\ell^2}$ and $\|\,.\,\|_{\mathbb{T}}$.

The discrete Fourier transform $\mathscr{F}_\varepsilon : \mathscr{L}^2\left(\mathbb{T}^d\right)\to\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ is defined by

$$(\mathscr{F}_\varepsilon f)(x) := \frac{1}{\sqrt{2\pi}^d}\int_{[-\pi,\pi]^d} e^{-ix\cdot\frac{\xi}{\varepsilon}} f(\xi)\,d\xi\,, \qquad f\in\mathscr{L}^2(\mathbb{T}^d) \tag{2.3}$$

with inverse $\mathscr{F}_\varepsilon^{-1} : \ell^2\left((\varepsilon\mathbb{Z})^d\right)\to\mathscr{L}^2\left(\mathbb{T}^d\right)$,

$$(\mathscr{F}_\varepsilon^{-1} v)(\xi) := \frac{1}{\sqrt{2\pi}^d}\sum_{x\in(\varepsilon\mathbb{Z})^d} e^{ix\cdot\frac{\xi}{\varepsilon}} v(x), \qquad v\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)\,, \tag{2.4}$$

where $x\cdot y := \langle x\,,\,y\rangle := \sum_{j=1}^d x_j y_j$ denotes the usual scalar product in $\mathbb{R}^d$ or $(\varepsilon\mathbb{Z})^d$ and we will often suppress the dot when the meaning is clear from the context.

In other words, the Fourier transform defined in (2.3) and (2.4) satisfies the Fourier inversion formulae

$$(\mathscr{F}_\varepsilon\mathscr{F}_\varepsilon^{-1}u)(x) \;=\; u(x)\,, \qquad u\in\ell^2\left((\varepsilon\mathbb{Z})^d\right) \tag{2.5}$$

$$(\mathscr{F}_\varepsilon^{-1}\mathscr{F}_\varepsilon f)(\xi) \;=\; f(\xi)\,, \qquad f\in\mathscr{L}^2(\mathbb{T}^d) \tag{2.6}$$

Furthermore $\mathscr{F}_\varepsilon$ is an isometry, i.e.,

$$\langle v\,,\,u\rangle_{\ell^2} = \left\langle \mathscr{F}_\varepsilon^{-1}v\,,\,\mathscr{F}_\varepsilon^{-1}u\right\rangle_{\mathbb{T}}\,, \qquad u,v\in\ell^2\left((\varepsilon\mathbb{Z})^d\right) \tag{2.7}$$

$$\langle f\,,\,g\rangle_{\mathbb{T}} = \langle\mathscr{F}_\varepsilon f\,,\,\mathscr{F}_\varepsilon g\rangle_{\ell^2}\,, \qquad f,g\in\mathscr{L}^2(\mathbb{T}^d)\,. \tag{2.8}$$

The equations (2.5), (2.6) and (2.7) are shown in Appendix A.1, equation (2.8) is a direct consequence of (2.6) and (2.7).

We denote by $\langle f\,,\,g\rangle_{\mathscr{L}^2} := \int_{\mathbb{R}^d}\overline{f}(\xi)g(\xi)\,d\xi$ the scalar product on $\mathscr{L}^2(\mathbb{R}^d)$, the space of square integrable functions on $\mathbb{R}^d$, and we introduce on $\mathscr{L}^2(\mathbb{R}^d)$ the $\varepsilon$-scaled Fourier transform

$$(F_\varepsilon^{-1}f)(\xi) \;:=\; (\varepsilon\sqrt{2\pi})^{-d}\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}\xi\cdot x} f(x)\,dx \tag{2.9}$$

$$(F_\varepsilon u)(x) \;:=\; (\sqrt{2\pi})^{-d}\int_{\mathbb{R}^d} e^{-\frac{i}{\varepsilon}\xi\cdot x}u(\xi)\,d\xi\,,$$

where compared to the usual Fourier transform the roles of $x$ and $\xi$ are interchanged. We notice that for any $f,g\in\mathscr{L}^2(\mathbb{R}^d)$

$$\left\langle F_\varepsilon^{-1}f\,|\,F_\varepsilon^{-1}g\right\rangle_{\mathscr{L}^2(\mathbb{R}^d_\xi)} = \varepsilon^{-d}\,\langle f\,|\,g\rangle_{\mathscr{L}^2(\mathbb{R}^d_x)} \tag{2.10}$$

We denote the set of the natural numbers with zero by $\mathbb{N}=\{0,1,2,\dots\}$ and the set of the natural numbers without zero by $\mathbb{N}^*=\{1,2,\dots\}$.

Furthermore $\mathcal{M}(n\times m,\mathbb{K})$ denotes the space of $n\times m$-matrices with elements in $\mathbb{K}$.
The domain of an operator $A$ is denoted by $\mathscr{D}(A)$.

**2.1.2. Pseudo-differential operators on the lattice** $(\varepsilon\mathbb{Z})^d$**.** We introduce the notion of symbol spaces including the small parameter $\varepsilon\in(0,1]$, where the symbols are allowed to include $\varepsilon$ not only directly but also as scaling parameter, as described in Dimassi-Sjöstrand [**16**]. Since the phase space is given by $(\varepsilon\mathbb{Z})^d\times\mathbb{T}^d$, the relation between the operators and their symbols is given by use of the discrete Fourier transformation defined in (2.4),(2.3).

For the general theory of microlocal analysis, we refer to Grigis-Sjöstrand [**24**], Robert [**50**] and Hörmander [**41**], where symbol spaces and spaces of associated pseudo-differential operators are introduced.

A symbolic calculus is introduced in Appendix B.

Definition 2.1. (a) *A function $m:\mathbb{R}^d\times\mathbb{T}^d\to[0,\infty)$ is called an order function, if there exist constants $C_0,N_1>0$, such that*

$$m(x,\xi)\leq C_0\langle x-y\rangle^{N_1}m(y,\eta)\,,\qquad x,y\in\mathbb{R}^d,\ \xi,\eta\in\mathbb{T}^d\,,$$

*where we used the notation $\langle x\rangle:=\sqrt{1+|x|^2}$.*

(b) *For an order function $m$ on $\mathbb{R}^d\times\mathbb{T}^d$, the symbol space $S(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ consists of all $a\in\mathscr{C}^\infty(\mathbb{R}^d\times\mathbb{T}^d)$, for which for all $\alpha,\beta\in\mathbb{N}^d$ there is a constant $C_{\alpha,\beta}$ such that*

$$|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)|\leq C_{\alpha,\beta}m(x,\xi)\,,\qquad x\in\mathbb{R}^d,\ \xi\in\mathbb{T}^d\,,$$

*where as usual $\partial_x^\alpha:=\partial_{x_1}^{\alpha_1}\dots\partial_{x_d}^{\alpha_d}$. We often write $S(m)$, if the underlying space is clear.*

(c) *The Fréchet-Semi-Norms of a symbol $a\in S(m)$ are defined as*

$$\|a\|_{\alpha,\beta}:=\sup_{x,\xi}\frac{|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)|}{m(x,\xi)}\,.$$

(d) *If the symbol $a(x,\xi;\varepsilon)$ depends on a small parameter $\varepsilon\in(0,1]$, $a$ is said to be in $S(m)$, if $a(\cdot\,;\varepsilon)$ is uniformly bounded in $S(m)$ for $\varepsilon$ varying in $(0,1]$. Let $S^k(m):=\varepsilon^kS(m)$ describe for $k\in\mathbb{R}$ the space of symbols of the form $\varepsilon^ka(x,\xi;\varepsilon)$ for $a\in S(m)$. For $\delta\in[0,1]$, the space $S^k_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ consists of functions $a(x,\xi;\varepsilon)$ on $\mathbb{R}^d\times\mathbb{T}^d\times(0,1]$, belonging to $S(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ for every fixed $\varepsilon$ and satisfying*

$$|\partial_x^\alpha\partial_\xi^\beta a(x,\xi;\varepsilon)|\leq C_{\alpha,\beta}m(x,\xi)\varepsilon^{k-\delta(|\alpha|+|\beta|)}\,,\quad x\in\mathbb{R}^d,\ \xi\in\mathbb{T}^d\,.$$

(e) *Let $a_j\in S^{k_j}_\delta(m), k_j\nearrow\infty$, then we write $a\sim\sum_{j=0}^\infty a_j$ if $a-\sum_{j=0}^N a_j\in S^{k_{N+1}}_\delta(m)$ for every $N\in\mathbb{N}$.*

(f) *A pseudo-differential operator $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a):\mathcal{K}\left((\varepsilon\mathbb{Z})^d\right)\longrightarrow\mathcal{K}'\left((\varepsilon\mathbb{Z})^d\right)$ is defined by*

$$\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)\,v(x):=(2\pi)^{-d}\sum_{y\in(\varepsilon\mathbb{Z})^d}\int_{[-\pi,\pi]^d}e^{\frac{i}{\varepsilon}(y-x)\xi}a(x,\xi;\varepsilon)v(y)\,d\xi\,,\tag{2.11}$$

*where $a\in S^k_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$,*

$$\mathcal{K}\left((\varepsilon\mathbb{Z})^d\right):=\{u:(\varepsilon\mathbb{Z})^d\to\mathbb{C}\mid u\text{ has compact support}\}\tag{2.12}$$

*and $\mathcal{K}'\left((\varepsilon\mathbb{Z})^d\right)$ denotes its dual with respect to $\langle\,.\,,\,.\,\rangle_{\ell^2}$.*

We give two important results concerning symbols and the associated operators, which are proven in Appendix B. The first (Lemma B.2) tells us, that the operator associated to a symbol via (2.11) can be extended continuously on a discrete version of a Schwartz-space.

Lemma 2.2. *Let $a\in S^0_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ and, for $\varepsilon>0$,*

$$s\left((\varepsilon\mathbb{Z})^d\right):=\left\{u:(\varepsilon\mathbb{Z})^d\to(\varepsilon\mathbb{Z})^d\;\Big|\;\|u\|_\alpha:=\sup_{x\in(\varepsilon\mathbb{Z})^d}\sum_{j=1}^d\left|x_j^{\alpha_j}u(x)\right|<\infty,\ \alpha\in\mathbb{N}^d\right\}.$$

*We consider on $s$ the natural topology $\tau$ associated to the family of semi-norms $\|\cdot\|_\alpha$.*
*Then the operator $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)$ associated to $a$ defined in* (2.11) *is continuous : $s\left((\varepsilon\mathbb{Z})^d\right)\longrightarrow s\left((\varepsilon\mathbb{Z})^d\right)$ with respect to $\tau$.*

If we consider only symbols, which are bounded (i.e. for which $m = \mathbf{1}$), we have an adapted version of the Calderon-Vaillancourt Theorem (Proposition B.8).

PROPOSITION 2.3. *Let $a \in S^r_\delta(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ with $0 \leq \delta \leq \frac{1}{2}$. Then there exists a constant $M > 0$ such that, for the associated operator $\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(a)$ given by (2.11) the estimate*

$$\| \operatorname{Op}^{\mathbb{T}^d}_\varepsilon(a)u\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq M\varepsilon^r \|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}$$

*holds for any $u \in s\left((\varepsilon\mathbb{Z})^d\right)$ and any $\varepsilon > 0$. $\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(a)$ can therefore be extended to a continuous operator: $\ell^2\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with $\|\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(a)\|_\infty \leq M\varepsilon^r$. Moreover one can choose $M$ depending only on a finite number of Frechet semi-norms of the symbol $a$.*

**2.1.3. Generalized Kinetic Energy.** As briefly described in the introduction, we assume the Hamilton operator $H_\varepsilon$ to consist of a multiplication operator, interpreted as potential energy, and a translation operator, taking the role of a (generalized) kinetic energy. Usually in classical mechanics the kinetic energy as phase space function is represented by $\xi^2$, where $\xi \in \mathbb{R}^d$ denotes the momentum variable. The associated operator derived by a quantization procedure is then given by $-\Delta$ (or $-\hbar^2\Delta$ in the case of an $\hbar$-scaled quantization).

We will now define what we mean by a (periodic) kinetic energy in a generalized sense.

DEFINITION 2.4. 1. *A real valued symbol $t \in S^0_0(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ is called a periodic kinetic energy function, if:*
   (a) *$t(x,\xi) \geq 0$ for all $x \in \mathbb{R}^d$ and $\xi \in \mathbb{T}^d$.*
   (b) *$t(x,\xi) = 0$ if and only if $\xi = 0$.*
   (c) *At $\xi = 0$, the function $t$ has for fixed $x \in \mathbb{R}^d$ an expansion*

$$t(x,\xi) = \langle \xi\, , \, B(x)\xi\rangle + O\left(|\xi|^3\right) \qquad \text{for } \ |\xi| \to 0\,, \tag{2.13}$$

   *where $B : \mathbb{R}^d \to \mathcal{M}(d \times d, \mathbb{R})$ is positive definite and symmetric.*
   (d) *For any $\varepsilon > 0$, the associated operator $\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(t)$ on the Hilbert space $\ell^2((\varepsilon\mathbb{Z})^d)$ with scalar product $\langle . \, , \, . \rangle_{\ell^2}$, defined by*

$$\mathcal{K} \ni v \mapsto \operatorname{Op}^{\mathbb{T}^d}_\varepsilon(t)v(x) := (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi} t(x,\xi)v(y)\, d\xi\,, \tag{2.14}$$

   *is positive and symmetric.*

   *We say that $t$ is the symbol associated to $\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(t)$. The operator $\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(t)$ is then called a discrete kinetic energy operator.*

2. *Let $S^0_0(m)(\mathbb{R}^{2d})$ denote the usual symbol space with respect to a small parameter as described in Appendix B.4.*

   *A real valued symbol $t \in S^0_0(m)\left(\mathbb{R}^{2d}\right)$, is called a kinetic energy function, if:*
   (a) *$t(x,\xi) \geq 0$ for all $x,\xi \in \mathbb{R}^d$.*
   (b) *$t(x,\xi) = 0$ if and only if $\xi = 0$.*
   (c) *At $\xi = 0$, the function $t$ has for fixed $x \in \mathbb{R}^d$ an expansion*

$$t(x,\xi) = \langle \xi\, , \, B(x)\xi\rangle + O\left(|\xi|^3\right) \qquad \text{for } \ |\xi| \to 0\,, \tag{2.15}$$

   *where $B : \mathbb{R}^d \to \mathcal{M}(d \times d, \mathbb{R})$ is positive definite and symmetric.*
   (d) *For any $\varepsilon > 0$, the associated operator $\operatorname{Op}_\varepsilon(t)$ on the Hilbert space $\mathscr{L}^2(\mathbb{R}^d)$ with the scalar product $\langle . \, , \, . \rangle_{\mathscr{L}^2}$, defined by*

$$\mathbb{C}^\infty_0(\mathbb{R}^d) \ni v \mapsto \operatorname{Op}_\varepsilon(t)v(x) := (\varepsilon 2\pi)^{-d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}(y-x)\xi} t(x,\xi)v(y)\, d\xi\, dx\,, \tag{2.16}$$

   *is positive and symmetric.*

   *The operator $\operatorname{Op}_\varepsilon(t)$ associated to a kinetic energy function is called a kinetic energy operator.*

3. *A pure multiplication operator is called a potential energy operator.*

REMARK 2.5. (a) *Since the periodic kinetic energy function $t$ is a function on $\mathbb{R}^d \times \mathbb{T}^d$, it can also be considered as a function on $\mathbb{R}^{2d}$, which is $2\pi$-periodic with respect to $\xi$. We denote this function also by $t$.*

*For any $x \in \mathbb{R}^d$ and $\varepsilon > 0$, the function $\xi \mapsto t(x,\xi)$ has a Fourier expansion*

$$t(x,\xi) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x) e^{-\frac{i}{\varepsilon}\gamma\cdot\xi} \, . \tag{2.17}$$

*There exists a function*

$$\tilde{a} : \mathbb{Z}^d \times \mathbb{R}^d \ni (y,x) \mapsto \tilde{a}_y(x) \in \mathbb{C} \, , \quad \textit{such that} \quad a_\gamma(x) = \tilde{a}_{\frac{\gamma}{\varepsilon}}(x) \, . \tag{2.18}$$

*Since $t \in \mathbb{C}^\infty\left(\mathbb{R}^d \times \mathbb{T}^d\right)$, it follows from Lemma A.1 in Appendix A.1 that for fixed $x \in \mathbb{R}^d$ there exists a constant $C > 0$ such that for all $n \in \mathbb{N}$ and for all $\varepsilon > 0$*

$$\| \, | \, . \, |^n a_.(x) \|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq C \, . \tag{2.19}$$

*Thus (2.17) converges for each fixed $x \in (\varepsilon\mathbb{Z})^d$.*

(b) *If $t \in S_0^0(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$, i.e., if $t$ is bounded, then the estimate (2.19) holds uniformly with respect to $x$. Furthermore it follows from Proposition 2.3 that in this case the associated operator $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(t)$ is bounded and can therefore be defined on the whole space $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$.*

(c) *The discrete kinetic energy operator acts as a translation operator on $u \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ via*

$$\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(t) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x)\tau_\gamma \tag{2.20}$$

*(see Appendix A.3), where $\tau_\gamma u(x) := u(x+\gamma)$.*

(d) *The comparison of the expansion (2.17) of $t(x,\xi)$ with the assumption (2.13) yields*

$$\sum_{\eta \in \mathbb{Z}^d} a_{\varepsilon\eta}(x)\left(1 - i\eta\cdot\xi - \frac{1}{2}(\eta\cdot\xi)^2 + O\left(|\xi|^3\right)\right) = \langle \xi \, , \, B(x)\xi\rangle + f(x)O\left(|\xi|^3\right) \, ,$$

*thus for all $x \in (\varepsilon\mathbb{Z})^d$*

$$\sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x) = 0, \tag{2.21}$$

$$\sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x)\frac{i}{\varepsilon}\gamma_\nu = 0, \qquad \textit{for} \quad \nu \in \{1,\dots,d\} \tag{2.22}$$

$$-\frac{1}{2\varepsilon^2}\sum_\gamma a_\gamma(x)\gamma_\nu\gamma_\mu = B_{\nu\mu}(x) \qquad \textit{for} \quad \mu,\nu \in \{1,\dots,d\} \, , \tag{2.23}$$

*where $B$ is symmetric. Since $\langle v \, , \, B(x)v\rangle = -\sum_\gamma a_\gamma(x)(v\cdot\gamma)^2$, the matrix $B$ is moreover positive definite if $a_\gamma \leq 0$ for all $\gamma \neq 0$ and $\mathrm{span}\{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, a_\gamma < 0\} = \mathbb{R}^d$.*

In the next lemma, we will give conditions for $a_\gamma$ which ensure that $T_\varepsilon$ is positive and symmetric.

Lemma 2.6. *Let $\varepsilon > 0$ and let $T_\varepsilon = \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(t)$ be the unbounded operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with domain $\mathcal{K}((\varepsilon\mathbb{Z})^d)$, defined by*

$$T_\varepsilon u(x) := \sum_\gamma a_\gamma(x)u(x+\gamma) \, .$$

*Then*

(a) *$T_\varepsilon$ is symmetric if and only if $a_\gamma(x) = a_{-\gamma}(x+\gamma)$.*
(b) *$T_\varepsilon$ is positive if it is symmetric and $a_\gamma(x) \leq 0$ for $\gamma \neq 0$.*

Proof:

(a) $\Longleftarrow$:
By definition $T_\varepsilon$ is a symmetric operator if $\langle T_\varepsilon u \, , \, v\rangle_{\ell^2} = \langle u \, , \, T_\varepsilon v\rangle_{\ell^2}$ for any $u,v \in \mathscr{D}(T_\varepsilon)$, or equivalently,

$$\sum_{x,\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x)\overline{u}(x+\gamma)v(x) = \sum_{x,\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x)\overline{u}(x)v(x+\gamma) \, . \tag{2.24}$$

The right-hand side can through substitutions $\tilde{x} = x + \gamma$ and $\tilde{\gamma} = -\gamma$ be written as

$$\sum_{\tilde{x},\tilde{\gamma}\in(\varepsilon\mathbb{Z})^d} a_{-\tilde{\gamma}}(\tilde{x}+\tilde{\gamma})\overline{u}(\tilde{x}+\tilde{\gamma})v(\tilde{x}) \; . \tag{2.25}$$

Since the sum is taken over all $\tilde{x}$ and $\tilde{\gamma}$, these variables can be renamed to $x$ and $\gamma$. If $a_\gamma(x) = a_{-\gamma}(x+\gamma)$ for all $x$ and $\gamma$, we see at once that (2.25) is equal to the left-hand side of (2.24).
$\Longrightarrow$:
If $T_\varepsilon$ is symmetric, equation (2.24) holds for all $u, v \in \mathscr{D}(T_\varepsilon)$, so we can choose $u = \delta_{\tilde{y}}$ and $v = \delta_{\tilde{x}}$, where

$$\delta_x(y) = \begin{cases} 1\,, & x = y \\ 0\,, & \text{otherwise} \end{cases} \; .$$

By this choice, (2.24) yields

$$a_{\tilde{x}-\tilde{y}}(\tilde{y}) = a_{\tilde{y}-\tilde{x}}(\tilde{x})$$

and thus with $\gamma := \tilde{y} - \tilde{x}$ we are done.
(b) The operator $T_\varepsilon$ is positive if for all $u \in \mathscr{D}(T_\varepsilon)$

$$\langle T_\varepsilon u\,,\, u\rangle_{\ell^2} = \sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)u(x+\gamma)u(x) \geq 0\; .$$

The sum can be rewritten as

$$\sum_x \left\{ a_0(x)|u(x)|^2 + \sum_{\gamma\neq 0} a_\gamma(x)u(x+\gamma)u(x) \right\}$$

and by (2.21) this equals

$$\sum_x \sum_{\gamma\neq 0} a_\gamma(x) \left( u(x+\gamma)u(x) - |u(x)|^2 \right) \; .$$

By (a) and the substitution $\tilde{x}$ and $\tilde{\gamma}$ as in (2.25), we can transform this sum to

$$\begin{aligned} \langle T_\varepsilon u\,,\, u\rangle_{\ell^2} &= \frac{1}{2} \left\{ \sum_{\substack{x\\ \gamma\neq 0}} a_\gamma(x) \left( u(x+\gamma)u(x) - |u(x)|^2 \right) + \sum_{\substack{\tilde{x}\\ \tilde{\gamma}\neq 0}} a_{-\tilde{\gamma}}(\tilde{x}+\tilde{\gamma}) \left( u(\tilde{x})u(\tilde{x}+\tilde{\gamma}) - |u(\tilde{x}+\tilde{\gamma})|^2 \right) \right\} \\ &= -\frac{1}{2} \sum_{\substack{x\\ \gamma\neq 0}} a_\gamma(x) \left( u(x) - u(x+\gamma) \right)^2 \; . \end{aligned}$$

If $a_\gamma(x) \leq 0$ for $\gamma \neq 0$, the last term is obviously greater or equal to 0.

□

## 2.2. Harmonic Approximation of the Spectrum of $H_\varepsilon$

In this section we will show that under certain assumptions, outlined below in Hypothesis 2.7, the eigenvalues of the Hamilton operator $H_\varepsilon$ introduced in (1.1), acting on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, are given in the limit $\varepsilon \to 0$ by the eigenvalues of an adapted harmonic oscillator on $\mathscr{L}^2\left(\mathbb{R}^d\right)$.

### 2.2.1. Hypothesis and Stability Result.

HYPOTHESIS 2.7. *Let $H_\varepsilon = T_\varepsilon + V_\varepsilon$ denote a self adjoint operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, where:*

(a) *$T_\varepsilon$ is a discrete kinetic energy operator as introduced in Definition 2.4 with the further condition that the associated symbol $t$ belongs to the symbol class $S_0^0(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ in the sense of Definition 2.1.*

(b) *The potential energy $V_\varepsilon$ acts as the lattice restriction of a polynomially bounded multiplication operator $\widehat{V}_\varepsilon \in \mathscr{C}^\infty(\mathbb{R}^d)$ on $\mathscr{L}^2\left(\mathbb{R}^d\right)$, which has an expansion*

$$\widehat{V}_\varepsilon(x) = V_0(x) + \varepsilon\, V_1(x) + R_2(x;\varepsilon)\,, \tag{2.26}$$

*where $V_0, V_1$ belong to $\mathscr{C}^\infty(\mathbb{R}^d)$, $R_2 \in \mathscr{C}^\infty(\mathbb{R}^d \times (0, \varepsilon_0])$ for some $\varepsilon_0 > 0$ and has the property that for any compact set $K \subset \mathbb{R}^d$ there exists a constant $C_K$ such that $\sup_{x\in K} |R_2(x;\varepsilon)| \leq C_K\varepsilon^2$.*

*Furthermore there exist constants $R, C > 0$ such that $V_\varepsilon(x) > C$ for all $|x| \geq R$ and $\varepsilon \in (0, \varepsilon_0]$.*

(c) *$V_0 \geq 0$ and it takes the value 0 only at a finite number of points $\{x_j\}_{j=1}^m$, where its Hessian*

$$(\tilde{A}^j_{\nu\mu}) := \frac{1}{2}\left(\frac{\partial^2 V_0}{\partial x_\nu \partial x_\mu}(x_j)\right) \tag{2.27}$$

*is positive definite (i.e. the absolute minima are non-degenerate). We call the minima $\{x_j\}_{j=1}^m$ of $V_0$ potential wells.*

For $t \in S_0^0(\mathbf{1})$ it follows from Proposition 2.3, that $T_\varepsilon$ is bounded, thus $H_\varepsilon$ is self adjoint on the maximal domain of $V_\varepsilon$, i.e. $\mathscr{D}(H_\varepsilon) = \{u \in \ell^2((\varepsilon\mathbb{Z})^d) \,|\, V_\varepsilon u \in \ell^2((\varepsilon\mathbb{Z})^d)\}$.

REMARK 2.8. *Any function $f \in \mathscr{C}_0^\infty(\mathbb{R}^d_\xi)$, which is supported in $(-\pi, \pi)^d$, admits a unique $\mathscr{C}^\infty$ periodic continuation to $\mathbb{R}^d$. Thus any such $f$ can be considered as a function on the torus $\mathbb{T}^d$. We shall denote this function on $\mathbb{T}^d$ by $\tilde{f}$.*

Let $k \in \mathscr{C}_0^\infty\left(\mathbb{R}^d\right)$ be a cut-off function on $\mathbb{R}^d$ such that $k(\xi) = 1$ for $|\xi| \leq 2$ and $\operatorname{supp} k \subset (-\pi, \pi)^d$. Then the truncated quadratic approximation of $t$ given by

$$t_{\pi,q}(x, \xi) := \langle \xi\,,\, B(x)\xi\rangle\, k(\xi)\,, \qquad \xi \in \mathbb{R}^d,\, x \in \mathbb{R}^d, \tag{2.28}$$

can by Remark 2.8 be associated to $\tilde{t} \in S_0^0(\mathbf{1})(\mathbb{R}^d \times \mathbb{T}^d)$. The associated bounded operator on the lattice (see (2.11)) is denoted by $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{t}_{\pi,q}) =: T_{\varepsilon,q}$.

Moreover we define for a critical point $x_j$ of $V_0$ in the sense of Hypothesis 2.7

$$\tilde{t}_{\pi,q,j}(\xi) := \tilde{t}_{\pi,q}(x_j, \xi) \quad \text{and} \quad T_{\varepsilon,q,j} := \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{t}_{\pi,q,j})\,. \tag{2.29}$$

To compare $H_\varepsilon$ with an harmonic oscillator on $\mathscr{L}^2\left(\mathbb{R}^d\right)$, we associate to the periodic kinetic energy function $t$ a translation operator $\widehat{T} := \mathrm{Op}_\varepsilon(t)$ on $\mathbb{C}_0^\infty(\mathbb{R}^d)$ by identifying $t \in \mathbb{C}^\infty(\mathbb{R}^d \times \mathbb{T}^d)$ with the associated periodic function $t \in \mathbb{C}^\infty(\mathbb{R}^{2d})$. Then $\widehat{T}$ is given by

$$\widehat{T} := \mathrm{Op}_\varepsilon(t) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x)\tau_\gamma\,, \qquad x \in \mathbb{R}^d\,. \tag{2.30}$$

Thus $\widehat{T}$ induces the same translations on the square integrable functions on $\mathbb{R}^d$ as $T_\varepsilon$ on the lattice functions and we define the associated Hamilton operator $\widehat{H}_\varepsilon$ on $\mathscr{D}(\widehat{H}_\varepsilon) = \left\{u \in \mathscr{L}^2\left(\mathbb{R}^d\right) \,|\, \widehat{V}_\varepsilon u \in \mathscr{L}^2\left(\mathbb{R}^d\right)\right\}$ as

$$\widehat{H}_\varepsilon u(x) := \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x) u(x+\gamma) + \widehat{V}_\varepsilon(x) u(x)\,, \qquad u \in \mathscr{D}(\widehat{H}_\varepsilon)\,. \tag{2.31}$$

Contrary to the lattice case, it is possible to determine for the quadratic approximation $t_q(x, \xi) := \langle \xi\,,\, B(x)\xi\rangle$ of $t$ on $\mathbb{R}^d \times \mathbb{R}^d$ the action of the associated operator on $\mathscr{L}^2(\mathbb{R}^d)$ by

$$\widehat{T}_q := \mathrm{Op}_\varepsilon(t_q) = -\varepsilon^2 \sum_{\nu,\mu=1}^d B_{\nu\mu}(x)\partial_\nu\partial_\mu\,. \tag{2.32}$$

As in the periodic case, we define for fixed a potential well $x_j \in \mathbb{R}^d$ and for all $\xi \in \mathbb{R}^d$

$$t_{q,j}(\xi) := t_q(x_j, \xi) \quad \text{and} \quad \mathrm{Op}_\varepsilon(t_{q,j}) =: \widehat{T}_{q,j}\,. \tag{2.33}$$

REMARK 2.9. *We denote by $\mathscr{G}_{x_0} = (\varepsilon\mathbb{Z})^d + x_0$ the $\varepsilon$-scaled lattice, which is shifted to the point $x_0 \in \mathbb{R}^d$ (thus $x_0 \in \mathscr{G}_{x_0}$, but it may be that $0 \notin \mathscr{G}_{x_0}$).*

*Then $x + \gamma \in \mathscr{G}_{x_0}$ for any $x \in \mathscr{G}_{x_0}, x_0 \in \mathbb{R}^d$ and $\gamma \in (\varepsilon\mathbb{Z})^d$, thus if $\mathbf{1}_{\mathscr{G}_x}$ is defined as the restriction map to the lattice $\mathscr{G}_{x_0}$, it follows at once that $\tau_\gamma$ commutes with $\mathbf{1}_{\mathscr{G}_x}$. Since as a function of $x$, the operator $H_\varepsilon$ was assumed to be the restriction of an operator on $\mathbb{R}^d$, we can therefore consider $H_\varepsilon$ in the obvious way as an operator on $\mathcal{K}(\mathscr{G}_{x_0})$ and for any $u \in \mathscr{C}_0^\infty\left(\mathbb{R}^d\right)$, for any $x_0 \in \mathbb{R}^d$ and any $\varepsilon > 0$*

$$\left(\mathbf{1}_{\mathscr{G}_{x_0}}\, \widehat{H}_\varepsilon u\right)(x) = \left(H_\varepsilon\, \mathbf{1}_{\mathscr{G}_{x_0}}\, u\right)(x)\,, \qquad x \in \mathscr{G}_{x_0}\,. \tag{2.34}$$

By Hypothesis 2.7, the potential energy $\widehat{V}_\varepsilon$ has at a critical point $x_j$ for $|x - x_j| \to 0$ the expansion

$$\widehat{V}_\varepsilon(x) = V_0^j(x) + \varepsilon\, V_1(x_j) + \varepsilon\, O(|x - x_j|) + O(|x - x_j|^3) + R_2(x,\varepsilon) \tag{2.35}$$

and we set $V_\varepsilon^j(x) := V_0^j(x) + \varepsilon\, V_1(x_j)$ ,

where $V_0^j(x) := \Big\langle (x - x_j)\, ,\, \tilde{A}^j(x - x_j)\Big\rangle$ and $R_2 = O(\varepsilon^2)$.

Let $H_\varepsilon$ be an operator satisfying Hypothesis 2.7 and let $A^j := B_D^{\frac{1}{2}}\tilde{A}^j B_D^{\frac{1}{2}}$, where $\tilde{A}^j$ denotes the Hessian of $V_0$ at a critical point $x_j$ and $B_D$ is the diagonalization of $B(x_j)$ as described in Appendix A, Section A.2.

The main result of this chapter is the following theorem:

Theorem 2.10. *Let*

$$K_j := -\Delta + \langle x\, ,\, A^j x\rangle + V_1(x_j)\,, \qquad j = 1, \dots m$$

*denote self adjoint operators on* $\mathscr{L}^2\left(\mathbb{R}^d\right)$ *and* $K := \bigoplus_{j=1}^m K_j$ *denote a self adjoint operator on* $\bigoplus_{j=1}^m \mathscr{L}^2\left(\mathbb{R}^d\right)$*).*

*Then for any fixed* $n \in \mathbb{N}^*$ *and* $\varepsilon$ *sufficiently small,* $H_\varepsilon$ *has at least* $n$ *eigenvalues.*

*Counting multiplicity, we denote for* $n \in \mathbb{N}^*$ *the* $n$*-th eigenvalue of* $K$ *by* $e_n$ *and the* $n$*-th eigenvalue of* $H_\varepsilon$ *by* $E_n(\varepsilon)$*. Then in the limit* $\varepsilon \to 0$*,*

$$E_k(\varepsilon) = \varepsilon e_k + O\left(\varepsilon^{\frac{6}{5}}\right)\ . \tag{2.36}$$

Remark 2.11. *The operators* $K_j$ *are harmonic oscillators with the additional additive constant* $V_1(x_j)$*. Denoting by* $(\omega_\nu^j)^2$ *for* $\omega_\nu^j > 0$ *the eigenvalues of the matrix* $A^j$*, the eigenvalues of the operator* $K_j$ *are given by*

$$\sigma(K_j) = \left\{ e_{\alpha,j} = \sum_{\nu=1}^d \left(\omega_\nu^j(2\alpha_\nu + 1)\right) + V_1(x_j)\ \middle|\ \alpha \in \mathbb{N}^d \right\}\ . \tag{2.37}$$

*The spectrum* $\sigma(K)$ *of* $K$ *is the union* $\sigma(K) = \bigcup_{j=1}^m \sigma(K_j)$ *of the spectra* $\sigma(K_j)$ *for all* $j$*, i.e. for* $n$ *given as in the setting of Theorem 2.10, the correspondence* $(\alpha, j) \leftrightarrow n$ *is one-to-one. The normalized eigenfunctions of the operators* $K_j$ *associated to an eigenvalue* $e_{\alpha,j}$ *are given by*

$$g_{\alpha,K_j}(x) = h_\alpha(x)e^{-\varphi_0^j(x)}\,, \qquad \alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d\,, \tag{2.38}$$

*where* $h_\alpha(x) = h_{\alpha_1}\cdot h_{\alpha_2}\cdot \dots \cdot h_{\alpha_d}$ *and each* $h_{\alpha_\mu}$ *denotes a one-dimensional Hermite polynomial*

$$h_l(t) = \frac{(-1)^l}{\sqrt{2^l l!}\pi^{\frac{1}{4}}} e^{t^2}\left(\frac{d}{dt}\right)^l e^{-t^2} \tag{2.39}$$

*with* $l = \alpha_\nu$*. We assume* $h_\alpha$ *to be normalized in the sense that the* $\mathscr{L}^2$*-norm of* $g_{\alpha,K_j}$ *is equal to unity. The phase function is given by*

$$\varphi_0^j(x) := \frac{1}{2}\sum_{\nu=1}^d \omega_\nu^j \langle x\, ,\, y_\nu^j\rangle^2\,, \tag{2.40}$$

*where* $y_\nu^j \in \mathbb{R}^d$*,* $(\nu = 1, \dots, d)$ *is an orthonormal basis in* $\mathbb{R}^d$ *of eigenvectors of* $A^j$*.*

**2.2.2. Lemmata concerning the Proof of Theorem 2.10.** The strategy of the proof is to restrict the Hamilton operator $H_\varepsilon$ to small $\varepsilon^{\frac{2}{5}}$-scaled neighborhoods of its critical points in $x$ and $\xi$, i.e. to neighborhoods of $\{(x_j, 0)\}_{j=1}^m$ in phase space. Then the restricted discrete operator can be compared with a corresponding continuous operator acting on $\mathscr{L}^2(\mathbb{R}^d)$.

We follow in part the ideas of the proof of Theorem 11.1 in Cycon-Froese-Kirsch-Simon [**15**] on the quasi-classical eigenvalue limit of a Schrödinger operator. But in contrast to the Schrödinger setting described in this proof, where the kinetic operator is given by the Laplacian on $\mathbb{R}^d$, the discrete operator $T_\varepsilon$ depends on both the position and the momentum and acts on a different space than the harmonic oscillator. The first point consists in localizing the operator simultaneously with respect to $x$ and $\xi$, which is done by use of a version of microlocal calculus adapted to the discrete setting as invented in Appendix B. The idea is to "quantize" the symbol of the operator multiplied with cut-off functions with respect to $x$ and $\xi$. By Proposition B.8, the uniform estimates for the symbol can be used to get norm-estimates for the associated operators.

The starting point of the proof lies in the construction of a partition of unity. This is done in such a way that it permits us to treat separately the neighborhoods of the minima and the region outside of these neighborhoods.

Let $\chi$ be a $\mathscr{C}_0^\infty(\mathbb{R}^d)$-function with the properties

(a) $0 \leq \chi \leq 1$,
(b) $\chi(x) = 1$ if $|x| \leq 1$,
(c) $\chi(x) = 0$ if $|x| \geq 2$,
(d) $\sqrt{\mathbf{1} - \chi^2}$ is a $\mathscr{C}^\infty(\mathbb{R}^d)$-function.

We define functions which localize in $\varepsilon^{\frac{2}{5}}$-scaled neighborhoods of the minima $x_j$, $1 \leq j \leq m$, by

$$\chi_{j,\varepsilon}(x) := \chi\left(\varepsilon^{-\frac{2}{5}}(x - x_j)\right), \qquad x \in \mathbb{R}^d. \tag{2.41}$$

For $\varepsilon$ sufficiently small, $\operatorname{supp}\chi_{j,\varepsilon} \cap \operatorname{supp}\chi_k = \emptyset$ for $k \neq j$. Thus by (d), the function

$$\chi_{0,\varepsilon} := \sqrt{\mathbf{1} - \sum_{j=1}^m \chi_{j,\varepsilon}^2(x)}$$

localizing outside of the wells, is an element of $\mathscr{C}^\infty(\mathbb{R}^d)$ for $\varepsilon$ sufficiently small. Clearly by these definitions $\sum_{l=0}^m \chi_{l,\varepsilon}^2 = \mathbf{1}$.

Using this partition of unity, we can find an estimate in sup-norm for the error, which arises by replacing the potential energy operator $V_\varepsilon$ introduced in (2.26) in an $\varepsilon$-scaled neighborhood of $x_j$ by its quadratic approximation $V_\varepsilon^j(x) = V_0^j(x) + \varepsilon V_1(x_j)$.

For $1 \leq j \leq m$ we get with the notation $V_1^j(x) := V_1(x_j)$

$$\begin{aligned} \left\|\chi_{j,\varepsilon}\left(\left(V_0 - V_0^j\right) + \varepsilon\left(V_1 - V_1^j\right)\right)\chi_{j,\varepsilon}\right\|_\infty &\leq \sup_{x\in\operatorname{supp}(\chi_{j,\varepsilon})}\left|\left(V_0 - V_0^j\right)(x)\right| + \varepsilon\left|\left(V_1 - V_1^j\right)(x)\right| \\ &= O\left(\varepsilon^{\frac{6}{5}}\right), \end{aligned} \tag{2.42}$$

because $(V_0(x) - V_0^j(x)) = O\left(|x - x_j|^3\right)$ and $(V_1 - V_1^j)(x) = O(|x - x_j|)$ as $x \to 0$ and since $|x - x_j| = O\left(\varepsilon^{\frac{2}{5}}\right)$ for $x \in \operatorname{supp}(\chi_{j,\varepsilon})$. Thus by (2.35) we get the estimate

$$\left\|\chi_{j,\varepsilon}\left(\widehat{V}_\varepsilon - V_\varepsilon^j\right)\chi_{j,\varepsilon}\right\|_\infty = O\left(\varepsilon^{\frac{6}{5}}\right). \tag{2.43}$$

In this context, we just mention that in the framework of the calculus of pseudo-differential operators introduced in Appendix B it is possible to consider $T_\varepsilon$ simultaneously localized in configuration and momentum space. To this end we define a cut-off function $\phi_0 \in \mathscr{C}_0^\infty\left(\mathbb{R}^d\right)$, using the original cut-off function $\chi$, by

$$\phi_{0,\varepsilon}(\xi) := \chi(\varepsilon^{-\frac{2}{5}}\xi), \qquad \xi \in \mathbb{R}^d \tag{2.44}$$

and $\phi_{1,\varepsilon} := \sqrt{\mathbf{1} - \phi_{0,\varepsilon}^2}$.

To $\phi_{0,\varepsilon}$ we can associate a function $\tilde{\phi}_{0,\varepsilon} \in \mathscr{C}_0^\infty(\mathbb{T}^d)$ on the torus (see Remark 2.8). Let

$$\tilde{\phi}_{0,\varepsilon}(\xi) := \phi_{0,\varepsilon}(\xi), \qquad \xi \in [-\pi, \pi]^d \tag{2.45}$$

and its periodic continuation for $\xi \in \mathbb{R}^d$. Then we set $\tilde{\phi}_{1,\varepsilon}(\xi) := \sqrt{\mathbf{1} - \tilde{\phi}_{0,\varepsilon}^2} \in \mathscr{C}^\infty(\mathbb{T}^d)$, which gives $\tilde{\phi}_{0,\varepsilon}^2 + \tilde{\phi}_1^2 = \mathbf{1}$.

The functions $\tilde{\phi}_{j,\varepsilon}$ can be considered as elements of $S_{\frac{2}{5}}^0(\mathbb{R}^d \times \mathbb{T}^d)$ with associated operator $\operatorname{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{j,\varepsilon})$. The statement of Proposition B.9 is the estimate

$$\left\|\chi_{j,\varepsilon}\operatorname{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})\left(T_\varepsilon - T_{\varepsilon,q,j}\right)\operatorname{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})\chi_{j,\varepsilon}\right\|_\infty = O\left(\varepsilon^{\frac{6}{5}}\right), \tag{2.46}$$

where $\|.\|_\infty$ denotes the operator norm. The estimate (2.46) suggests the definition

$$\widehat{H}^j := \widehat{T}_{q,j} + V_0^j + \varepsilon V_1(x_j) \tag{2.47}$$

as a model operator on $\mathscr{L}^2(\mathbb{R}^d)$, which is a good approximation of $\widehat{H}_\varepsilon$ and $H_\varepsilon$ respectively for small neighborhoods of $\xi = 0$ and $x = x_j$, i.e. for a localization in the configuration and momentum space. As shown in Appendix A.2, $\widehat{H}^j$ is unitary equivalent to

$$H^j := -\varepsilon^2\Delta + \big\langle (x-x_j)\,,\, A^j(x-x_j)\big\rangle + \varepsilon\, V_1(x_j)\,, \tag{2.48}$$

where $A^j$ is defined as in Theorem 2.10. By scaling, $H^j$ is unitary equivalent to $\varepsilon K_j$ (see Appendix A.4). Thus the spectrum of $H^j$ is given by $\varepsilon\,\sigma(K_j)$ and the eigenfunctions are

$$g_{\alpha j}(x) = \varepsilon^{-\frac{d}{4}} h_\alpha\left(\tfrac{x-x_j}{\sqrt{\varepsilon}}\right) e^{-\varphi_0^j(\frac{x-x_j}{\sqrt{\varepsilon}})}\,. \tag{2.49}$$

The following lemma gives estimates on the error terms which occur by decomposing $H_\varepsilon$ with respect to the partition of unity introduced above into a sum of Dirichlet operators. It is a generalization of the IMS-localization formula for Schrödinger operators described for example in Cycon-Froese-Kirsch-Simon [**15**].

LEMMA 2.12. *Let $H_\varepsilon = T_\varepsilon + V_\varepsilon$ satisfy Hypothesis 2.7 and denote by $V_\varepsilon^j$ the quadratic approximation of $V_\varepsilon$ defined in (2.35).*

*Let $\chi_{j,\varepsilon}\,, 0\leq j\leq m$ and $\tilde\phi_{k,\varepsilon}\,, k=0,1$ be given by (2.41) and (2.45) respectively and denote by $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{k,\varepsilon})$ the associated operator. Then the following estimates hold in operator norm.*

(a)

$$H_\varepsilon = \sum_{j=0}^m \chi_{j,\varepsilon}\, H_\varepsilon\, \chi_{j,\varepsilon} + O\left(\varepsilon^{\frac{6}{5}}\right)\,.$$

(b)

$$T_\varepsilon + V_\varepsilon^j = \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon})(T_\varepsilon+V_\varepsilon^j)\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon}) + \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{1,\varepsilon})(T_\varepsilon+V_\varepsilon^j)\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{1,\varepsilon}) + O\left(\varepsilon^{\frac{6}{5}}\right)\,.$$

The proof of Lemma 2.12 is done by use of the microlocal calculus introduced in Appendix B, in particular Lemma B.10 and Proposition B.8. But we should mention that at this point, it would still be possible to give a proof by direct calculation, avoiding the symbolic calculus. This is shown in Appendix A.6.

Proof of Lemma 2.12:

(a):
Since by definition $\sum_{j=0}^m \chi_{j,\varepsilon}^2 = \mathbf{1}$, we can split $H_\varepsilon$ in the following way

$$H_\varepsilon = \frac{1}{2}\sum_{j=0}^m \chi_{j,\varepsilon}^2\, H_\varepsilon + \frac{1}{2}H_\varepsilon \sum_{j=0}^m \chi_{j,\varepsilon}^2 = \sum_{j=0}^m \chi_{j,\varepsilon}\, H_\varepsilon\, \chi_{j,\varepsilon} + \frac{1}{2}\sum_{j=0}^m [\chi_{j,\varepsilon}, [\chi_{j,\varepsilon}, H_\varepsilon]]\,. \tag{2.50}$$

To show the assertion, we thus have to estimate the double commutators. To this end, we first observe, that $t\in S_0^0(\mathbf{1})$ and $\chi_j\in S_{\frac{2}{5}}^0(\mathbf{1})$, $j=0,\dots m$. Furthermore $\chi_j$ commutes with $V_\varepsilon$, thus it is sufficient to analyze the symbol of the double commutator with $t$. It follows from Lemma B.10, that $[\chi_{j,\varepsilon}, [\chi_{j,\varepsilon}, t]_\#]_\# \in S_{\frac{2}{5}}^{\frac{6}{5}}(\mathbf{1})$. By Proposition B.8, this induces the stated result for the norm of the corresponding operator.

(b):
The arguments are quite similar to (a), but we need to consider the expansions for the symbolic double commutator, since the quadratic potential $V_\varepsilon^j$ is not bounded, but $V_\varepsilon^j\in S_0^0(|x|^2)$. Thus the general result on the symbol class of the double commutator given in Lemma B.10 is not sufficient. By Lemma B.10, the double commutator in the symbolic calculus with $\alpha,\alpha_1,\alpha_2\in\mathbb{N}^d$ for $k=0,1$ can be written as

$$[\tilde\phi_k(\xi), [\tilde\phi_k(\xi), (t+V_\varepsilon^j)(x,\xi)]_\#]_\# = \sum_{|\alpha|=2}(i\varepsilon)^{|\alpha|}\left(\partial_x^\alpha(t+V_\varepsilon^j)\right)(x,\xi)\sum_{\alpha_1+\alpha_2=\alpha}\left(\partial_\xi^{\alpha_1}\tilde\phi_k\right)\left(\partial_\xi^{\alpha_2}\tilde\phi_k\right)(\xi) + R_3\,.$$

Now we use that $t\in S_0^0(1)$ and $\tilde\phi_k\in S_{\frac{2}{5}}^0(1)$ and furthermore that the second derivative of the quadratic term $V_\varepsilon^j$ is constant. Thus all the summands are bounded, of order $\varepsilon^{2-\frac{4}{5}}$ and the $\varepsilon$-order in lowered by $\frac{2}{5}$ with each differentiation. Thus all these terms are elements of $S_{\frac{2}{5}}^{\frac{6}{5}}(\mathbf{1})$. By Lemma

B.10, the remainder $R_3$ depends linearly on a finite number of derivatives $\partial_x^\beta(h+V_\varepsilon^j)$ with $|\beta|\geq 3$ (which is bounded) and $\left(\partial_\xi^{\beta_1}\tilde\phi_k\right)\left(\partial_\xi^{\beta_2}\tilde\phi_k\right)$ with $|\beta_1|+|\beta_2|\geq 3$. Thus it is an element of $S^{\frac{9}{5}}_{\frac{2}{5}}(\mathbf{1})$. We therefore get $[\tilde\phi_k(\xi),[\tilde\phi_k(\xi),(t+V_\varepsilon^j)(x,\xi)]_\#]_\#\in S^{\frac{6}{5}}_{\frac{2}{5}}(\mathbf{1})$, yielding by Proposition B.8 the stated norm estimate for the associated operator.

□

In order to analyze the eigenvalues of $H_\varepsilon$, one would usually try to compute the matrix elements of $H_\varepsilon$ with respect to the basis of eigenfunctions. Since we do not know the eigenfunctions of $H_\varepsilon$, we work with the harmonic oscillator eigenfunctions $g_{\alpha j}$ introduced in (2.49), and restrict them to the lattice $(\varepsilon\mathbb{Z})^d$. We denote these restricted functions, which are elements of $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, by $g_{\alpha j}^\varepsilon$.

The functions $g_{\alpha j}$ defined in (2.49) are localized near the well $x_j$ for $j=1,\dots,m$ and decrease exponentially fast with respect to the phase function $\varphi_0^j$. Thus the difference between the matrix element $\langle g_{\alpha j}\,,\,H_\varepsilon g_{\beta l}\rangle_{\ell^2}$ for $H_\varepsilon$ and the one for the operator localized at the well $x_j$ by use of the cut-off function $\chi_{j,\varepsilon}$ is small. This and similar estimates for the potential and kinetic energy operators are the subject of the following lemma.

LEMMA 2.13. *Let $H_\varepsilon$ and $T_\varepsilon$ be given as in Hypothesis 2.7, $V_\varepsilon^j$ by (2.35). Let $\chi_{j,\varepsilon}$, $1\leq j\leq m$ as well as $\tilde\phi_{0,\varepsilon}$ and $\phi_{0,\varepsilon}$ denote the cut-off functions defined in (2.41), (2.44) and (2.45) respectively. Let $\widehat{T}_{q,j}$ denote the quadratic approximation of $\widehat{T}$ at the point $x_j$ as given in (2.33). Let $g_{\alpha j}^{(\varepsilon)}$ denote the eigenfunctions of the harmonic oscillator defined in (2.49) (or their restriction to the lattice). Then for $\varepsilon\to 0$:*

(a)
$$\left|\left\langle g_{\alpha j}^\varepsilon\,,\,H_\varepsilon g_{\beta l}^\varepsilon\right\rangle_{\ell^2}-\left\langle \chi_{j,\varepsilon}g_{\alpha j}^\varepsilon\,,\,H_\varepsilon\chi_{j,\varepsilon}g_{\beta l}^\varepsilon\right\rangle_{\ell^2}\right|=O\left(\varepsilon^{\frac{6}{5}}\right)\,. \tag{2.51}$$

(b) *There exists a constant $c>0$ such that*
$$\left|\left\langle g_{\alpha j}\,,\,V_\varepsilon^j g_{\beta l}\right\rangle_{\mathscr{L}^2}-\left\langle \chi_{j,\varepsilon}g_{\alpha j}\,,\,V_\varepsilon^j\chi_{j,\varepsilon}g_{\beta l}\right\rangle_{\mathscr{L}^2}\right|=O\left(e^{-c\varepsilon^{-\frac{1}{5}}}\right)\,.$$

(c)
$$\left|\left\langle \chi_{j,\varepsilon}g_{\alpha j}^\varepsilon\,,\,T_\varepsilon\,\chi_{j,\varepsilon}g_{\beta l}^\varepsilon\right\rangle_{\ell^2}-\left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon})\chi_{j,\varepsilon}g_{\alpha j}^\varepsilon)\,,\,T_\varepsilon\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon})\chi_{j,\varepsilon}g_{\beta l}^\varepsilon\right\rangle_{\ell^2}\right|=O\left(\varepsilon^{\frac{6}{5}}\right)\,. \tag{2.52}$$

(d) *There exists a constant $c>0$ such that*
$$\left|\left\langle g_{\alpha j}\,,\,\widehat{T}_{q,j}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}-\left\langle \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon})\chi_{j,\varepsilon}g_{\alpha j}\,,\,\widehat{T}_{q,j}\,\mathrm{Op}_\varepsilon(\phi_{0,\varepsilon})\chi_{j,\varepsilon}g_{\beta l}\right\rangle_{\mathscr{L}^2}\right|=O\left(e^{-c\varepsilon^{-\frac{1}{5}}}\right)\,.$$

Proof of Lemma 2.13:

(a):

By Lemma 2.12
$$\begin{aligned}&\left|\left\langle g_{\alpha j}^\varepsilon\,,\,H_\varepsilon g_{\beta j}^\varepsilon\right\rangle_{\ell^2}-\left\langle \chi_{j,\varepsilon}g_{\alpha j}^\varepsilon\,,\,H_\varepsilon\chi_{j,\varepsilon}g_{\beta j}^\varepsilon\right\rangle_{\ell^2}\right| \\ &\qquad=\left|\sum_{x\in(\varepsilon\mathbb{Z})^d}\sum_{k\neq j}\chi_k(x)g_{\alpha j}^\varepsilon(x)(T_\varepsilon+V_\varepsilon)\chi_k(x)g_{\beta j}^\varepsilon(x)\right|+O\left(e^{\frac{6}{5}}\right).\end{aligned} \tag{2.53}$$

We consider the kinetic and potential term separately, starting with the potential term $V_\varepsilon$. By substituting $(\mathbf{1}-\chi_{j,\varepsilon}^2)$ on its support by 1, we get
$$\begin{aligned}\left|\sum_{x\in(\varepsilon\mathbb{Z})^d}(\mathbf{1}-\chi_{j,\varepsilon}^2)V_\varepsilon(x)g_{\alpha j}^\varepsilon(x)g_{\beta l}^\varepsilon(x)\right| &\leq \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ |x-x_j|\geq\varepsilon^{\frac{2}{5}}}}\left|V_\varepsilon(x)g_{\alpha j}^\varepsilon(x)g_{\beta l}^\varepsilon(x)\right| \\ &\leq C\varepsilon^{-\frac{d}{4}}\sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ |x-x_j|\geq\varepsilon^{\frac{2}{5}}}}\left|V_\varepsilon(x)g_{\alpha j}^\varepsilon(x)\right|\,,\end{aligned}$$

for some $C > 0$, where we used that $g_{\beta l} = O(\varepsilon^{-\frac{d}{4}})$ for the last step. Setting $u = x - x_j$ where $u \in \mathscr{G}_{x_j}$ (see Remark 2.9), the right hand side is for some polynomial $p$ bounded from above by

$$C\varepsilon^{-\frac{d}{2}} \sum_{|u|\geq \varepsilon^{\frac{2}{5}}} \left| V_\varepsilon(u + x_j) h_\alpha\left(\tfrac{u}{\sqrt{\varepsilon}}\right) e^{-\frac{|u|^2}{\varepsilon}} \right| \leq C\varepsilon^{-\frac{d}{2}} \sum_{|u|\geq \varepsilon^{\frac{2}{5}}} |p(u)| e^{-\frac{|u|^2}{\varepsilon}} ,$$

since the potential energy was assumed to be bounded by a polynomial in Hypothesis 2.7. This yields for some $c > 0$

$$\left| \sum_{x\in(\varepsilon\mathbb{Z})^d} (\mathbf{1} - \chi_{j,\varepsilon}^2) V_\varepsilon(x) g_{\alpha j}^\varepsilon(x) g_{\beta l}^\varepsilon(x) \right| = O\left(e^{-|c|\varepsilon^{-\frac{1}{5}}}\right) . \tag{2.54}$$

In order to estimate the kinetic term, we use $g_{\beta l} = O(\varepsilon^{-\frac{d}{4}})$ and the fact that for some $C > 0$ $\sum_\gamma |a_\gamma(x)| \leq C$ uniform with respect to $x$. Thus by the substitution $u = x - x_j$ we get

$$\begin{aligned} &\left| \sum_{x\in(\varepsilon\mathbb{Z})^d} \sum_{k\neq j} \chi_k(x) g_{\alpha j}^\varepsilon(x) \sum_\gamma a_\gamma(x)\chi_k(x+\gamma) g_{\beta l}^\varepsilon(x+\gamma) \right| \\ &\qquad \leq C'\varepsilon^{-\frac{d}{2}} \sum_{|u|\geq \varepsilon^{\frac{2}{5}}} \left| h_\alpha\left(\tfrac{u}{\sqrt{\varepsilon}}\right) e^{-\frac{|u|^2}{\varepsilon}} \right| = O\left(e^{-|c|\varepsilon^{-\frac{1}{5}}}\right) . \end{aligned} \tag{2.55}$$

Inserting (2.54) and (2.55) in (2.53) shows the stated estimate.

(b):

By the definition of the scalar product in $\mathscr{L}^2\left(\mathbb{R}^d\right)$ and the substitution of $\mathbf{1} - \chi_{j,\varepsilon}^2$ by $\mathbf{1}$ on its support, we get

$$\begin{aligned} &\left| \left\langle g_{\alpha j} \, , \, V_\varepsilon^j g_{\beta l} \right\rangle_{\mathscr{L}^2} - \left\langle \chi_{j,\varepsilon} g_{\alpha j} \, , \, V_\varepsilon^j \chi_{j,\varepsilon} g_{\beta l} \right\rangle_{\mathscr{L}^2} \right| \\ &\quad = \left| \int_{\mathbb{R}^d} \left( V_\varepsilon^j(x) - \chi_{j,\varepsilon} V_\varepsilon^j \chi_{j,\varepsilon}(x) \right) g_{\alpha j}(x) g_{\beta l}(x)\, dx \right| \leq \int_{|x-x_j|\geq \varepsilon^{(2/5)}} \left| g_{\alpha j}(x) V_\varepsilon^j(x) g_{\beta l}(x) \right| \, dx \end{aligned}$$

Using again $g_{\beta l} = O(\varepsilon^{-\frac{d}{4}})$ together with the substitution $u = x - x_j$ and the exponential decay of $g_{\alpha j}$, right hand side can for some polynomial $p$ be estimated from above by

$$c\varepsilon^{-\frac{d}{2}} \int_{|u|\geq \varepsilon^{\frac{2}{5}}} p(|u|) e^{-C\frac{|u|^2}{\varepsilon}} \, d|u| = O\left(e^{-\frac{C}{2}\varepsilon^{-\frac{1}{5}}}\right) ,$$

which proves the stated result.

(c):

To prove this statement, we sum by parts to increase the order in $\varepsilon$ of the error term.

By Lemma 2.12,

$$\begin{aligned} &\left| \left\langle \chi_{j,\varepsilon} g_{\alpha j}^\varepsilon \, , \, T_\varepsilon \, \chi_{j,\varepsilon} g_{\beta l}^\varepsilon \right\rangle_{\ell^2} - \left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon}) \chi_{j,\varepsilon} g_{\alpha j}^\varepsilon \, , \, T_\varepsilon \, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon}) \chi_{j,\varepsilon} g_{\beta l}^\varepsilon \right\rangle_{\ell^2} \right| \\ &\quad = \left| \left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{1,\varepsilon}) \chi_{j,\varepsilon} g_{\alpha j}^\varepsilon \, , \, T_\varepsilon \, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{1,\varepsilon}) \chi_{j,\varepsilon} g_{\beta l}^\varepsilon \right\rangle_{\ell^2} \right| + O\left(\varepsilon^{\frac{6}{5}}\right) \end{aligned} \tag{2.56}$$

By equation (2.7) and the definition of the symbol $t$

$$\left| \left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{1,\varepsilon}) \chi_{j,\varepsilon} g_{\alpha j}^\varepsilon \, , \, T_\varepsilon \, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{1,\varepsilon}) \chi_{j,\varepsilon} g_{\beta l}^\varepsilon \right\rangle_{\ell^2} \right| = \left| \left\langle \tilde{\phi}_{1,\varepsilon} \mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon} g_{\alpha j}^\varepsilon) \, , \, t\, \tilde{\phi}_{1,\varepsilon} \mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon} g_{\beta l}^\varepsilon) \right\rangle_{\mathbb{T}} \right| . \tag{2.57}$$

This gives by Definition (2.2)

$$\begin{aligned} &\left| \left\langle \tilde{\phi}_{1,\varepsilon} \mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon} g_{\alpha j}^\varepsilon) \, , \, t\, \tilde{\phi}_{1,\varepsilon} \mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon} g_{\beta l}^\varepsilon) \right\rangle_{\mathbb{T}} \right| \\ &\qquad \leq \int_{[-\pi,\pi]^d} \left| \tilde{\phi}_{1,\varepsilon}(\xi)\, t(x,\xi) \tilde{\phi}_{1,\varepsilon}(\xi) \, (\overline{\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g_{\alpha j}^\varepsilon})(\xi) (\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g_{\beta l}^\varepsilon)(\xi) \right| \, d\xi \, . \end{aligned} \tag{2.58}$$

Now again by replacing the function $\tilde{\phi}_{1,\varepsilon}$ on its support by $\mathbf{1}$, we get

$$\int\limits_{[-\pi,\pi]^d} \left|\tilde{\phi}_{1,\varepsilon}(\xi)\, t(x,\xi)\tilde{\phi}_{1,\varepsilon}(\xi)\,(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon_{\alpha j}})(\xi)(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon_{\beta l})(\xi)\right| d\xi \le \int\limits_{\substack{[-\pi,\pi]^d\\ |\xi|\ge\varepsilon^{\frac{2}{5}}}} \left|t(x,\xi)\,(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon_{\alpha j}})(\xi)(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon_{\beta l})(\xi)\right| d\xi\,. \tag{2.59}$$

We now estimate the product of the Fourier transforms. By the definition (2.4) of the inverse Fourier transform,

$$(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon_{\alpha j}})(\xi) = \frac{1}{\sqrt{2\pi}^d}\sum_{y\in(\varepsilon\mathbb{Z})^d} e^{-\frac{i}{\varepsilon}\xi\cdot y}\chi_{j,\varepsilon}(y)g^\varepsilon_{\alpha j}(y)\,.$$

To analyze this series and the complex conjugate with $g_{\beta l}$ respectively, we use summation by parts, which allows us to obtain any order in $\varepsilon$ by repeating this procedure several times. To this end we use the discrete Laplace operator $\Delta_\varepsilon$ in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ (see equation (2.125) and Appendix A.3)

$$(\Delta_\varepsilon f)(x) := \left(\sum_{\nu=1}^d(\tau_{\varepsilon e_\nu}+\tau_{-\varepsilon e_\nu}) - 2d\right) f(x)\,. \tag{2.60}$$

The operator $\Delta_\varepsilon$ is symmetric in $\ell^2((\varepsilon\mathbb{Z})^d)$, i.e.,

$$\langle f\,,\,\Delta_\varepsilon h\rangle_{\ell^2} = \langle \Delta_\varepsilon f\,,\,h\rangle_{\ell^2}\,,\qquad f,h\in\ell^2((\varepsilon\mathbb{Z})^d)\,. \tag{2.61}$$

In order to use (2.61) to obtain an estimate for (2.59), we have to find a function $h\in\ell^2((\varepsilon\mathbb{Z})^d)$ such that $e^{\pm\frac{i}{\varepsilon}x\cdot\xi} = \Delta_\varepsilon h(x)$. Since

$$\Delta_\varepsilon e^{\pm\frac{i}{\varepsilon}x\cdot\xi} = -\left(2d - 2\sum_{\nu=1}^d\cos(\xi_\nu)\right)e^{\pm\frac{i}{\varepsilon}x\cdot\xi}\,,$$

we have the representation

$$e^{\pm\frac{i}{\varepsilon}x\cdot\xi} = -\left(2d - 2\sum_{\nu=1}^d\cos(\xi_\nu)\right)^{-1}\Delta_\varepsilon e^{\pm\frac{i}{\varepsilon}x\cdot\xi}\,. \tag{2.62}$$

From (2.62) and (2.61) it follows that

$$\sum_{x\in(\varepsilon\mathbb{Z})^d}\chi_{j,\varepsilon}(x)g^\varepsilon_{\alpha j}(x)e^{\pm\frac{i}{\varepsilon}x\cdot\xi} = -\left(2d - 2\sum_{\nu=1}^d\cos(\xi_\nu)\right)^{-1}\sum_{x\in(\varepsilon\mathbb{Z})^d}(\Delta_\varepsilon\chi_{j,\varepsilon}g^\varepsilon_{\alpha j})(x)e^{\pm\frac{i}{\varepsilon}x\cdot\xi}\,. \tag{2.63}$$

We estimate the first factor on the right hand side of (2.63) in the region $\xi\in[-\pi,\pi]^d$ with $|\xi|\ge\varepsilon^{\frac{2}{5}}$. From the inequality $\pi^2(1-\cos\xi_\nu)\ge\xi_\nu^2$ for $|\xi_\nu|\le\pi$ it follows that

$$\frac{1}{\sum_{\nu=1}^d(2-2\cos(\xi_\nu))} \le \frac{\pi^2}{2\sum_{\nu=1}^d\xi_\nu^2} = \frac{\pi^2}{2|\xi|^2}\,.$$

Since we have to estimate in (2.59) the product of two Fourier transforms, we estimate the square of this factor. We thus have for $|\xi|\ge\varepsilon^{\frac{2}{5}}$ and $|\xi_\nu|\le\pi\,,\nu\in\{1,\dots,d\}$

$$\left(\frac{1}{\sum_{\nu=1}^d(2-2\cos(\xi_\nu))}\right)^2 \le \left(\frac{\pi^2}{2\varepsilon^{\frac{4}{5}}}\right)^2 = \frac{\pi^4}{2}\varepsilon^{-\frac{8}{5}}\,. \tag{2.64}$$

To find an estimate for the remaining series on the right hand side of (2.63), we use the differentiability of the functions $\chi_{j,\varepsilon}g_{\alpha j}$ and their Taylor expansion, setting $y := \frac{x}{\sqrt{\varepsilon}}$ and $z := \varepsilon^{-\frac{2}{5}}x$ and

$$g_{\alpha j}(x) = \varepsilon^{-\frac{d}{4}}\tilde{g}_{\alpha j}(\varepsilon^{-\frac{1}{2}}x)\qquad\text{and}\qquad \chi_{j,\varepsilon}(x) = \tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}x)\,, \tag{2.65}$$

since $g_{\alpha j}$ is scaled by $\varepsilon^{-\frac{1}{2}}$ and $\chi_j$ is scaled by $\varepsilon^{-\frac{2}{5}}$. This yields

$$\partial_{x_\nu}\left(\chi_{j,\varepsilon}g_{\alpha j}\right)(x) = \varepsilon^{-\frac{d}{4}}\left(\varepsilon^{-\frac{1}{2}}\left[\chi_{j,\varepsilon}(x)\left(\partial_{y_\nu}\tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}x)\right] + \varepsilon^{-\frac{2}{5}}\left[\tilde{g}_{\alpha j}(\varepsilon^{-\frac{1}{2}}x)\left(\partial_{z_\nu}\tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}x)\right]\right) \tag{2.66}$$

We thus have

$$|\chi_{j,\varepsilon} g_{\alpha j}(x \pm \varepsilon e_\nu) - \chi_{j,\varepsilon} g_{\alpha j}(x)| \leq \varepsilon^{-\frac{d}{4}} \Big| \pm \Big\{ \varepsilon^{\frac{1}{2}} \left[ \chi_{j,\varepsilon}(x) \left(\partial_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}} x) \right] + \varepsilon^{\frac{3}{5}} \left[ \left(\partial_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}} x) \tilde{g}_{\alpha j}(\varepsilon^{-\frac{1}{2}} x) \right] \Big\}$$
$$+ \sup_{t\in[0,1]} \frac{\varepsilon}{2} \left[ \chi_{j,\varepsilon}(x \pm t\varepsilon e_\nu) \left(\partial^2_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x \pm t\varepsilon e_\nu)) \right]$$
$$+ \frac{1}{2} \varepsilon^{\frac{11}{10}} \left[ \left(\partial_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x \pm t\varepsilon e_\nu)) \left(\partial_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x \pm t\varepsilon e_\nu)) \right]$$
$$+ \frac{1}{2} \varepsilon^{\frac{6}{5}} \left[ \left(\partial^2_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x \pm t\varepsilon e_\nu)) \tilde{g}_{\alpha j}(\varepsilon^{-\frac{1}{2}}(x \pm t\varepsilon e_\nu)) \right] \Big| .$$

Since the first derivatives cancel, the term $\Delta_\varepsilon \chi_{j,\varepsilon} g^\varepsilon_{\alpha j}(x)$ can thus by (2.66) be estimated as follows:

$$\left|\Delta_\varepsilon \chi_{j,\varepsilon} g^\varepsilon_{\alpha j}(x)\right| = \left| \sum_{\nu=1}^d (\chi_{j,\varepsilon} g_{\alpha j}(x + \varepsilon\, e_\nu) - \chi_{j,\varepsilon} g_{\alpha j}(x)) + (\chi_{j,\varepsilon} g_{\alpha j}(x - \varepsilon\, e_\nu) - \chi_{j,\varepsilon} g_{\alpha j}(x)) \right|$$
$$= \varepsilon^{-\frac{d}{4}} \frac{\varepsilon}{2} \sum_{\nu=1}^d \Big\{ \sup_{t\in[0,1]} \left| \chi_{j,\varepsilon}(x + \varepsilon\, e_\nu) \left(\partial^2_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x + \varepsilon\, e_\nu)) \right|$$
$$+ \left| \varepsilon^{\frac{1}{10}} \left(\partial_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x + \varepsilon\, e_\nu)) \left(\partial_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x + \varepsilon\, e_\nu)) \right|$$
$$+ \left| \varepsilon^{\frac{1}{5}} \left(\partial^2_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x + \varepsilon\, e_\nu)) \tilde{g}_{\alpha j})(\varepsilon^{-\frac{1}{2}}(x + \eta\varepsilon e_\nu)) \right|$$
$$+ \left| \chi_{j,\varepsilon}(x - \varepsilon\, e_\nu) \left(\partial^2_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x - \varepsilon\, e_\nu)) \right|$$
$$+ \left| \varepsilon^{\frac{1}{10}} \left(\partial_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x - \varepsilon\, e_\nu)) \left(\partial_{y_\nu} \tilde{g}_{\alpha j}\right)(\varepsilon^{-\frac{1}{2}}(x - \varepsilon\, e_\nu)) \right|$$
$$+ \left| \varepsilon^{\frac{1}{5}} \left(\partial^2_{z_\nu} \tilde{\chi}_{j,\varepsilon}\right)(\varepsilon^{-\frac{2}{5}}(x - \varepsilon\, e_\nu)) \tilde{g}_{\alpha j}(\varepsilon^{-\frac{1}{2}}(x - \eta\varepsilon e_\nu)) \right| \Big\} \quad (2.67)$$

The cut-off functions and the eigenfunctions $g_{\alpha j}$ of the harmonic oscillator are together with all their derivatives summable. Thus the series on the right hand side of (2.63) is bounded and by (2.67) of order $\varepsilon^{1-\frac{d}{4}}$. Since all the estimates were independent of the choice of $(\alpha j)$, we get by (2.64) for some $C > 0$

$$\left| \overline{(\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon_{\alpha j})}(\xi) (\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon_{\beta l})(\xi) \right| = O\left(\varepsilon^{\frac{2}{5} - \frac{d}{2}}\right) \quad (2.68)$$

Thus with one summation by parts, we gain a factor $\varepsilon^{\frac{2}{5}}$. Iteration this procedure $N$ times and estimating the derivatives of $g_{\alpha j}$ and $\chi_{j,\varepsilon}$ by the supremum over the intervals $I_{\nu N} = [x - N\varepsilon e_\nu, x + N\varepsilon e_\nu]$, which is bounded and summable with respect to $x$, we gain the factor $\varepsilon^{\frac{2N}{5}}$. The integration in (2.59) yields bounded terms, thus

$$\int\limits_{\substack{[-\pi,\pi]^d \\ |\xi|\geq\varepsilon^{\frac{2}{5}}}} t(z,\xi)\, \frac{1}{(2\pi)^d} \left| \overline{(\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon_{\alpha j})}(\xi) (\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon_{\beta l})(\xi) \right| d\xi = O\left(\varepsilon^{\frac{2N}{5} - \frac{d}{2}}\right), \quad N \in \mathbb{N}$$

and by the equations (2.56), (2.57) and (2.58), we have the stated result.
(d):
We split this estimate in two steps. At first, similar to the proof of point (a), we estimate

$$\left| \left\langle g_{\alpha j}\,,\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \widehat{T}_{q,j}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon})\, g_{\beta l} \right\rangle_{\mathscr{L}^2} - \left\langle g_{\alpha j}\,,\, \chi_{j,\varepsilon}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \widehat{T}_{q,j}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \chi_{j,\varepsilon}\, g_{\beta l} \right\rangle_{\mathscr{L}^2} \right|$$
$$\leq \int_{|x - x_j| \geq \varepsilon^{-\frac{2}{5}}} \left| g_{\alpha j}(x) \left( \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \widehat{T}_{q,j}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \right) g_{\beta l}(x) \right| \leq C e^{-c\varepsilon^{-\frac{1}{5}}} .$$

Here we used that the derivatives of the eigenfunctions are bounded and that the eigenfunctions are exponentially decreasing.
As second step we analyze the difference

$$\left| \left\langle g_{\alpha j}\,,\, \widehat{T}_{q,j}\, g_{\beta l} \right\rangle_{\mathscr{L}^2} - \left\langle g_{\alpha j}\,,\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \widehat{T}_{q,j}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon})\, g_{\beta l} \right\rangle_{\mathscr{L}^2} \right| = \left| \left\langle g_{\alpha j}\,,\, \mathrm{Op}_\varepsilon(\phi_{1,\varepsilon})^2 \widehat{T}_{q,j}\, g_{\beta l} \right\rangle_{\mathscr{L}^2} \right| .$$

Similarly to (2.57), by using Parseval‘s equation we estimate the last term,

$$\left|\left\langle g_{\alpha j}\,,\,\mathrm{Op}_\varepsilon(\phi_{1,\varepsilon})^2\widehat{T}_{q,j}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}\right| = \left|\left\langle F_\varepsilon^{-1}g_{\alpha j}\,,\,\phi_{1,\varepsilon}^2\widehat{T}_{q,j}\,F_\varepsilon^{-1}g_{\beta l}\right\rangle_{\mathscr{L}^2}\right|$$
$$\leq \int_{|\xi|\geq\varepsilon^{\frac{2}{5}}}\left|\left(F_\varepsilon^{-1}g_{\alpha j}\right)(\xi)t_{qj}(\xi)\left(F_\varepsilon^{-1}g_{\beta l}\right)(\xi)\right|\,d\xi \leq Ce^{c\varepsilon^{-\frac{1}{5}}}\,,$$

where in the last step we used that the Fourier transform of the Gauss function is again a Gauss function, and thus the Fourier transforms of the eigenfunctions and its derivatives are exponentially decreasing and bounded as the eigenfunctions are.

□

Since Theorem 2.10 compares the eigenvalues of a self adjoint unbounded operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with the eigenvalues of the harmonic oscillator, which is an unbounded self adjoint operator on $\mathscr{L}^2\left(\mathbb{R}^d\right)$, we have to compare some matrix elements with respect to the scalar product $\langle .\,,\,.\rangle_{\ell^2}$ with those with respect to $\langle .\,,\,.\rangle_{\mathscr{L}^2}$. How this can be done is shown in the next lemma, giving an estimate for the difference of these terms.

Lemma 2.14. *Let $T_{\varepsilon,q,j}$ and $\widehat{T}_{q,j}$ be defined in (2.29) and (2.33) respectively and let $V_\varepsilon^j$ be given by (2.35). Let $f,g\in\mathscr{L}^2\left(\mathbb{R}^d\right)$ denote normalized eigenfunctions of the harmonic oscillator given in (2.48) (of the form (2.49)) and $f^\varepsilon, g^\varepsilon\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ their restrictions to the lattice. Let $\chi_{j,\varepsilon}$, $1\leq j\leq m$, $\tilde{\phi}_{0,\varepsilon}$ and $\phi_0$ be the cut-off functions defined in (2.41), (2.45) and (2.44). Then for $\varepsilon$ sufficiently small*

(a)

$$\left\langle\chi_{j,\varepsilon}f^\varepsilon\,,\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})T_{\varepsilon,q,j}\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})\,\chi_{j,\varepsilon}g^\varepsilon\right\rangle_{\ell^2}$$
$$= \varepsilon^{-d}\left(\left\langle\chi_{j,\varepsilon}f\,,\,\mathrm{Op}_\varepsilon(\phi_0)\widehat{T}_{q,j}\,\mathrm{Op}_\varepsilon(\phi_0)\,\chi_{j,\varepsilon}g\right\rangle_{\mathscr{L}^2} + O\left(\varepsilon^{\frac{6}{5}}\right)\right)\,.$$

(b)

$$\left\langle f^\varepsilon\,,\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g^\varepsilon\right\rangle_{\ell^2} = \varepsilon^{-d}\left(\left\langle f\,,\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g\right\rangle_{\mathscr{L}^2} + O\left(\varepsilon^{\frac{13}{10}}\right)\right)\,.$$

Proof of Lemma 2.14:

(a):
By use of the isometry of the Fourier transform (2.7) and the symbol $t_{\pi,q,j}$ associated to $T_{\varepsilon,q,j}$, we get

$$\left\langle\chi_{j,\varepsilon}f^\varepsilon\,,\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})T_{\varepsilon,q,j}\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_{0,\varepsilon})\chi_{j,\varepsilon}g^\varepsilon\right\rangle_{\ell^2} = \left\langle\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}f^\varepsilon)\,,\,\tilde{\phi}_{0,\varepsilon}t_{\pi,q,j}\tilde{\phi}_{0,\varepsilon}\,\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}g^\varepsilon)\right\rangle_{\mathbb{T}}$$
$$= \int_{[-\pi,\pi]^d}\tilde{\phi}_{0,\varepsilon}(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}f^\varepsilon})(\xi)t_{\pi,q,j}(\xi)\left(\tilde{\phi}_{0,\varepsilon}\left(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon\right)\right)(\xi)\,d\xi\,. \quad (2.69)$$

Since for $\varepsilon$ small enough $\tilde{\phi}_{0,\varepsilon}|_{[-\pi,\pi]^d} = \phi_0|_{[-\pi,\pi]^d}$ and $\phi_0(x)=0$ for $x\in\mathbb{R}^d\setminus[-\pi,\pi]^d$, we can within the integral replace $\tilde{\phi}_{0,\varepsilon}$ by $\phi_0$ and extend then the range of the integral to $\mathbb{R}^d$. Furthermore for $\varepsilon$ small enough we can identify $t_{\pi,q,j}$ and $t_{q,j}$ on the support of $\phi_0$, thus

$$\int_{[-\pi,\pi]^d}\tilde{\phi}_{0,\varepsilon}(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}f^\varepsilon})(\xi)t_{\pi,q,j}(\xi)\left(\tilde{\phi}_{0,\varepsilon}\left(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon\right)\right)(\xi)\,d\xi$$
$$= \int_{\mathbb{R}^d}\phi_0(\xi)(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}f^\varepsilon})(\xi)t_{q,j}(\xi)\phi_0(\xi)\,(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi)\,d\xi\,. \quad (2.70)$$

The right hand side of (2.70) can, by addition of $a-a$ with

$$a := \phi_0(\xi)(\overline{F_\varepsilon^{-1}\chi_{j,\varepsilon}f})(\xi)t_{q,j}(\xi)\phi_0(\xi)\left((\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi) + (F_\varepsilon^{-1}\chi_{j,\varepsilon}g)(\xi)\right)\,,$$

be decomposed to the sum

$$\int_{\mathbb{R}^d} \phi_0(\xi) \left( \overline{(\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} f^\varepsilon)}(\xi) - \overline{(F_\varepsilon^{-1} \chi_{j,\varepsilon} f)}(\xi) \right) t_{q,j}(\xi)\, \phi_0(\xi)\, (\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon)(\xi)\, d\xi$$
$$+ \int_{\mathbb{R}^d} \phi_0(\xi) (\overline{F_\varepsilon^{-1} \chi_{j,\varepsilon} f})(\xi))\, t_{q,j}(\xi)\, \phi_0(\xi)\, ((\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} g^\varepsilon)(\xi) - (F^{-1} \chi_{j,\varepsilon} g)(\xi))\, d\xi$$
$$+ \int_{\mathbb{R}^d} \phi_0(\xi) (\overline{F_\varepsilon^{-1} \chi_{j,\varepsilon} f})(\xi))\, t_{q,j}(\xi)\, \phi_0(\xi)\, (F_\varepsilon^{-1} \chi_{j,\varepsilon} g)(\xi)\, d\xi\,. \quad (2.71)$$

The last summand in (2.71) can be understood as a scalar product in $\mathscr{L}^2(\mathbb{R}^d_\xi)$ and is, by the "Parseval" relation (2.10) for the quantized Fourier transform (2.9), equal to the remaining term on the right hand side of (a).

We therefore have to estimate the first two terms on the right hand side of (2.71), where we separately treat the factors in the integral. Using the identity $\varepsilon^d = \int_{[x,x+\varepsilon[^d} dy$ and the definitions (2.9) of $F_\varepsilon^{-1}$ and (2.4) of $\mathscr{F}_\varepsilon^{-1}$, we rewrite the first factor in the first summand. Thus the identity of $f^\varepsilon$ and $g^\varepsilon$ with $f$ and $g$ respectively on the points of the lattice yields

$$\phi_0(\xi) \left( \overline{(\mathscr{F}_\varepsilon^{-1} \chi_{j,\varepsilon} f^\varepsilon)}(\xi) - \overline{(F_\varepsilon^{-1} \chi_{j,\varepsilon} f)}(\xi) \right)$$
$$= \phi_0(\xi) \left(\varepsilon\sqrt{2\pi}\right)^{-d} \sum_{x \in (\varepsilon\mathbb{Z})^d} \int_{[x,x+\varepsilon[^d} \left( e^{\frac{i}{\varepsilon} x\cdot\xi} \chi_{j,\varepsilon} f(x) - e^{\frac{i}{\varepsilon} y\cdot\xi} \chi_{j,\varepsilon} f(y) \right) dy$$
$$= \phi_0(\xi) \left(\varepsilon\sqrt{2\pi}\right)^{-d} \sum_{x \in (\varepsilon\mathbb{Z})^d} \int_{[x,x+\varepsilon[^d} \left( (e^{\frac{i}{\varepsilon} x\cdot\xi} - e^{\frac{i}{\varepsilon} y\cdot\xi}) \chi_{j,\varepsilon} f(x) - e^{\frac{i}{\varepsilon} y\cdot\xi} (\chi_{j,\varepsilon} f(y) - \chi_{j,\varepsilon} f(x)) \right) dy\,. \quad (2.72)$$

For the first summand in (2.72), we use that $|\xi| \leq 2\varepsilon^{\frac{2}{5}}$ on $\operatorname{supp} \phi_0$, thus with $Q_x = [x, x+\varepsilon]^d$

$$\left| e^{\frac{i}{\varepsilon} x\xi} - e^{\frac{i}{\varepsilon} y\xi} \right| \leq \sup_{y \in Q_x} \left| \tfrac{1}{\varepsilon}(x-y)\cdot\xi \right| = O\left(\varepsilon^{\frac{2}{5}}\right)\,.$$

Since the resulting term is independent of $y$, we use again $1 = \varepsilon^{-d} \int_{[x,x+\varepsilon]^d} dy$ to get

$$\phi_0(\xi) \left(\varepsilon\sqrt{2\pi}\right)^{-d} \left| \sum_{x \in (\varepsilon\mathbb{Z})^d} \int_{[x,x+\varepsilon[^d} (e^{\frac{i}{\varepsilon} x\cdot\xi} - e^{\frac{i}{\varepsilon} y\cdot\xi}) \chi_{j,\varepsilon} f(x)\, dy \right|$$
$$\leq \phi_0(\xi) \sqrt{2\pi}^{-d} \varepsilon^{\frac{2}{5}} C \sum_{x \in (\varepsilon\mathbb{Z})^d} \chi_{j,\varepsilon} |f(x)|\,. \quad (2.73)$$

Since $f$ was supposed to be a normalized eigenfunction of the harmonic oscillator, i.e. scaled with $\varepsilon^{-\frac{1}{2}}$ and normalized with a factor $\varepsilon^{-\frac{d}{4}}$, the last sum can be estimated with the substitution $x = \varepsilon v$ and

$$f(x) = \varepsilon^{-\frac{d}{4}} \tilde{f}(x/\sqrt{\varepsilon}) \quad (2.74)$$

as

$$\sum_{x \in (\varepsilon\mathbb{Z})^d} \chi_{j,\varepsilon} |f(x)| \leq \varepsilon^{-\frac{d}{4}} \sum_{v \in \mathbb{Z}^d} |\tilde{f}(\sqrt{\varepsilon} v)| = \varepsilon^{-\frac{3d}{4}} \left( \varepsilon^{\frac{d}{2}} \sum_{v \in \mathbb{Z}^d} |\tilde{f}(\sqrt{\varepsilon} v)| \right) \quad (2.75)$$

Now we notice, that by the definition of the Riemannian integral

$$\lim_{\varepsilon \to 0} \left( \varepsilon^{\frac{d}{2}} \sum_{v \in \mathbb{Z}^d} |\tilde{f}(\sqrt{\varepsilon} v)| \right) = \int_{\mathbb{R}^d} |\tilde{f}(u)|\, du\,, \quad (2.76)$$

which is a constant independent of $\varepsilon$.

By inserting (2.76) into (2.75), we get the estimate

$$\sum_{x \in (\varepsilon\mathbb{Z})^d} \chi_{j,\varepsilon} |f(x)| = O\left(\varepsilon^{-\frac{3d}{4}}\right)\,. \quad (2.77)$$

Inserted in (2.73), this yields

$$\phi_0(\xi)\left(\varepsilon\sqrt{2\pi}\right)^{-d}\left|\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon[^d}(e^{\frac{i}{\varepsilon}x\cdot\xi}-e^{\frac{i}{\varepsilon}y\cdot\xi})\chi_{j,\varepsilon}f(x)\,dy\right|\leq\phi_0(\xi)C\varepsilon^{\frac{2}{5}-\frac{3d}{4}}\;. \tag{2.78}$$

To estimate the second summand on the right hand side of (2.72), we use $|x_k-y_k|\leq\varepsilon$ for all $k$. In order to take the scaling of $f$ and $\chi_j$ with respect to $\varepsilon$ into account, we set $u:=\frac{x}{\sqrt{\varepsilon}}$ and $z:=x\varepsilon^{-\frac{2}{5}}$. This yields for $\tilde{f}$ and $\tilde{\chi}_j$ as defined in (2.74) and (2.75) respectively with $I_\nu(x)=[x,x+\varepsilon e_\nu[$

$$|\chi_{j,\varepsilon}f(y)-\chi_{j,\varepsilon}f(x)|\leq\varepsilon^{-\frac{d}{4}}d\sqrt{\varepsilon}\sum_{\nu=1}^{d}\sup_{w\in I_\nu}\left|\chi_{j,\varepsilon}(w)\left(\partial_{u_\nu}\tilde{f}\right)(\varepsilon^{-\frac{1}{2}}w)+\varepsilon^{\frac{1}{10}}\left(\partial_{z_\nu}\tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}w))\right)\tilde{f}(\varepsilon^{-\frac{1}{2}}w)\right|. \tag{2.79}$$

Again the resulting term does not depend on $y$, therefore by (2.79)

$$\begin{aligned}\left|\phi_0(\xi)\left(\varepsilon\sqrt{2\pi}\right)^{-d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon[^d}e^{\frac{i}{\varepsilon}y\cdot\xi}(\chi_{j,\varepsilon}f(y)-\chi_{j,\varepsilon}f(x))\,dy\right|&\\ \leq\phi_0(\xi)\sqrt{2\pi}^{-d}\varepsilon^{-\frac{d}{4}}d\sqrt{\varepsilon}C&\\ \times\sum_{x\in(\varepsilon\mathbb{Z})^d}\sum_{\nu=1}^{d}\sup_{w\in[x,x+\varepsilon e_\nu]}\left|\chi_{j,\varepsilon}(w)\left(\partial_{u_\nu}\tilde{f}\right)(\varepsilon^{-\frac{1}{2}}w)+\varepsilon^{\frac{1}{10}}\left(\partial_{z_\nu}\tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}w)\right)\tilde{f}(\varepsilon^{-\frac{1}{2}}w)\right|&\end{aligned} \tag{2.80}$$

Since the derivative of $f$ is of the same structure as $f$ itself, we have by the arguments leading to (2.75)

$$\begin{aligned}&\varepsilon^{-\frac{d}{4}}\sum_{x\in(\varepsilon\mathbb{Z})^d}\sum_{\nu=1}^{d}\sup_{w\in[x,x+\varepsilon e_\nu]}\left|\chi_{j,\varepsilon}(w)\left(\partial_{u_\nu}\tilde{f}\right)(\varepsilon^{-\frac{1}{2}}w)+\left(\partial_{z_\nu}\tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}w)\right)\tilde{f}(\varepsilon^{-\frac{1}{2}}w)\right|\\ &\quad\leq C\varepsilon^{-\frac{3d}{4}}\varepsilon^{\frac{d}{2}}\sum_{\nu=1}^{d}\sum_{y\in\mathbb{Z}^d}\sup_{w\in[y,y+e_\nu]}\left\{\left|\left(\partial_{u_\nu}\tilde{f}\right)\right|+\left|\tilde{f}\right|\right\}(\varepsilon^{\frac{1}{2}}w)\\ &\quad\leq C\varepsilon^{-\frac{3d}{4}}\sum_{\nu=1}^{d}\left\{\varepsilon^{\frac{d}{2}}\sum_{y\in\mathbb{Z}^d}\sup_{w\in[y,y+1]^d}\left|\partial_{u_\nu}\tilde{f}\right|(\varepsilon^{\frac{1}{2}}w)+\varepsilon^{\frac{d}{2}}\sum_{y\in\mathbb{Z}^d}\sup_{w\in[y,y+1]^d}\left|\tilde{f}\right|(\varepsilon^{\frac{1}{2}}w)\right\}\end{aligned} \tag{2.81}$$

It follows by (2.76) (see the construction of the Riemannian integral) that both summands on the right hand side of (2.81) tend to a finite limit and are therefore bounded by constants independent of $\varepsilon$, thus

$$\varepsilon^{-\frac{d}{4}}\sum_{x\in(\varepsilon\mathbb{Z})^d}\sum_{\nu=1}^{d}\sup_{w\in[x,x+\varepsilon e_\nu]}\left|\chi_{j,\varepsilon}(w)\left(\partial_{u_\nu}\tilde{f}\right)(\varepsilon^{-\frac{1}{2}}w)+\varepsilon^{\frac{1}{10}}\left(\partial_{z_\nu}\tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}w)\right)\tilde{f}(\varepsilon^{-\frac{1}{2}}w)\right|=O\left(\varepsilon^{-\frac{3d}{4}}\right) \tag{2.82}$$

Inserted in (2.80), this leads for some $C>0$ to

$$\left|\phi_0(\xi)\left(\varepsilon\sqrt{2\pi}\right)^{-d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon[^d}e^{\frac{i}{\varepsilon}y\cdot\xi}(\chi_{j,\varepsilon}f(y)-\chi_{j,\varepsilon}f(x))\,dy\right|\leq C\phi_0(\xi)\varepsilon^{\frac{1}{2}-\frac{3d}{4}} \tag{2.83}$$

Inserting (2.83) and (2.78) into (2.72) yields

$$\phi_0(\xi)\left|(\overline{\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}f^\varepsilon})(\xi)-(\overline{F_\varepsilon^{-1}\chi_{j,\varepsilon}f})(\xi)\right|=O\left(\varepsilon^{\frac{2}{5}-\frac{3d}{4}}\right)\,. \tag{2.84}$$

For the first summand in (2.71), we use the estimate $\sup_\xi\phi_0(\xi)t_{q,j}(\xi)\leq c\varepsilon^{\frac{4}{5}}$, which follows from the fact that $t_{q,j}$ is quadratic with respect to $\xi$ together with the scaling of the support of $\phi_0$. This yields together with (2.84)

$$\begin{aligned}\Big|\int_{\mathbb{R}^d}\phi_0(\xi)\left(\overline{(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}f^\varepsilon)}(\xi)-\overline{(F_\varepsilon^{-1}\chi_{j,\varepsilon}f)}(\xi)\right)\, t_{q,j}(\xi)\,\phi_0(\xi)\,(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi)\,d\xi\Big|\\ \leq C\varepsilon^{\frac{2}{5}-\frac{3d}{4}}\int_{\mathbb{R}^d}|\phi_0(\xi)t_{q,j}(\xi)|\left|\phi_0(\xi)(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi)\right|\,d\xi\\ \leq C\varepsilon^{\frac{6}{5}-\frac{3d}{4}}\int_{\mathbb{R}^d}\left|\phi_0(\xi)(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi)\right|\,d\xi\ = O\left(\varepsilon^{\frac{6}{5}-d}\right)\,.\end{aligned}$$

In the last step, we used that $g$ and its Fourier transform are of order $\varepsilon^{-\frac{d}{4}}$.

The second summand in (2.71) can be treated using the same arguments, so

$$\int_{\mathbb{R}^d}\phi_0(\xi)(\overline{F_\varepsilon^{-1}\chi_{j,\varepsilon}f})(\xi))\,t_{q,j}(\xi)\,\phi_0(\xi)\,((\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}g^\varepsilon)(\xi)-(F_\varepsilon^{-1}\chi_{j,\varepsilon}g)(\xi))\,d\xi = O\left(\varepsilon^{\frac{6}{5}-d}\right)\,,\tag{2.85}$$

which by (2.71) proves (a) of Lemma 2.14.

(b):

Writing the scalar product similarly to equation (2.71) using the identity $\varepsilon^d=\int_{[x,x+\varepsilon[^d}dy$, we get

$$\begin{aligned}\left\langle f^\varepsilon\,,\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g^\varepsilon\right\rangle_{\ell^2} &= \sum_{x\in(\varepsilon\mathbb{Z})^d}f^\varepsilon(x)\,(\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g^\varepsilon)(x) = \qquad (2.86)\\ &=\frac{1}{\varepsilon^d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon[^d}\left\{(f(x)-f(y))\,(\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g)(x)+\right.\\ &\qquad\left.+f(y)\,\left((\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}g)(x)-(\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}g)(y)\right)+f(y)\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g(y)\right\}\,dy\,.\end{aligned}$$

The functions arising in the last summand are all defined on $\mathbb{R}^d$, the sum of integrals on the lattice cells can therefore be combined to an integral on $\mathbb{R}^d$, which by definition is equal to the scalar product in $\mathscr{L}^2(\mathbb{R}^d)$ multiplied by the factor $\varepsilon^{-d}$. Similar to the proof of (a) it remains to estimate the first two terms.

In order to estimate the second factor in the first summand on the right hand side of (2.86), we observe in (2.35) that $V_\varepsilon^j$ is of second order in $x-x_j$ and that the term constant in $x$ is of order $\varepsilon$. Since we have $|x-x_j|^2\leq 4\varepsilon^{\frac{4}{5}}$ for all $x\in\operatorname{supp}(\chi)$, this gives for some $C>0$ the estimate $\sup_{x\in\mathbb{R}^d}\left|\chi_jV_\varepsilon^j\chi_j(x)\right|\leq C\varepsilon^{\frac{4}{5}}$ for the cut potential, thus

$$\begin{aligned}\varepsilon^{-d}\left|\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon)^d}(f(x)-f(y))\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g(x)\,dy\right|\\ \leq\varepsilon^{\frac{4}{5}-d}C\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon)^d}|f(x)-f(y)|\,|g(x)|\,dy\end{aligned}$$

Setting $u=\frac{x}{\sqrt{\varepsilon}}$ and $I_\nu(u)=[u,u+\sqrt{\varepsilon}e_\nu[$, a Taylor expansion at the point $x$ yields for $\tilde f$ defined in (2.74)

$$|f(x)-f(y)|\leq\varepsilon^{\frac{1}{2}-\frac{d}{4}}\sum_{\nu=1}^d\sup_{z\in I_\nu(u)}|(\partial_{u_\nu}\tilde f)(z)|\,.\tag{2.87}$$

Thus by (2.87) and with $\tilde g$ defined similar to $\tilde f$

$$\begin{aligned}&\varepsilon^{-d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon)^d}|f(x)-f(y)|\,|g(x)|\,dy\\ &\qquad\leq C\varepsilon^{\frac{1}{2}-\frac{d}{2}}\sum_{\nu=1}^d\sum_{x\in(\varepsilon\mathbb{Z})^d}\sup_{z\in[x,x+\varepsilon[^d}|\partial_{u_\nu}\tilde f|(\varepsilon^{-\frac{1}{2}}z)|\tilde g|(\varepsilon^{-\frac{1}{2}}x)\,\varepsilon^{-d}\int_{[x,x+\varepsilon[^d}dy\\ &\qquad\leq C\varepsilon^{\frac{1}{2}-d}\sum_{\nu=1}^d\varepsilon^{\frac{d}{2}}\sum_{v\in\mathbb{Z}^d}\sup_{z\in[v,v+1[^d}|\partial_{u_\nu}\tilde f||\tilde g|(\varepsilon^{\frac{1}{2}}z)\,,\end{aligned}\tag{2.88}$$

where in the last step we used the substitution $v = \varepsilon x$. By (2.76), the sum is bounded by a constant independent of $\varepsilon$, thus we get

$$\varepsilon^{-d} \sum_{x\in(\varepsilon\mathbb{Z})^d} \int_{[x,x+\varepsilon)^d} |f(x) - f(y)|\, |g(x)|\, dy = O\left(\varepsilon^{\frac{1}{2}-d}\right) . \tag{2.89}$$

Inserting (2.89) in (2.87) yields

$$\varepsilon^{-d} \left| \sum_{x\in(\varepsilon\mathbb{Z})^d} \int_{[x,x+\varepsilon)^d} (f(x) - f(y))\, \chi_{j,\varepsilon} V_\varepsilon^j \chi_{j,\varepsilon}\, g(x)\, dy \right| = O\left(\varepsilon^{\frac{13}{10}-d}\right) . \tag{2.90}$$

The second term in equation (2.86) can be shown by similar arguments to be of the same order with respect to $\varepsilon$, which completes the proof of the second part of the lemma. □

There is now still one estimate needed for the proof of Theorem 2.10. It concerns the error, which is made by replacing the $x$-dependent quadratic approximation $\widehat{T}_q$ of the kinetic energy by the operator fixed at the well (and thus constant with respect to $x$).

LEMMA 2.15. *Let $\widehat{T}_q$ and $\widehat{T}_{q,j}$ be given by (2.32) and (2.33) respectively for $1 \le j \le m$. Let $\chi_{j,\varepsilon}$ be the cut-off function defined in (2.41) and $f, g$ denote normalized eigenfunctions of the harmonic oscillator given in (2.48), then*

$$\left| \left\langle f\, ,\, \chi_{j,\varepsilon}\, \widehat{T}_q\, \chi_{j,\varepsilon}\, g \right\rangle_{\mathscr{L}^2} - \left\langle f\, ,\, \chi_{j,\varepsilon}\, \widehat{T}_{q,j}\, \chi_{j,\varepsilon}\, g \right\rangle_{\mathscr{L}^2} \right| = O\left(\varepsilon^{\frac{7}{5}}\right) .$$

Proof:
By the definitions of the operators

$$\left| \left\langle f\, ,\, \chi_{j,\varepsilon}\, (\widehat{T}_q - \widehat{T}_{q,j})\, \chi_{j,\varepsilon}\, g \right\rangle_{\mathscr{L}^2} \right| = \left| \left\langle f\, ,\, \chi_{j,\varepsilon}\, \varepsilon^2 \textstyle\sum_{\nu,\mu} (B_{\nu\mu}(x) - B_{\nu\mu}(x_j)) \partial_\nu \partial_\mu\, \chi_{j,\varepsilon}\, g \right\rangle_{\mathscr{L}^2} \right| .$$

As $g$ is scaled by $\frac{x}{\sqrt{\varepsilon}}$,

$$\|\varepsilon^2 \partial_\nu \partial_\mu \chi_{j,\varepsilon} g\|_{\mathscr{L}^2} = O(\varepsilon) .$$

Since $|x| \le 2\varepsilon^{\frac{2}{5}}$ in the support of $\chi_{j,\varepsilon}$, we have $B_{\nu\mu}(x) - B_{\nu\mu}(x_j) = O\left(\varepsilon^{\frac{2}{5}}\right)$, which together with the preceding estimate proves the lemma by the Schwarz inequality. □

**2.2.3. Proof of Theorem 2.10.** We split the proof of the theorem in two parts by estimating the term $\frac{E_n(\varepsilon)}{\varepsilon}$ in the limit $\varepsilon \to 0$ from above (2.91) and from below (2.101) by $e_n$, which together give the equality (2.36).

**Estimate from above:**

$$\frac{E_n(\varepsilon)}{\varepsilon} \le e_n + O\left(\varepsilon^{\frac{1}{5}}\right) \qquad \text{for} \quad \varepsilon \to 0 . \tag{2.91}$$

The statement (2.91) can be shown using the preceding Lemmata and estimates.
At first we use the points (a) and (c) in Lemma 2.13, leading to the estimate

$$\begin{aligned} \left\langle g^\varepsilon_{\alpha j}\, ,\, H_\varepsilon\, g^\varepsilon_{\beta l} \right\rangle_{\ell^2} &= \left\langle g^\varepsilon_{\alpha j}\, ,\, \chi_{j,\varepsilon} H_\varepsilon \chi_{j,\varepsilon}\, g^\varepsilon_{\beta l} \right\rangle_{\ell^2} + O\left(\varepsilon^{\frac{6}{5}}\right) \\ &= \left\langle g^\varepsilon_{\alpha j}\, ,\, \chi_{j,\varepsilon}\, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon}) T_\varepsilon\, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon}) \chi_{j,\varepsilon}\, g^\varepsilon_{\beta l}) \right\rangle_{\ell^2} + \left\langle g^\varepsilon_{\alpha j}\, ,\, \chi_{j,\varepsilon} V_\varepsilon \chi_{j,\varepsilon}\, g^\varepsilon_{\beta l} \right\rangle_{\ell^2} + O\left(\varepsilon^{\frac{6}{5}}\right) . \end{aligned} \tag{2.92}$$

By Proposition B.9 in Appendix B, localized at the critical points with respect to $x$ and $\xi$ simultaneously, $T_\varepsilon$ can (modulo terms of order $\varepsilon^{\frac{6}{5}}$) be replaced by its quadratic approximation $T_{\varepsilon,q,j}$ at the point $x_j$. Furthermore by (2.43) we can replace $V_\varepsilon$ localized at $x_j$ by the quadratic approximation $V_\varepsilon^j$ given in (2.35). Thus

$$\begin{aligned} &\left\langle g^\varepsilon_{\alpha j}\, ,\, H_\varepsilon\, g^\varepsilon_{\beta l} \right\rangle_{\ell^2} \\ &\quad = \left\langle g^\varepsilon_{\alpha j}\, ,\, \chi_{j,\varepsilon}\, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon}) T_{\varepsilon,q,j}\, \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon})\, \chi_{j,\varepsilon} g^\varepsilon_{\beta l} \right\rangle_{\ell^2} + \left\langle g^\varepsilon_{\alpha j}\, ,\, \chi_{j,\varepsilon} V_\varepsilon^j \chi_{j,\varepsilon}\, g^\varepsilon_{\beta l} \right\rangle_{\ell^2} + O\left(\varepsilon^{\frac{6}{5}}\right) \\ &\quad = \varepsilon^{-d} \left( \left\langle g_{\alpha j}\, ,\, \chi_{j,\varepsilon}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \widehat{T}_{q,j}\, \mathrm{Op}_\varepsilon(\phi_{0,\varepsilon}) \chi_{j,\varepsilon} g_{\beta l} \right\rangle_{\mathscr{L}^2} + \left\langle g_{\alpha j}\, ,\, \chi_{j,\varepsilon} V_\varepsilon^j \chi_{j,\varepsilon}\, g_{\beta l} \right\rangle_{\mathscr{L}^2} + O\left(\varepsilon^{\frac{6}{5}}\right) \right) , \end{aligned}$$

where for the second step, the transition from (functions and scalar product in) $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ to $\mathscr{L}^2\left(\mathbb{R}^d\right)$, we used Lemma 2.14,(a) and (b).

Point (d) and (e) of Lemma 2.13 yield

$$\left\langle g_{\alpha j}\,,\,\chi_{j,\varepsilon}\operatorname{Op}_\varepsilon(\phi_{0,\varepsilon})\widehat{T}_{q,j}\,\operatorname{Op}_\varepsilon(\phi_{0,\varepsilon})\chi_{j,\varepsilon}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}+\left\langle g_{\alpha j}\,,\,\chi_{j,\varepsilon}V_\varepsilon^j\chi_{j,\varepsilon}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}=\left\langle g_{\alpha j}\,,\,\widehat{T}_{q,j}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}+\left\langle g_{\alpha j}\,,\,V_\varepsilon^j\,g_{\beta l}\right\rangle_{\mathscr{L}^2}+O\left(\varepsilon^{\frac{6}{5}}\right)\,. \tag{2.93}$$

By use of Appendix A.2, we can perform a coordinate transformation to pass over from $\widehat{H}^j$ given by (2.47) to the diagonalized $H^j$ given by (2.48), therefore

$$\left\langle g_{\alpha j}\,,\,\widehat{T}_{q,j}\,g_{\beta l}\right\rangle_{\mathscr{L}^2}+\left\langle g_{\alpha j}\,,\,V_\varepsilon^j\,g_{\beta l}\right\rangle_{\mathscr{L}^2}=\left\langle g_{\alpha j}\,,\,\widehat{H}^j\,g_{\beta l}\right\rangle_{\mathscr{L}^2}=\left\langle g_{\alpha j}\,,\,H^j\,g_{\beta l}\right\rangle_{\mathscr{L}^2}\,. \tag{2.94}$$

Since $H^jg_{\alpha j}=\varepsilon e_{n(\alpha,j)}g_{\alpha j}$, the estimates (2.92) to (2.94) can be combined to give

$$\left\langle g^\varepsilon_{\alpha j}\,,\,H_\varepsilon\,g^\varepsilon_{\beta l}\right\rangle_{\ell^2}=\varepsilon^{-d}\left(\varepsilon\,e_{m(\alpha,j)}\delta_{m(\alpha,j),n(\beta,l)}+O\left(\varepsilon^{\frac{6}{5}}\right)\right)\,, \tag{2.95}$$

where $m(\alpha,j)$ and $n(\beta,l)$ are the numbers of the eigenvalues corresponding to the pairs $(\alpha,j)$ and $(\beta,l)$. The estimate (2.91) follows from (2.95), if we use the Min-Max-formula for a fixed, sufficiently small $\varepsilon$. Choose $(n-1)$ linear independent elements $\zeta_1,\dots\zeta_{n-1}$ of the domain of $H_\varepsilon$ and define

$$Q(\zeta_1,\dots\zeta_{n-1}):=\inf\left\{\langle\psi\,,\,H_\varepsilon\,\psi\rangle_{\ell^2}\;|\;\psi\in\mathscr{D}(H_\varepsilon),\;\|\psi\|=1,\;\psi\in[\zeta_1,\dots\zeta_{n-1}]^\perp\right\} \tag{2.96}$$

and

$$E_n(\varepsilon):=\sup_{\zeta_1,\cdots\zeta_{n-1}}Q(\zeta_1,\dots\zeta_{n-1})\,. \tag{2.97}$$

By Theorem B.12 in Appendix B.5, which is an analog of Persson's Theorem on the infimum of the essential spectrum in the discrete setting, Hypothesis 2.7 ensures that $\inf\sigma_{ess}(H_\varepsilon)\geq c>0$. Since $E_n(\varepsilon)$ is by (2.95) of order $\varepsilon$, it belongs for $\varepsilon$ small enough to the discrete spectrum. Thus the Min-Max principle shows that $E_1(\varepsilon)\leq E_2(\varepsilon)\leq\ldots\leq E_n(\varepsilon)$ are the first (ordered by magnitude) $n$ eigenvalues of $H_\varepsilon$.

For $\lambda>0$ we can choose $\zeta_1,\dots\zeta_{n-1}$, such that

$$E_n(\varepsilon)\leq Q(\zeta_1,\dots\zeta_{n-1})+\lambda\,. \tag{2.98}$$

To deal with the factor $\varepsilon^{-d}$ in (2.95), we use the estimate

$$\left\langle g^\varepsilon_{\alpha j}\,,\,g^\varepsilon_{\beta l}\right\rangle_{\ell^2}=\varepsilon^{-d}\left(\langle g_{\alpha j}\,,\,g_{\beta l}\rangle_{\mathscr{L}^2}+O(\sqrt{\varepsilon})\right)\,, \tag{2.99}$$

which follows from the following considerations. Similar to the proof of Lemma 2.14, we use the identity $\varepsilon^d=\int_{[x,x+\varepsilon[^d}dy$, to write

$$\begin{aligned}\langle f^\varepsilon\,,\,g^\varepsilon\rangle_{\ell^2}&=\sum_{x\in(\varepsilon\mathbb{Z})^d}f^\varepsilon(x)\,g^\varepsilon(x)\\&=\frac{1}{\varepsilon^d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\int_{[x,x+\varepsilon[^d}\left\{(f(x)-f(y))\,g(x)+f(y)\,(g(x)-g(y))+f(y)g(y)\right\}\,dy\,.\end{aligned}$$

The last summand is equal to the scalar product in $\mathscr{L}^2(\mathbb{R}^d)$ multiplied by the factor $\varepsilon^{-d}$. By (2.89), the first two summands in the integral are of order $\varepsilon^{\frac{1}{2}-d}$, thus (2.99) is shown.

It follows from (2.99) that for $\varepsilon>0$ sufficiently small, the functions $g^\varepsilon_{\alpha j}\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ are linearly independent. Thus the functions associated to the first $n$ eigenvalues of $H^j$ span an $n$-dimensional space, which we denote by $\mathscr{M}_n$. Then $\mathscr{N}:=\mathscr{M}_n\cap[\zeta_1,\dots\zeta_{n-1}]^\perp$ is at least one dimensional. Thus there exists a function $\psi\in\mathscr{N}$ with $\|\psi\|=1$ and it follows from (2.95) and (2.96) that

$$Q(\zeta_1,\dots\zeta_{n-1})\leq\langle\psi\,,\,H_\varepsilon\,\psi\rangle_{\ell^2}\leq\;\varepsilon\,e_n+O\left(\varepsilon^{\frac{6}{5}}\right) \tag{2.100}$$

Since $\lambda$ is arbitrary, we have by (2.97) and (2.100)

$$E_n(\varepsilon)\leq\varepsilon\,e_n+O\left(\varepsilon^{\frac{6}{5}}\right)$$

proving (2.91).

**Estimate from below:**

$$\frac{E_n(\varepsilon)}{\varepsilon} \geq e_n + O\left(\varepsilon^{\frac{1}{5}}\right) \qquad \text{for} \quad \varepsilon \to 0 \tag{2.101}$$

As in the first part of the proof, we will use the cut-off functions $\chi_{j,\varepsilon}$ and $\tilde{\phi}_k$ defined in (2.41) and (2.45) (which are scaled by $\varepsilon^{-\frac{2}{5}}$) and the corresponding function $\phi_k$ on $\mathbb{R}^d$.

Let $l \leq n-1$ such that $e_n = e_{n-1} = \ldots = e_{l+1} > e_l$, where $e_r$ denotes the $r$-th eigenvalue of $K$ for $r \in \mathbb{N}^*$ and $e_0 := -\infty$. Let $e \in (e_l, e_n)$, particularly $e \notin \sigma(\bigoplus_j K_j)$. Then we claim that there exists a constant $C > 0$ such that

$$\langle \psi \,,\, H_\varepsilon \,\psi\rangle_{\ell^2} \geq \varepsilon\, e \langle \psi \,,\, \psi\rangle_{\ell^2} + \langle \psi \,,\, R_l \,\psi\rangle_{\ell^2} - C\|\psi\|^2_{\ell^2}\varepsilon^{\frac{6}{5}}\,, \qquad \psi \in \mathscr{D}(H_\varepsilon)\,, \tag{2.102}$$

for some symmetric operator $R_l$ with $\operatorname{rank} R_l \leq l$. This implies (2.101). To see this implication, let $\psi \in \mathscr{M}_n$ with $\|\psi\| = 1$. From the Mini-Max-formula it follows

$$E_n(\varepsilon) \geq \langle \psi \,,\, H_\varepsilon \,\psi\rangle_{\ell^2} \,. \tag{2.103}$$

On the other hand there exists a $\psi \in \mathscr{M}_n \cap \ker R_l$, since $\dim\ker\left(R_l|_{\mathscr{M}_n}\right) \geq 1$. For this $\psi$ the inequality (2.102) yields

$$\langle \psi \,,\, H_\varepsilon \,\psi\rangle_{\ell^2} \geq \varepsilon\, e + O\left(\varepsilon^{\frac{6}{5}}\right) \,. \tag{2.104}$$

which together with (2.103) gives (2.101). It therefore suffices to show (2.102).

By Lemma 2.12, $H_\varepsilon$ splits as

$$H_\varepsilon = \sum_{j=1}^m \chi_{j,\varepsilon} H_\varepsilon \chi_{j,\varepsilon} + \chi_{0,\varepsilon} H_\varepsilon \chi_{0,\varepsilon} + O\left(\varepsilon^{\frac{6}{5}}\right)\,, \tag{2.105}$$

where the estimate on the error term in the following estimates is understood with respect to operator norm. $\chi_{0,\varepsilon}$ is supported in the region outside of the wells, thus $|x - x_j| > \varepsilon^{\frac{2}{5}}$ for $1 \leq j \leq m$ and $x \in \operatorname{supp}\chi_{0,\varepsilon}$. Since the potential is of second order in $x$ or of order $\varepsilon$, we have for $\varepsilon$ sufficiently small and $e < e_n$

$$\chi_{0,\varepsilon} H_\varepsilon \chi_{0,\varepsilon} \geq \chi_{0,\varepsilon} V_\varepsilon \chi_{0,\varepsilon} \geq \varepsilon\, e\, \chi^2_{0,\varepsilon} \,. \tag{2.106}$$

In the neighborhoods of the wells, (2.43) allows to approximate the potential by the quadratic term, therefore (2.43) and (2.106) give

$$H_\varepsilon \geq \sum_{j=1}^m \chi_{j,\varepsilon}(T_\varepsilon + V^j_\varepsilon)\chi_{j,\varepsilon} + \varepsilon\, e\, \chi^2_{0,\varepsilon} + O\left(\varepsilon^{\frac{6}{5}}\right) \,. \tag{2.107}$$

In the first summand we introduce the partition of unity (2.45) in momentum space and get by Lemma 2.12

$$\begin{aligned}\sum_{j=1}^m \chi_{j,\varepsilon}(T_\varepsilon + V^j_\varepsilon)\chi_{j,\varepsilon} &= \sum_{j=1}^m \chi_{j,\varepsilon}(x)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_0)(T_\varepsilon + V^j_\varepsilon)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_0)\chi_{j,\varepsilon}(x) + \\ &\quad + \sum_{j=1}^m \chi_{j,\varepsilon}(x)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1)(T_\varepsilon + V^j_\varepsilon)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1)\chi_{j,\varepsilon}(x) + O\left(\varepsilon^{\frac{6}{5}}\right) \,.\end{aligned} \tag{2.108}$$

By use of the norm estimates for the operator localized simultaneously with respect to $x$ and $\xi$ given in Proposition B.9 (Appendix B), it is modulo terms of order $O\left(\varepsilon^{\frac{6}{5}}\right)$ possible to replace $T_\varepsilon$ by $T_{\varepsilon,q,j}$ in the region localized at $\xi = 0$ and $x = x_j$. The function $\tilde{\phi}_1$ is supported in the exterior region with $|\xi| > \varepsilon^{\frac{2}{5}}$, thus we have by arguments similar to those leading to (2.106)

$$\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1)(T_\varepsilon + V^j_\varepsilon)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1) \geq \varepsilon\, e\, \operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1)^2 \,. \tag{2.109}$$

Substituting (2.109) in (2.108), replacing $T_\varepsilon$ by $T_{\varepsilon,q,j}$ in the first summand of (2.108) and substituting the resulting equation in (2.107) yields

$$\begin{aligned}H_\varepsilon &\geq \sum_{j=1}^m \chi_{j,\varepsilon}(x)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_0)\left(T_{\varepsilon,q,j} + V^j_\varepsilon\right)\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_0)\chi_{j,\varepsilon}(x) \\ &\quad + \varepsilon\, e \sum_{j=1}^m \chi_{j,\varepsilon}(x)\left(\operatorname{Op}^{\mathbb{T}^d}_\varepsilon(\tilde{\phi}_1)\right)^2\chi_{j,\varepsilon}(x) + \varepsilon\, e\chi^2_{0,\varepsilon} + O\left(\varepsilon^{\frac{6}{5}}\right) \,.\end{aligned} \tag{2.110}$$

By the isometry of the Fourier transform the expectation value of the first summand of (2.110) can be written as

$$\sum_{j=1}^m \left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_0)\chi_{j,\varepsilon}(x)\psi\,,\,(T_{\varepsilon,q,j}+V_\varepsilon^j)\ \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_0)\chi_{j,\varepsilon}(x)\psi\right\rangle_{\ell^2} \tag{2.111}$$
$$=\sum_{j=1}^m \left\langle \tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,(t_{\pi,q,j}+\mathscr{F}_\varepsilon^{-1}V_\varepsilon^j\mathscr{F}_\varepsilon)\,\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}}.$$

The cut-off function $\tilde\phi_0$ restricts the integration from the torus to the neighborhood of the origin scaled by $\varepsilon^{-\frac{2}{5}}$. For $\varepsilon$ sufficiently small we therefore can pass from the scalar product in $\mathscr{L}^2\left(\mathbb{T}^d\right)$ defined in (2.2) to the scalar product in $\mathscr{L}^2\left(\mathbb{R}^d\right)$, if we simultaneously replace $\tilde\phi_0$ by $\phi_0$ and $t_{\pi,q,j}$ by $t_{q,j}$. This follows from the fact, that the range of the integral is in both cases restricted to the support of $\phi_0$. Changing variables as described in Appendix A.2, we can pass from $\widehat{H}^j$ to $H^j$. Moreover $\mathscr{F}_\varepsilon^{-1}V_\varepsilon^j\mathscr{F}_\varepsilon = F_\varepsilon^{-1}V_\varepsilon^jF_\varepsilon$ and $F_\varepsilon\langle\xi\,,\,\xi\rangle F_\varepsilon^{-1}=-\varepsilon^2\Delta$, thus we get, for $j=0,\dots m$,

$$\left\langle \tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,(t_{\pi qj}+\mathscr{F}_\varepsilon^{-1}V_\varepsilon^j\mathscr{F}_\varepsilon)\,\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}} \tag{2.112}$$
$$=\left\langle \phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,(F_\varepsilon^{-1}H^jF_\varepsilon)\,\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathscr{L}^2}.$$

We introduce the spectral decomposition of $F_\varepsilon^{-1}H^jF_\varepsilon$ and denote by $l_j$ the number of eigenvalues of $H^j$ below $e$. Thus $e_{l_j}\le e_l<e$ for all $j$ and $\sum_{j=1}^m l_j=l$. By replacing all eigenvalues $e_{k_j}>e$ of $H^j$ by $e$ we get

$$(F_\varepsilon^{-1}H^jF_\varepsilon)=\varepsilon\sum_{k_j}e_{k_j}\Pi^j_{k_j}\ge\varepsilon\sum_{k_j\le l_j}e_{k_j}\,\Pi^j_{k_j}+\varepsilon\,e\,(\mathbf{1}-\sum_{k_j\le l_j}\Pi^j_{k_j})\,, \tag{2.113}$$

where $\Pi^j_{k_j}$ denotes the projection on the eigenspace to the $k_j$-th eigenvalue of $H^j$. Inserting (2.113) into the right hand side of (2.112) and going back to the scalar product on $\mathscr{L}^2\left(\mathbb{T}^d\right)$ again by replacing $\phi_0$ by $\tilde\phi_0$ yields

$$\sum_{j=1}^m \left\langle \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_0)\chi_{j,\varepsilon}(x)\psi\,,\,(T_{\varepsilon,q,j}+V_\varepsilon^j)\ \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_0)\chi_{j,\varepsilon}(x)\psi\right\rangle_{\ell^2}$$
$$\ge\sum_{j=1}^m\Big\{\left\langle\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,\varepsilon\textstyle\sum_{k_j}(e_{k_j}-e)\Pi^j_{k_j}\tilde\phi_0\mathscr{F}_\varepsilon{}^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}}$$
$$+\varepsilon\,e\left\langle\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}}\Big\} \tag{2.114}$$

Thus by (2.114) together with (2.110) there exists a constant $C>0$ such that

$$\langle\psi\,,\,H_\varepsilon\,\psi\rangle_{\ell^2}\ge\varepsilon\,e\sum_{j=1}^m\left\langle\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,\tilde\phi_0\mathscr{F}_\varepsilon{}^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}} \tag{2.115}$$
$$+\sum_{j=1}^m\left\langle\tilde\phi_0\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,(\varepsilon\textstyle\sum_{k\le l_j}(e_k-e)\Pi^j_k)\,\tilde\phi_0\mathscr{F}_ep^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}}$$
$$+\varepsilon\,e\sum_{j=1}^m\left\langle\tilde\phi_1\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\,,\,\tilde\phi_1\mathscr{F}_\varepsilon^{-1}(\chi_{j,\varepsilon}\psi)\right\rangle_{\mathbb{T}}$$
$$+\varepsilon\,e\left\langle(\mathscr{F}_\varepsilon^{-1}\chi_{0,\varepsilon}\psi)\,,\,(\tilde\phi_0^2+\tilde\phi_1^2)(\mathscr{F}_\varepsilon{}^{-1}\chi_{0,\varepsilon}\psi)\right\rangle_{\mathbb{T}}-C\varepsilon^{\frac{6}{5}}\|\psi\|^2_{\ell^2}.$$

The introduction of $\tilde\phi_0^2+\tilde\phi_1^2=\mathbf{1}$ in the last summand allows us to combine this term with the first and third summand. Since $\mathrm{rank}(A+B)\le\mathrm{rank}\,A+\mathrm{rank}\,B$ and $\mathrm{rank}\,\Pi^j_{k_j}=1$, the operators in the scalar products contributing to the second summand has rank $l_j$. The restriction by the cut-off functions does not increase the rank and moreover $\sum_{j=1}^m l_j=l$, thus the rank of the operator defined by

$$R_l:=\sum_{j=1}^m(\mathscr{F}_\varepsilon{}^{-1}\chi_{j,\varepsilon}\mathscr{F}_\varepsilon)\tilde\phi_0\sum_{k\le l_j}(\varepsilon(e_k-e)\Pi^j_k)\tilde\phi_0(\mathscr{F}_\varepsilon{}^{-1}\chi_{j,\varepsilon}\mathscr{F}_\varepsilon)$$

is at most equal to $l$. The right hand side of equation (2.115) can therefore for some $C > 0$ be written as

$$\varepsilon\, e \sum_{j=0}^{m} \Big\langle \tilde{\phi}_0(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}\psi)\,,\, \tilde{\phi}_0(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}\psi)\Big\rangle_{\mathbb{T}} + \big\langle \mathscr{F}_\varepsilon^{-1}\psi\,,\, R_l\,({\mathscr{F}_\varepsilon}^{-1}\psi)\big\rangle_{\mathbb{T}}$$
$$+\,\varepsilon\, e \sum_{j=0}^{m} \Big\langle \tilde{\phi}_{1,\varepsilon}(\mathscr{F}_\varepsilon^{-1}\chi_{j,\varepsilon}\psi)\,,\, \tilde{\phi}_{1,\varepsilon}({\mathscr{F}_\varepsilon}^{-1}\chi_{j,\varepsilon}\psi)\Big\rangle_{\mathbb{T}} - C\varepsilon^{\frac{6}{5}}\|\psi\|^2_{\ell^2}\,. \quad (2.116)$$

Again the first and third summand can be combined so that the cut-off functions in both spaces add up to **1**. We thus get by (2.115) and (2.116) that for some $C > 0$

$$\langle \psi\,,\, H_\varepsilon\,\psi\rangle_{\ell^2} \geq \varepsilon\, e\langle \psi\,,\, \psi\rangle_{\ell^2} + \langle \psi\,,\, A_l\psi\rangle_{\ell^2} - C\varepsilon^{\frac{6}{5}}\|\psi\|^2_{\ell^2}\,, \quad (2.117)$$

where $A_l := {\mathscr{F}_\varepsilon}^{-1} R_l \mathscr{F}_\varepsilon$ is again an operator of at least rank $l$, because the rank of an operator is not changed by taking the Fourier transform. Thus it is shown that (2.102) holds and by the considerations at the beginning of the second part of the proof, the assertion (2.101) follows. Combined with (2.91), this completes the proof of Theorem 2.10.

□

## 2.3. Probabilistic Operator

Returning to the situation described in the introduction, we will show the applicability of Theorem 2.10 to Hamilton operators appearing in the discussion of questions connected to the thermodynamic limit of the dynamics in metastable mean field spin chains.

To this end we have to check wether the operators induced by a Markov chain, which we call probabilistic operators, satisfy the conditions described in Hypothesis 2.7.

First we describe a general notion of a probabilistic operator, then we give an example and analyze it more precisely.

Let us consider a family $\{\mu_\varepsilon\}_{\varepsilon\in(0,\varepsilon_0]}$ such that the function $\mu_\varepsilon : (\varepsilon\mathbb{Z})^d \to (0,1]$ denotes a probability measure on the lattice $(\varepsilon\mathbb{Z})^d$. Then a Markov chain is described by means of a "transition matrix" $P_\varepsilon : (\varepsilon\mathbb{Z})^d \times (\varepsilon\mathbb{Z})^d \to [0,1]$, where $P_\varepsilon(x,y)$ is interpreted as the probability of the transition from $x \in (\varepsilon\mathbb{Z})^d$ to $y \in (\varepsilon\mathbb{Z})^d$. $P_\varepsilon$ is a stochastic matrix, thus

$$\sum_{y\in(\varepsilon\mathbb{Z})^d} P_\varepsilon(x,y) = 1\,, \qquad x \in (\varepsilon\mathbb{Z})^d\,. \quad (2.118)$$

We assume that $P_\varepsilon$ satisfies the detailed balance condition, i.e.

$$\mu_\varepsilon(x)P_\varepsilon(x,y) = \mu_\varepsilon(y)P_\varepsilon(y,x)\,. \quad (2.119)$$

Then $(1 - P_\varepsilon)$ defines a self adjoint diffusion operator on $\ell^2\left((\varepsilon\mathbb{Z})^d, \mu_\varepsilon\right)$ via

$$(1 - P_\varepsilon)u(x) = u(x) - \sum_{y\in(\varepsilon\mathbb{Z})^d} P_\varepsilon(x,y)u(y)\,.$$

In fact $P_\varepsilon$ is a bounded operator on $\ell^2((\varepsilon\mathbb{Z})^d, \mu_\varepsilon)$ with $\|P_\varepsilon\| = 1$. To see this, we first notice that by (2.118)

$$|P_\varepsilon u(x)|^2 = \left(\sum_{y\in(\varepsilon\mathbb{Z})^d} P_\varepsilon(x,y)\right)\left(\sum_{\gamma} P_\varepsilon(x,y)|u(y)|^2\right)$$
$$= \sum_{\gamma} P_\varepsilon(x,y)|u(y)|^2\,.$$

This yields by (2.119), the Fubini-Theorem and again (2.118)

$$\begin{aligned}\|P_\varepsilon u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d,\mu_\varepsilon)} &= \sum_{x\in(\varepsilon\mathbb{Z})^d}\mu_\varepsilon(x)|P_\varepsilon u(x)|^2 = \sum_x \mu_\varepsilon(x)\sum_y P_\varepsilon(x,y)|u(y)|^2\\ &= \sum_y\left(\sum_x P_\varepsilon(y,x)\right)\mu_\varepsilon(y)|u(y)|^2\\ &= \|u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d,\mu_\varepsilon)}\ .\end{aligned}$$

The symmetry follows from (2.119), since for $u,v\in\ell^2((\varepsilon\mathbb{Z})^d,\mu_\varepsilon)$

$$\begin{aligned}\langle u\,,\,P_\varepsilon v\rangle_{\ell^2((\varepsilon\mathbb{Z})^d,\mu_\varepsilon)} &= \sum_{x\in(\varepsilon\mathbb{Z})^d}\mu_\varepsilon(x)u(x)\sum_{y\in(\varepsilon\mathbb{Z})^d}P_\varepsilon(x,y)v(y)\\ &= \sum_y\sum_x \mu_\varepsilon(y)P_\varepsilon(y,x)u(x)v(y) = \langle P_\varepsilon u\,,\,v\rangle_{\ell^2((\varepsilon\mathbb{Z})^d,\mu_\varepsilon)}\end{aligned}$$

Conjugation with respect to the measure $\mu_\varepsilon$ induces a bounded self adjoint operator $H_\varepsilon := \mu_\varepsilon^{\frac{1}{2}}(1-P_\varepsilon)\mu_\varepsilon^{-\frac{1}{2}}$ on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, whose restriction to $\mathcal{K}((\varepsilon\mathbb{Z})^d)$ is given by

$$H_\varepsilon u(x) = u(x) - \mu_\varepsilon^{\frac{1}{2}}(x)\sum_\gamma P_\varepsilon(x,x+\gamma)\mu_\varepsilon^{-\frac{1}{2}}(x+\gamma)u(x+\gamma)\ ,\quad u\in\mathcal{K}((\varepsilon\mathbb{Z})^d) \tag{2.120}$$

Note that $\mathcal{K}((\varepsilon\mathbb{Z})^d)$ is dense in $\ell^2((\varepsilon\mathbb{Z})^d)$ and $H_\varepsilon$ is linear continuous and is therefore completely determined by (2.120). In the following we will supress the mention to the $\varepsilon$-dependance of $\mu_\varepsilon$ by writing simply $\mu$.

To get the standard form $H_\varepsilon = T_\varepsilon + V_\varepsilon$, where $T_\varepsilon$ is a discrete kinetic operator in the sense of Definition 2.4 and $V_\varepsilon$ is a potential energy, we use (2.118) and add $a-a$ with $a := \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)u(x)$ to get

$$\begin{aligned}H_\varepsilon u(x) &= \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x)u(x) - \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)u(x)\\ &\quad+\sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)u(x) - \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}u(x+\gamma)\\ &= \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)(u(x)-u(x+\gamma))\\ &\qquad+\sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\left(\mu^{-\frac{1}{2}}(x)-\mu^{-\frac{1}{2}}(x+\gamma)\right)u(x)\ .\end{aligned}$$

Then $H_\varepsilon = T_\varepsilon + V_\varepsilon$, where

$$\begin{aligned}T_\varepsilon(x) &:= \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)(\mathbf{1}-\tau_\gamma)\\ V_\varepsilon(x) &:= \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\left(\mu^{-\frac{1}{2}}(x)-\mu^{-\frac{1}{2}}(x+\gamma)\right)\ .\end{aligned}$$

Comparing $T_\varepsilon$ with the Fourier expansion (2.20) for a general discrete kinetic energy operator, the Fourier coefficients are given by

$$a_0(x) = \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)\geq 0 \tag{2.121}$$

$$a_\gamma(x) = -\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)\ ,\quad \gamma\neq 0\ . \tag{2.122}$$

Thus we see that in the case of probabilistic operators, the condition $a_\gamma\leq 0$ for $\gamma\neq 0$, which by Lemma 2.6, (b) insures the positivity of $T_\varepsilon$, is always fulfilled. The detailed balance condition for $P_\varepsilon$ ensures the symmetry of $T_\varepsilon$ as follows. By (2.119)

$$\begin{aligned}\mu^{\frac{1}{2}}(x)a_\gamma(x) &= -\mu(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma) =\\ &= -\mu(x+\gamma)P_\varepsilon(x+\gamma,x)\mu^{-\frac{1}{2}}(x+\gamma) =\\ &= -\mu^{\frac{1}{2}}(x+\gamma)P_\varepsilon(x+\gamma,x)\ .\end{aligned}$$

On the other hand,

$$\begin{aligned} \mu^{\frac{1}{2}}(x)a_{-\gamma}(x+\gamma) &= -\mu^{\frac{1}{2}}(x)\mu^{\frac{1}{2}}(x+\gamma)P_\varepsilon(x+\gamma,x)\mu^{-\frac{1}{2}}(x) = \\ &= -\mu^{\frac{1}{2}}(x+\gamma)P_\varepsilon(x+\gamma,x)\ , \end{aligned}$$

thus $a_\gamma(x) = a_{-\gamma}(x+\gamma)$ and by Lemma 2.6,(a) the operator $T_\varepsilon$ is symmetric. Therefore $T_\varepsilon$ is a discrete kinetic energy operator in the sense of Definition 2.4, if the first three conditions on the associated phase space function $t$ are fulfilled. Writing $t(x,\xi)$ in the form (2.17), these conditions follow from the fact that

$$a_0 - \sum_{\gamma\neq 0} a_\gamma = 0 \tag{2.123}$$

for $a_0, a_\gamma$ given by (2.121) and (2.122) respectively. (2.123) gives at once, that $t(x,0)=0$ and by the sign of $a_\gamma$

$$\begin{aligned} t(x,\xi) &= a_0 + \sum_{\gamma\neq 0} a_\gamma e^{-\frac{i}{\varepsilon}\gamma\cdot\xi} \geq a_0 - \sum_{\gamma\neq 0} |a_\gamma(x)||e^{-\frac{i}{\varepsilon}\gamma\cdot\xi}| \geq \\ &\geq a_0 - \sum_{\gamma\neq 0}|a_\gamma(x)| = \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma = 0 \end{aligned}$$

Since on the other hand for each $\xi \neq 0$ there exist $\gamma \neq 0$ such that $e^{-\frac{i}{\varepsilon}\gamma\cdot\xi} \neq 1$, the function $t$ is strictly positive for $\xi \neq 0$. As discussed in Remark 2.5, (d), the matrix $B$ is symmetric and since for $\gamma \neq 0$ all $a_\gamma$ are smaller or equal to zero, it is positive definite. Thus the kinetic energy operator of a probabilistic operator is a discrete kinetic energy in the sense of Definition 2.4, if the stochastic terms $\mu$ and $P_\varepsilon$ can be interpreted as lattice restrictions of functions in $\mathscr{C}^\infty\left(\mathbb{R}^d\right)$.

By acting with $T_\varepsilon$ on $\mu^{\frac{1}{2}}$ and multiplying with $\mu^{-\frac{1}{2}}$, we get

$$\begin{aligned} \mu^{-\frac{1}{2}}(x)\left(T_\varepsilon\mu^{\frac{1}{2}}\right)(x) &= \mu^{-\frac{1}{2}}(x)\sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\mu^{-\frac{1}{2}}(x+\gamma)\left(\mu^{\frac{1}{2}}(x)-\mu^{\frac{1}{2}}(x+\gamma)\right) = \\ &= \sum_{\gamma\neq 0}\mu^{\frac{1}{2}}(x)P_\varepsilon(x,x+\gamma)\left(\mu^{-\frac{1}{2}}(x+\gamma)-\mu^{-\frac{1}{2}}(x)\right)\ , \end{aligned}$$

and thus for a general probabilistic operator, the potential energy can be written in terms of the kinetic energy and the measure $\mu_\varepsilon$ as

$$V_\varepsilon(x) = -\mu_\varepsilon^{-\frac{1}{2}}(x)\left(T_\varepsilon\mu_\varepsilon^{\frac{1}{2}}\right)(x)\ . \tag{2.124}$$

The assumptions on $V_0$ given in Hypothesis 2.7 must be reflected in the form of the measure $\mu$ and the transition matrix $P_\varepsilon$. In the following, we will analyze an example, where $\mu_\varepsilon$ is the Boltzmann measure induced by terms of a free energy functional $F$.

We assume that we can associate an smooth energy functional $F:\mathbb{R}^d \longrightarrow \mathbb{R}$ to the configuration space, the "free energy" of the system, having only non-degenerate critical points. Then we can associate to each lattice point $x\in(\varepsilon\mathbb{Z})^d$ the Boltzmann measure $\mu_\varepsilon(x) := Z_\varepsilon^{-1}e^{-\frac{F(x)}{\varepsilon}}$ with the state sum $Z_\varepsilon = \sum_x e^{-\frac{F(x)}{\varepsilon}}$ as normalizing factor. We define a transition matrix $P_\varepsilon$ on $(\varepsilon\mathbb{Z})^d$, where the only transitions which are allowed, are those to neighboring lattice points, by

$$P_\varepsilon(x,x+\gamma) := \begin{cases} \frac{\sqrt{\mu(x+\gamma)}}{\sqrt{\mu(x)}} & ,|\gamma| = \varepsilon \\ 0 & ,|\gamma|>\varepsilon \\ 1-\sum_{\gamma>0}\frac{\sqrt{\mu(x+\gamma)}}{\sqrt{\mu(x)}} & ,\gamma = 0. \end{cases}$$

As described in the general case, kinetic and potential energy of the induced Hamilton operator $H_\varepsilon = T_\varepsilon + V_\varepsilon$ are given by

$$T_\varepsilon := 2d - \sum_{\nu=1}^{d}(\tau_{\varepsilon e_\nu} + \tau_{-\varepsilon e_\nu}) = -\Delta_\varepsilon \tag{2.125}$$

equal to the discrete Laplacian defined in (2.60) and

$$V_\varepsilon = \sum_{|\gamma|=\varepsilon}\mu^{-\frac{1}{2}}(\tau_\gamma\mu^{\frac{1}{2}}) - 2d = -\mu^{-\frac{1}{2}}(T_\varepsilon\mu^{\frac{1}{2}})\ .$$

By Appendix A.3 the symbol associated to (2.125) is

$$t(\xi) = 2d - 2\sum_{\nu=1}^{d} \cos(\xi_\nu), \qquad \xi \in \mathbb{T}^d,$$

therefore the Taylor expansion of $t$ at $\xi = 0$ is

$$t(\xi) = 2d - 2\sum_{\nu=1}^{d} \left(1 - \frac{\xi_\nu^2}{2} + \frac{\xi_\nu^4}{4!} + O\left(|\xi|^6\right)\right)$$

and thus has the form assumed in Definition 2.4.

The potential energy can be computed as

$$\begin{aligned} V_\varepsilon(x) &= -e^{\frac{F(x)}{2\varepsilon}} (T_\varepsilon\, e^{-\frac{F(x)}{2\varepsilon}}) \\ &= -2d + \sum_{\nu=1}^{d} e^{\frac{F(x)}{2\varepsilon}} \left(e^{-\frac{F(x+\varepsilon e_\nu)}{2\varepsilon}} + e^{-\frac{F(x-\varepsilon e_\nu)}{2\varepsilon}}\right). \end{aligned} \tag{2.126}$$

To verify equations (2.26) and (2.35) for this potential, we make a Taylor expansion of $F(x \pm \varepsilon e_\nu)$ at $x$ to get

$$\begin{aligned} V_\varepsilon &= -2d + \sum_{\nu=1}^{d} \left(e^{-\frac{1}{2\varepsilon}(\partial_\nu F(x)\varepsilon + \frac{1}{2}\partial_\nu^2 F(x)\varepsilon^2 + O(\varepsilon^3))} + e^{-\frac{1}{2\varepsilon}(-\partial_\nu F(x)\varepsilon + \frac{1}{2}\partial_\nu^2 F(x)\varepsilon^2 + O(\varepsilon^3))}\right) \\ &= -2d + \sum_{\nu=1}^{d} \left(e^{-\frac{1}{2}\partial_\nu F(x)} + e^{\frac{1}{2}\partial_\nu F(x)}\right) e^{-\frac{1}{4}\partial_\nu^2 F(x)\varepsilon + O(\varepsilon^2)}. \end{aligned} \tag{2.127}$$

Expanding the second factor at zero, this yields

$$V_\varepsilon = -2d + \sum_{\nu=1}^{d} \left(e^{-\frac{1}{2}\partial_\nu F(x)} + e^{\frac{1}{2}\partial_\nu F(x)}\right)\left(1 - \tfrac{1}{4}\partial_\nu^2 F(x)\varepsilon + O(\varepsilon^2)\right).$$

Using the equality of the first bracket to the term $2\cosh\left(\frac{1}{2}\partial_\nu F(x)\right)$, we get

$$V_\varepsilon = -2d + 2\sum_{\nu=1}^{d} \left(\cosh\left(\tfrac{1}{2}\partial_\nu F(x)\right) - \tfrac{1}{4}\partial_\nu^2 F(x)\varepsilon \cosh\left(\tfrac{1}{2}\partial_\nu F(x)\right) + O(\varepsilon^2)\right).$$

From $\cosh(2x) = 1 + 2\sinh^2(x)$ for the first summand and $\partial_\nu(\sinh(f(x))) = \partial_\nu(f(x))\cosh(f(x))$ for the second it follows that

$$V_\varepsilon = \sum_{\nu=1}^{d} \left(4\sinh^2\left(\tfrac{1}{4}\partial_\nu F(x)\right) - \varepsilon\,\partial_\nu\left(\sinh\left(\tfrac{1}{2}\partial_\nu F(x)\right)\right) + O(\varepsilon^2)\right) =: V_0(x) + \varepsilon\, V_1(x) + O(\varepsilon^2)$$

with

$$\begin{aligned} V_0(x) &= \sum_{\nu=1}^{d} 4\sinh^2\left(\tfrac{1}{4}\partial_\nu F(x)\right)\} \\ V_1(x) &= -\sum_{\nu=1}^{d} \partial_\nu\left(\sinh\left(\tfrac{1}{2}\partial_\nu F(x)\right)\right). \end{aligned}$$

Thus the potential can be written in the form (2.26). By an expansion at the potential wells, which are the extremals of the free energy, up to the order $\varepsilon^2$, we get

$$\begin{aligned} V_\varepsilon(x - x_j) = \sum_{\nu,\mu=1}^{d} \left(2\sum_{\eta=1}^{d} (\partial_\nu\partial_\eta(F(x_j))\partial_\mu\partial_\eta(F(x_j)))(x - x_j)_\nu (x - x_j)_\mu\right) + \\ + p_3(|x - x_j|) - \varepsilon\sum_{\eta=1}^{d} \partial_\eta^2 F(x_j) + O(\varepsilon^2), \end{aligned}$$

therefore by setting $(A^j_{\nu\mu}) := 2\sum_{\eta=1}^{d}(\partial_\nu\partial_\eta(F(x_j))\partial_\mu\partial_\eta(F(x_j)))$, the quadratic approximation of $V_\varepsilon$ takes the form (2.35), if the critical points of the free energy are non-degenerate. The absolute minima of the potential energy correspond to the minima of the free energy while the saddle points of the free energy induce minima of $V_\varepsilon$, which are higher by a term of order $\varepsilon$. If we assume, that $F$ tends to $\infty$ at least as $|x|^2$ for $|x| \to \infty$, then $V_\varepsilon$ is bounded from below and strictly positive for $|x|$ large enough as follows from (2.126). Therefore Hamilton operator under consideration therefore fulfills the assumptions of Theorem 2.10.

Thus the spectrum of $H_\varepsilon$ converges in the limit of infinitely many elements of the spin chain to the spectrum of the direct sum of the associated harmonic oscillators $H^j_{os}$ at the wells $x_j$, where

$$H^j_{os}u(x) = -\Delta u(x) + \left( 2\sum_{\eta=1}^{d} \left(\langle \nabla\partial_\eta(F(x_j))\, ,\, (x - x_j)\rangle\right)^2 - \varepsilon \sum_{\eta=1}^{d} \partial_\eta^2 F(x_j) \right) .$$

CHAPTER 3

# Construction of asymptotic expansions

This chapter is mainly concerned with the analysis of $\widehat{H}_\varepsilon$, the Hamilton operator on $\mathscr{L}^2\left(\mathbb{R}^d\right)$ associated to the discrete Hamiltonian $H_\varepsilon$. We construct asymptotic expansions of WKB-type for the eigenfunctions and eigenvalues of $\widehat{H}_\varepsilon$ in the neighborhood of one fixed potential well. The restriction of these quasi-modes to any $\varepsilon$-scaled lattice $\mathscr{G}_x = (\varepsilon\mathbb{Z})^d + x$ as described in Remark 2.9 are then quasi-modes for the discrete Hamiltonian $H_\varepsilon$ for the same eigenvalues.

## 3.1. Hypothesis and motivation

Motivated by the form of the eigenfunctions of the harmonic oscillator, we will make the ansatz, that the eigenfunctions in the classically forbidden regions are exponentially decreasing. In Section 3.2 this approach results in the eikonal equation as leading order of the eigenvalue problem. We can associate to the eikonal equation an energy function. It turns out to be $-t(x, i\xi) - V_0(x)$.
To obtain these improvements of the stability result proved in Chapter 2, it is necessary to refine the assumptions for the Hamilton operator $H_\varepsilon$ and thus $\widehat{H}_\varepsilon$.

Hypothesis 3.1. 1. *Let $H_\varepsilon = T_\varepsilon + V_\varepsilon$ be a self adjoint operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with associated phase space symbol $h_\varepsilon(x,\xi;\varepsilon) := t(x,\xi) + \widehat{V}_\varepsilon$, such that:*

(a) *$t \in S_0^0(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ is a periodic kinetic energy function in the sense of Definition 2.4. Regarding $t$ as a function on $\mathbb{R}^d \times \mathbb{R}^d$, which is periodic with respect to $\xi$, we assume furthermore that the function $\mathbb{R}^d \ni \xi \mapsto t(x,\xi)$ is even and has an analytic continuation to $\mathbb{C}^d$.*

(b) *The potential energy $V_\varepsilon$ is the lattice restriction of a function $\widehat{V}_\varepsilon \in \mathscr{C}^\infty(\mathbb{R}^d)$, which has an expansion*

$$\widehat{V}_\varepsilon(x) = \sum_{l=0}^{N} \varepsilon^l V_l(x) + R_{N+1}(x;\varepsilon)\,, \tag{3.1}$$

*where $V_\ell \in \mathscr{C}^\infty(\mathbb{R}^d)$. In addition $R_{N+1} \in \mathscr{C}^\infty(\mathbb{R}^d \times (0,\varepsilon_0])$ and for any compact set $K \subset \mathbb{R}^d$ there exists a constant $C_K$ such that $\sup_{x\in K} |R_{N+1}(x;\varepsilon)| \leq C_K \varepsilon^{N+1}$.*

c) *We assume that there exist constants $R, C > 0$ such that $V_\varepsilon(x) > C$ for all $|x| \geq R$ and $\varepsilon \in (0,\varepsilon_0]$. Furthermore $V_0(x)$ has exactly one, strictly non-degenerate, minimum at $x_1 = 0$ with the value $V_0(0) = 0$.*

2. *Let $\mathrm{Op}_\varepsilon(h_\varepsilon) =: \widehat{H}_\varepsilon = \widehat{T} + \widehat{V}_\varepsilon$ denote a self adjoint operator on $\mathscr{L}^2(\mathbb{R}^d)$, where we identified the symbol $h_\varepsilon$ on $\mathbb{R}^d \times \mathbb{T}^d$ with the periodic symbol on $\mathbb{R}^d \times \mathbb{R}^d$.*

Remark 3.2. (a) *It follows from the Hypothesis, that $V_0$ expands at $x = 0$ as*

$$V_0(x) = \langle x\,,\, Ax\rangle + \sum_{k\geq 3}^{N} W_k(x) + O\left(|x|^{N+1}\right) = V_0^1(x) + V_s(x) \quad \textit{where} \tag{3.2}$$
$$V_0^1(x) := \langle x\,,\, Ax\rangle\,,$$

*$W_k$ denotes a homogeneous polynomial of order $k$ and $A$ is symmetric. $V_0^1(x)$ denotes the harmonic oscillator potential described in Chapter 2 with critical point $x_1 = 0$.*

(b) *If the value of $V_0$ at the minimum $x_1 = 0$ is $E_0$, the potential can be replaced by $V_0 - E_0$ to fulfill the hypothesis.*

(c) *Since the constructions in this chapter are all done on $\mathbb{R}^d$, the particular choice $x_1 = 0$ is arbitrary. This choice is done only to simplify the notation and may be changed just by translation to any other point.*

(d) *We will use the notation* $h_0(x,\xi) := t(x,\xi) + V_0(x)$ *for the symbol of the zero order part of* $H_\varepsilon$ *with respect to* $\varepsilon$.

(e) *Since the periodic function* $\xi \mapsto t(x,\xi)$ *is assumed to be even with respect to* $\xi \mapsto -\xi$, *it has the representation*

$$t(x,\xi) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x) \cos\left(\tfrac{1}{\varepsilon}\gamma \cdot \xi\right), \qquad x \in \mathbb{R}^d,\, \xi \in \mathbb{R}^d\,. \tag{3.3}$$

*This leads to the fact, that its Taylor expansion at the point* $\xi = 0$ *is even, i.e. we have*

$$t(x,\xi) = \langle \xi\,,\, B(x)\xi\rangle + \sum_{\substack{|\alpha|=2n\\ n\geq 2}} B_\alpha(x)\xi^\alpha\,, \quad \xi \in \mathbb{T}^d\,, \quad x \in \mathbb{R}^d \tag{3.4}$$

*where* $\xi^\alpha := \xi_1^{\alpha_1} \ldots \xi_d^{\alpha_d}$, $\alpha \in \mathbb{N}_0^d$ *and* $B_\alpha$ *are real valued functions on* $\mathbb{R}^d$.

(f) *The assumption on the analytic continuation on* $\mathbb{R}^d \times \mathbb{C}^d$ *implies that the Fourier transforms* $a_\gamma$ *decay exponentially with respect to* $\gamma$, *more precisely it follows from Proposition A.3 in Appendix A.1, that for any* $c > 0$ *there exists a constant* $C$ *such that* $\| e^{\frac{c|.|}{\varepsilon}} a_.(x)\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq C$ *uniformly with respect to* $x \in \mathbb{R}^d$.

Remark 3.3. *We will reduce the discussion to the case where the quadratic terms in the potential and kinetic energy are diagonalized simultaneously at the point* $x_1$ *as described in Appendix A.2. We thus choose coordinates, such that for the symbol* $t$ *the quadratic term in* $\xi$ *at* $x_1$ *is the scalar product and* $V_0^1(x) = \sum_{\nu=1}^d \lambda_\nu^2 x_\nu^2$ *with* $\lambda_\nu > 0$ *for* $0 \leq \nu \leq d$.

As described in Section 2.2.2, the associated harmonic oscillator

$$H^1(x, \varepsilon D) := -\varepsilon^2\Delta + V_0^1(x) + \varepsilon V_1(0)\,, \qquad x \in \mathbb{R}^d\,,$$

as defined in (2.48) for $j = 1$, approximates $H_\varepsilon$ and $\widehat{H}_\varepsilon$ near the well $x_1 = 0$ in the limit $\varepsilon \to 0$. The eigenfunctions of $H^1$ are given by (2.49) with

$$\varphi_0(x) := \varphi_0^1(x) = \sum_{\nu=1}^d \frac{\lambda_\nu}{2} x_\nu^2\,, \qquad x \in \mathbb{R}^d\,, \tag{3.5}$$

which solves the harmonic eikonal equation $|\nabla\varphi_0(x)|^2 = V_0^1(x)$.
This suggests looking for a formal symbol $a(x,\varepsilon)$ and a real valued continuous function $\varphi(x)$ such that

$$u(x,\varepsilon) = a(x,\varepsilon)e^{-\frac{\varphi(x)}{\varepsilon}}$$

is a formal eigenfunction for $H_\varepsilon$.
The aim of this chapter is to show that we can find a positive $\mathscr{C}^\infty$-function $\varphi(x)$ on $\mathbb{R}^d$, asymptotic sums

$$\widetilde{E}_j(\varepsilon) \sim \sum_{k\in\mathbb{N}/2} \varepsilon^k E_{jk}\,, \qquad j = 1, \ldots, m$$

where $\varepsilon E_{j0}$ is an eigenvalue of $H^1$ with multiplicity $m$, and corresponding asymptotic sums

$$a_j(x,\varepsilon) \sim \sum_{\substack{k\in\mathbb{Z}/2\\ k\geq -M}} \varepsilon^k a_{jk}(x), \quad a_{jk} \in \mathscr{C}^\infty(\mathbb{R}^d)\,, \tag{3.6}$$

such that in a neighborhood $\mathscr{O}'$ of 0

$$(\widehat{H}_\varepsilon - \varepsilon\widetilde{E}_j(\varepsilon))\left(a_j(x,\varepsilon)e^{-\frac{\varphi(x)}{\varepsilon}}\right) = O\left(\varepsilon^\infty\right) e^{-\frac{\varphi(x)}{\varepsilon}}\,. \tag{3.7}$$

for $\varepsilon \to 0$. Then from (2.34) it follows that the restriction of these quasi-modes to any $\varepsilon$-scaled lattice $\mathscr{G}_{x_0}$, $x_0 \in \mathbb{R}^d$ satisfy the same equation with $\widehat{H}_\varepsilon$ replaced by the discrete operator $H_\varepsilon$ acting on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$.

### 3.2. Solution of the Eikonal Equation

If we formally compute the left hand side of (3.7) and expand the coefficients of $e^{-\frac{\varphi(x)}{\varepsilon}}$ in powers of $\varepsilon$, the equation of order zero determines the function $\varphi$. The order zero term of the conjugated potential energy is $V_0$, since $\widehat{V}_\varepsilon$ commutes with $e^{\frac{\varphi(x)}{\varepsilon}}$. The conjugated kinetic term is for $u \in \mathscr{L}^2\left(\mathbb{R}^d\right)$ given by

$$
\begin{aligned}
e^{\frac{\varphi}{\varepsilon}}\widehat{T}e^{-\frac{\varphi}{\varepsilon}}u(x) &= e^{\frac{\varphi(x)}{\varepsilon}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)e^{-\frac{\varphi(x+\gamma)}{\varepsilon}}u(x+\gamma)\\
&= \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)e^{\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))}u(x+\gamma)\,.
\end{aligned}
$$

If in addition $u \in \mathscr{C}^1\left(\mathbb{R}^d\right)$ and $\varphi \in \mathscr{C}^2\left(\mathbb{R}^d\right)$, using the Taylor expansion of $\varphi(x+\gamma)$ and $u(x+\gamma)$ at $x$, the last sum is equal to

$$
\begin{aligned}
&\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)e^{\frac{1}{\varepsilon}(-\gamma\cdot\nabla\varphi(x)-\sum_{\nu\mu}\gamma_\nu\gamma_\mu\int_0^1\partial_\mu\partial_\nu(\varphi(x+t\gamma))(1-t)\,dt}\left(u(x)+\int_0^1\nabla u(x+t\gamma)\cdot\gamma\,dt\right)\\
&=\sum_{y\in\mathbb{Z}^d}\tilde{a}_y(x)e^{-y\cdot\nabla\varphi(x)}e^{-\varepsilon\sum_{\nu\mu}y_\nu y_\mu\int_0^1\partial_\mu\partial_\nu(\varphi(x+t\varepsilon y))(1-t)\,dt}\left(u(x)+\varepsilon\int_0^1\nabla u(x+t\varepsilon y)\cdot y\,dt\right)
\end{aligned}
\tag{3.8}
$$

for $\tilde{a}_y$ defined in (2.18). The term of order zero in $\varepsilon$ can therefore by the assumption on the analytic extension of $t$ to $D_c$ be understood as

$$
\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)e^{-\frac{1}{\varepsilon}\gamma\cdot\nabla\varphi(x)}u(x) = t(x,-i\nabla\varphi(x))\,. \tag{3.9}
$$

Since $t(x,\xi)$ was assumed to be even with respect to $\xi\mapsto-\xi$, we have $t(x,-i\nabla\varphi(x)) = t(x,i\nabla\varphi(x))$ and therefore $t(x,i\xi)$ is real valued. In particular we have by (3.3) the representation

$$
t(x,i\xi) = \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\frac{\gamma\cdot\xi}{\varepsilon}\,,\qquad x,\xi\in\mathbb{R}^d\,.
$$

The resulting order zero part of (3.7) is given by

$$
t(x,i\nabla\varphi(x)) + V_0(x) = 0\,. \tag{3.10}
$$

We call (3.10) the eikonal equation (it is the generalization of the harmonic eikonal equation mentioned above).
By this procedure we have derived a new energy function

$$
\tilde{h}_0(x,\xi) := -h_0(x,i\xi) = -t(x,i\xi) - V_0(x)\,, \tag{3.11}
$$

where the sign is chosen in such a way that the kinetic energy function $-t(x,i\xi)$ is positive.
We shall prove that there exists a unique positive $\mathscr{C}^\infty$-function $\varphi$ defined in a neighborhood $\Omega$ of 0, solving (3.10), such that $\varphi$ has an expansion as asymptotic series

$$
\varphi(x)\sim\varphi_0(x)+\sum_{k\geq1}\varphi_k(x)\,,\qquad x\in\Omega\,, \tag{3.12}
$$

where $\varphi_0$ is given by (3.5) and each $\varphi_k$ is an homogeneous polynomial of order $k+2$, (i.e. $\varphi(x)-\varphi_0(x) = O(|x|^3)$ for $|x|\to0$).
Following Helffer ([**29**]), the idea of the proof is to determine $\varphi$ as generating function of a lagrangian manifold $\Lambda_+ = \{(x,\nabla\varphi(x))\,|\,(x,\xi)\in\mathscr{N}\}$ lying in the "energy shell" $\tilde{h}_0^{-1}(0)$, where $\mathscr{N}$ is a neighborhood of $(0,0)$. By Hypothesis 3.1, $\tilde{h}_0$ expands in a neighborhood of $(0,0)$ in $T^*\mathbb{R}^d$ as

$$
\tilde{h}_0(x,\xi) = \langle\xi\,,\,B(x)\xi\rangle - \sum_{\nu=1}^d\lambda_\nu^2x_\nu^2 + O\left(|\xi|^3+|x|^3\right)\,. \tag{3.13}
$$

Thus by the symmetry of the matrix $B$, the Hamiltonian vector field of $\tilde{h}_0$ in a neighborhood of $(0,0)$ expands as

$$\begin{aligned} X_{\tilde{h}_0} &= 2\sum_{\nu=1}^{d}\left(\sum_{\mu=1}^{d} B_{\nu\mu}(x)\xi_\mu \frac{\partial}{\partial x_\nu} + \left(\lambda_\nu^2 x_\nu + \sum_{\mu,\eta=1}^{d} \frac{\partial B_{\mu\eta}}{\partial x_\nu}(x)\xi_\mu\xi_\eta\right)\frac{\partial}{\partial \xi_\nu}\right) + O\left(|\xi|^2+|x|^2\right) = \\ &= 2\sum_{\nu=1}^{d}\left(\sum_{\mu=1}^{d} B_{\nu\mu}(x)\xi_\mu \frac{\partial}{\partial x_\nu} + \lambda_\nu^2 x_\nu \frac{\partial}{\partial \xi_\nu}\right) + O\left(|\xi|^2+|x|^2\right) . \end{aligned} \tag{3.14}$$

We assume $B(0) = \mathbf{1}$ as in Remark 3.3, thus the linearization of $X_{\tilde{h}_0}$ at the critical point $(0,0)$ yields the fundamental matrix

$$L := DX_{\tilde{h}_0}(0,0) = 2\begin{pmatrix} & 0 & & 1 & & 0 \\ & & & & \ddots & \\ & & & 0 & & 1 \\ \lambda_1^2 & & 0 & & & \\ & \ddots & & & 0 & \\ 0 & & \lambda_d^2 & & & \end{pmatrix} . \tag{3.15}$$

$L$ has the eigenvalues $\pm 2\lambda_\nu \, , \nu = 1, \ldots d$.
An eigenvector $(x,\xi)$ with respect to $\pm\lambda_\nu$ fulfills $\xi_\nu = \pm\lambda_\nu x_\nu$. By $\Lambda_\pm^0$ we denote the positive (resp. negative) eigenspace of $L$. $\Lambda_\pm^0$ can be characterized as the phase space subsets, which consist of all points $(x,\xi)$ such that $e^{-tL}(x,\xi) \to 0$ for $t \to \pm\infty$. Moreover, $\Lambda_\pm^0$ are Lagrangian subspaces of $T_{(0,0)}(T^*\mathbb{R}^d)$ of the form $\xi = \pm\nabla\varphi_0(x)$ with $\varphi_0$ defined in (3.5).

Denote by $F_t$ the flow of the hamiltonian vector field $X_{\tilde{h}_0}$. Then the Local Stable Manifold Theorem ([**2**]) tells us, that there is an open neighborhood $\mathscr{N}$ of $(0,0)$, such that the two submanifolds

$$\Lambda_\pm\left(X_{\tilde{h}_0}, (0,0)\right) := \left\{ (x,\xi) \in T^*\mathbb{R}^d \,\middle|\, F_t(x,\xi) \to (0,0) \quad \text{for} \quad t \to \mp\infty \right\} \tag{3.16}$$

exist and are unique in $\mathscr{N}$. They are called stable ($\Lambda_-$) and unstable ($\Lambda_+$) manifold of $X_{\tilde{h}_0}$ of the critical point $(0,0)$. Moreover they are of dimension $d$ and tangent to $\Lambda_\pm^0$ at $(0,0)$ (i.e. $T_{(0,0)}(\Lambda_\pm) = \Lambda_\pm^0$). $\Lambda_+$ and $\Lambda_-$ are contained in $\tilde{h}_0^{-1}(0)$, because $\tilde{h}_0(F_t(x,\xi)) = \tilde{h}_0(x,\xi)$.

In order to show that the tangent spaces at each point $(x,\xi) \in \Lambda_\pm$ are Lagrangian linear subspaces of $T_{(x,\xi)}(T^*\mathbb{R}^d)$ (in which case we call $\Lambda_\pm$ Lagrangian manifolds in $T^*\mathbb{R}^d$), we have to show, that the canonical symplectic form $\omega = \sum_{j=1}^d d\xi_j \wedge dx_j$ vanishes for all $u, v \in T_{(x,\xi)}(\Lambda_\pm)$. The Hamiltonian flow leaves the symplectic form invariant, we therefore find for $(u,v) \in T_{(x,\xi)}(\Lambda_+)$

$$\omega_{(x,\xi)}(u,v) = \omega_{F_t(x,\xi)}((DF_t)u, (DF_t)v) .$$

In the limit $t \to -\infty$, the elements of $T_{(x,\xi)}(\Lambda_+)$ lie in the lagrangian plane $\Lambda_+^0$, where the symplectic form vanishes, thus $\omega_{(x,\xi)}(u,v) = 0$ for all $(u,v) \in T_{(x,\xi)}(\Lambda_+)$.

The projection $(x,\xi) \mapsto x$ defines a diffeomorphism of $\mathscr{N} \cap \Lambda_+$ onto a sufficiently small neighborhood $\Omega$ of $0$ in $\mathbb{R}^d$. Therefore we can parameterize $\Lambda_+$ as the set of points $(x_1, \ldots x_d, \Psi_1(x), \ldots \Psi_d(x))$ with $\Psi_\nu \in \mathscr{C}^\infty(\Omega)$. Since $\Lambda_+$ is Lagrangian, we can deduce $\frac{\partial \Psi_\nu}{\partial x_\mu} = \frac{\partial \Psi_\mu}{\partial x_\nu}$ and there exists a function $\varphi \in \mathscr{C}^\infty(\Omega)$ with

$$\nabla\varphi(x) = \Psi(x) \quad \text{and} \quad \varphi(0) = 0 .$$

Since $T_{(0,0)}(\Lambda_\pm) = \Lambda_\pm^0$, the leading order term of this function $\varphi$ is equal to $\varphi_0$, thus $\varphi$ can be written as (3.12). Furthermore $\varphi$ solves the eikonal equation (3.10), because $\Lambda_+ \subset \tilde{h}_0^{-1}(0)$.

Remark 3.4. *With the ansatz (3.12), we have a constructive procedure to iteratively find the terms $\varphi_k$.*
*The coefficients of the eikonal equation (3.10) of the lowest order in $x$ vanish and the coefficients belonging to higher orders in $x$ iteratively fix the $\varphi_k$.*

*To this end, we expand $B(x)$ and $B_\alpha(x)$ at $x=0$ as*

$$B(x) = \mathbf{1} + \left(\sum_{\nu=1}^{d} \frac{\partial B_{\mu\eta}}{\partial x_\nu}(0) x_\nu\right) + O\left(|x|^2\right) =: \mathbf{1} + (DB)(0)\, x + O\left(|x|^2\right) \tag{3.17}$$

$$B_\alpha(x) = B_\alpha(0) + \sum_{\nu=1}^{d} \frac{\partial B_\alpha}{\partial x_\nu}(0) x_\nu + O\left(|x|^2\right) =: B_\alpha(0) + (DB_\alpha)(0)\, x + O\left(|x|^2\right)\,. \tag{3.18}$$

*The third order equation*

$$-\langle \nabla\varphi_0\,,\, (DB(0)\, x)\nabla\varphi_0\rangle - 2\sum_{\nu=0}^{d} \lambda_\nu x_\nu \tfrac{\partial \varphi_1}{\partial x_\nu}(x) + W_3(x) = 0\,, \qquad x\in\Omega$$

*fixes $\varphi_1$ for a given $W_3$, the fourth order*

$$-2\langle \nabla\varphi_0\,,\, ((DB)(0)\, x)\nabla\varphi_1\rangle + \sum_{|\alpha|=4} B_\alpha (\nabla\varphi_0)^\alpha - 2\sum_{\nu=0}^{d} \lambda_\nu x_\nu \tfrac{\partial\varphi_2}{\partial x_\nu}(x) - \sum_{\nu=0}^{d}\left(\tfrac{\partial \varphi_1}{\partial x_\nu}\right)^2 + W_4(x) = 0$$

*is an equation for $\varphi_2$ and the higher orders in $\varphi$ are inductively given by the higher order parts of the eikonal equation, which all take the form*

$$\left(\sum_{\nu=1}^{d} \lambda_\nu x_\nu \tfrac{\partial}{\partial x_\nu}\right)\varphi_k(x) = v_{k+2}(x)\,, \qquad x\in\Omega\,,$$

*with $v_k = O(|x|^k)$ for $|x|\to 0$.*

## 3.3. Transformation of the variable and formal symbol spaces

In order to find WKB-expansions there are, as in the setting of usual Schrödinger operators, two possible strategies to deal with the degeneracy of eigenvalues in the harmonic approximation. The first is an FBI-transformation of the eigenfunctions as described for example in Helffer-Sjöstrand [**33**]. The second method, which we are going to use, is the conjugation of the eigenfunctions with the exponential weight $e^{-\frac{\varphi(x)}{\epsilon}}$ and the coordinate change $y = \frac{x}{\sqrt{\varepsilon}}$. This procedure is used for example in Klein-Schwarz [**45**].

Definition 3.5. *Let $\psi$ denote any real valued function on $\mathbb{R}^d$.*
*We introduce an $\varepsilon$-dependent unitary map*

$$U_\varepsilon(\psi) : \mathscr{L}^2\left(\mathbb{R}^d, dx\right) \to \mathscr{L}^2\left(\mathbb{R}^d, e^{-2\frac{\psi(\sqrt{\varepsilon}y)}{\varepsilon}}dy\right) =: \mathscr{H}_\psi$$

*by*

$$(U_\varepsilon(\psi)f)(y) = \varepsilon^{\frac{d}{4}} e^{\frac{\psi(\sqrt{\varepsilon}y)}{\varepsilon}} f(\sqrt{\varepsilon}y)\,. \tag{3.19}$$

Then, for $\widehat{H}_\varepsilon$ as described in Hypothesis 3.1,

$$\widehat{G}_{\varepsilon,\psi} := \frac{1}{\varepsilon}\, U_\varepsilon(\psi)\widehat{H}_\varepsilon U_\varepsilon^{-1}(\psi) \tag{3.20}$$

defines a self adjoint operator on $\mathscr{H}_\psi$, whose domain contains the set of all polynomials, if $\psi\geq C|x|$ for some $C>0$ and for all large $x$.

We are going to apply the dilation defined in (3.20) to a function $\tilde\varphi\in\mathscr{C}^\infty(\mathbb{R}^d)$, which is constructed as follows.

Hypothesis 3.6. *Let $\tilde{\emptyset}$ denote a neighborhood of 0 such that the function $\varphi\in\mathscr{C}^\infty(\tilde{\emptyset})$ constructed in the previous section fulfills the eikonal equation inside of $\tilde{\emptyset}$ and such that for any $\delta>0$ and for some $C>0$ the estimate $|\nabla\varphi(x)|\geq C$ holds for $x\in\tilde{\emptyset}\setminus\{|x|\leq\delta\}$.*

*We consider some set $\emptyset$ such that $\overline{\emptyset}\subset\tilde{\emptyset}$ and define a smooth cut-off function $\chi$ supported in $\tilde{\emptyset}$ such that $\chi(x)=1$ for any $x\in\emptyset$.*

*Then we set for any $\delta>0$*

$$\tilde\varphi(x) := \chi\varphi(x) + \delta(1-\chi)|x|\,.$$

Henceforth we write $\widehat{G}_\varepsilon := \widehat{G}_{\varepsilon,\varphi}$.

We will now give an expansion of $\widehat{G}_\varepsilon$ with respect to $\sqrt{\varepsilon}$. To this end, we consider the Taylor expansion $\mathcal{T}_0 h_\varepsilon$ of $h_\varepsilon$ at the point $(0,0) \in \mathbb{R}^{2d}$. To this Taylor expansion, we can associate an operator $\mathcal{T}_0 \widehat{H}_\varepsilon := \mathrm{Op}_\varepsilon(\mathcal{T}_0 h_\varepsilon)$. We shall obtain a formal series $G := \mathcal{T}_0 \widehat{G}_\varepsilon$ by expanding $\frac{1}{\varepsilon} U_\varepsilon(\tilde{\varphi}) \mathcal{T}_0 \widehat{H}_\varepsilon U_\varepsilon^{-1}(\tilde{\varphi})$ as amplified below.

Proposition 3.7. *The Taylor expansion at the phase space point* $(0,0)$ *of* $\widehat{G}_\varepsilon$ *defined in (3.20) is given by*

$$\mathcal{T}_0 \widehat{G}_\varepsilon = \sum_{k \in \frac{\mathbb{N}}{2}} \varepsilon^k G_k \,, \tag{3.21}$$

*where*

$$G_k = b_{k,0}(y) + \sum_{|\gamma|=1}^{2k+2} b_{k,\gamma}(y) \partial_y^\gamma \,. \tag{3.22}$$

*Here* $b_{k,0}$ *is a polynomial of degree* $m \leq 2k$ *and* $b_{k,\gamma}$ *for* $|\gamma| \neq 0$ *are polynomials of degree* $m \leq 2k + 2 - |\gamma|$. *They are even (odd) with respect to* $y \mapsto -y$ *for even (odd)* $m$.

Before we prove Proposition 3.7, we introduce the following formal symbol spaces, to give an algebraic sense to the expansion (3.21).

Let for $n \in \mathbb{N}^*$

$$\mathcal{K}_{\frac{1}{n}} := \left\{ \mu = \sum_{j \in \frac{\mathbb{Z}}{n}} \mu_j \varepsilon^j \;\middle|\; \mu_j \in \mathbb{C} \quad \text{and} \quad c_\mu := \inf\{ j \,|\, \mu_j \neq 0\} > -\infty \right\} \tag{3.23}$$

$$\mathcal{V} := \left\{ p = \sum_{j \in \frac{\mathbb{Z}}{2}} p_j \varepsilon^j \;\middle|\; p_j \in \mathbb{C}[y] \quad \text{and} \quad c_p := \inf\{ j \,|\, p_j \neq 0\} > -\infty \right\} . \tag{3.24}$$

Defining componentwise addition and multiplication by the Cauchy product, i.e,

$$\mu_1 \cdot \mu_2 = \left( \sum_{k \in \frac{\mathbb{Z}}{n}} a_k \varepsilon^k \right) \cdot \left( \sum_{l \in \frac{\mathbb{Z}}{n}} b_l \varepsilon^l \right) = \sum_{m \in \frac{\mathbb{Z}}{n}} \sum_{k+l=m} (a_k b_l) \varepsilon^m = \mu_3 \,, \qquad \mu_1, \mu_2, \mu_3 \in \mathcal{K}_{\frac{1}{n}} \,,$$

$\mathcal{K}_{\frac{1}{n}}$ becomes a field of formal Laurent series with final principal part and $\mathcal{V}$ is a vector space over $\mathcal{K}_{\frac{1}{2}}$. We can associate to $\widehat{G}_\varepsilon$ a well defined operator $G$ on $\mathcal{V}$ by setting for $\mathcal{V} \ni p = \sum_{\substack{j \geq k \\ j \in \frac{\mathbb{Z}}{2}}} \varepsilon^j p_j$,

$$Gp(y) = \sum_{j \geq k} \varepsilon^j \mathcal{T}_0 \widehat{G}_\varepsilon p_j(y) = \sum_{j \geq k} \varepsilon^j \sum_{r \in \frac{\mathbb{N}}{2}} \varepsilon^r G_r p_j(y) = \sum_{j+r=l \geq k} \varepsilon^l G_r p_j(y) \in \mathcal{V} \,. \tag{3.25}$$

Remark 3.8. (a) *As a map on* $\mathbb{C}[y]$ *(the polynomial ring over* $\mathbb{C}$*),* $G_k$ *raises the degree of a polynomial by* $2k$ *and preserves (or changes) the parity with respect to* $y \mapsto -y$ *according to the sign* $(-1)^{2k}$. *This follows at once from the degree and parity of the polynomials* $b_{k,0}$ *and* $b_{k,\gamma}$ *in the representation of* $G_k$.

(b) *The term of order zero is given more precisely by*

$$G_0 = \Delta_y \tilde{\varphi}_0(y) + \sum_{\nu=1}^{d} (2(\partial_{y_\nu} \tilde{\varphi}_0(y)) \partial_{y_\nu}) - \Delta_y + V_1(0) \tag{3.26}$$

*This will be shown after the proof of Proposition 3.7.*

Proof of Proposition 3.7:

*Step 1:*

To show equation (3.21), we start by analyzing the terms arising from the potential energy $\widehat{V}_\varepsilon$. We have

$$\frac{1}{\varepsilon} U_\varepsilon(\tilde{\varphi}) \widehat{V}_\varepsilon U_\varepsilon^{-1}(\tilde{\varphi}) f(y) = \frac{1}{\varepsilon} \widehat{V}_\varepsilon(\sqrt{\varepsilon} y) f(y)$$

and expanding $V_i(\sqrt{\varepsilon}y)$, $i \in \mathbb{N}$, at $y = 0$, we get

$$\mathcal{T}_0 V_0(\sqrt{\varepsilon}y) = \varepsilon \sum_{j=1}^{d} \lambda_j^2 y_j^2 + \sum_{k\geq 3} \varepsilon^{\frac{k}{2}} W_k(y) \tag{3.27}$$
$$\varepsilon^l \mathcal{T}_0 V_l(\sqrt{\varepsilon}y) = \varepsilon^l V_l(0) + \varepsilon^{l+\frac{1}{2}} D_x V_l|_{x=0} y + \sum_{k\geq 2} \varepsilon^{\frac{k+2l}{2}} q_{l,k}(y) \,, \qquad l \in \mathbb{N}\,,$$

where $q_{l,k}$ are monomials in $y$ of order $k \in \mathbb{N}$. The formal power series $\mathcal{T}_0 \widehat{V}_\varepsilon$ is defined by the formal sum of terms given in (3.27). Thus if $q_{l,k}$ denotes for each $l \in \mathbb{N}$ a monomial of order $k$ in $y$ for $k \geq 2$ and zero otherwise and $W_2(y) := \sum_{\nu=1}^{d} \lambda_\nu^2 y_\nu^2$, we have

$$\frac{1}{\varepsilon}\mathcal{T}_0 \widehat{V}_\varepsilon(\sqrt{\varepsilon}y) = \sum_{j\in\mathbb{N}} \Bigg[ \varepsilon^j \Bigg( W_{2j+2}(y) + \sum_{1\leq l\leq j-1} (q_{l,(2j-2l)}(y)) + V_{j+1}(0) \Bigg) + $$
$$+ \varepsilon^{\frac{2j+1}{2}} \Bigg( W_{2j+3}(y) + \sum_{1\leq lj-\frac{1}{2}} (q_{l,(2j+1-2l)}(y)) + D_x V_{j+1}|_{x=0} y \Bigg) \Bigg] = \sum_{k\in\frac{\mathbb{N}}{2}} \varepsilon^k p_k(y) \tag{3.28}$$

where $p_k$ denotes a polynomial of degree $2k{+}2$. Each power $k$ of $\varepsilon$ can be written as a sum $k = l{+}m$ with $k, l \in \frac{\mathbb{N}}{2}$ and $m \in \mathbb{N}$. Here $l$ arises as $(\varepsilon y^2)^l$ by the transformation of variables and $m$ describes the power in $\varepsilon$ belonging to $V_m$. Thus any combination of $l$ and $m$ with $l + m = k$ results in one of the summands in the coefficient of $\varepsilon^k$ and is a monomial in $y$ of order $2l$. Since $m \in \mathbb{N}$, we have $2k{+}2 = 2l \mod 2$ and thus all summands in the polynomial $p_k$ have the same parity, i.e. $p_k$ is even (odd) if $2k{+}2$ is even (odd) (this is equivalent to the statement, that $k$ is an integer (half-integer)).

*Step 2:*
Now we investigate the coefficients in the expansion of the kinetic energy $\widehat{T}$ after conjugation with $U_\varepsilon(\tilde{\varphi})$.

We start by analyzing a differential operator $(\varepsilon\partial)^\alpha$ conjugated with the exponential weight $e^{\frac{\tilde{\varphi}}{\varepsilon}}$. By the Leibnitz formula, each derivative $\partial_\alpha$ acting on the product of $e^{-\frac{\tilde{\varphi}}{\varepsilon}}$ and $g$ splits into a derivative $\partial_\beta$ acting on the exponential and a derivative $\partial_\gamma$ with $\gamma = \alpha - \beta$ acting on $g$. In general, we have the formula

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}} \varepsilon^{|\alpha|} \partial_x^\alpha e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} g\left(\frac{x}{\sqrt{\varepsilon}}\right) = \varepsilon^{|\alpha|} \left( \frac{1}{\sqrt{\varepsilon}}\partial_y - \frac{1}{\varepsilon}\nabla\tilde{\varphi}(\sqrt{\varepsilon}\,.\,) \right)^\alpha g(\,.\,)\Big|_{y=\frac{x}{\sqrt{\varepsilon}}} . \tag{3.29}$$

For the exponential term, we get with $\beta, k_j \in \mathbb{N}^d$

$$\partial_x^\beta \left( e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right) = e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \sum_{n=1}^{|\beta|} \varepsilon^{-n} (-1)^n \sum_{\beta=k_1+\ldots+k_n} \prod_{j=1}^{n} \partial_x^{k_j} \tilde{\varphi}(x) \,. \tag{3.30}$$

To get the resulting lowest order in $\varepsilon$ for fixed $n$ after the transformation of the variable $x$ to $y = \frac{x}{\sqrt{\varepsilon}}$, we have to find the lowest order of $\tilde{\varphi}$ in $x$. Since $\tilde{\varphi}$ can by (3.12) be written as asymptotic series, where the first term is quadratic in $x$, each factor in the product on the right hand side of (3.30) with a first derivative of $\tilde{\varphi}$, i.e. with $|k_j| = 1$, which starts linear in $x$, leads to one positive order $\sqrt{\varepsilon}$. Higher derivatives of $\tilde{\varphi}$ start with a constant term, thus the variable transformation of these factors has no effect on the lowest order in $\varepsilon$ of the resulting product.

Introducing for a fixed $n$ and decomposition $\beta = k_1 + \ldots + k_n$ the notation $m_p := \#\{k_j \in \mathbb{N}^d \,|\, |k_j| = p\}$, where $1 \leq p \leq |\beta|$, we get $-n + \frac{m_1}{2}$ as resulting order in $\varepsilon$. The integer $m_p$ denotes the number of factors which are derivatives of $\tilde{\varphi}$ of order $p$. Thus for $\beta, \gamma, k_j \in \mathbb{N}^d$ the left hand side of (3.29) is equal to

$$\sum_{\beta+\gamma=\alpha} \partial_y^\gamma g(y) \sum_{n=1}^{|\beta|} \sum_{\beta=\sum k_j} \varepsilon^{|\alpha|-\frac{|\gamma|}{2}-n+\frac{m_1}{2}} \prod_{j=1}^{n} \left(\partial_y^{k_j}\tilde{\varphi}\right)(y) \,. \tag{3.31}$$

To get the lowest $\varepsilon$-order, we have to analyze the possible combinations of $n$ and $m_1$, which depends of $(k_1, \ldots, k_n)$.
It follows from the definition of $m_p$, that $n = \sum_{p=1}^{|\beta|} m_p$ and in addition $\sum_{j=1}^{n} |k_j| = \sum_{p=1}^{|\beta|} p\, m_p =$

$|\beta|$.

By the discussion above, the leading terms of the right hand side of (3.29) after the transformation from $x$ to $\sqrt{\varepsilon}y$ and multiplication with $\varepsilon^{-1}$ (which occurs in the transformation from $\widehat{H}_\varepsilon$ to $\widehat{G}_\varepsilon$) are of order

$$\varepsilon^{|\alpha|-1-\frac{|\gamma|}{2}-n+\frac{m_1}{2}}\,. \tag{3.32}$$

Let $n = |\beta| - l$ for $1 \leq l < |\beta|$, then the possible values for $m_1$ are

$$(n-l)_+ \leq m_1 \leq n-1\,, \quad \text{where} \quad (n-l)_+ := \max\{n-l, 0\}\,. \tag{3.33}$$

For $n = |\beta|$ it follows at once that $m_1 = n$. If $l < \frac{|\beta|}{2}$, then at least $n-1$ factors on the right hand side of (3.30) must be first derivatives of $\tilde{\varphi}$. If $n \leq \frac{|\beta|}{2}$, then it is possible that the number $m_1$ of first order derivatives is zero. By (3.33) and with $n = |\beta| - l$, we can estimate the term $-n + \frac{m_1}{2}$ as follows

$$-n + \frac{m_1}{2} \geq -n + \frac{(n-l)_+}{2} \geq \begin{cases} -|\beta| + l + \frac{1}{2}(|\beta| - l - l) = -\frac{|\beta|}{2} & \text{for} \quad 0 \leq l < \frac{|\beta|}{2} \\ -|\beta| + l \geq -\frac{|\beta|}{2} & \text{for} \quad \frac{|\beta|}{2} \leq l < |\beta| \end{cases}. \tag{3.34}$$

The full exponent of $\varepsilon$ can therefore be estimated by

$$|\alpha| - 1 - \frac{|\gamma|}{2} - \frac{|\beta|}{2} = \frac{|\alpha|}{2} - 1\,. \tag{3.35}$$

The lowest order in $\varepsilon$ resulting from a differential operator $(\varepsilon D)^\alpha$ is thus $\varepsilon^{\frac{|\alpha|}{2}-1}$. Since the kinetic energy starts with a second order derivative, we see that no negative orders in $\varepsilon$ occur and we start with $\varepsilon^0$.

From the preceding discussion, we get

$$\begin{aligned} &\frac{1}{\varepsilon}U_\varepsilon(\tilde{\varphi})\left(B_\alpha(x)(\varepsilon D_x)^\alpha\right)U_\varepsilon(\tilde{\varphi})^{-1} = \\ &\qquad = B_\alpha(\sqrt{\varepsilon}y)\sum_{\gamma+\beta=\alpha}\sum_{n=1}^{|\beta|}\sum_{\sum k_j=\beta}\varepsilon^{|\alpha|-1-n-\frac{|\gamma|}{2}}\prod_{j=1}^n\left(\partial_x^{k_j}\tilde{\varphi}\right)(\sqrt{\varepsilon}y)\partial_y^\gamma\,. \end{aligned}$$

Since the lowest order of $\tilde{\varphi}$ in $x$ is two (see Section 3.2), we have for fixed $n$ and decomposition $[k] := (k_1, \dots, k_n)$ with $\sum_j k_j = \beta$, as already mentioned above,

$$\mathcal{T}_0\prod_{j=1}^n\partial_x^{k_j}\tilde{\varphi}(\sqrt{\varepsilon}y) = a_{m_1}(y)\varepsilon^{\frac{m_1}{2}} + \sum_{l\in\mathbb{N}^*}a_{m_1+l}(y)\varepsilon^{\frac{m_1+l}{2}}\,,$$

where $a_k$ denotes a homogeneous polynomial of order $k$. By use of the Taylor expansion of $B_\alpha$ given in (3.17) and (3.18), this leads to

$$\begin{aligned} \mathcal{T}_0 B_\alpha(\sqrt{\varepsilon}y)\prod_{j=1}^n\partial_x^{k_j}\tilde{\varphi}(\sqrt{\varepsilon}y) &= \left(\sum_{l\in\mathbb{N}}\sum_{|\beta|=l}\partial_k^\beta B_\alpha(0)\varepsilon^{\frac{l}{2}}y^\beta\right)\left(a_{m_1}(y)\varepsilon^{\frac{m_1}{2}} + \sum_{l\in\mathbb{N}^*}a_{m_1+l}(y)\varepsilon^{\frac{m_1+l}{2}}\right) = \\ &= \sum_{l\in\mathbb{N}}\varepsilon^{\frac{m_1+l}{2}}b_{m_1+l}(y)\,, \end{aligned}$$

where $b_k$ denotes a homogeneous polynomial in $y$ of order $k$. By (3.33), it follows with $l = |\beta| - n$ that $(n-l)_+ = (2n - |\beta|)_+$, thus we can conclude denoting by $(n-1, n) = n-1$ for $n < |\beta|$ and $(n-1, n) = n$ for $n = |\beta|$

$$\mathcal{T}_0\frac{1}{\varepsilon}U_\varepsilon(\tilde{\varphi})\left(B_\alpha(x)(\varepsilon D_x)^\alpha\right)U_\varepsilon(\tilde{\varphi})^{-1} = \sum_{\gamma+\beta=\alpha}\sum_{n=1}^{|\beta|}\sum_{m_1=(2n-|\beta|)_+}^{(n-1,n)}\sum_{l\in\mathbb{N}}\varepsilon^{|\alpha|-1-n+\frac{m_1+l-|\gamma|}{2}}b_{m_1+l}(y)\partial_y^\gamma$$

and therefore

$$\mathcal{T}_0\frac{1}{\varepsilon}U_\varepsilon(\tilde{\varphi})\left(\mathcal{T}_0\widehat{T}(x,\varepsilon D)\right)U_\varepsilon(\tilde{\varphi})^{-1} = \sum_{\substack{|\alpha|=2n\\ n\geq 1}}\sum_{\gamma+\beta=\alpha}\sum_{n=1}^{|\beta|}\sum_{m_1=(2n-|\beta|)_+}^{(n-1,n)}\sum_{l\in\mathbb{N}}\varepsilon^{|\alpha|-1-n+\frac{m_1+l-|\gamma|}{2}}b_{m_1+l}(y)\partial_y^\gamma\,. \tag{3.36}$$

*Step 3:*

In the last step we are going to combine the terms resulting from the kinetic and potential energy.

In equation (3.36), the term with $|\gamma| = 0$ and $n = |\beta|$ is given by $t(x, i\nabla\tilde{\varphi})$ as described in the beginning of Section 3.2. Thus by the eikonal equation (3.10) it follows that in a neighborhood of $x = 0$ this term cancels with the potential term $\varepsilon^{-1}V_0(\sqrt{\varepsilon}y)$ leading to the summands $W_k$ in (3.28). Thus the remaining potential term is given by

$$\begin{aligned}\mathcal{T}_0\frac{1}{\varepsilon}(\widehat{V}_\varepsilon - V_0)(\sqrt{\varepsilon}y) &= V_1(0) + \varepsilon V_2(0) + \sum_{j\geq 2}\Bigg[\varepsilon^j\Bigg(V_{j+1}(0) + \sum_{1\leq l\leq j-1} q_{l,(2j-2l)}(y)\Bigg) \\ &\quad + \varepsilon^{\frac{2j+1}{2}}\Bigg(\langle\nabla V_{j+1}(0)\,,\,y\rangle + \sum_{1\leq l\leq j-\frac{1}{2}} q_{l,(2j+1-2l)}(y)\Bigg)\Bigg] \\ &= \sum_{k\in\frac{\mathbb{N}}{2}}\varepsilon^k p_k(y)\,, \end{aligned} \tag{3.37}$$

where $p_k$ denotes a polynomial of order $(2k-2)_+$.

The combination of the transformed potential and kinetic energy described in (3.37) and (3.36) therefore yields

$$\begin{aligned}\mathcal{T}_0\widehat{G}_\varepsilon &= \mathcal{T}_0\frac{1}{\varepsilon}U_\varepsilon(\tilde{\varphi})(\phi)\mathcal{T}_0\widehat{H}_\varepsilon U_\varepsilon(\tilde{\varphi})^{-1} \\ &= \sum_{m\in\mathbb{N}}\varepsilon^{\frac{m}{2}}p_{m-2}(y) + \sum_{\substack{|\alpha|=2n\\ n\geq 1}}\sum_{\gamma+\beta=\alpha}\sum_{n=1}^{\min\{|\beta|,|\alpha|-1\}}\sum_{m_1=(2n-|\beta|)_+}^{(n-1,n)}\sum_{l\in\mathbb{N}}\varepsilon^{|\alpha|-1-n+\frac{m_1+l-|\gamma|}{2}}b_{m_1+l}(y)\partial_y^\gamma \\ &=: \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r G_r(y,\partial_y)\,,\end{aligned}$$

where $p_k$ is even (odd) with respect to $y \mapsto -y$, if $k$ is even (odd).

In order to get the stated result, we collect the terms with the fixed order $r$ in $\varepsilon$. For these terms the kinetic part must satisfy

$$r = |\alpha| - 1 - n + \frac{m_1 + l + |\gamma|}{2}\,, \tag{3.38}$$

which is coupled with $b_{m_1+l}$ and a differential operator $\partial_y^\gamma$. Equation (3.38) yields

$$m_1 + l = 2r + 2(1 + n - |\alpha|) + |\gamma|\,.$$

Thus for fixed $|\gamma|$ the polynomial has fixed parity, since $1+n-|\alpha| \in \mathbb{Z}$ and therefore $2(1+n-|\alpha|)$ is even for all possible combinations of $|\alpha|$ and $n$. The maximal order for the polynomials results for $n = \min\{|\beta|, |\alpha|-1\} = \min\{|\alpha|-|\gamma|, |\alpha|-1\}$ in

$$m = \begin{cases} 2r + 2(1+|\alpha|-|\gamma|-|\alpha|) + |\gamma| = 2r+2-|\gamma|\,, & |\gamma| > 0 \\ 2r + 2(1+|\alpha|-1-|\alpha|) = 2r\,, & |\gamma| = 0\end{cases}.$$

For $|\gamma| \geq 0$, the coefficient of $\partial_y^\gamma$ is therefore a polynomial of order $2r+2-|\gamma|$ which is even (odd) with respect to $y \mapsto -y$, if $2r+2-|\gamma|$ is even (odd). For $|\gamma| = 0$, the polynomial is even. For fixed order $\varepsilon^r$, the maximal degree $|\gamma|_{\max}$ of differentiation occurs for $m_1 + l = 0$ (the coefficient is then constant), since $|\gamma| = 2r+2-(m_1+l)$ and therefore $|\gamma|_{\max} = 2r+2$.
The resulting term of the transformation of the kinetic energy can therefore be written as

$$\mathcal{T}_0\frac{1}{\varepsilon}U_\varepsilon(\tilde{\varphi})\left(\mathcal{T}_0\widehat{T}(x,\varepsilon D)\right)U_\varepsilon(\tilde{\varphi})^{-1} - t(x,-i\nabla\phi) = \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r\left(a_{2r}(y) + \sum_{|\gamma|=1}^{2r+2}a_{2r+2-|\gamma|}(y)\partial_y^\gamma\right)\,, \tag{3.39}$$

where $a_k(y)$ denotes a polynomial of degree $k$ which is even (odd) with respect to $y \mapsto -y$, if $k$ is even (odd).
The term for the potential energy given in (3.37) can be included into the term for $|\gamma| = 0$, since the polynomials $p_k$ are of order $2k-2$ in $y$ for $k \geq 2$ and of order zero otherwise and obey the

same parity properties as the polynomials $a_{2r}$, as discussed below (3.28). Thus

$$\begin{aligned} \mathcal{T}_0\widehat{G}_\varepsilon &= \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r p_r(y) + \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r\left(a_{2r} + \sum_{|\gamma|=1}^{2r+2} a_{2r+2-|\gamma|}(y)\partial_y^\gamma\right) \\ &= \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r\left(b_{2r}(y) + \sum_{|\gamma|=1}^{2r+2} b_{2r+2-|\gamma|}(y)\partial_y^\gamma\right) =: \sum_{r\in\frac{\mathbb{N}}{2}}\varepsilon^r G_r \end{aligned}$$

with

$$G_r = b_{2r}(y) + \sum_{|\gamma|=1}^{2r+2} b_{2r+2-|\gamma|}(y)\partial_y^\gamma\,,$$

as stated in the proposition.

□

Proof of Remark 3.8,(b):
From equations (3.35) and (3.27) it follows that the term of order $\varepsilon^0$ results only from the transformation of the quadratic part of the kinetic energy evaluated at $x = 0$ (the lowest order term in the $\varepsilon$-expansion of $B(x)$), the quadratic part of the potential energy and the the constant $V_1(0)$. Again by use of the eikonal equation (3.10) the terms $V_0^1(x)$ and $|\nabla\tilde{\varphi}_0(x)|^2$ cancel. As remarked we chose coordinates such that $B(0) = \mathbf{1}$, these terms can therefore be calculated directly, which by the chain and product rule or with (3.29) leads to (3.26).

□

We shall define a sesqui-linear form on $\mathcal{V}$ with values in $\mathcal{K}_{\frac{1}{2}}$ (where complex conjugation is understood componentwise), which is formally given by

$$\langle p\,,\,q\rangle_{\mathcal{V}} = \int_{\mathbb{R}^d}^f \overline{p(\varepsilon,y)}q(\varepsilon,y)\left[e^{-2\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}}\right]_f dy\,, \tag{3.40}$$

where $\left[e^{-2\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}}\right]_f$ respectively $\int^f$ indicates, that we are dealing with formal expansions with respect to powers in $\varepsilon$. To this end, using (3.12), we define real polynomials $\o_k \in \mathbb{R}[y]$ by $\o_0 := 1$ and

$$\left[e^{-2\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}}\right]_f =: e^{-\sum_{\nu=1}^d\lambda_\nu y_\nu^2}\left(1 + \sum_{k\in\frac{\mathbb{N}^*}{2}}\varepsilon^k\o_k(y)\right)\,. \tag{3.41}$$

Then

$$\o_j(y) = \sum_{l=1}^{2j}\sum_{\substack{k_1+\ldots+k_l=j\\ k_i\in\frac{\mathbb{N}^*}{2}}}\frac{(-2)^l}{l!}\tilde{\varphi}_{2k_1}(y)\ldots\tilde{\varphi}_{2k_l}(y)\,, \tag{3.42}$$

which is a sum of homogeneous polynomials of degree $2j + 2l$ with parity $(-1)^{2j}$.
By the expansion (3.41) and the special structure of the elements of $\mathcal{V}$, we can now give a definition of the sesqui-linear form in $\mathcal{V}$.

Definition 3.9. *For $p = \sum_{j\in\frac{\mathbb{Z}}{2}} p_j\varepsilon^j$ and $q = \sum_{j\in\frac{\mathbb{Z}}{2}} q_j\varepsilon^j$ in $\mathcal{V}$ we define the sesqui-linear form $\langle .\,,\,.\rangle_{\mathcal{V}} : \mathcal{V}\times\mathcal{V}\to\mathcal{K}_{\frac{1}{2}}$ by*

$$\langle p\,,\,q\rangle_{\mathcal{V}} := \sum_{i\in\frac{\mathbb{Z}}{2}}\varepsilon^i\sum_{j+k+l=i}\int_{\mathbb{R}^d}\overline{p_j(y)}q_k(y)\o_l(y)e^{-\sum_{\nu=1}^d\lambda_\nu y_\nu^2}\,dy\,. \tag{3.43}$$

Note that $\langle p\,,\,q\rangle_{\mathcal{V}}$ depends only on the Taylor expansion of $\varphi$ at 0.

Lemma 3.10. *The sesqui-linear form defined in (3.43) is non-degenerate, i.e,*

$$\langle p\,,\,q\rangle_{\mathcal{V}} = 0 \quad \textit{for all} \quad p\in\mathcal{V} \quad \textit{implies} \quad q = 0\,. \tag{3.44}$$

Proof:
We have to show that for every $q \neq 0$ there exists a $p$ such that the sesqui-linear form does not vanish.
If $q \neq 0$ we have $q = \sum_{j\geq k} q_j \varepsilon^j$, $k, j \in \frac{\mathbb{Z}}{2}$ for some $k$. Defining $p := \varepsilon^k q_k$ (we could also choose $p = q$ to get the stated result), the lowest order occurring in the sesqui-linear form is $2k$, and the coefficient to this order is given by

$$\int_{\mathbb{R}^d} |q_k|^2 e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2}\, dy > 0\,.$$

Since all other combinations lead to higher orders in $\varepsilon$, this term can not be cancelled.

□

We shall show that $G$ is a symmetric operator with respect to $\langle .\,,\,.\rangle_{\mathcal{V}}$.

Proposition 3.11. *Let $G$ be the operator* (3.25) *on $\mathcal{V}$ induced by $\widehat{G}_\varepsilon$ defined in (3.20) and let $\langle .\,,\,.\rangle_{\mathcal{V}}$ be the non-degenerate sesqui-linear form introduced in Definition 3.9.
Then for all $p, q \in \mathcal{V}$*

$$\langle p\,,\, Gq\rangle_{\mathcal{V}} = \langle Gp\,,\, q\rangle_{\mathcal{V}}\,.$$

Proof:
We will denote by $Y = \mathbb{C}[y]$ the set of all polynomials in $y$, considered as a subset of the form domain of $\widehat{G}_\varepsilon$ for $\varepsilon > 0$. This can canonically be identified with the subset $\mathcal{Y}$ of all polynomials in $\mathcal{V}$.
By the linearity of the sesqui-linear form, it is sufficient to prove the proposition for $p, q \in \mathcal{Y}$.
We need the following lemma:

Lemma 3.12. *Let $p, q \in Y$ . Then the following holds.*

(a) *For all $y \in \mathbb{R}^d$ and for $\varepsilon_0$ sufficiently small, the function*

$$\sqrt{\varepsilon} \mapsto F(y, \sqrt{\varepsilon}) := \overline{p(y)}(\widehat{G}_\varepsilon q)(y) e^{-\frac{2\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} \tag{3.45}$$

*is well defined as a $\mathscr{C}^\infty$-function of $\sqrt{\varepsilon} \in [0, \sqrt{\varepsilon_0}]$.*

(b) *For all $z \in \mathbb{R}^d$ and $N \in \mathbb{N}$ the function defined in (3.45) satisfies*

$$\begin{aligned} \lim_{\varepsilon\to 0} \partial^N_{\sqrt{\varepsilon}} F(y, \sqrt{\varepsilon}) &= \sum_{j=0}^N \binom{N}{j} \overline{p(y)} (G_{\frac{j}{2}} q)(y) \emptyset_{\frac{N-j}{2}}(y) e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2} \\ &=: \partial^N_{\sqrt{\varepsilon}=0} F(y, \sqrt{\varepsilon})\,. \end{aligned} \tag{3.46}$$

(c)

$$J(\sqrt{\varepsilon}) := \int_{\mathbb{R}^d} F(y, \sqrt{\varepsilon})\, dy \tag{3.47}$$

*defines a function in $\mathscr{C}^\infty([0, \varepsilon_0))$, for which*

$$J^{(N)}(0) = \int_{\mathbb{R}^d} \partial^N_{\sqrt{\varepsilon}=0} F(y, \sqrt{\varepsilon})\, dy, \qquad N \in \mathbb{N}\,. \tag{3.48}$$

Proof of Lemma 3.12:
(a): This follows from the Definition (3.20) of $\widehat{G}_\varepsilon$ and the fact that the solution of the eikonal equation $\tilde{\varphi}(x)$ is $\mathscr{C}^\infty$ in some neighborhood $\emptyset$ of 0.

(b): We use the Taylor expansion (3.41) for the exponential factor and the expansion of $\widehat{G}_\varepsilon$ given by (3.21) and (3.22). These combined with the Leibnitz rule give directly the term in (3.46).

(c): By use of Definition (3.20) and $y = \frac{x}{\sqrt{\varepsilon}}$ one has

$$\begin{aligned} J(\sqrt{\varepsilon}) = \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \overline{p(y)} (U_\varepsilon(\tilde{\varphi}) \widehat{H}_\varepsilon U_\varepsilon(\tilde{\varphi})^{-1} q)(y) e^{-\frac{2\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}}\, dy = \\ = \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \overline{p\left(\tfrac{x}{\sqrt{\varepsilon}}\right)} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}_\varepsilon \left( q\left(\tfrac{x}{\sqrt{\varepsilon}}\right) e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right) dx\,, \end{aligned} \tag{3.49}$$

thus $J \in \mathscr{C}^\infty(\mathbb{R} \setminus \{0\})$. In order to show (3.48) we split the region of integration by introducing cut-off functions $\zeta_0, \zeta_1$ such that $\zeta_0 \in \mathscr{C}_0^\infty(\mathbb{R}^d)$, $\zeta_0(x) = 1$ for $|x| \leq \eta$ and $\zeta_0 + \zeta_1 = \mathbf{1}$. Here $\eta$ is chosen such that $\{|x| \leq \eta\} \subset \emptyset$ for $\emptyset$ as introduced in Hypothesis 3.6 We get

$$J(\sqrt{\varepsilon}) = \Big( \int_{\mathbb{R}^d} \zeta_0(\sqrt{\varepsilon} y) \overline{p(y)} (\widehat{G}_\varepsilon q)(y) e^{-\frac{2\tilde{\varphi}(\sqrt{\varepsilon} y)}{\varepsilon}} )\, dx + \\ + \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \zeta_1(x) \overline{p\left(\tfrac{x}{\sqrt{\varepsilon}}\right)} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}_\varepsilon \left( q\left(\tfrac{x}{\sqrt{\varepsilon}}\right) e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right) dx \Big) . \quad (3.50)$$

To find an estimate for the second term, we notice that by Hypothesis 3.1 we have $\widehat{H}_\varepsilon = \widehat{T} + \widehat{V}_\varepsilon$, where $\widehat{T}$ is bounded and $\widehat{V}_\varepsilon$ is a multiplication operator, which is polynomially bounded. Thus $\widehat{H}_\varepsilon \left( q\left(\frac{x}{\sqrt{\varepsilon}}\right) e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right) =: u_\varepsilon(x)$ is an element of $\mathscr{L}^2(\mathbb{R}^d)$ and $\|u_\varepsilon\|_{\mathscr{L}^2}$ is at most of order $\varepsilon^{-k}$ for some finite $k \geq 0$ depending on the dimension $d$.

By the assumptions on $\tilde{\varphi}$ we have $\tilde{\varphi}(x) \geq C|x|$ on the support of $\zeta_1$, thus by the Cauchy-Schwarz inequality

$$\begin{aligned} \left| \int_{\mathbb{R}^d} \zeta_1(x) \overline{p\left(\tfrac{x}{\sqrt{\varepsilon}}\right)} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}_\varepsilon \left( q\left(\tfrac{x}{\sqrt{\varepsilon}}\right) e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right) dx \right| &\leq \int_{|x|\geq\eta} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} |\overline{p(\tfrac{x}{\sqrt{\varepsilon}})}| |u_\varepsilon(x)|\, dx \\ &\leq \|u_\varepsilon\|_{\mathscr{L}^2} \left( \int_{|x|\geq\eta} e^{-\frac{2\tilde{\varphi}(x)}{\varepsilon}} |\overline{p(\tfrac{x}{\sqrt{\varepsilon}})}|^2\, dx \right)^{\frac{1}{2}} \\ &= O\left( e^{-\frac{\eta}{2\varepsilon}} \right) \end{aligned} \quad (3.51)$$

We shall now prove the assertion (3.48) by induction in $N$.

For $N = 0$ we have to analyze the limit $\varepsilon \to 0$ of $J(\sqrt{\varepsilon})$ as given in (3.50). In order to show (3.48), it remains by (3.51) to show, that we can interchange integration and $\lim_{\varepsilon\to 0}$ in the first term on the right hand side of (3.50). This can be done by use of the Dominated convergence theorem, since there exist constants $C, D > 0$ such that for any $\varepsilon \in [0, \varepsilon_0]$ the integrand is bounded as

$$\left| \zeta_0(x) \overline{p(y)} (\widehat{G}_\varepsilon q)(y) e^{-\frac{2\tilde{\varphi}(\sqrt{\varepsilon} y)}{\varepsilon}} \right| \leq C e^{-\frac{|y|^2}{D}} . \quad (3.52)$$

In order to see this, we write $\widehat{G}_\varepsilon$ by use of $\widehat{H}_\varepsilon$ as described above and use the Taylor expansion of $e^{\frac{\varphi}{\varepsilon}} \widehat{T} e^{-\frac{\varphi}{\varepsilon}} u$ given in (3.8) and the expansion of $V_\varepsilon$. By (3.9) and the eikonal equation (3.10), the term of order $\varepsilon^{-1}$ on the left hand side of (3.52) vanishes on the support of $\zeta_0$. The remaining potential term $\zeta_0(V_\varepsilon - V_0)$ is by assumption polynomially bounded, thus (3.52) is obvious for this term. In order to analyze the remaining kinetic term, we use that it can by (3.8) be written as

$$\zeta_0(x) \sum_{\eta\in\mathbb{Z}^d} \tilde{a}_\eta(x) e^{-\eta\cdot\nabla\varphi(x)} e^{-\varepsilon \sum_{\nu\mu} \eta_\nu \eta_\mu \int_0^1 \partial_\mu \partial_\nu (\varphi(x+t\varepsilon\eta))(1-t)\, dt} \int_0^1 \nabla u(x + t\varepsilon\eta) \cdot \eta\, dt \quad (3.53)$$

for $\tilde{a}_\eta$ defined in (2.18). The idea is to split the sum on the right hand side of (3.53) for some $R > 0$ in the part with $|\eta| \leq R$, which is bounded by some constant depending on $R$, and the part with $|\eta| > R$. For the second part, we use that by Hypothesis 3.6 and (3.12), the second derivative of $\tilde{\varphi}$ is positive definite inside of $\emptyset$ and homogeneous of order $-1$ outside of $\tilde{\emptyset}$. Thus by the exponential decay of $a_\gamma$, this part of the sum is bounded as well. This yields (3.52).

We therefore can deduce that $J \in \mathscr{C}^0(\mathbb{R})$ and that it satisfies (3.48) for $N = 0$, i.e.,

$$J(0) = \lim_{\varepsilon\to 0} J(\sqrt{\varepsilon}) = \int_{\mathbb{R}^d} \lim_{\varepsilon\to\ 0} F(y, \sqrt{\varepsilon})\, dy .$$

It remains to show that for arbitrary $N$ the assumption (3.48) for $N-1$ and $J \in \mathscr{C}^{N-1}(\mathbb{R})$ imply

$$J^{(N)}(0) = \int_{\mathbb{R}^d} \partial^N_{\sqrt{\varepsilon}=0} F(y, \sqrt{\varepsilon})\, dy = \lim_{\varepsilon\to 0} J^{(N)}(\sqrt{\varepsilon}) \quad (3.54)$$

The second equality then gives $J \in \mathscr{C}^N(\mathbb{R})$. We have by (3.51)

$$J^{(N-1)}(\sqrt{\varepsilon}) = \partial^{N-1}_{\sqrt{\varepsilon}} \int_{|y|\leq\frac{\eta}{\sqrt{\varepsilon}}} F(y, \sqrt{\varepsilon})\, dy + O\left(e^{-\frac{\eta}{\varepsilon}}\right) = \int_{|y|\leq\frac{\eta}{\sqrt{\varepsilon}}} \partial^{N-1}_{\sqrt{\varepsilon}} F(y, \sqrt{\varepsilon})\, dy + O\left(e^{-\frac{\eta}{2\varepsilon}}\right) . \quad (3.55)$$

and by the induction hypothesis, we have (3.55) also for $\sqrt{\varepsilon}=0$. Thus

$$\lim_{\varepsilon\to 0}\frac{1}{\sqrt{\varepsilon}}\left(J^{(N-1)}(\sqrt{\varepsilon})-J^{(N-1)}(0)\right)=$$
$$\lim_{\varepsilon\to 0}\frac{1}{\sqrt{\varepsilon}}\int_{|y|\leq\frac{\eta}{\sqrt{\varepsilon}}}\left(\partial^{N-1}_{\sqrt{\varepsilon}}F(y,\sqrt{\varepsilon})-\partial^{N-1}_{\sqrt{\varepsilon}=0}F(y,\sqrt{\varepsilon})\right)dy+O\left(e^{-\frac{\eta}{2\varepsilon}}\right). \quad (3.56)$$

Using (3.46) and the fact that each $G_k$ maps polynomials to polynomials, we find as above an integrable upper bound for the integrand, which is independent of $\varepsilon$. Thus again by the Dominated convergence theorem, the right hand side of (3.56) is equal to

$$\int_{|y|\leq\frac{\eta}{\sqrt{\varepsilon}}}\partial^{N}_{\sqrt{\varepsilon}=0}F(y,\sqrt{\varepsilon})\,dy+O\left(e^{-\frac{\eta}{2\varepsilon}}\right)=\int_{\mathbb{R}^d}\partial^{N}_{\sqrt{\varepsilon}=0}F(y,\sqrt{\varepsilon})\,dy\,.$$

This gives the first equality in (3.54).
In order to obtain the second equality, we use (3.55) with $N-1$ replaced by $N$ and again the Dominated convergence theorem. □

We come back to the proof of Proposition 3.11.
In order to use the symmetry of $\widehat{G}_\varepsilon$ on $\mathscr{H}_{\tilde{\varphi}}$, we define a function on $\mathbb{R}_+$ by

$$\left\langle p\,,\,\widehat{G}q\right\rangle_{\mathscr{H}_{\tilde{\varphi}}}(\sqrt{\varepsilon}):=\left\langle p\,,\,\widehat{G}_\varepsilon q\right\rangle_{\mathscr{H}_{\tilde{\varphi}}},\quad p,q\in Y\,. \quad (3.57)$$

By Lemma 3.12, the function defined in (3.57) is $\mathscr{C}^\infty([0,\varepsilon_0])$. If we denote the set of such functions by $\mathcal{F}$, (3.57) yields a well defined map

$$\left\langle .\,,\,\widehat{G}\,.\right\rangle_{\mathscr{H}_{\tilde{\varphi}}}:Y\times Y\to\mathcal{F}\,.$$

Denoting by $T:\mathcal{F}\to\mathcal{K}_{\frac{1}{2}}$ the map which assigns to each $f\in\mathcal{F}$ its Taylor expansion in $\sqrt{\varepsilon}$, it follows from Lemma 3.12 and from the definitions of $G$ and of the sesqui-linear form in $\mathcal{V}$, that the diagram

$$\begin{array}{ccc} Y\times Y & \xrightarrow{\left\langle .\,,\,\widehat{G}.\right\rangle_{\mathscr{H}_{\tilde{\varphi}}}} & \mathcal{F} \\ \downarrow & & \downarrow T \\ \mathcal{Y}\times\mathcal{Y} & \xrightarrow{\langle .\,,\,G.\rangle_{\mathcal{V}}} & \mathcal{K}_{\frac{1}{2}} \end{array}$$

is commutative. Since for $\left\langle\widehat{G}\,.\,,\,.\right\rangle_{\mathscr{H}_{\tilde{\varphi}}}$ and $\langle G\,.\,,\,.\rangle_{\mathcal{V}}$ we have the analogous diagram, the proposition is traced back to the symmetry of $\widehat{G}$ on $\mathscr{H}_{\tilde{\varphi}}$. □

## 3.4. Construction of asymptotic expansions

In this section we construct formal asymptotic expansions for the eigenfunctions and eigenvalues of $\widehat{H}_\varepsilon$, solving the spectral problem to arbitrary high order in $\varepsilon$.
First we recall that the operator $\varepsilon G_0$ on $\mathscr{H}_\varphi$, given in (3.26), is unitary equivalent to the harmonic oscillator

$$H^0(\varepsilon)=-\varepsilon^2\Delta+\sum_{\nu=1}^{d}\lambda_\nu^2x_\nu^2+V_1(0)\,, \quad (3.58)$$

where the unitary transformation $U_\varepsilon(\varphi_0)$ is defined in (3.19). Therefore the spectrum of $G_0$ is given by (2.37) with $\omega^j_\nu$ replaced by $\lambda_\nu$.
The eigenfunctions of $H^0(\varepsilon)$ are the functions $g_{\alpha,0}$ defined in (2.49) with $\varphi_0$ introduced in (3.5), thus the $\mathscr{H}_\varepsilon$-normalized eigenfunctions of $\varepsilon G_0$ are given by

$$\left(U_\varepsilon(\varphi_0)g_{\alpha,0}\right)(y)=h_\alpha(y)\,, \quad (3.59)$$

where $h_\alpha$ denotes as in Remark 2.11 the product of Hermite polynomials $h_{\alpha_\nu}\in\mathbb{R}[y_\nu]$. Since $h_k(-x)=(-1)^kh_k(x)$, it follows that $h_\alpha$ is even (respectively odd), if $|\alpha|$ is even (resp. odd).

In order to get an expression for the resolvent of the full operator $G$ on $\mathcal{V}$, we notice that for $z \notin \sigma(G_0)$ the resolvent $R_0(z) = (G_0 - z)^{-1}$ is well defined on polynomials and hence on $\mathcal{V}$.

LEMMA 3.13. *Let $z \notin \sigma(G_0)$ and $p, q \in \mathcal{V}$. Then*

(a) *the inverse of $(G - z) : \mathcal{V} \to \mathcal{V}$ is given by the formal von Neumann series*

$$R(z) := \sum_{k=0}^{\infty} \left[ -R_0(z) \sum_{j \in \frac{\mathbb{N}^*}{2}} \varepsilon^j G_j \right]^k R_0(z) = - \sum_{j \in \frac{\mathbb{N}}{2}} \varepsilon^j r_j(z) \qquad \textit{with} \tag{3.60}$$

$$r_j := \sum_{\substack{k+l=j \\ k \in \mathbb{N}, l \in \frac{\mathbb{N}^*}{2}}} \left(-R_0 G_l\right)^k R_0 \,.$$

(b)

$$\langle p\,,\, R(z) q \rangle_{\mathcal{V}} = \langle R(\bar{z}) p\,,\, q \rangle_{\mathcal{V}}\,. \tag{3.61}$$

(c) *For $r_j$ defined in* (3.60)

$$\langle p\,,\, r_j(z) q \rangle_{\mathcal{V}} = \langle r_j(\bar{z}) p\,,\, q \rangle_{\mathcal{V}}, \qquad j \in \tfrac{\mathbb{N}}{2}\,. \tag{3.62}$$

Proof:

(a): $R_0(z)$ and $G_j$ map polynomials to polynomials and raise the degree only by a finite order depending on $j$ (see Remark 3.8). Thus they are linear operators in $\mathcal{V}$ and the same is true for each summand in the von Neumann expansion. For each $j \in \frac{\mathbb{N}}{2}$ the operator $r_j$ is a finite sum of compositions of $R_0$ and $G_k$, where the order of $G_k$ is at most equal to $j$. Thus $r_j$ is a bounded operator in $\mathcal{V}$.

In order to show that the series is well defined we have to show that with the notation $G_+ := \sum_{j \in \frac{\mathbb{N}^*}{2}} \varepsilon^j G_j$ the partial sums

$$S_n = \sum_{k=0}^{n} [-R_0(z) G_+]^k = \frac{1 - (-R_0 G_+)^{n+1}}{1 + R_0(z) G_+}$$

converge. Using the metric $M$ and the norm $\|\,.\,\|_{\mathcal{V}}$ on $\mathcal{V}$ respectively defined in Appendix A.7 by means of an $\varepsilon$-adic valuation, we will show that $\{S_n\}_{n \in \mathbb{N}}$ is a Cauchy sequence. Let $n > m$, $n, m, k \in \mathbb{N}$ and $u \in \mathcal{V}$ fixed with $\|u\|_{\mathcal{V}} = \varepsilon^k$. Then by the properties of the $\varepsilon$-adic valuation on $\mathcal{K}_{\frac{1}{2}}$

$$\begin{aligned} &M\left( \left( \frac{-(-R_0 G_+)^{n+1}}{1 + R_0(z) G_+} \right) u, \left( \frac{-(-R_0 G_+)^{m+1}}{1 + R_0(z) G_+} \right) u \right) \le \\ &\le \max_{j \in \{n, m\}} \left\{ \left( v_\varepsilon \left( \left\langle \tfrac{(-R_0(z) G_+)^{j+1}}{1 + R_0(z) G_+} u\,,\, \tfrac{(-R_0(z) G_+)^{j+1}}{1 + R_0(z) G_+} u \right\rangle_{\mathcal{V}} \right) \right)^{\frac{1}{2}} \right\} = \\ &= \varepsilon^{\frac{2k + n + 1 - 1}{2}} = \|u\|_{\mathcal{V}}\, \varepsilon^{\frac{n}{2}}\,, \end{aligned}$$

because $R_0(z) G_+$ raises the order in $\varepsilon$ by $\frac{1}{2}$. Thus in this formal sense of expansions with respect to $\varepsilon^{\frac{1}{2}}$, the mentioned sequence is Cauchy in the given metric and the series converges to $(1 + R_0(z) G_+)^{-1}$.

In order to verify that $R(z) = (G - z)^{-1}$, we analyze

$$R(z)(G - z) = \sum_{k=0}^{\infty} [-R_0(z) G_+]^k R_0(z) (G_0 + G_+ - z)\,. \tag{3.63}$$

The right hand side of equation (3.63) is equal to

$$\begin{aligned} &(1 + R_0(z) G_+)^{-1} R_0(z) (G_0 - z) + (1 + R_0(z) G_+)^{-1} R_0(z) G_+ = \\ &\qquad = (1 + R_0(z) G_+)^{-1} (1 + R_0(z) G_+) = \mathbf{1} \end{aligned}$$

and thus $R(z)$ is the left inverse of $G - z$. Applying $(G - z)$ from the left to $R(z)$, we get

$$\begin{aligned} &(G - z) R(z) = (G_0 - z + G_+)(R_0(z) - R_0(z) G_+ R_0(z) + \ldots) = \\ &\quad = \mathbf{1} - G_+ R_0(z) + G_+ R_0(z) G_+ R_0(z) - \ldots + G_+ R_0(z) - G_+ R_0(z) G_+ R_0(z) + \ldots = \mathbf{1}\,. \end{aligned}$$

and therefore $R(z)$ is the inverse of $(G-z)$.

(b): By use of $R(z)(G-z) = \mathbf{1} = (G-z)R(z)$ and Proposition 3.11, we can write

$$\langle p\,,\, q\rangle_{\mathcal{V}} = \langle p\,,\,(G-z)R(z)q\rangle_{\mathcal{V}} = \langle (G-\bar{z})p\,,\, R(z)q\rangle_{\mathcal{V}}$$

and

$$\langle p\,,\, q\rangle_{\mathcal{V}} = \langle R(\bar{z})(G-\bar{z})p\,,\, q\rangle_{\mathcal{V}}\,.$$

This proves the second statement.

(c): This follows directly from the expansion (3.60).

□

In the following we will use the resolvent operator $R(z)$ to define a spectral projection for $G$ associated to an eigenvalue of the harmonic oscillator, i.e. of $G_0$.

By (3.60) $R(z)$ is determined on the polynomials and hence on $\mathcal{V}$ by the action of the operators $r_j(z) : \mathcal{V} \to \mathcal{V}$ on the Hermite polynomials, which form a basis in $\mathcal{Y}$ and thus in $\mathcal{V}$.

It follows from Proposition 3.7, that $G_j$ raises the degree of each polynomial by $2j$, thus there exist real numbers $c^j_{\alpha\beta}$ such that for all $\alpha, \beta \in \mathbb{N}_0^d$, $j \in \frac{\mathbb{N}}{2}$ we have

$$G_j h_\alpha = \sum_{|\beta|\leq|\alpha|+2j} c^j_{\alpha\beta} h_\beta \tag{3.64}$$

and from (3.64) together with (3.60) we can conclude, that there exist rational functions $d^j_{\alpha\beta}(z)$ with poles at most at the elements of the spectrum of $G_0$ for which

$$r_j(z) h_\alpha = \sum_{|\beta|\leq|\alpha|+2j} d^j_{\alpha\beta}(z) h_\beta\,. \tag{3.65}$$

Let $E$ be an eigenvalue of $G_0$ with multiplicity $m$ and let $\Gamma(E)$ be a circle in the complex plane around $E$, oriented counterclockwise, such that all other eigenvalues of $G_0$ lie outside of it.
Then since $r_j(z)$ is for each $j \in \frac{\mathbb{N}}{2}$ well defined on $\mathcal{V}$ and depends meromorphically of $z$, we can define for $p = \sum_{k\geq M} \varepsilon^k p_k \in \mathcal{V}$

$$\Pi_E p := \sum_{k+l=j\in\frac{\mathbb{N}}{2}} \varepsilon^j \frac{1}{2\pi i} \oint\limits_{\Gamma(E)} r_l(z) p_k\, dz\,. \tag{3.66}$$

We denote this operator by

$$\Pi_E = -\frac{1}{2\pi i} \oint\limits_{\Gamma(E)} (G-z)^{-1}\, dz\,.$$

In the Schrödinger setting, such an operator describes the projection to the eigenspaces of all eigenvalues of $G$ inside of $\Gamma$.

Proposition 3.14. *Let $E \in \sigma(G_0)$ with multiplicity $m$.*
*Then the operator $\Pi_E$ defined in (3.66) is a symmetric projection in $\mathcal{V}$ of dimension $m$, which commutes with $G$.*

Proof:
*Symmetry:*

The symmetry of $\Pi_E$ is a consequence of (3.62):

$$\Big\langle p\,,\, \oint_{\Gamma(E)} r_j(z)\, dz q\Big\rangle_{\mathcal{V}} = -\Big\langle \oint_{\Gamma(E)} r_j(z)\, dz p\,,\, q\Big\rangle_{\mathcal{V}}\,,$$

where the negative sign results from the conjugation of $z$. Since we defined $\Pi_E$ with an additional $i$, the sign will not change and with linearity of the scalar product the symmetry of $\Pi_E$ follows at once.

$\Pi_E^2 = \Pi_E$:
Let $\tilde{z} \notin \operatorname{Int}\Gamma(E)$, where $\operatorname{Int}\Gamma(E)$ denotes the interior of $\Gamma(E)$. Then

$$(G-\tilde{z})^{-1}\Pi_E = -(G-\tilde{z})^{-1}\frac{1}{2\pi i}\oint\limits_{\Gamma(E)} (G-z)^{-1}\, dz = -\frac{1}{2\pi i}\oint\limits_{\Gamma(E)} (G-\tilde{z})^{-1}(G-z)^{-1}\, dz \tag{3.67}$$

and using the resolvent equation $\big((G-\tilde z)^{-1}-(G-z)^{-1}\big)=(\tilde z-z)(G-\tilde z)^{-1}(G-z)^{-1}$ the last term is equal to

$$-\frac{1}{2\pi i}\oint\limits_{\Gamma(E)}\frac{1}{\tilde z-z}\left((G-\tilde z)^{-1}-(G-z)^{-1}\right)dz=$$

$$=-(G-\tilde z)^{-1}\frac{1}{2\pi i}\oint\limits_{\Gamma(E)}\frac{1}{\tilde z-z}\,dz+\frac{1}{2\pi i}\oint\limits_{\Gamma(E)}\frac{1}{\tilde z-z}(G-z)^{-1}\,dz=$$

$$=-\frac{1}{2\pi i}\oint\limits_{\Gamma(E)}\frac{1}{z-\tilde z}(G-z)^{-1}\,dz\,. \tag{3.68}$$

To get the last equality we used the fact, that $\tilde z$ lies outside of $\Gamma(E)$ and thus the first integral term vanishes. Now let $\tilde\Gamma(E)$ be another circle around $E$, which lies in the exterior of $\Gamma(E)$, such that in the interior of $\tilde\Gamma(E)$ are no other eigenvalues of $G_0$ too. Choosing $\tilde z\notin \operatorname{Int}\Gamma(E)$ with $\tilde z\in\operatorname{Int}\tilde\Gamma(E)$ and using (3.67), (3.68) we get

$$\begin{aligned}\Pi_E^2 &= \frac{1}{4\pi^2}\oint\limits_{\tilde\Gamma(E)}(G-\tilde z)^{-1}\,d\tilde z\oint\limits_{\Gamma(E)}(G-z)^{-1}\,dz=\\ &=\frac{1}{4\pi^2}\oint\limits_{\Gamma(E)}(G-z)^{-1}\oint\limits_{\tilde\Gamma(E)}\frac{1}{z-\tilde z}\,d\tilde z\,dz=-\frac{1}{2\pi i}\oint\limits_{\Gamma(E)}(G-z)^{-1}\,dz=\Pi_E\,.\end{aligned}$$

$\operatorname{rank}\Pi_E=m$:

We introduce the set

$$I_E:=\left\{\alpha\in\mathbb N^d\;\middle|\;G_0h_\alpha=Eh_\alpha\right\}=:\{\alpha^1,\dots,\alpha^m\} \tag{3.69}$$

numbering the $m$ Hermite polynomials with eigenvalue (energy) $E$ for $G_0$. As a consequence of the representation (3.60) (recall $r_0(z)=R_0(z)$) and of the definition (3.66), we can write for $\alpha\in I_E$

$$\Pi_Eh_\alpha=h_\alpha+\sum_{j\in\frac{\mathbb N^*}{2}}\varepsilon^jp_j \tag{3.70}$$

for some polynomials $p_j\in\mathbb C[y]$ of degree less than or equal to $|\alpha|+2j$ (this follows from (3.65)). Since the Hermite polynomials form a basis, (3.70) implies that the functions $\Pi_Eh_{\alpha^k}$, $k=1,\dots m$, are linearly independent over $\mathcal K_{\frac12}$. Thus their span has dimension $m$. It remains to show that this span coincides with the range of $\Pi_E$, i.e., we have to show that for all $\beta\in\mathbb N_0^d$ there exist $\mu_\alpha\in\mathcal K_{\frac12}$, $\alpha\in I_E$, such that

$$\Pi_Eh_\beta=\sum_{\alpha\in I_E}\mu_\alpha h_\alpha\,. \tag{3.71}$$

The case $\beta\in I_E$ is trivial, so let $\beta\notin I_E$, then

$$\Pi_Eh_\beta=\sum_{j\in\frac{\mathbb N^*}{2}}\varepsilon^jp_j \tag{3.72}$$

for some $p_j\in\mathbb C[y]$. Since the Hermite polynomials form a basis in $\mathbb C[y]$, the polynomial $p_{\frac12}$ expands to

$$p_{\frac12}=\sum_{\alpha\in I_E}c_\alpha h_\alpha+\sum_{\gamma\notin I_E}c_\gamma h_\gamma\,. \tag{3.73}$$

Applying $\Pi_E$ on both sides of (3.72) and using $\Pi_E^2=\Pi_E$, (3.73) and again (3.72) for the second equality, we get

$$\Pi_Eh_\beta=\varepsilon^{\frac12}\sum_{\alpha\in I_E}c_\alpha\Pi_Eh_\alpha+\varepsilon^{\frac12}\sum_{\gamma\notin I_E}c_\gamma\Pi_Eh_\gamma+\sum_{\substack{j\geq1\\ j\in\frac{\mathbb N^*}{2}}}\varepsilon^j\Pi_Ep_j=\varepsilon^{\frac12}\sum_{\alpha\in I_E}c_\alpha\Pi_Eh_\alpha+\sum_{\substack{j\geq1\\ j\in\frac{\mathbb N^*}{2}}}\varepsilon^j\tilde p_j$$

for $\tilde p_j\in\mathbb C[y]$. Thus by expanding the terms of the next order we gain the order $\varepsilon^{\frac12}$ in the remaining term and inductively obtain $\mu_\alpha\in\mathcal K_{\frac12}$ satisfying equation (3.71).

$\Pi_E G = G\Pi_E$:
This follows from the fact that $G$ commutes with $R(z)$ together with the definition (3.66).

□

The aim of the following construction is to find an orthonormal basis in $\operatorname{Ran}\Pi_E$, such that $G|_{\operatorname{Ran}\Pi_E}$ is represented by a symmetric $m\times m$-Matrix $M=(M_{ij})$ with $M_{ij}\in\mathcal{K}_{\frac{1}{2}}$.
To this end, we rename the spectral projections of the eigenfunctions belonging to the eigenvalue $E$ by $f_j := \Pi_E h_{\alpha^j}$, $\alpha^j \in I_E$. Then equation (3.70) and Definition 3.9 for the sesqui-linear form in $\mathcal{V}$ imply

$$\langle f_i\,,\,f_j\rangle_{\mathcal{V}} = \delta_{ij} + \sum_{k\in\frac{\mathbb{N}^*}{2}} \varepsilon^k\gamma_k, \qquad 1\le i,j\le m\,, \qquad \gamma_k\in\mathbb{R}\,, \tag{3.74}$$

since the Hermite polynomials are orthogonal and the $g_{\alpha^j,0}$ are normalized in the $\mathscr{L}^2$-norm. Defining $F=(F_{ij}) := (\langle f_i\,,\,f_j\rangle_{\mathcal{V}})$, $F$ is symmetric, because the $f_k$ are real functions. The symmetric matrix $B := F^{-\frac{1}{2}}$ is given by a binomial series (using the Taylor series for $(1+x)^{-\frac{1}{2}}$ at 0, which is convergent for $x<1$) and if all matrix elements $F_{ij}$ are in $\mathcal{K}_{\frac{1}{n}}$, the same is true for all $B_{ij}$. Then

$$e := (e_1,\dots,e_m) := (f_1,\dots,f_m)B =: fB \tag{3.75}$$

defines an orthonormal basis $\{e_1,\dots e_m\}$ of $\operatorname{Ran}\Pi_E$ (the orthonormalization of $\{f_1,\dots,f_m\}$), because

$$(fB)^t(fB) = Bf^tfB = F^{-\frac{1}{2}}FF^{-\frac{1}{2}} = \mathbf{1}\,.$$

In this basis, the matrix $M=(M_{ij})$ of $G|_{\operatorname{Ran}\Pi_E}$ is given by

$$M = e^tGe = Bf^tGfB = BF^GB\,, \tag{3.76}$$

where $F^G_{kl} := \langle f_k\,,\,Gf_l\rangle_{\mathcal{V}} \in \mathcal{K}_{\frac{1}{2}}$. Thus $M$ is a finite symmetric matrix with entries in $\mathcal{K}_{\frac{1}{2}}$. Using the Propositions 3.7 and 3.14, the equations (3.64) and (3.74) and the fact, that $\varepsilon^{\frac{d}{4}}h_{\alpha^j}$, $\alpha^j\in I_E$, are the eigenfunctions of $G_0$ for the eigenvalue $E$, we can conclude

$$F^G_{ij} = E\delta_{ij} + \sum_{k\in\frac{\mathbb{N}^*}{2}} \varepsilon^k\mu_k \qquad \mu_k\in\mathbb{R}\,. \tag{3.77}$$

It is shown in [**45**], that $\mathcal{K} := \bigcup_{n\in\mathbb{N}}\mathcal{K}_{\frac{1}{n}}$ is algebraically closed, thus any $m\times m$-matrix with entries in $\mathcal{K}$ possesses $m$ eigenvalues in $\mathcal{K}$, counted with their algebraic multiplicity. By the following theorem, which is proven in the appendix of [**45**], it actually follows that the eigenvalues of matrices with entries in the ring $\mathcal{K}_{\frac{1}{n}}$ also lie in $\mathcal{K}_{\frac{1}{n}}$.

THEOREM 3.15. *Let $M$ be a hermitian $m\times m$-matrix with elements in $\mathcal{K}_{\frac{1}{n}}$ for some $n\in\mathbb{N}$. Then the eigenvalues $E_1,\dots E_m$ are in $\mathcal{K}_{\frac{1}{n}}$ with real coefficients, and the highest negative power occurring in their expansion is bounded by the highest negative power in the expansions of $M_{ij}$. Furthermore the associated eigenvectors $u_j\in(\mathcal{K}_{\frac{1}{n}})^m$ can be chosen to be orthonormal in the natural inner product.*

We can conclude from Theorem 3.15 and the special form of the elements of $M$ defined in (3.76) that this matrix possesses $m$ (not necessarily distinct) eigenvalues in $\mathcal{K}_{\frac{1}{2}}$ of the form

$$E_j(\varepsilon) = E + \sum_{k\in\frac{\mathbb{N}^*}{2}} \varepsilon^kE_{jk} = \sum_{k\in\frac{\mathbb{N}}{2}} \varepsilon^kE_{jk}\,, \quad j=1,\dots m \tag{3.78}$$

where $E_{j0}=E$ and the corresponding eigenfunctions are

$$\psi_j(\varepsilon) = \sum_{k\in\frac{\mathbb{N}}{2}} \varepsilon^k\psi_{jk}\,. \tag{3.79}$$

From (3.70) and the fact that every eigenfunction can be written as linear combination

$$\psi = \sum_{\alpha\in I_E} \lambda_\alpha\Pi_Eh_\alpha \tag{3.80}$$

with coefficients $\lambda_\alpha$ without negative powers in $\sqrt{\varepsilon}$, it follows that the maximal degree of $\psi_{jk}\in\mathbb{C}[y]$ is given by $\max_{\alpha\in I_E}(|\alpha|+2k)$.

Using the several parity results in the preceding propositions, we can prove the next proposition about the absence of half integer terms in the energy expansion.

Proposition 3.16. *Let all $\alpha \in I_E$ have the same parity (i.e., $|\alpha|$ is either even for all $\alpha \in I_E$ or odd for all $\alpha \in I_E$), where $I_E$ is defined in (3.69). Let $M$ denote the matrix specified in equation (3.76) and $E_j(\varepsilon)$ its eigenvalues given in (3.78). Then $M_{ij} \in \mathcal{K}_1$ and $E_j(\varepsilon) \in \mathcal{K}_1$ for $1 \le i, j \le m$.*

Proof:
By Theorem 3.15 we know that if $M_{ij} \in \mathcal{K}_1$, the same is true for the eigenvalues $E_j(\varepsilon)$, so it suffices to prove the proposition for $M_{ij}$. By equation (3.76), $M = BF^G B$ where $B = \left(\langle f_i\,,\, f_j\rangle_{\mathcal{V}}\right)^{-\frac{1}{2}}$ and $F^G = (\langle f_k\,,\, Gf_l\rangle_{\mathcal{V}})$.
In order to distinguish between the indices arising in the expansions and those numbering different eigenfunctions, we will change the notation during this proof to $f_\alpha = \varepsilon^{\frac{d}{4}}\Pi_E h_\alpha$ and $F^G_{\alpha\beta}$ for $\alpha, \beta \in I_E$.
We start by proving that $\langle f_\alpha\,,\, f_\beta\rangle_{\mathcal{V}} \in \mathcal{K}_1$. By definition (3.66) the coefficients in the power series of $f_\alpha$ are given by

$$f_{\alpha j} = \frac{1}{2\pi i}\oint_\Gamma r_j(z) h_\alpha\, dz\,. \tag{3.81}$$

The $r_j(z)$ are determined by $G_j$ and $R_0(z)$, and since $G_j$ changes the parity of a polynomial in $\mathbb{C}[y]$ by the factor $(-1)^{2j}$, $j \in \frac{\mathbb{N}^*}{2}$ (see Remark 3.8), we can conclude by the definition of $R_0(z)$ that $r_j(z)$ changes the parity by $(-1)^{2j}$ as well. Using that the parity of $h_\alpha$ is given by $(-1)^{|\alpha|}$, we obtain $(-1)^{|\alpha|+2j}$ as parity of $f_{\alpha j}$. By Definition 3.9 we have

$$\langle f_\alpha\,,\, f_\beta\rangle_{\mathcal{V}} = \sum_{n\in\frac{\mathbb{Z}}{2}} \varepsilon^n \sum_{\substack{j,k,l\in\frac{\mathbb{Z}}{2}\\ j+k+l=n}} \int_{\mathbb{R}^d} f_{\alpha j}(y) f_{\beta k}(y) \o_l(y) e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2}\, dy\,.$$

We shall show that for $2n$ odd (and thus for $n$ half-integer), each summand vanishes. For fixed $j,k,l$ the integral will vanish if the entire integrand is odd. According to (3.42) the parity of $\o_l$ is $(-1)^{2l}$, the scalar product therefore vanishes if $(|\alpha|+2j+|\beta|+2k+2l)$ is odd. Since by assumption $\alpha$ and $\beta$ have the same parity, $|\alpha|+|\beta|$ is even and so $2(j+k+l) = 2n$ has to be odd, which occurs if $n$ is half-integer. This shows that $\langle f_\alpha\,,\, f_\beta\rangle_{\mathcal{V}} \in \mathcal{K}_1$ and the same is true for $B_{\alpha\beta}$ by definition.
It remains to show the same result for $F^G_{\alpha\beta}$ given by

$$\langle f_\alpha\,,\, Gf_\beta\rangle_{\mathcal{V}} = \sum_{n\in\frac{\mathbb{Z}}{2}} \varepsilon^n \sum_{\substack{j,k,l,r\in\frac{\mathbb{Z}}{2}\\ j+k+l+r=n}} \int_{\mathbb{R}^d} f_{\alpha j}(y) G_r f_{\beta k}(y) \o_l(y) e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2}\, dy\,.$$

The operator $G_r$ changes the parity by $(-1)^{2r}$ as already mentioned, so as before the integral vanishes if $j+k+l+r = n$ is half integer.

□

## 3.5. Construction of Asymptotic Expansions in $x$ and $\varepsilon$

In this section we will construct formal asymptotic expansions in our original variable $x$ and associate $\mathscr{C}^\infty$-functions to them by use of a Borel-procedure.

**3.5.1. Expansion with respect to the original variable.** We will now return to our original variable $x = \sqrt{\varepsilon}y$. Substituting it in equation (3.79) and rearranging with respect to powers in $\sqrt{\varepsilon}$ yields

$$\psi_j(y,\varepsilon) = \sum_{k\in\frac{\mathbb{N}}{2}} \varepsilon^k \psi_{jk}(y) = \sum_{k\in\frac{\mathbb{N}}{2}} \varepsilon^k \psi_{jk}\left(\frac{x}{\sqrt{\varepsilon}}\right) =: \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\ge -N}} \varepsilon^l \widehat{a}_{jl}(x) \tag{3.82}$$

and we set

$$\widehat{a}_j(x,\varepsilon) := \psi_j\left(\frac{x}{\sqrt{\varepsilon}}, \varepsilon\right) = \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\ge -N}} \varepsilon^l \widehat{a}_{jl}(x)\,. \tag{3.83}$$

The order of $\psi_{jk}$ as a polynomial in $y$ is $M = \max_{\alpha\in I_E}(|\alpha| + 2k)$, giving rise the order $-\frac{M}{2}$ in $\varepsilon$ after the substitution $x = \sqrt{\varepsilon}y$. Thus the order of $\varepsilon^k\psi_{jk}$ is $-N = k - \frac{M}{2} = -\max_{\alpha\in I_E}\frac{|\alpha|}{2}$ independent of $k$. It is then clear that $N = 1$ if $E$ denotes the lowest eigenvalue.

In general, $\widehat{a}_{jl}$ is a formal power series in $x$, because for every fixed $l$ there exists a smallest $h$, such that only $\psi_{jk}$ with $k \geq h$ contribute (for example $\widehat{a}_{j,-N}$ consists of the highest power terms of all $\psi_{jk}$ respectively).

The lowest order in $x$ of $\widehat{a}_{jl}$ is determined by the order in $y$ of the first contributing function $\psi_{jh}$, which results in the power $\varepsilon^l$ (looking again at our example, we see that for $\widehat{a}_{j,-N}$ the lowest order in $x$ is $2N = \max_{\alpha\in I_E} |\alpha|$, for $\widehat{a}_{j,-N+1}$ the lowest order is $2N-1$ and for $\widehat{a}_{jl}$ with $l \geq 0$, the lowest order is given by the lowest order term of $\psi_{jl}$, which is zero). We denote by $\mathcal{A}$ the set of formal symbols $\widehat{a}_j$ given by a power series as in (3.83) with arbitrary $N$. Then $\mathcal{A}$ is a vector space over $\mathcal{K}_{\frac{1}{2}}$, on which

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}_\varepsilon e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}}$$

acts as an operator with eigenfunctions $\widehat{a}_j$, where $\widehat{H}_\varepsilon$ fulfills Hypothesis 3.1 and $\tilde{\varphi}$ is constructed in Hypothesis 3.6. The following theorem will summarize these results and give a condition on the absence of half integer terms in the expansion.

THEOREM 3.17. *Let $E$ be an eigenvalue with multiplicity $m$ of the harmonic approximation $G_0$ of $\widehat{G}_\varepsilon$ given in (3.26). Let $\widehat{H}_\varepsilon$ be a Hamilton operator satisfying Hypothesis 3.1 and $\tilde{\varphi}$ be the real function described in Hypothesis 3.5.*

(a) *Then the operator $e^{\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}_\varepsilon e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}}$ has an orthonormal system of $m$ eigenfunctions $\widehat{a}_j$ of the form (3.83) in $\mathcal{A}$, where the lowest order monomial in $\widehat{a}_{jl} \in \mathbb{C}[[x]]$ is of degree $\max\{-2l, 0\}$.*
*The associated eigenvalues are*

$$\varepsilon E_j(\varepsilon) = \varepsilon \left( E + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk} \right) .$$

(b) *If $|\alpha|$ is even (resp. odd) for all $\alpha \in I_E$, then all half integer (resp. integer) terms in the expansion (3.83) of the eigenfunctions with respect to $x$ vanish.*

Proof:

(a): This point is already shown in the discussion succeeding equation (3.83).

(b): By equation (3.80) and Proposition 3.16 together with Theorem 3.15 we can write any eigenfunction $\psi$ as a linear combination of $\Pi_E h_\alpha$ with coefficients in $\mathcal{K}_1$, thus we get explicitly

$$\psi\left(\frac{x}{\sqrt{\varepsilon}}\right) = \sum_{\alpha\in I_E} \sum_{\substack{j\in\mathbb{N}_0 \\ k\in\frac{\mathbb{N}}{2}}} \varepsilon^{j+k} \lambda_{\alpha j} f_{\alpha k}\left(\frac{x}{\sqrt{\varepsilon}}\right) .$$

As discussed below (3.81), the polynomials $f_{\alpha k}$ are of degree $(|\alpha| + 2k)$ in $y$, thus they have the order $\varepsilon^{-(k+\frac{|\alpha|}{2})}$ and the parity of $|\alpha| + 2k$, since they consist of monomials of order $|\alpha| + 2k - 2l$, $0 \leq 2l \leq |\alpha| + 2k$, $l \in \mathbb{N}$. If we combine the powers in $\varepsilon$ arising in the sum, we get $\varepsilon^{j+l-\frac{|\alpha|}{2}}$, where $j$ and $l$ are both integer. If $|\alpha|$ is even, the whole exponent is integer, if it is odd the exponent is half integer. So if one of these assumptions is true for all $\alpha \in I_E$, there remain no half integer respectively integer terms. Since the transition to $\widehat{a}_j$ is just a reordering, this is also true for $\widehat{a}_j$.
□

**3.5.2. Approximate Eigenfunctions.** As a first step, to analyze the spectrum of $H_\varepsilon$ as an operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, we construct quasi-modes, i.e., $\mathscr{C}^\infty$-functions $a_{jl}$ and real numbers $\tilde{E}_{jl}$, such that asymptotic sums of them solve (3.7) to arbitrary high polynomial order in $x$ and $\varepsilon$ in a sufficiently small neighborhood $\mathcal{O}'$ of 0 (independent of $\varepsilon$).
For $\widehat{a}_j$ given by (3.83), we can use the Theorem of Borel (see for example Grigis, Sjöstrand [**24**]) with respect to $x$, to find $\mathscr{C}^\infty$-functions $\tilde{\widehat{a}}_{jl}$ possessing $\widehat{a}_{jl}$ as Taylor series at zero and to define a

formal asymptotic series in a neighborhood $\varnothing'$ of 0 by

$$\tilde{\hat{a}}_j(x,\varepsilon) := \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\geq -N}} \varepsilon^l \tilde{\hat{a}}_{jl}(x) .$$

Then

$$e^{\frac{\tilde\varphi(x)}{\varepsilon}}(H_\varepsilon - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\tilde{\hat{a}}_j(x,\varepsilon) = b_j(x,\varepsilon) , \tag{3.84}$$

where $b_j(x,\varepsilon) = \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\geq -N}} \varepsilon^l b_{jl}(x)$ has the property, that each $b_{jl}$ vanishes to infinite order at $x = 0$. It remains to show that it is possible to modify the functions $\tilde{\hat{a}}_{jl}$ by uniquely determined functions $\tilde b_{jl}$ vanishing at zero to infinite order, such that for the resulting functions $\tilde a_{jl} := \tilde{\hat{a}}_{jl} - \tilde b_{jl}$, the formal series

$$\tilde a_j(x,\varepsilon) := \sum_{\substack{l\geq -N\\ l\in\mathbb{Z}/2}} \varepsilon^l \tilde a_{jl}(x) \tag{3.85}$$

solves for $x\in\varnothing'$ the equation

$$e^{\frac{\tilde\varphi(x)}{\varepsilon}}(H_\varepsilon - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\tilde a_j(x,\varepsilon) = 0 .$$

To this end, we have to show that the equation

$$e^{\frac{\tilde\varphi(x)}{\varepsilon}}(H_\varepsilon - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\tilde b_j(x,\varepsilon) = b_j(x,\varepsilon) .$$

has a unique formal power solution $\tilde b_j(x,\varepsilon) \sim \sum \varepsilon^l \tilde b_{jl}(x)$ with coefficients $\tilde b_{jl} \in \mathscr{C}^\infty(\varnothing')$ vanishing to infinite order at $x = 0$. The equation of order zero is the eikonal equation already mentioned in Section 3.2, vanishing identically in $\varnothing'$ for the appropriate choice of $\tilde\varphi$. All higher order equations are called transport equations and determine for given initial conditions order by order the functions $\tilde b_{jl}$. We must show that they have unique solutions and that the solutions are $\mathscr{C}^\infty$. By the definition of $T_\varepsilon$ and the assumptions in Hypothesis 3.1, we have

$$e^{\frac{\tilde\varphi(x)}{\varepsilon}}\left[T_\varepsilon + V_\varepsilon - \varepsilon\left(E + \sum_{k\in\mathbb{N}/2}\varepsilon^k E_{jk}\right)\right]e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\sum_{\substack{l\geq -N\\ l\in\mathbb{Z}/2}}\varepsilon^l \tilde b_{jl}(x) =$$

$$= \sum_{\substack{l\geq -N\\ l\in\mathbb{Z}/2}}\varepsilon^l\left\{\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}\left[a_\gamma(x)e^{\frac{1}{\varepsilon}(\tilde\varphi(x)-\tilde\varphi(x+\gamma))}\tilde b_{jl}(x+\gamma,\varepsilon)\right] + \sum_{k\in\mathbb{N}_0/2}\varepsilon^k\left(V_k(x) - \varepsilon E_{jk}\right)\tilde b_{jl}(x,\varepsilon)\right\} .$$

To get the different orders in $\varepsilon$ of the kinetic term, we expand $\tilde\varphi$ and $\tilde b_{jl}$ at $x$ and set $\eta := \frac{\gamma}{\varepsilon}\in\mathbb{Z}^d$. For appropriate $t, t'\in[0,1]$

$$\frac{1}{\varepsilon}\left(\tilde\varphi(x) - \tilde\varphi(x+\varepsilon\eta)\right) = -\nabla\tilde\varphi(x)\cdot\eta - \frac{\varepsilon}{2}\sum_{\nu,\mu=1}^d \eta_\nu\eta_\mu\partial_\nu\partial_\mu\tilde\varphi(x) - \frac{\varepsilon^2}{6}\sum_{\alpha,\nu,\mu=1}^d \eta_\alpha\eta_\nu\eta_\mu\partial_\alpha\partial_\nu\partial_\mu\tilde\varphi(x+t\varepsilon\eta)$$

and

$$\tilde b_{jl}(x+\varepsilon\eta) = \tilde b_{jl}(x) + \varepsilon\eta\cdot\nabla\tilde b_{jl}(x) + \varepsilon^2\sum_{\nu,\mu=1}^d \eta_\nu\eta_\mu\partial_\nu\partial_\mu\tilde b_{jl}(x+t'\varepsilon\eta) .$$

In addition, we use the expansion of the exponential function at zero to get

$$e^{\frac{1}{\varepsilon}(\tilde\varphi(x)-\tilde\varphi(x+\gamma))} = e^{-\nabla\tilde\varphi(x)\cdot\eta}\left(1 - \frac{\varepsilon}{2}\sum_{\nu,\mu=1}^d\eta_\nu\eta_\mu\partial_\nu\partial_\mu\tilde\varphi(x) + \frac{\varepsilon^2}{4}\left(\sum_{\nu,\mu=1}^d\eta_\nu\eta_\mu\partial_\nu\partial_\mu\tilde\varphi(x)\right)^2 - O\left(\varepsilon^4\right)\right)\times$$
$$\times\left(1 - \frac{\varepsilon^2}{6}\sum_{\alpha,\nu,\mu=1}^d \eta_\alpha\eta_\nu\eta_\mu\partial_\alpha\partial_\nu\partial_\mu\tilde\varphi(x+t\varepsilon\eta) + O\left(\varepsilon^4\right)\right)\left(1 + O\left(\varepsilon^3\right)\right) .$$

The lowest order equation is that of order $-N$. By the eikonal equation, the left hand side vanishes and the same argument applies for the $-N+\frac{1}{2}$ order equation. The first non-vanishing term arises from the action of the first order part of the conjugated operator on the function $\tilde{b}_{j,-N}(x)$,which is for $\tilde{a}$ defined in (2.18)

$$\left\{\sum_{\eta\in\mathbb{Z}^d}\tilde{a}_\eta(x)e^{-\nabla\tilde{\varphi}(x)\cdot\eta}\left(\eta\cdot\nabla-\frac{1}{2}\sum_{\nu,\mu=1}^{d}\eta_\nu\eta_\mu\partial_\nu\partial_\mu\tilde{\varphi}(x)\right)+V_1(x)-E\right\}\tilde{b}_{j,-N}(x)=b_{j,-N}\,. \tag{3.86}$$

This equation takes the form

$$\left(\mathcal{P}(x,\partial_x)+f(x)\right)u(x)=v(x) \tag{3.87}$$

for the differential operator

$$\mathcal{P}(x,\partial_x):=\sum_{\eta\in\mathbb{Z}^d}\tilde{a}_\eta(x)e^{-\nabla\tilde{\varphi}(x)\cdot\eta}\eta\cdot\nabla\,, \tag{3.88}$$

which is well defined by the polynomial decrease of $a_\gamma$ (see Remark 3.2). The next and all higher order equations result from the action of the first order part of the conjugated operator given in (3.86) on the respective highest order part of $\tilde{b}_j$, which for the $k$-th order is the term $\tilde{b}_{j,k-1}$. Additionally to the first order equation, a term is produced by the action of higher orders of the conjugated operator on lower order parts of $\tilde{b}_j$. Since these lower order terms are already determined by the preceding transport equations, this additional part can be treated as an additional inhomogeneity of (3.87). Thus all transport equation take the form

$$\left(\mathcal{P}(x,\partial_x)+f(x)\right)u(x)=v(x) \tag{3.89}$$

with $f,v\in\mathscr{C}^\infty(\emptyset')$ and $v$ vanishing to infinite order at $x=0$ by the construction of the formal series (3.83). The differential operator $\mathcal{P}$ defined in (3.88) is of the form $\langle Z\,,\,\nabla\rangle$ for the vector field $Z(x)=(z_1(x),\dots,z_d(x))$ given by

$$z_\nu(x)=\sum_{\eta\in\mathbb{Z}^d}\tilde{a}_\eta(x)e^{-\nabla\tilde{\varphi}(x)\cdot\eta}\eta_\nu\quad.$$

Using (2.22) we see that $x=0$ is a critical point of the vector field $Z$. In order to linearize at zero, we compute

$$\partial_{x_\mu}z_\nu(0)=\sum_{\eta\in\mathbb{Z}^d}\Big[(\partial_{x_\mu}\tilde{a}_\eta)(0)e^{-\nabla\tilde{\varphi}(0)\cdot\eta}\eta_\nu-\tilde{a}_\eta(0)e^{-\nabla\tilde{\varphi}(0)\cdot\eta}\partial_{x_\mu}(\langle\nabla\tilde{\varphi}\,,\,\eta\rangle)(0)\eta_\nu\Big]\,.$$

Since for $x\in\emptyset$ the phase function $\tilde{\varphi}$ is given by (3.12), we get $\nabla\tilde{\varphi}(0)=0$ and $\partial_{x_\mu}(\nabla\tilde{\varphi}\eta)(0)=\lambda_\mu\eta_\mu$. In Hypothesis 3.1 we assumed the kinetic energy to vary at least quadratic in $x$, thus the first derivative of $a_{\varepsilon\eta}$ vanishes and

$$\partial_{x_\mu}z_\nu(0)=-\sum_{\eta\in\mathbb{Z}^d}\tilde{a}_\eta(0)\lambda_\mu\eta_\mu\eta_\nu\,.$$

By (2.23) and since we chose coordinates such that $B(0)=\mathbf{1}$ as described in Remark 3.3, we get

$$-\sum_{\eta\in\mathbb{Z}^d}\tilde{a}_\eta(0)\eta_\mu\eta_\nu\lambda_\mu=\begin{cases}\lambda_\mu>0 & \text{for}\quad\nu=\mu\\ 0 & \text{for}\quad\nu\neq\mu\,.\end{cases}$$

Therefore the linearization of $Z$ at 0 is $Z_0:=(z_{10},\dots,z_{d0})$ with $z_{\nu 0}(x)=\lambda_\nu x_\nu$ and the corresponding differential operator is given by

$$\mathcal{P}_0(x,\partial_x)=\sum_{\nu=1}^{d}\lambda_\nu x_\nu\partial_{x_\nu}$$

with $\lambda_\nu>0$ for $\nu=1,\dots,d$. Now we are in the state to use the results in Dimassi-Sjöstrand [**16**] (Proposition 3.5) and Helffer [**29**] (Proposition 2.3.7), which tell us, that under the given assumptions the differential equation (3.89) has a unique $\mathscr{C}^\infty$-solution in a sufficiently small neighborhood $\emptyset'$ of suitable shape (star-shaped in the notion of Dimassi-Sjöstrand [**16**]) vanishing to infinite order at $x=0$. We briefly recall the proof for the existence and uniqueness of solutions of the partial differential equation (3.89) using the method of integrating along the characteristics of the vector field $Z$. We denote by $]-\infty,0]\ni t\mapsto\gamma(t)$ the integral curve of $Z$, i.e.,

$$\dot{\gamma}(t)=Z(\gamma(t))\,,\quad\text{with}\quad\gamma(0)=x_0\in\emptyset'\,, \tag{3.90}$$

for some $x_0 \in \mathcal{O}' \setminus \{0\}$. Formally this integral curve is given by $\gamma(t) = e^{tZ}(x_0),\ t \le 0$. By (3.90) we get

$$\dot u(\gamma(t)) = \langle \dot\gamma(t)\,,\, \nabla u(\gamma(t))\rangle = \langle Z\,,\,\nabla u\rangle(\gamma(t)) = \mathcal{P}(x,\partial_x)u(\gamma(t)) = v(\gamma(t)) - fa(\gamma(t))$$

Since all eigenvalues of the linearized vector field $Z_0$ are strictly positive, it follows by the theory of ordinary differential equations, that $\gamma(t)$ approaches 0 exponentially fast for $t \to -\infty$, i.e., $|\gamma(t)| \le Ce^{-\frac{|t|}{C}}|x_0|$ for arbitrary small suitable $\mathcal{O}'$. The inhomogeneity $v$ is a $\mathscr{C}^\infty$-function vanishing at 0 to infinite order, thus by the preceding estimate $v(\gamma(t)) = O\left(e^{-C|t|}\right)$ for every $C > 0$ and we have a unique $\mathscr{C}^\infty$-solution $u$ of (3.89) with $u = O\left(|x|^\infty\right)$. Thus the formal power series $\tilde a_j(x,\varepsilon)$ defined in (3.85) solves in $\mathcal{O}'$ the equation

$$(\widehat H_\varepsilon - \varepsilon \tilde E_j(\varepsilon))\left(\tilde a_j(x,\varepsilon)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\right) = 0\,, \quad \tilde E_j(\varepsilon) = E + \sum_{k\in\frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk}\,.$$

Again by a Borel procedure, but now with respect to $\varepsilon$, we can find a function $a_j' \in \mathscr{C}^\infty\left(\mathcal{O}' \times [0,\infty)\right)$ representing the asymptotic sum $\tilde a_j(x,\varepsilon)$ given in (3.85), which we denote by

$$a_j'(x,\varepsilon) \sim \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\ge -N}} \varepsilon^l \tilde a_{jl}(x)\,. \tag{3.91}$$

In order to get a function, which is defined on $\mathbb{R}^d \times [0,\infty)$, we multiply with a cut-off function $k \in \mathscr{C}_0^\infty(\mathbb{R}^d)$, with $\operatorname{supp} k \subset \mathcal{O}'$ and such that for some $\tilde{\mathcal{O}}, \overline{\tilde{\mathcal{O}}} \subset \mathcal{O}'$ we have $k(x) = 1$ for $x \in \tilde{\mathcal{O}}$. We denote the resulting function $a_j \in \mathscr{C}_0^\infty\left(\mathbb{R}^d \times [0,\infty)\right)$ by

$$a_j(x,\varepsilon) := k(x)a_j'(x,\varepsilon) \sim k(x) \sum_{\substack{l\in\frac{\mathbb{Z}}{2}\\ l\ge -N}} \varepsilon^l \tilde a_{jl}(x)\,. \tag{3.92}$$

Analogously we define a real number $E_j(\varepsilon)$ as an asymptotic sum

$$E_j(\varepsilon) \sim E + \sum_{k\in\frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk}\,. \tag{3.93}$$

We have therefore proven the main part of the following theorem.

THEOREM 3.18. *Let, for $\varepsilon > 0$, $\widehat H_\varepsilon$ and $H_\varepsilon$ respectively be an Hamilton operator satisfying Hypothesis 3.1. As described in Hypothesis 3.6, we choose a real function $\tilde\varphi$ and a star shaped neighborhood $\mathcal{O}'$ of 0.*

*Let $\varepsilon E$ be an eigenvalue of the harmonic approximation $H^0$ of $H_\varepsilon$ given in* (3.58) *with multiplicity $m$ and for $j = 1,\dots,m$ let the functions $a_j \in \mathscr{C}_0^\infty\left(\mathbb{R}^d \times [0,\infty)\right)$ be as defined in* (3.92)*, where the cut-off function $k$ is supported in $\mathcal{O}'$ and $k(x) = 1$ for $x \in \tilde{\mathcal{O}}$ for some neighborhood $\mathcal{O}$ of 0 with $\overline{\tilde{\mathcal{O}}} \subset \mathcal{O}'$. Then the functions $a_j$ and the real numbers $E_j$ defined in* (3.93) *solve the equation*

$$(\widehat H_\varepsilon - \varepsilon E_j(\varepsilon))\left(a_j(x,\varepsilon)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\right) = O\left(\varepsilon^\infty\right)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\,, \quad (x\in\tilde{\mathcal{O}},\ \varepsilon\to 0)\,. \tag{3.94}$$

*For any $x_0 \in \mathbb{R}^d$, the restriction $\mathbf{1}_{\mathscr{G}_{x_0}} a_j(x,\varepsilon)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}$ of the approximate eigenfunctions to the lattice $\mathscr{G}_{x_0} = (\varepsilon\mathbb{Z})^d + x_0$ are approximate eigenfunctions for the operator $H_\varepsilon$ with respect to the same approximate eigenvalues, i.e.,*

$$(H_\varepsilon - \varepsilon E_j(\varepsilon))\,\mathbf{1}_{\mathscr{G}_{x_0}}\left(a_j(x,\varepsilon)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\right) = \mathbf{1}_{\mathscr{G}_{x_0}} O\left(\varepsilon^\infty\right)e^{-\frac{\tilde\varphi(x)}{\varepsilon}}\,, \quad (x\in\tilde{\mathcal{O}}\cap\mathscr{G}_{x_0},\ \varepsilon\to 0)\,. \tag{3.95}$$

Proof:

To make the step from $\widehat H_\varepsilon$ acting on $\mathscr{C}_0^\infty\left(\mathbb{R}^d\right)$ to the operator $H_\varepsilon$ acting on lattice functions $\mathcal{K}\left((\varepsilon\mathbb{Z})^d\right)$, we use that $\mathscr{G}_{x_0}$, the lattice shifted to any point $x_0 \in \mathbb{R}^d$ in the sense that $x_0 \in \mathscr{G}_{x_0}$, is invariant under the action of $\widehat H_\varepsilon$ as discussed in Remark 2.9. Thus the restriction to the lattice commutes with $\widehat H_\varepsilon$ and the action of the restriction operator $\mathbf{1}_{\mathscr{G}_{x_0}}$ to (3.94) yields (3.95) by use of (2.34).

Remark 3.19. *It follows from the construction given in* (3.83) *that the constant $N$ denoting the lowest order in $\varepsilon$ in the expansion* (3.92) *is given by* $N = \max_{\alpha \in I_E} \frac{|\alpha|}{2}$. *Here* $I_E := \left\{ \alpha \in \mathbb{N}^d \,\middle|\, G_0 h_\alpha = E h_\alpha \right\}$*, where $E$ denotes an eigenvalue (energy) of the harmonic oscillator $G_0$, giving the zero order term in the expansion* (3.93)*. Furthermore, $h_\alpha$ denote the associated eigenfunctions, which were shown to be products of the hermite polynomials introduced in* (2.39)*.*
*It follows at once that in the case of the bottom of the spectrum, i.e., if $E = 1$, the associated eigenfunctions are the constant function $h_0$ and therefore $N = 0$ in this case.*

CHAPTER 4

# Finsler Distance associated to $H_\varepsilon$

In this chapter, we define the notion of a metric and distance function adapted to the Hamilton operator $H_\varepsilon$, which describes the decay rate of the eigenfunctions of a Dirichlet operator associated to $H_\varepsilon$ and extends the solution of the eikonal equation outside of a neighborhood $\Omega$ of one well. Analog to the construction of Agmon [**3**] for Schrödinger operators, the idea is to find a metric, such that the geodesics with respect to this metric are equal to the base integral curves of the Hamilton vector field, but since $T_\varepsilon$ is a translation operator we have to use the notion of a Finsler metric instead of a Jacobi metric.
In Chapter 6, we will use this distance function on $\mathbb{R}^d$, to replace the locally defined quasi modes of $H_\varepsilon$ constructed in Chapter 3 by globally defined functions.

In the following definitions we introduce the general notion of a Finsler manifold, where the distance is defined via variation over the length of curves as in the Riemannian setting. For the theory of Finsler manifolds we refer to the detailed description for example in Bao-Chern-Shen [**6**] (from which we adopt the notation), Asanov [**5**] Abate-Patrizio [**1**] and Giaquinta-Hildebrandt [**22**].

For a manifold $M$ we denote by $T_xM$ the tangent space at the base point $x \in M$ and by $TM$ the tangent bundle of $M$. We denote an element of $TM$ by $(x, v)$ where $x \in M$ and $v \in T_xM$ such that the projection $\pi : TM \to M$ is given by $\pi(x, v) = x$. The cotangent space $T^*_xM$ at $x \in M$ is the dual space of $T_xM$, the cotangent bundle is denoted by $T^*M$ and analog to the tangent bundle its elements are written as $(x, \xi)$. The projection $\pi^* : T^*M \to M$ is then given by $\pi^*(x, \xi) = x$. Sometimes the tangent space $T_xM = \pi^{-1}(x)$ and the cotangent space $T^*_xM = (\pi^*)^{-1}(x)$ are called fibre over $x$.

The canonical pairing between an element $v \in T_xM$ and $\xi \in T^*_xM$ is written as $v \cdot \xi$.

For a local coordinate system $(x_1, \dots, x_d) : U \to \mathbb{R}^d$, where $U \in M$ open, the induced coordinate bases of $TM$ and $T^*M$ are given by $\partial_{x_\nu}$ and $dx_\nu$, $\nu = 1, \dots d$ respectively. An element $(x, v) \in \pi^{-1}(U) \subset TM$ can then be written in local coordinates $(x_1, \dots, x_d, v_1, \dots, v_d)$, where $v = \sum_{\nu=1}^d v_\nu \partial_{x_\nu}$ and analogously an element $(x, \xi)$ of the cotangent bundle can be written as $(x_1, \dots, x_d, \xi_1, \dots, \xi_d)$ for $\xi = \sum_\nu \xi_\nu dx_\nu$. If $f$ is a function on $M$ or $TM$, then we use the same letter for the associated function in $\mathbb{R}^d$ with respect to local coordinates.

## 4.1. Definition and Properties of Finsler Manifold and Finsler Metric

Definition 4.1. *Let $M$ denote a $d$-dimensional $\mathscr{C}^\infty$-manifold, $TM$ its tangent bundle and $TM \setminus \{0\} := \{(x, v) \in TM \,|\, v \neq 0\}$ the slit tangent bundle.*

(a) *A (Lagrange)-function $F : TM \to [0, \infty)$ is called a Finsler function on $M$, if:*
  1) *$F$ is of class $\mathscr{C}^\infty(TM \setminus \{0\})$.*
  2) *It satisfies the homogeneity condition $F(x, \lambda v) = \lambda F(x, v)$ for $\lambda > 0$, i.e. $F$ is positive homogeneous of order 1 in each fibre $T_xM$.*
  3) *$F(x, v) > 0$ for $v \neq 0$.*

(b) *A Finsler function $F$ is said to be absolutely homogeneous, if*
  4) *it satisfies the condition $F(x, \lambda v) = |\lambda| F(x, v)$ for all $\lambda \in \mathbb{R}$,*

  *i.e. if it is absolute homogeneous of order 1 with respect to the fibre variable.*

(c) *A manifold together with a Finsler function, $(M, F)$, is called Finsler manifold.*

In our setting, only absolutely homogeneous Finsler functions arise.
A Finsler function induces a curve length on $M$ as follows.

Definition 4.2. (a) *A curve $\gamma : [a, b] \to M$, $\quad t \mapsto \gamma(t)$ on $M$ is called regular, if it is $\mathscr{C}^2$ and the velocity $\dot\gamma(t) \neq 0$ for all $t \in [a, b]$, where $\dot\gamma(t) := \frac{d}{dt}\gamma(t) \in T_{\gamma(t)}M$.*

(b) *We denote by* $\Gamma_{a,b}(x_1,x_2)$ *the collection of all regular curves* $\gamma$ *on* $M$ *which are parameterized over* $[a,b]$ *and satisfy* $\gamma(a)=x_1$ *and* $\gamma(b)=x_2$*. Then* $\Gamma_{a,b}(x_1,x_2)$ *is a Banach-manifold (for the notion of manifolds of maps and the construction of coordinate charts see for example Klingenberg* [**46**] *or Hamilton* [**26**]*).*

(c) *For any Finsler function* $F$ *on* $M$*, the curve length* $s_F:\Gamma_{a,b}(x_1,x_2)\to\mathbb{R}$ *associated to* $F$ *is defined as*

$$s_F(\gamma):=\int_a^b F(\gamma(t),\frac{d}{dt}\gamma(t))\,dt\,.$$

(d) *For any* $\delta>0$*, a regular variation of* $\gamma\in\Gamma_{a,b}(x_1,x_2)$ *is a* $\mathscr{C}^2$*-map* $\gamma_\delta:[a,b]\times(-\delta,\delta)\to M$*, such that* $\gamma_\delta(t,0)=\gamma(t)$ *for all* $t\in[a,b]$ *and* $\gamma_\delta(.,u)$ *is regular for each* $u\in(-\delta,\delta)$*.*

*A regular variation of* $\gamma$ *with fixed endpoints (i.e. with* $\gamma_\delta(a,u)=x_1$ *and* $\gamma_\delta(b,u)=x_2$ *for all* $u\in(-\delta,\delta)$*) can be considered as a map* $\gamma_\delta:(-\delta,\delta)\to\Gamma_{a,b}(x_1,x_2)$*, i.e. as a* $\mathscr{C}^2$*-curve in* $\Gamma_{a,b}(x_1,x_2)$ *passing the point* $\gamma$ *for the parameter value* $u=0$*.*

*Therefore the tangent space of* $\Gamma_{a,b}(x_1,x_2)$ *at a point* $\eta$ *is given by*

$$T_\eta\Gamma_{a,b}(x_1,x_2)=\{\partial_u\eta_\delta|_{u=0}\,|\,\eta_\delta\quad\text{is a regular variation of}\quad\eta\quad\text{with fixed endpoints}\}\,. \tag{4.1}$$

(e) *The tangential of the curve length* $s_F$ *with respect to a Finsler function* $F$ *at a point* $\eta$ *is a mapping* $ds_F|_\eta:T_\eta\Gamma_{a,b}(x_1,x_2)\to T_{s_F(\eta)}\mathbb{R}$*, which is given by* $ds_F|_\eta(\partial_u\eta_\delta|_{u=0})=\partial_u s_F(\eta_\delta)|_{u=0}$*.*

$ds_F$ *is called the first variation of curve length in Finsler geometry.*

(f) *A regular curve* $\gamma\in\Gamma_{a,b}(x_1,x_2)$ *is called a geodesic with respect to the Finsler function* $F$ *(or a Finsler geodesic), if* $ds_F|_\gamma=0$*, i.e. if* $\partial_u s_F(\gamma_\delta)|_{u=0}=0$ *for all regular variations* $\gamma_\delta$ *of* $\gamma$ *with fixed endpoints.*

Remark 4.3. (a) *The curve length* $s_F(\gamma)$ *of* $\gamma$ *is well defined, because by condition 2) for* $F$ *(the positive homogeneity with respect to* $v$*, Def.4.1,(a)2)) the integral is independent of the parametrization of the curve.*

(b) *In the book of Agmon* [**3**]*, the curve length in Finsler geometry is defined with respect to the wider class of absolutely continuous curves. ( A complex curve* $\gamma$ *on the interval* $[a,b]$ *is absolute continuous, if for all* $\varepsilon>0$ *there exists a* $\delta>0$ *such that* $\sum_{j=1}^n|\gamma(\beta_j)-\gamma(\alpha_j)|<\varepsilon$ *for all* $n\in\mathbb{N}$ *and disjoint segments* $(\alpha_1,\beta_1),\dots(\alpha_n,\beta_n)$ *which satisfy* $\sum_{j=1}^n|\beta_j-\alpha_j|<\delta$*.)*

*These curves are not differentiable in the usual sense, but it is shown in Rudin* [**52**]*, Thm.7.18, that if* $\gamma$ *is absolutely continuous, then it is differentiable almost everywhere on* $[a,b]$*,* $\dot\gamma\in\mathscr{L}^1$ *and* $\gamma(t)-\gamma(a)=\int_a^t\dot\gamma(s)\,ds$*.*

*The restriction to the class of* $\mathscr{C}^2$*-curves is adapted to the definition given by Abate-Patrizio* [**1**]*, allowing to use the results given there.*

(c) *Since the point* $\eta\in\Gamma_{a,b}(x_1,x_2)$ *is a curve on* $M$*, any tangent vector* $\partial_u\eta_\delta|_{u=0}\in T_\eta\Gamma_{a,b}(x_1,x_2)$ *at* $\eta$ *can be considered as a vector field* $\partial_u\eta_\delta|_{u=0}(.)$ *along* $\eta(.)\subset M$*, i.e. as a function* $\partial_u\eta_\delta|_{u=0}:[a,b]\to TM$ *such that* $\partial_u\eta_\delta|_{u=0}(t)\in T_{\eta(t)}M$*. Since the variation* $\eta_\delta$ *was assumed to have fixed endpoints, it follows that* $\partial_u\eta_\delta|_{u=0}(a)=\partial_u\eta_\delta|_{u=0}(b)=0$*.*

If the manifold $M$ is connected, the notion of the integral length of a curve suggests to define the distance between two points as the infimum of the distance over all regular curves joining these points.

Definition 4.4. *Let* $(M,F)$ *denote a Finsler manifold.*

(a) *The Finsler distance* $d_F(x_1,x_2):M\times M\to[0,\infty]$ *between the points* $x_1$ *and* $x_2$ *is defined by*

$$d_F(x_1,x_2):=\inf_{\gamma\in\Gamma_{0,1}(x_1,x_2)}s_F(\gamma)\,.$$

*If* $\Gamma_{0,1}(x_1,x_2)$ *is empty, the distance is defined to be infinity.*

(b) *A geodesic* $\gamma$ *between two points* $x_1$ *and* $x_2$ *is called minimal, if* $s_F(\gamma)=d(x_1,x_2)$*.*

In Lemma 4.8 we will show, that in the case of an absolutely homogeneous Finsler function, this distance is actually a metric on $M$.

REMARK 4.5. *A function $g \in \mathscr{C}^\infty(TM, \mathbb{R})$ is called a Riemannian metric if for each $x \in M$ its restriction $g_x : T_xM \to \mathbb{R}$ to the fibre over $x$ is a positive definite quadratic form and therefore induces a scalar product. Defining $g_{ij(x)} := g_x(\partial_{x_i}, \partial_{x_j})$, in local coordinates the Riemannian metric is therefore given by a covariant two-tensor*

$$ds^2 = g = \sum_{i,j=1}^{d} g_{ij(x)} dx_i \otimes dx_j \qquad \text{with} \quad g_{ij(x)} = g_{ji(x)} \;. \tag{4.2}$$

*Each Riemannian metric $g$ induces a Finsler function via $F_g(x,v) := \sqrt{g_x(v,v)}$, thus each Riemannian manifold is a Finsler manifold. In local coordinates $F_g$ is determined by*

$$F_g^2(x_1, \ldots, x_d, v_1, \ldots, v_d) = \sum_{i,j} g_{ij(x)} v_i v_j \tag{4.3}$$

*and thus*

$$g = \sum_{i,j} \partial^2_{v_i v_j} \left(\frac{1}{2} F_g^2\right) dx_i \otimes dx_j \;. \tag{4.4}$$

*Then for any regular curve $\gamma : [0,1] \to M$, the curve length with respect to $F = F_g$ defined in Definition 4.2 is equal to the Riemannian curve length, i.e. $s_{F_g}(\gamma) = \int |\dot\gamma(t)|\, dt$, with $|\dot\gamma(t)|^2 := g_{\gamma(t)}(\dot\gamma(t), \dot\gamma(t))$ and the Finsler distance $d_{F_g}$ given in Definition 4.4 is thus equal to the Riemannian distance.*

*In a weak sense there is an inverse of this connection between Riemannian and Finsler manifolds. For a given Finsler function $F$, equation (4.4) with $F$ instead of $F_g$ defines a symmetric covariant 2-tensor $g_F$. The elements of the matrix $(g_{ij}(x,v))$ determined by (4.3) again with a general Finsler function at the place of $F_g$, are then depending not only on the base variable $x$ but also on the tangent vector $v$. In local coordinates, $g_{ij}$ can for a general Finsler function be defined as*

$$g_{ij} := \frac{\partial^2}{\partial v_i \partial v_j}\left(\frac{1}{2}F^2\right) = F \frac{\partial^2 F}{\partial v_i \partial v_j} + \frac{\partial F}{\partial v_i}\frac{\partial F}{\partial v_j} \;. \tag{4.5}$$

DEFINITION 4.6. *We denote by $SM := TM/\sim_S$ the sphere bundle, where*

$$(x,v) \sim_S (y,w)\,, \quad \text{if} \quad x = y \quad \text{and} \quad v = \lambda w \quad \text{for any} \quad \lambda > 0\,.$$

*By $PTM$ we denote the projective bundle of $TM$, i.e. $PTM = TM/\sim_P$, where*

$$(x,v) \sim_P (y,w)\,, \quad \text{if} \quad x = y \quad \text{and} \quad v = \lambda w \quad \text{for any} \quad \lambda \neq 0\,.$$

Since $F$ is positive (or absolutely) homogeneous of degree one in $v$, the functions $g_{ij}$ are homogeneous of degree zero in $v$ and are thus functions on the sphere (or projective) bundle respectively.

REMARK 4.7. *In the literature, the definition of the Finsler function is sometimes slightly different concerning the positivity (Definition 4.1,a)3)). Instead of positivity of $F$, strong convexity of $F$ is required, i.e. the matrix $(g_{ij}(x,v))$ defined in (4.5) is assumed to be positive definite. By use of the homogeneity condition, this follows from the positivity of $F$ as can be seen by the following considerations.*

*A function $F$ which is homogeneous of order 1, fulfills by the Euler Theorem the relations*

$$\sum_{i=1}^{d} v_i \frac{\partial F}{\partial v_i} = F \quad \text{and} \quad \sum_{i=1}^{d} v_i \frac{\partial^2 F}{\partial v_i \partial v_j} = 0\,. \tag{4.6}$$

*The second equation follows from the first by differentiation. To verify the positive definiteness of $g$, we have to analyze the term*

$$\sum_{i,j=1}^{d} g_{ij} v_i v_j = \sum_{i,j=1}^{d} \left(F \frac{\partial^2 F}{\partial v_i \partial v_j} v_i v_j + \frac{\partial F}{\partial v_i}\frac{\partial F}{\partial v_j} v_i v_j\right)\,.$$

*By (4.6), the first summand on the right hand side vanishes and the second is again by the Euler theorem equal to $F^2$. Thus by the positiveness of the Finsler function except for $v = 0$, the matrix $g$ is positive definite. Since by definition $F \geq 0$, the two assumptions are equivalent.*

*It is shown in Bao-Chern-Shen* [**6**]*, that additional properties of a Finsler function are*

$$F(x, v+\tilde{v}) \leq F(x,v) + F(x,\tilde{v}), \quad (x,v),(x,\tilde{v}) \in TM \qquad \textit{Triangle inequality} \tag{4.7}$$

$$\sum_{i=1}^{d} w_i \frac{\partial F}{\partial v_i}(v) \leq F(w), \quad w, v \in T_xM,\ v \neq 0 \qquad \textit{Fundamental inequality} \tag{4.8}$$

*In* (4.8) *equality holds if and only if* $w = \alpha v$ *for some* $\alpha \geq 0$.

In the next lemma some elementary properties of the Finsler distance are described. For a detailed proof of (b) we again refer to Bao-Chern-Shen [**6**], Lemma 6.2.1.

Lemma 4.8. *Let* $(M, F)$ *be a Finsler Manifold and* $d_F$ *the Finsler distance as defined in Definition 4.4.*

(a) $d_F$ *obeys the following two properties of a metric space.*
   i) $d_F(x_1, x_2) \geq 0$*, where equality holds if and only if* $x_1 = x_2$.
   ii) $d_F(x_1, x_3) \leq d_F(x_1, x_2) + d_F(x_2, x_3)$
   *If in addition the Finsler function* $F$ *is absolutely homogeneous, then*
   iii) $d_F(x_1, x_2) = d_F(x_2, x_1)$.
   *For an absolutely homogeneous Finsler function,* $(M, d_F)$ *is thus a metric space.*

(b) *At every point* $x \in M$ *there exists a local coordinate system* $\phi : \overline{U} \to \mathbb{R}^d$*, with the following properties for some* $c > 1$*:*
   i) *The closure of* $U$ *is compact,* $\phi(x) = 0$ *and* $\phi$ *maps* $U$ *diffeomorphically onto an open ball of* $R^d$.
   ii) *For all* $v = \sum_i v_i \partial_{x_i} \in T_xM$ *and* $x \in \overline{U}$

$$\frac{|v|}{c} \leq F(x,v) \leq c|v| \qquad \textit{and} \qquad F(x,-v) \leq c^2 F(x,v)\ ,$$

   *where* $|v| = \sqrt{\sum_i v_i^2}$.
   iii) *Given any* $x_0, x_1 \in U$*, we have*

$$\frac{1}{c}|\phi(x_1) - \phi(x_0)| \leq d_F(x_0, x_1) \leq c|\phi(x_1) - \phi(x_0)|\ .$$

   iv) *For every pair of points* $x_0, x_1 \in U$*, we have*

$$\frac{1}{c^2} d_F(x_1, x_0) \leq d_F(x_0, x_1) \leq c^2 d_F(x_1, x_0)\ .$$

Proof:

(a) i) follows directly from the strict positivity of $F$.
   ii) The right-hand side is given by the minimum over all curves joining $x_1$ and $x_3$ and hitting $x_2$ while on the left-hand side the minimum is taken over all curves from $x_1$ to $x_3$. Thus on the right-hand side we take the minimum over a smaller set and the inequality follows.
   iii) The absolute homogeneity of $F$ yields $F(x,v) = F(x,-v)$. Therefore the original integral is equal to the reversed one from the end point to the starting point which proves the given statement.

(b) This part is identical to Bao-Chern-Shen [**6**], Lemma 6.2.1, and we refer to the proof given there.

□

### 4.2. Finsler Function adapted to a hyperregular Hamiltonian

To define a Finsler distance, which is adapted to the given physical context, we introduce a Legendre transformation with respect to a Hamilton function $h$ on the cotangent bundle $T^*M$, which allows to pass from covectors (momentum variables), denoted by $\xi$, to vectors (velocity variables) denoted by $v$ and vice versa. To this end, we need the notion of fibre derivatives, hyperconvexity and hyperregularity of $h$. It is shown in Proposition 4.12, that hyperconvexity of $h$ is a sufficient condition for hyperregularity.

DEFINITION 4.9. (a) *Let $M$ be a manifold and $f \in \mathscr{C}^\infty(T^*M, \mathbb{R})$. Denote by $f_x$ the restriction $f|_{T_x^*M}$ of $f$ to the fibre $T_x^*M$ over $x$. Then the map $\mathcal{D}_F f : T^*M \to TM$ defined by $\mathcal{D}_F f(x,\xi) := Df_x(\xi)$, is called the fibre derivative of $f$.*

*We sometimes use the notation $\mathcal{D}_F f(x,\xi) = D_\xi f(x,\xi)$.*

(b) *Along the same lines the fibre derivative of a function $g \in \mathscr{C}^\infty(TM, \mathbb{R})$ is defined as $\mathcal{D}_F g : TM \to T^*M$, $\quad \mathcal{D}_F g(x,v) := Dg_x(v)$.*

(c) *Let $G_x : T_x^*M \times T_xM \to \mathbb{R}$ denote the canonical pairing $G_x(\xi, v) := \xi \cdot v (= \xi(v))$. We denote by $G$ the function on $M$, that associates to each $x \in M$ the function $G_x$.*

(d) *A function $f : SM \to TM$ is called strictly fibre preserving, if $f([(x,u)]) \in [(x,u)]$ (i.e. if for each $[(x,u)] := \{(x,v) \,|\, v = \lambda u,\ \lambda > 0\} \in SM$ there exists a $\lambda > 0$ such that $f([(x,u)]) = (x, \lambda u)$).*

(e) *A smooth function $h : T^*M \to \mathbb{R}$ (or $L : TM \to \mathbb{R}$) is said to be hyperregular, if its fibre derivative $\mathcal{D}_F h : T^*M \to TM$ (or $\mathcal{D}_F L : TM \to T^*M$) is a diffeomorphism.*

REMARK 4.10. (a) *The derivative $Df_x(\xi)$ maps $T_\xi(T_x^*M)$ linearly to $T_{f_x(\xi)}\mathbb{R}$. Since $T_x^*M$ and $\mathbb{R}$ are vector spaces, they are isomorphic to their tangent spaces $T_\xi(T_x^*M)$ and $T_{f_x(\xi)}\mathbb{R}$ respectively. Thus $Df_x(\xi)$ can be considered as bounded linear functional on $T_x^*M$, i.e. as an element of $T_xM$. It follows immediately from Definition 4.9, that $\mathcal{D}_F f$ is a fibre preserving smooth mapping. For $h \in \mathscr{C}^\infty(T^*M, \mathbb{R})$ we will in the following often use the notation*

$$\xi_h(x,v) := (\mathcal{D}_F h)^{-1}(x,v) \quad \text{and} \quad v_h(x,\xi) := \mathcal{D}_F h(x,\xi)\ . \tag{4.9}$$

(b) *In local coordinates $(x_1, \ldots, x_d)$ the canonical pairing $G_x$ is given by*

$$G_x(\xi_1, \ldots, v_d) = \sum_{\nu=1}^d \xi_\nu v_\nu\ .$$

DEFINITION 4.11. *Let $V$ be a normed vectorspace and $L$ a real valued function on $V$.*

(a) *$L$ is called convex, if for all $v_1, v_2 \in V$ and $\lambda \in [0,1]$*

$$L(\lambda v_1 + (1-\lambda)v_2) \le \lambda L(v_1) + (1-\lambda)L(v_2)\ . \tag{4.10}$$

(b) *If furthermore $L \in \mathscr{C}^2(V)$, it is called strictly convex, if $D^2L|_{v_0}(v,v) > 0$ for all $v_0, v \in V$, i.e. if the bilinear map $D^2L|_{v_0}$ on $V$ is positive definite.*

(c) *We call $L \in \mathscr{C}^2(V)$ hyperconvex, if there exists a constant $\alpha > 0$ such that*

$$D^2L|_{v_0}(v,v) \ge \alpha \|v\|^2 \quad \text{for all} \quad v_0, v \in V\ .$$

As in the case of functions on $\mathbb{R}^n$, convexity of $L$ implies that the bilinear map $D^2L|_{v_0}$ is non-negative. This can be seen as follows. Define for any fixed $v_1, v_2 \in V$ the function $f : [0,1] \to \mathbb{R}$ by setting $f(t) := L(tv_1 + (1-t)v_2)$. Then $f$ is convex, since for any $\lambda, s, t \in [0,1]$

$$\begin{aligned} f(\lambda t + (1-\lambda)s) &= L((\lambda t + (1-\lambda)s)v_1 + (1 - (\lambda t + (1-\lambda)s))t) \\ &= L(\lambda(tv_1 + (1-t)v_2) + (1-\lambda)(sv_1 + (1-s)v_2)) \\ &\le \lambda L(tv_1 + (1-t)v_2) + (1-\lambda)L(sv_1 + (1-s)v_2) \\ &= \lambda f(t) + (1-\lambda)f(s)\ . \end{aligned}$$

Thus $f'$ is increasing,

$$f(t) - f(s) \ge f'(s)(t-s) \tag{4.11}$$

and therefore

$$(t-s)(f'(t) - f'(s)) \ge 0 \quad \text{and} \quad f''(t) \ge 0\,, \quad s,t \in [0,1] \tag{4.12}$$

By the definition of $f$, from (4.11) follows

$$L(tv_1 + (1-t)v_2) - L(sv_1 + (1-s)v_2) \ge DL(sv_1 + (1-s)v_2)(v_1 - v_2)(t-s)$$

and in particular by setting $t = 1$ and $s = 0$

$$L(v_1) - L(v_2) \ge DL(v_2)(v_1 - v_2)\ . \tag{4.13}$$

The second estimate in (4.12) yields

$$f''(t) = D^2L|_{(tv_1 + (1-t)v_2)}[(v_1 - v_2), (v_1 - v_2)] \ge 0\ . \tag{4.14}$$

Furthermore, if $L$ is strictly convex, the inequality in (4.10) and (4.12) is strict. Thus again by the definition of $f$ it follows from (4.12) that

$$(t-s)\left(DL(tv_1+(1-t)v_2)(v_1-v_2)-DL(sv_1+(1-s)v_2)(v_1-v_2)\right)>0\,.$$

In particular, setting $t=1$ and $s=0$, we have

$$\left(DL(v_1)-DL(v_2)\right)(v_1-v_2)>0 \tag{4.15}$$

The following Proposition gives a connection between hyperconvexity and hyperregularity.

Proposition 4.12. *If a real valued function $h\in\mathscr{C}^\infty(T^*M)$ is hyperconvex in each fibre $T_x^*M$, it is hyperregular.*

Proof:

The fibre derivative $\mathcal{D}_Fh:T^*M\to TM$ is a global diffeomorphism, if it is a local diffeomorphism and bijective.

By definition, $\mathcal{D}_Fh$ is fibre preserving, thus with respect to local coordinates at $(x_0,\xi_0)$, its derivative is given by the $2d\times 2d$-matrix

$$D\mathcal{D}_Fh|_{(x_0,\xi_0)}=\begin{pmatrix}\mathbf{1} & 0\\ * & M\end{pmatrix}\,,\quad\text{where}\quad M=D^2_\xi h|_{(x_0,\xi_0)}\,. \tag{4.16}$$

Since $h$ was assumed to be hyperconvex in each fibre, $M$ is positive definite and thus it follows from (4.16), that $\mathcal{D}_Fh$ is a local diffeomorphism (Inverse Function Theorem).

Since $\mathcal{D}_Fh$ is by definition fibre preserving, i.e. it is the identity map with respect to the base point $x\in M$, it is sufficient to show the bijectivity of the function $Dh_x:T_x^*M\to T_xM$ for all $x\in M$.

Thus we fix any $x\in M$ and analyze $Dh_x$. Since $h_x$ is strictly convex for each $x\in M$, the inequality

$$(\xi-\eta)\left(Dh_x(\xi)-Dh_x(\eta)\right)>0\,,\qquad \xi,\eta\in T_x^*M,\,\eta\neq\xi$$

holds by (4.15). Thus $\xi\neq\eta$ implies $Dh_x(\xi)\neq Dh_x(\eta)$, and therefore $\mathcal{D}_Fh(x,.)=Dh_x$ is injective.

To show the surjectivity, we first consider for any $v_0\in T_xM$ the solution $v:[0,1]\to T_xM$ of the initial value problem

$$\dot v(t)=v_0\,,\qquad v(0)=0\,, \tag{4.17}$$

which obviously fulfills $v(t)=tv_0$ and $v(1)=v_0$. The idea is now to show, that there exists a curve $\xi:[0,1]\to T_x^*M$, such that $\xi(1)$ is the pre-image of $v_0$ with respect to $Dh_x$, i.e. such that $Dh_h(\xi(1))=v_0$.

If we can establish, that the initial value problem

$$v_0=\frac{d}{dt}Dh_x(\xi(t))=D^2h_x(\xi(t))\cdot\dot\xi(t)\,,\qquad \xi(0)=0\,. \tag{4.18}$$

has a solution $\xi(t)$ for all $t\in[0,1]$, then

$$v_0=\int_0^1 D^2h_x(\xi(t))\cdot\dot\xi(t)\,dt=Dh_x(\xi(1))-Dh_x(\xi(0))=Dh_x(\xi(1))\,.$$

Thus the existence of a solution of (4.18) for any $v_0\in T_xM$ and all $t\in[0,1]$ implies the surjectivity of $Dh_x$.

Since from the hyperconvexity it follows that $D^2h_x|_{\xi(t)}>0$, there exists at each point $\xi(t)$ of the curve the inverse $\left(D^2h_x|_{\xi(t)}\right)^{-1}$ of the linearization of $Dh_x$ at $\xi(t)$, thus (4.18) can be rewritten as

$$\dot\xi(t)=\left(D^2h_x|_{\xi(t)}\right)^{-1}\cdot v_0\,,\qquad \xi(0)=0\,. \tag{4.19}$$

The differential equation is thus of the form $\dot\xi=F(\xi)$ for the vector field $F$ on $T_x^*M$ given by $F(\xi)=\left(D^2h_x|_\xi\right)^{-1}\cdot v_0$. Since $h\in\mathscr{C}^\infty(T^*M)$, the vector field $F$ is locally Lipschitz for all $\xi\in T_x^*M$, thus it follows from the Picard-Lindelöf Theorem (see for example Walter [**61**], page 61, Theorem 7), that the initial value problem (4.19) has for any $v_0\in T_xM$ a solution, which either exists for all $t\geq 0$ or becomes infinity for a finite value of $t$.

In order to exclude, that the curve $\xi$ reaches infinity for some $t<1$, which means that the curve does not exist on the whole interval $[0,1]$, we need the hyperconvexity of $h$. We choose a norm $\|.\|_{T_x^*M}$ on $T_x^*M$ and denote by $\|.\|_{T_xM}$ the norm on $T_xM$, which is induced by duality. Since for fixed $\eta \in T_x^*M = T_\xi(T_x^*M)$ the second derivative $D^2h_x|_\xi(\eta)$ can be seen as linear form on $T_x^*M$, i.e. as an element of $T_xM$, it follows by the hyperconvexity of $h$, that there exists a constant $\alpha > 0$ such that for all $\xi \in T_x^*M$

$$\|D^2h_x|_\xi(\eta)\|_{T_xM} = \sup_{\mu \in T_x^*M} \frac{|D^2h_x|_\xi(\eta,\mu)|}{\|\mu\|_{T_x^*M}} \geq \frac{|D^2h_x|_\xi(\eta,\eta)|}{\|\eta\|_{T_x^*M}} \geq \alpha\|\eta\|_{T_x^*M}\,, \quad \eta \in T_\xi(T_x^*M) \tag{4.20}$$

and therefore

$$\|v\|_{T_xM} = \|D^2h_x|_\xi \left(D^2h_x|_\xi\right)^{-1}(v)\|_{T_xM} \geq \alpha\| \left(D^2h_x|_\xi\right)^{-1}(v)\|_{T_x^*M}\,, \qquad v \in T_xM\,. \tag{4.21}$$

(4.19) together with (4.21) yields

$$\|\dot{\xi}(t)\|_{T_x^*M} = \| \left(D^2h_x|_{\xi(t)}\right)^{-1}(v_0)\|_{T_x^*M} \leq \frac{1}{\alpha}\|v_0\|\,, \tag{4.22}$$

i.e. the velocity of the curve $\xi$ is bounded. Therefore $\|\xi(t)\| < \infty$ for $t < \infty$, i.e. the curve exists for all $t \in [0,1]$ and $\mathcal{D}_Fh(\xi(1)) = v_0$.
Thus for any $v_0 \in T_xM$ there exists a pre-image with respect to $\mathcal{D}_Fh(x,.) = Dh_x$, given by $\xi(1)$, where $\xi : [0,1] \to T_x^*M$ is the solution of (4.19). This shows the surjectivity of $Dh_x$.

Together with the injectivity of $Dh_x$ and the fact that $\mathcal{D}_Fh$ is a local diffeomorphism, it follows that $\mathcal{D}_Fh$ is a global diffeomorphism.

□

REMARK 4.13. *We define for any hyperregular Hamiltonian $h \in \mathscr{C}^\infty(T^*M)$ the energy function $E_h$ on $TM$ by*

$$E_h(x,v) := h \circ (\mathcal{D}_Fh)^{-1}(x,v)(= h(x,\xi_h(x,v)) \tag{4.23}$$

*and the action*

$$A_h : TM \to \mathbb{R}\,, \quad A_h(x,v) := G_x\left((\mathcal{D}_Fh)^{-1}(x,v), v\right)(= \xi_h(x,v)\cdot v)\,, \tag{4.24}$$

*where the fibre derivative $\mathcal{D}_Fh$ and the canonical pairing $G_x$ are introduced in Definition 4.9. Then it is shown in Abraham-Marsden* [**2**]*, Prop.3.6.7, that the Lagrange function*

$$L_h : TM \to \mathbb{R} \quad \text{defined by} \quad L_h(x,v) = A_h(x,v) - E_h(x,v) \tag{4.25}$$

*(the Legendre transform of $h$) is hyperregular on $TM$ and*

$$\begin{aligned} \mathcal{D}_FL_h(x,v) &= D_vA_h(x,v) - D_vE_h(x,v) \\ &= D_v\xi_h(x,v)\cdot v + \xi_h(x,v) - D_\xi h(x,\xi_h(x,v))\cdot D_v\xi_h(x,v) \\ &= D_v\xi_h(x,v)\cdot v + \xi_h(x,v) - v\cdot D_v\xi_h(x,v) \\ &= \xi_h(x,v) = (\mathcal{D}_Fh)^{-1}(x,v) \end{aligned} \tag{4.26}$$

*In fact* [**2**]*, Theorem 3.6.9 states, that the hyperregular Lagrangians on $TM$ and the hyperregular Hamiltonians on $T^*M$ are in bijection.*

*Later on we will use, that in particular by* (4.24) *and* (4.26)

$$A_h(x,v) = \mathcal{D}_FL_h(x,v)\cdot v\,. \tag{4.27}$$

*We recall some standard facts of classical mechanics, which are proven for example in Abraham-Marsden* [**2**].

*Let $h$ be a hyperregular Hamilton function. Then $(\gamma(t),\xi(t)) \in T^*M$ is an integral curve of the hamiltonian vector field $X_h$ in $T^*M$ if and only if it satisfies Hamilton's equations*

$$\begin{aligned} \frac{d\gamma}{dt}(t) &= D_\xi h(\gamma(t),\xi(t))(= \mathcal{D}_Fh(\gamma(t),\xi(t)) \\ \frac{d\xi}{dt}(t) &= D_\gamma h(\gamma(t),\xi(t))\,. \end{aligned} \tag{4.28}$$

*If $L_h$ is the associated Lagrange function defined by* (4.25)*, then $(\gamma(t),\dot\gamma(t)) = (\gamma(t),\mathcal{D}_Fh(\gamma(t),\xi(t)))$ on the tangent bundle is an integral curve of the Lagrangian vector field $X_L$ in $TM$ and satisfies Lagrange's equation*

$$D_\gamma L_h(\gamma(t),\dot\gamma(t)) = \frac{d}{dt}D_{\dot\gamma}L_h(\gamma(t),\dot\gamma(t))\,. \tag{4.29}$$

*On the other hand if a curve $(\gamma, \dot\gamma)$ in $TM$ satisfies Lagrange's equation (4.29), then the associated curve $(\gamma, \mathcal{D}_F L_h(\gamma(t), \dot\gamma(t)))$ on the cotangent bundle $T^*M$ is an integral curve of the hamiltonian vector field $X_h$.*

Definition 4.14. *For a smooth manifold $M$, a $\mathscr{C}^\infty$-function $h : T^*M \to \mathbb{R}$ and $E_0 \in \mathbb{R}$, we define the set of singular points $S_h(E_0)$ by*

$$S_h(E_0) := \{x \in M \mid h(x,0) = E_0\}\,.$$

*Since $S_h(E_0)$ is the level set of a smooth function $h(.,0)$ on $M$, it is closed. Thus $\widetilde{M} := M \setminus S_h(E_0)$ is again a smooth manifold.*

*Let $\pi_s : TM \to SM$ denote the projection $\pi_s(x,v) = [x,v]$, where $[x,v] := \{(y,u) \in TM \mid \exists\lambda > 0 : (y,u) = (x, \lambda v)\}$.*

Proposition 4.15. *Let $M$ be a d-dimensional smooth manifold and $h \in \mathscr{C}^\infty(T^*M)$ be even, hyperregular and strictly convex in each fibre $T_x^*M$.*

*Furthermore we assume that $h(.,0) : M \to \mathbb{R}$ is bounded from above and we set $E_0 \geq \max_{x\in M} h(x,0)$ and $S_h(E_0)$, $\widetilde{M}$ as described in Definition 4.14.*

i) *Then there exists a strictly fibre preserving $\mathscr{C}^\infty$-function $\tau_{E_0} : S\widetilde{M} \to T\widetilde{M}$, which is uniquely determined by the condition*

$$h \circ (\mathcal{D}_F h)^{-1} \circ \tau_{E_0} = E_0\,. \tag{4.30}$$

ii) *Let $\tilde\tau_{E_0} := \tau_{E_0} \circ \pi_S : T\widetilde{M} \to T\widetilde{M}$ and let $\ell_{h,E_0} : T\widetilde{M} \to \mathbb{R}$ be defined by*

$$\ell_{h,E_0}(x,v) := G_x\left((\mathcal{D}_F h)^{-1} \circ \tilde\tau_{E_0}(x,v), v\right)\,.$$

*Then $\ell_{h,E_0}$ is an absolutely homogeneous Finsler function on $\widetilde{M}$.*

iii) *For any regular curve $\gamma : [a,b] \to \widetilde{M}$, there exists a $\mathscr{C}^1$-function $\lambda : [a,b] \to \mathbb{R}_+$, such that*

$$\tilde\tau_{E_0}(\gamma(t), \dot\gamma(t)) = (\gamma(t), \lambda(t)\dot\gamma(t))\,.$$

Remark 4.16. (a) *Since by Proposition 4.15 the Finsler function $\ell_{h,E_0}$ is defined only on $\widetilde{M} = M \setminus S(E_0)$, we call $(M, \ell_{h,E_0})$ a Finsler manifold with singularities.*

(b) *It is possible to analyze an arbitrary energy value $E_0$ (i.e. which not necessarily fulfills the condition $E_0 \geq \max h(x,0)$), by changing the definition of $\widetilde{M}$ to $\widetilde{M}_n := M \setminus \{x \in M \mid E_0 \leq h(x,0)\}$.*

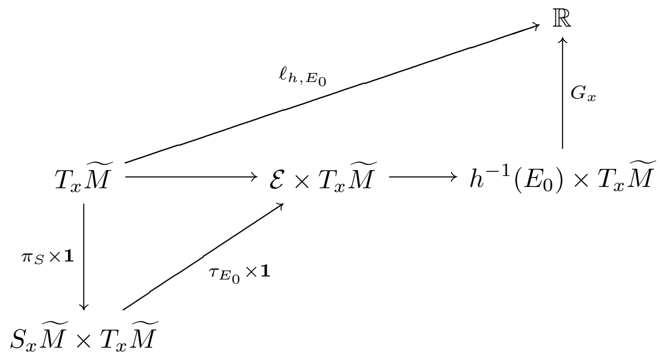
(c) *If we extend $\ell_{h,E_0}$ continuously from $\widetilde{M}$ to $M$ by setting $\ell_{h,E_0}(x,v) = 0$ for $x \in S(E_0)$, the associated distance $d_l$ is well defined on all of $M$. Nevertheless contrary to the case of a Finsler manifold without singularities (as described for example in Bao-Chern-Shen [**6**]), the geodesic curves with respect to $\ell_{h,E_0}$ may have kinks at the singular points.*

(d) *Geometrically, the function $\tilde\tau_{E_0}$ projects an element $(x,v)$ of the tangent bundle $T\widetilde{M}$ to an element $(x, \lambda v)$ (for $\lambda > 0$ suitable) in the $(2d-1)$-dimensional submanifold $\mathcal{E}$ of $TM$, which is determined by the condition $E_h|_{\mathcal{E}} = E_0$, i.e.*

$$\tilde\tau_{E_0}(x,v) \in \mathcal{E} := E_h^{-1}(E_0)\,. \tag{4.31}$$

*Therefore physically $\mathcal{E}$ can be interpreted as energy shell of the system for a given fixed energy $E_0$.*

(e) *Schematically the functions occurring in Lemma 4.15 are illustrated in the following diagram.*




$$v \xrightarrow{\tilde{\tau}_{E_0}\times \mathbf{1}} (\tilde{v}, v) \xrightarrow{(\mathcal{D}_F h)^{-1}\times \mathbf{1}} (\xi_h(\tilde{v}), v)$$

(f) *With the notation* (4.9) *it follows from the definition of $G_x$ (Def. 4.9), that $\ell_{h,E_0}(x,v)$ can be written as*

$$\ell_{h,E_0}(x,v) = \xi_h(x,\tilde{v}) \cdot v \quad \textit{where} \quad (x,\tilde{v}) = \tilde{\tau}_{E_0}(x,v) \in \mathcal{E} \ . \tag{4.32}$$

(g) *In the special case of a Schrödinger operator, i.e. if $h(x,\xi) = \frac{1}{2}\xi^2 + V(x)$, the fibre derivative is given by $v := D_\xi h(x,\xi) = \xi$ and thus $\ell_{h,E_0}(x,v) = \tilde{v} \cdot v$.*

To prove Proposition 4.15, we need the following lemma on the strict monotonicity of the energy function $E_h$ with respect to the modulus of the velocity.

LEMMA 4.17. *In the setting of Proposition 4.15 fix $x \in \widetilde{M}$ and $u \in T_x\widetilde{M}$ with $u \neq 0$. Then for $E_h : TM \to \mathbb{R}$ defined by (4.23), the function*

$$E_u : [0,\infty) \to \mathbb{R} \ , \qquad E_u(\lambda) := E_h(x, \lambda u)$$

*is strictly increasing. Furthermore $E_u(0) \leq E_0$ and $\lim_{\lambda\to\infty} E_u(\lambda) = \infty$.*

Proof of Lemma 4.17:

Since $Dh_x(0) = 0$ for all $x \in M$, it is clear that $v_h(x,0) = 0$ and vice versa, thus

$$E_u(0) = E_h(x,0) = h(x,0) \leq \max_{x\in M} h(x,0) \leq E_0 \ , \quad (x \in \widetilde{M} = M \setminus S(E_0)) \ .$$

To show that $E_u$ is strictly increasing, we will analyze the derivative of $E_u$ for $\lambda > 0$.
Since for fixed $x \in M$ by definition $\mathcal{D}_F h(x,\xi) = Dh_x(\xi)$, we have by the chain rule

$$\frac{dE_u}{d\lambda}|_\lambda = Dh_x|_{(Dh_x)^{-1}(\lambda u)} \cdot D\left(Dh_x\right)^{-1}|_{\lambda u}(u) \ . \tag{4.33}$$

We use the notation $\xi_h(x,v) = (Dh_x)^{-1}(v)$ (see Remark 4.10) and notice that $Dh_x|_{\xi_h(x,v)}$ maps the tangent space $T_{\xi_h}T^*_xM$ linearly to $T_{h(x,\xi_h)}\mathbb{R}$, and these spaces are isomorphic to $T^*_xM$ and $\mathbb{R}$ respectively as described in Remark 4.10. Thus $Dh_x|_{\xi_h(x,v)}$ can be interpreted as an element of $T_xM$. Since the fibre derivative of $h$ at the point $\xi$ is by definition given by $\mathcal{D}_F h(x,\xi) = Dh_x(\xi) \in T_xM$ it follows that

$$Dh_x|_{\xi_h(x,v)} = \mathcal{D}_F h\left[\left(\mathcal{D}_F h\right)^{-1}(x,v)\right] = v \,. \tag{4.34}$$

To analyze the second term on the right hand side of (4.33), we use that the Lagrange function $L_h : TM \to \mathbb{R}$ associated to $h$ as defined in Remark 4.13 is strictly convex in each fibre and $\mathcal{D}_F L_h(x,v) = \left(\mathcal{D}_F h\right)^{-1}(x,v)$. Together with (4.34) this yields

$$\frac{dE_u}{d\lambda}|_\lambda = \lambda u \cdot D_v \mathcal{D}_F L_h|_{(x,\lambda u)}(u) = \lambda\, D^2 L_{h,x}|_{\lambda u}(u,u) \ , \tag{4.35}$$

where we used for the second equality, that the derivative of $\mathcal{D}_F L_h|_{(x,v)}$ with respect to $v$ (which by definition is given by $D^2 L_{h,x}|_v$) is on the one hand a linear map from $T_xM$ to $T_x^*M$ and on the other hand by the duality of $T_xM$ and $T_x^*M$ a bilinear form on $T_xM$.

It follows immediately from (4.35) together with the strict convexity of $L_h$, that the the first derivative of $E_u$ is strictly positive for $\lambda \in (0,\infty)$ and thus $E_u$ is strictly increasing.
The fact that $E_u$ is unbounded, i.e. that $\lim_{\lambda\to\infty} E_u(\lambda) = \infty$, can be seen as follows. From the convexity of $h$ and since $h(x,\xi) \geq h(x,0) = -V_0(x)$ for all $\xi \in T^*M$, it follows that $\lim_{|\xi|\to\infty} h(x,\xi) = \infty$. Since $h$ is hyperregular, the mapping $\mathcal{D}_F h(x,.) = Dh_x : T_xM \to T_x^*M$ is a global diffeomorphism. Thus for any norm $\|.\|_{T_xM}$ on $T_xM$ and the induced norm $\|.\|_{T_x^*M}$ on $T_x^*M$, we have $\|Dh_x(v_n)\|_{T_x^*M} \to \infty$ for any sequence $(v_n)$ in $T_xM$ satisfying $\|v_n\|_{T_xM} \to \infty$.

In fact if this would not be the case, there would exist a sequence $(v_n)$ in $T_xM$ with $\|v_n\|_{T_xM} \to \infty$, but at least for a subsequence $(v_{n_k})$ there exists a constant $R > 0$ such that $\|Dh_x(v_{n_k})\|_{T_x^*M} \leq R$. Setting $v_{n_k} = (Dh_x)^{-1}(\xi_{n_k})$, this would lead to $\|\xi_{n_k}\|_{T_x^*M} \leq R$, but $\|(Dh_x)^{-1}(\xi_{n_k})\|_{T_xM} \to \infty$, which is a contradiction to $\|(Dh_x)^{-1}(\xi_{n_k})\|_{T_xM} \leq \max_{\|\xi\|_{T_x^*M}\leq R} \|(Dh_x)^{-1}(\xi_{n_k})\|_{T_xM} =: M < \infty$.

Thus

$$\lim_{\lambda\to\infty} E_u(\lambda) = \lim_{\lambda\to\infty} h(x,\xi_h(x,\lambda u)) = \lim_{\|\xi\|\to\infty} h(x,\xi) = \infty \ .$$

□

Proof of Proposition 4.15:

i) From Lemma 4.17 it follows that for fixed $x \in \widetilde{M}$, each ray $[(x,u)] = \{(x,v)\,|\, v = \lambda u, \lambda > 0\} \in S\widetilde{M}$ intersects the hypersurface $\mathcal{E}_x := E_h^{-1}(E_0) \cap T_x\widetilde{M}$ in exactly one point. In fact since $E_u(\lambda) = E_h(x,\lambda u)$ is strictly increasing, it is injective and thus there exists at most one $\lambda$ such that $E_u(\lambda) = E_0$.

On the other hand, since $E_u(0) \leq E_0$ and $\lim_{\lambda\to\infty} E_u(\lambda) = \infty$, there is by the Intermediate Value Theorem at least on value $\lambda$ with $E_u(\lambda) = E_0$.

Thus for each ray $[(x,u)]$ there is exactly one point $(x,\lambda u) \in T_x\widetilde{M}$ such that $E_h(x,\lambda u) = E_0$. Since for each $v \in T_xM$ there is exactly on ray $[x,u] \in S_xM$, it is therefore clear that for each $x \in \widetilde{M}$ the mapping $\tau_{E_0,x} : S_x\widetilde{M} \to \mathcal{E}_x$, given by $\tau_{E_0,x}([(x,u)]) = (x,\lambda u)$ is a bijection and thus $\tau_{E_0} : S\widetilde{M} \to T\widetilde{M}$ is in fact a parametrization of $\widetilde{\mathcal{E}} = E_h^{-1}(E_0) \cap T\widetilde{M}$ by $S\widetilde{M}$. Furthermore it follows immediately from the construction of $\tau_{E_0}$, that $\tau_{E_0}[(x,u)] = (x,\lambda u)$ for some $\lambda > 0$, i.e. $\tau_{E_0}$ is strictly fibre preserving.

To analyze the regularity of $\tau_{E_0}$, we will use the Implicit Function Theorem (on subsets of $\mathbb{R}^{2d}$). First we choose at any point $[x_0,u_0] \in S\widetilde{M}$ and $(x_0,v_0) \in T\widetilde{M}$ local coordinates. There exist open neighborhoods $U([x_0,u_0]) \subset S\widetilde{M}$ and $O(x_0,v_0) \subset T\widetilde{M}$ and open sets $V \subset \mathbb{R}^{2d-1}$ and $I \subset \mathbb{R}_+$, such that the coordinate maps

$$\phi : U([x_0,u_0]) \to V\ , \quad \phi([x,u]) =: s$$

and

$$\psi : O(x_0,v_0) \to V \times I\ , \quad \psi(x,v) = (s,\lambda)$$

are diffeomorphisms. Then we define the functions

$$\widehat{\tau}_{E_0} := \psi \circ \tau_{E_0} \circ \phi^{-1} : V \to V \times I \quad \text{and} \quad \widehat{E}_h := E_h \circ \psi^{-1} : V \times I \to \mathbb{R}\,.$$

It follows at once from the regularity of $h$ and $\mathcal{D}_F h$, that $\widehat{E}_h$ is a $\mathscr{C}^\infty$- function and by the considerations above, there is for each $s_0 \in V$ exactly one point $(s_0,\lambda_0) \in V \times \mathbb{R}_+$ such that

$$\widehat{E}_h(s_0,\lambda_0) = E_0\ . \tag{4.36}$$

Furthermore $\frac{d\widehat{E}_h}{d\lambda}(s_0,\lambda_0) > 0$ for all $(s_0,\lambda_0) \in V \times \mathbb{R}_+$ by Lemma 4.17. Thus by the Implicit Function Theorem there exists for each $s_0 \in V$ a neighborhood $\mathcal{N}(s_0) \subset V$ and a $\mathscr{C}^\infty$-function $\widehat{\lambda} : \mathcal{N}(s_0) \to \mathbb{R}_+$, such that $\widehat{E}_h(s,\widehat{\lambda}(s)) = E_0$ for all $s \in \mathcal{N}(s_0)$.

Since by construction $\widehat{\tau}_{E_0}(s) = (s,\widehat{\lambda}(s))$, i.e. $\widehat{\tau}_{E_0} = \mathbf{1}_V \times \widehat{\lambda}$, it follows at once that $\widehat{\tau}_{E_0}$ and the associated map $\tau_{E_0}$ are $\mathscr{C}^\infty$-functions.

iii) Since the function $\widehat{\lambda}$ constructed above by use of the Implicit Function Theorem is $\mathscr{C}^\infty$, it follows at once, that

$$\lambda : [a,b] \to \mathbb{R}_+\ , \qquad \lambda(t) := \widehat{\lambda} \circ \phi_t \circ \pi_S(\gamma(t),\dot{\gamma}(t)))$$

is $\mathscr{C}^1$, if $\gamma$ is regular. The function $\phi_t$ denotes the coordinate system associated to the point $[\gamma(t), \dot{\gamma}(t)]$.

ii) To show that $\ell_{h,E_0} : T\widetilde{M} \to \mathbb{R}$ is a Finsler function on $\widetilde{M}$, we check the defining properties.

1) The regularity $\ell_{h,E_0} \in \mathscr{C}^\infty(T\widetilde{M} \setminus \{0\})$ follows from the fact that $h$ is hyperregular (then $\mathcal{D}_F h$ is a diffeomorphism), the function $\tilde{\tau}_{E_0}$ is $\mathscr{C}^\infty$ and the definition of $G_x$ as pairing.

2) To show the positive homogeneity of $\ell_{h,E_0}$, i.e. that $\ell_{h,E_0}(x, \lambda v) = \lambda \ell_{h,E_0}(x, v)$ holds for all $\lambda > 0$, we notice that by construction $\tilde{\tau}_{E_0}(x, \lambda v) = \tilde{\tau}_{E_0}(x, v)$ for any $\lambda > 0$. Thus $(\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}$ is homogeneous of order zero in each fibre. Since $G_x(\xi, v) = \xi \cdot v$ is bilinear, it follows that

$$\ell_{h,E_0}(x, \lambda v) = G_x\left((\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}(x, \lambda v), \lambda v\right) = \lambda G_x\left((\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}(x, v), v\right) = \lambda \ell_{h,E_0}(x, v)$$

and thus $l$ is positive homogeneous of order one in each fibre.

3) To show the strict positivity of $\ell_{h,E_0}$ for $v \neq 0$, we define

$$a_h = A_h \circ \mathcal{D}_F h \,:\, T^*M \to \mathbb{R}\,, \qquad a_h(x, \xi) = \xi \cdot v_h(x, \xi) = \xi \cdot \mathcal{D}_F h(x, \xi)\,.$$

Since $h$ was assumed to be strictly convex in each fibre, the associated fibre derivative $\mathcal{D}_F h(x, \xi) = Dh_x(\xi)$ fulfills by (4.15) for $\xi, \eta \in T^*_x M$ with $\eta \neq \xi$ the relation

$$(\xi - \eta) \cdot (\mathcal{D}_F h(x, \xi) - \mathcal{D}_F h(x, \eta)) > 0\,.$$

Therefore choosing $\xi = -\eta$ and using that $h$ is even in each fibre (and thus $\mathcal{D}_F h$ is odd), yields

$$2\xi \cdot (\mathcal{D}_F h(x, \xi) - \mathcal{D}_F h(x, -\xi)) = 4\xi \cdot \mathcal{D}_F h(x, \xi) = 4a_h(x, \xi) > 0\,, \quad \text{for} \quad \xi \neq 0\,.$$

Since $h$ is even and strictly convex, it takes its absolute minimum at $\xi = 0$ (see Remark 4.21) and thus $\mathcal{D}_F h(x, 0) = 0$. Since furthermore $\mathcal{D}_F h$ is a global diffeomorphism, we get $(\mathcal{D}_F h)^{-1}(x, v) \neq 0$ for $v \neq 0$ and therefore

$$A_h(x, v) = a_h(x, (\mathcal{D}_F h)^{-1}(x, v)) > 0 \tag{4.37}$$

Setting $\tilde{\tau}_{E_0}(x, v) = (x, \tilde{v})$, it follows from the fact that $\tau_{E_0}$ is strictly fibre preserving, that there exists a $\lambda > 0$ such that $v = \lambda \tilde{v}$. Thus it follows from (4.37) and the linearity of $G_x$ with respect to each variable, that for $v \neq 0$

$$\begin{aligned}
\ell_{h,E_0}(x, v) &= G_x\left((\mathcal{D}_F h)^{-1}(x, \tilde{v}), v\right) = G_x\left((\mathcal{D}_F h)^{-1}(x, \tilde{v}), \lambda \tilde{v}\right) \\
&= \lambda G_x\left((\mathcal{D}_F h)^{-1}(x, \tilde{v}), \tilde{v}\right) = \lambda A_h(x, \tilde{v}) > 0\,.
\end{aligned}$$

and it is obvious by the definition of $G_x$ that $\ell_{h,E_0}(x, v) = 0$ if $v = 0$.

4) It remains to show that $\ell_{h,E_0}$ is not only positive, but absolute homogeneous of order one.

Since $\tau_{E_0}$ was assumed to be strictly fibre preserving, $\tilde{\tau}_{E_0}(x, v) = (x, \lambda v)$ where $\lambda > 0$. Since $h$ is even in each fibre, the derivative $\mathcal{D}_F h$ is odd and the same is true for the inverse $(\mathcal{D}_F h)^{-1}$. Thus for $(x, v) \in \mathcal{E}_x$

$$h \circ (\mathcal{D}_F h)^{-1}(x, -v) = h \circ (-\mathcal{D}_F h)^{-1}(x, v) = h \circ (\mathcal{D}_F h)^{-1}(x, v) = E_0\,, \tag{4.38}$$

where the second equality follows from the fact that $h$ is even. From (4.38) it follows that $(x, -v) \in \mathcal{E}$ if $(x, v) \in \mathcal{E}$, i.e. each fibre $\mathcal{E}_x$ of the energy shell is symmetric around $v = 0$. Thus if $\lambda v \in \mathcal{E}_x$ for $\lambda > 0$ suitable and $x \in \widetilde{M}$ fixed, then

$$\tilde{\tau}_{E_0}(-v) = \lambda(-v) = -\lambda v = -\tilde{\tau}_{E_0}(v)\,. \tag{4.39}$$

By the fact that $(\mathcal{D}_F h)^{-1}$ is odd, the bilinearity of $G_x$ and (4.39) we can conclude for any fixed $x \in \widetilde{M}$

$$\begin{aligned}
\ell_{h,E_0}(-v) &= G_x\left((\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}(-v), (-v)\right) = -G_x\left((\mathcal{D}_F h)^{-1}(-\tilde{\tau}_{E_0}(v)), v\right) \\
&= -G_x\left((-(\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}(v)), v\right) = G_x\left((\mathcal{D}_F h)^{-1} \circ \tilde{\tau}_{E_0}(v), v\right) = \ell_{h,E_0}(v)\,.
\end{aligned} \tag{4.40}$$

From (4.40) it follows that $\ell_{h,E_0}$ is even in each fibre and thus the absolute homogeneity follows from the positive homogeneity: for any $\lambda \in \mathbb{R}$

$$\ell_{h,E_0}(x, \lambda v) = \ell_{h,E_0}(x, |\lambda| v) = |\lambda| \ell_{h,E_0}(x, v)\,.$$

□

### 4.3. Finsler Geodesics as base integral curves of the associated vector field

By Proposition 4.15 each hyperregular Hamilton function on the cotangent bundle, which is strictly convex and even in each fibre and is bounded from above for $\xi = 0$, induces a metric structure on the base manifold.

The following proposition establishes the connection between geodesics with respect to the Finsler function $\ell_{h,E_0}$ for a given hyperregular Hamiltonian $h$ and the integral curves of the associated hamiltonian vector field $X_h$. Our proof will use the Euler-Maupertuis principle (at least implicitly). This part of the proof below is adapted from Abraham-Marsden [**2**].

PROPOSITION 4.18. *For a hyperregular hamiltonian $h \in \mathscr{C}^\infty(T^*M)$ and $E_0$ as in Proposition 4.15, let $\ell_h(:= \ell_{h,E_0})$ denote the corresponding Finsler function on $\widetilde{M}$ as constructed in Proposition 4.15. Let $\gamma_0 : [a,b] \to \widetilde{M}$ be a base integral curve of the associated hamiltonian vector field $X_h$ with energy $E_0$ (i.e. $E_h(\gamma_0(t), \dot{\gamma}_0(t)) = E_0$ for all $t \in [a,b]$).*
*Then $\gamma_0$ is a geodesic on $\widetilde{M}$ with respect to $\ell_h$.*
*Conversely if $\gamma_0$ is a geodesic on $\widetilde{M}$ with respect to $\ell_h$ and energy $E_0$, then $\gamma_0$ is a base integral curve of $X_h$ (i.e. $(\gamma_0, \dot{\gamma}_0)$ is a solution of Lagrange´s equation* (4.29)*).*

Proof:
We denote the endpoints of $\gamma_0$ by $\gamma_0(a) = x_1$ and $\gamma_0(b) = x_2$ and by $\Gamma_{a,b}(x_1, x_2)$ as introduced in Definition 4.2 the Banach manifold of all regular curves joining $x_1$ and $x_2$, which are parameterized over the interval $[a,b]$. We set

$$\Gamma(x_1, x_2, [a,b], E_0) := \{(\gamma, \alpha) \mid \alpha : [a,b] \to \mathbb{R} \quad \text{is} \quad \mathscr{C}^2, \quad \frac{d}{dt}\alpha > 0\,, \quad \alpha(a) = 0\,,$$
$$\gamma \in \Gamma_{0,\alpha(b)}(x_1, x_2) \quad \text{such that} \quad E_h(\gamma(\alpha(t)), \dot{\gamma}(\alpha(t)) = E_0 \quad \text{for all} \quad t \in [a,b]\}\,, \quad (4.41)$$

thus $\Gamma(x_1, x_2, [a,b], E_0)$ is the set of all pairs $(\gamma, \alpha)$, where $\gamma$ is a regular curve on $\widetilde{M}$ joining the points $x_1$ and $x_2$ and $\alpha$ is a change of parameter. This change of parameter ensures, that the curve $(\gamma \circ \alpha, \dot{\gamma} \circ \alpha) \in TM$ (which is not equal to the lifted curve $(\gamma \circ \alpha, \frac{d}{dt}(\gamma \circ \alpha))$) lies on the energy shell $\mathcal{E} = E_h^{-1}(E_0)$.

As $\Gamma_{a,b}(x_1, x_2)$, the space $\Gamma(x_1, x_2, [a,b], E_0)$ is a Banach manifold. In fact, by setting $A := \{\alpha : [a,b] \to \mathbb{R} \mid \frac{d}{dt}\alpha > 0 \quad \text{and} \quad \alpha(a) = 0\}$, it is a subspace of $\Gamma_{a,b}(x_1, x_2) \times A$ as pre-image of $E_0$ with respect to the map

$$f : \Gamma_{a,b}(x_1, x_2) \times A \to \mathscr{C}^1([a,b], \mathbb{R}) \quad \text{defined by} \quad f(\gamma, \alpha) := E_h(\gamma \circ \alpha, \dot{\gamma} \circ \alpha)\,,$$

thus we consider $E_0 \in \mathbb{R}$ as the constant function $E_0(t) = E_0$. Since $E_h = h \circ (D_F h)^{-1}$, where $D_F h$ is a diffeomorphism with $D_F h(x, 0) = (x, 0)$, it follows from the assumption that $E_0 > \max_{x \in \widetilde{M}} E_h(x, 0)$. Since furthermore $h$ is strictly convex, it is clear that $DE_h(x, v) \neq 0$ for $v \neq 0$. Thus from the regularity of the elements of $\gamma \in \Gamma_{a,b}(x_1, x_2)$, i.e. since $\dot{\gamma}(t) \neq 0$ for all $t \in [a,b]$ it follows that $E_0$ is a regular value of $E_h$ and by the definition of $f$ it is regular value of $f$. Thus the pre-image $f^{-1}(E_0) = \Gamma(x_1, x_2, [a,b], E_0)$ is a submanifold of $\Gamma_{a,b}(x_1, x_2) \times A$. This follows by the fact, that the Inverse Function Theorem holds in Banach spaces (see Hamilton [**26**]).

*Step 1:*
We start the proof of Proposition 4.18 by constructing a diffeomorphism between $\Gamma_{a,b}(x_1, x_2)$ and $\Gamma(x_1, x_2, [a,b], E_0)$.

By Proposition 4.15, there exists for any $\eta \in \Gamma_{a,b}(x_1, x_2)$ a unique $\mathscr{C}^1$-function $\lambda : [a,b] \to \mathbb{R}_+$, such that

$$E_h \circ \tilde{\tau}_{E_0}(\eta(t), \dot{\eta}(t)) = E_h(\eta(t), \lambda(t)\dot{\eta}(t)) = E_0\,.$$

Set

$$\alpha(t) := \int_a^t \frac{1}{\lambda(s)}\, ds \quad \text{and} \quad \gamma = \eta \circ \alpha^{-1} : [\alpha(a), \alpha(b)] \to \widetilde{M}\,,$$

then $\alpha : [a,b] \to \mathbb{R}$ with $\dot\alpha > 0$ , $\alpha(a) = 0$ and from

$$\dot\eta(t) = \frac{d}{dt}\gamma(\alpha(t)) = \dot\gamma(\alpha(t)) \cdot \dot\alpha(t) ,$$

it follows that

$$E_h(\gamma(\alpha(t)), \dot\gamma(\alpha(t))) = E_h(\eta(t), \dot\eta(t)(\dot\alpha(t))^{-1}) = E_h(\eta(t), \lambda_t \dot\eta(t)) = E_0 , \tag{4.42}$$

i.e. $(\gamma,\alpha) \in \Gamma(\eta(a), \eta(b), [a,b], E_0)$. Thus it follows that to each curve $\eta \in \Gamma_{a,b}(x_1,x_2)$ on $\widetilde{M}$ there exists a pair $(\gamma,\alpha) \in \Gamma(\eta(a), \eta(b), [a,b], E_0)$, where $\eta = \gamma\circ\alpha$. The choice of the change of parameter $\alpha$ (and thus the choice of the pair $(\gamma,\alpha)$) is unique by the condition $\alpha(a) = 0$.

On the other hand, if we start with a pair $(\gamma,\alpha) \in \Gamma(x_1,x_2,[a,b],E_0)$, then by definition $E_h(\gamma(s), \dot\gamma(s)) = E_0$ with $s = \alpha(t)$. If we set $\eta := \gamma\circ\alpha : [a,b] \to \widetilde{M}$ it follows from (4.42), that

$$\tilde\tau_{E_0}(\eta(t), \dot\eta(t)) = (\eta(t), (\dot\alpha(t))^{-1}\dot\eta(t)) \qquad \text{and thus} \qquad \lambda_t = (\dot\alpha(t))^{-1} . \tag{4.43}$$

We can conclude that there is a bijection

$$b_{E_0} : \Gamma_{a,b}(x_1,x_2) \to \Gamma(x_1,x_2,[a,b],E_0)$$

between the Banach manifolds given by

$$b_{E_0}(\eta) = (\eta\circ\alpha^{-1}, \alpha) \quad \text{with} \quad \alpha(t) := \int_a^t (\lambda(s))^{-1}\, ds \quad \text{for} \quad \tilde\tau_{E_0}(\eta,\dot\eta) = (\eta, \lambda\dot\eta) . \tag{4.44}$$

As described in Definition 4.2, the tangent space of $\Gamma_{a,b}(x_1,x_2)$ at a point $\eta$ can be constructed using the notion of regular variations of $\eta$ with fixed endpoints as

$$T_\eta\Gamma_{a,b}(x_1,x_2) = \{\partial_u\eta_\delta|_{u=0} \,|\, \eta_\delta \quad \text{is a regular variation of} \quad \eta \quad \text{with fixed endpoints}\} .$$

Along the same lines we construct the tangent space of $\Gamma(x_1,x_2,[a,b],E_0)$ at a point $(\gamma,\alpha)$. We define a regular variation of $(\gamma,\alpha)$ as a $\mathscr{C}^2$-mapping $(\gamma,\alpha)_\delta : (-\delta,\delta) \to \Gamma(x_1,x_2,[a,b],E_0)$ passing the point $(\gamma,\alpha)$ for $u = 0$, therefore

$$\begin{aligned} T_{(\gamma,\alpha)}\Gamma(x_1,x_2,[a,b],E_0) = \{\partial_u(\gamma,\alpha)_\delta|_{u=0} \,|\, &(\gamma,\alpha)_\delta : (-\delta,\delta) \to \Gamma(x_1,x_2,[a,b],E_0) \\ &\text{is} \quad \mathscr{C}^2 \quad \text{with} \quad (\gamma,\alpha)_\delta(0) = (\gamma,\alpha)\} . \end{aligned}$$

The points in $\Gamma_{a,b}(x_1,x_2)$ and $\Gamma(x_1,x_2,[a,b],E_0)$ are curves on $M$ and $M\times\mathbb{R}$ respectively and variations of the curves on $M$ and $M\times\mathbb{R}$ are curves on $\Gamma_{a,b}(x_1,x_2)$ and $\Gamma(x_1,x_2,[a,b],E_0)$ respectively, in particular the variation $(\gamma,\alpha)_\delta$ can be considered as a mapping

$$(\gamma,\alpha)_\delta : [a,b]\times(-\delta,\delta) \to M\times\mathbb{R} , \qquad (\gamma,\alpha)_\delta(t,u) := (\gamma_\delta(\alpha_\delta(t,u),u), \alpha_\delta(t,u)) .$$

Therefore as described in Remark 4.3 the tangent vectors at the points $\eta$ and $(\gamma,\alpha)$ respectively can be considered as vector fields along the curves in $M$ and $M\times\mathbb{R}$. Thus $\partial_u\eta_\delta|_{u=0} \in T_\eta\Gamma_{a,b}(x_1,x_2)$ can be identified with the mapping $\partial_u\eta_\delta|_{u=0} : [a,b] \to TM$ and $\partial_u(\gamma,\alpha)_\delta|_{u=0} \in \Gamma(x_1,x_2,[a,b],E_0)$ can be considered as mapping $\partial_u(\gamma,\alpha)_\delta|_{u=0} : [a,b] \to T(M\times\mathbb{R})$, given by

$$\begin{aligned} \partial_u(\gamma,\alpha)_\delta|_{u=0}(t) &= \left(\frac{d}{du}\gamma_\delta(\alpha_\delta(t,u),u), \partial_u\alpha_\delta(t,u)\right)\Big|_{u=0} \qquad (4.45) \\ &= \left(\frac{d}{dt}\gamma_\delta(\alpha_\delta(t,u),u)\partial_u\alpha_\delta(t,u) + \partial_u\gamma_\delta(\alpha_\delta(t,u),u)|_{u=0}, \partial_u\alpha_\delta(t,u)|_{u=0}\right) . \end{aligned}$$

Since the values of a variation $(\gamma,\alpha)_\delta =: (\gamma_\delta,\alpha_\delta)$ are assumed to be elements of $\Gamma(x_1,x_2,[a,b],E_0)$, it follows that $\alpha_\delta(a,u) = 0$ for all $u \in (-\delta,\delta)$ and the variation $\gamma_\delta$ (which is not a regular variation in the sense of Definition 4.2, since the domain depends on the value of the variation $\alpha_\delta$) has fixed endpoints, i.e. $\gamma_\delta(\alpha_\delta(a,u),u) = \gamma_\delta(0,u) = x_1$ and $\gamma_\delta(\alpha_\delta(b,u),u) = x_2$ for all $u \in (-\delta,\delta)$. This leads to

$$\begin{aligned} \frac{d}{du}\gamma_\delta(0,u) &= \partial_u\gamma_\delta(0,u) + \partial_t\gamma_\delta(0,u)\cdot\partial_u\alpha_\delta(a,u) = 0 \qquad (4.46) \\ \frac{d}{du}\gamma_\delta(\alpha_\delta(b,u),u) &= \partial_u\gamma_\delta(\alpha_\delta(b,u),u) + \partial_t\gamma_\delta(\alpha_\delta(b,u),u)\cdot\partial_u\alpha_\delta(b,u) = 0 . \end{aligned}$$

The bijection $b_{E_0}$ defined in (4.44) is a diffeomorphism, if for all $\eta \in \Gamma_{a,b}(x_1,x_2)$ its differential at the point $\eta$

$$db_{E_0}|_\eta : T_\eta\Gamma_{a,b}(x_1,x_2) \to T_{b_{E_0}(\eta)}\Gamma(x_1,x_2,[a,b],E_0)$$

has no critical points, i.e. if $db_{E_0}|_\eta(w) \neq (0,0)$ for $w \neq 0$.

By definition

$$db_{E_0}|_\eta(\partial_u \eta_\delta|_{u=0}) = \partial_u b_{E_0}(\eta_\delta)|_{u=0} = \partial_u(\eta\circ\alpha^{-1},\alpha)_\delta|_{u=0} \tag{4.47}$$

and by the identification (4.45) of tangent vectors with vector fields along curves, we get using that by definition $\alpha_\delta^{-1}(\alpha_\delta(t,u),u)=t$ for all $u\in(-\delta,\delta)$

$$\begin{aligned} db_{E_0}|_\eta(\partial_u\eta_\delta|_{u=0}(t)) &= \left(\partial_u(\eta\circ\alpha^{-1})_\delta|_{u=0}, \partial_u\alpha_\delta|_{u=0}\right)(t) \\ &= \left(\frac{d}{du}\eta_\delta(\alpha_\delta^{-1}(\alpha_\delta(t,u),u),u)|_{u=0}, \partial_u\alpha_\delta(t,u)|_{u=0}\right) \\ &= \left(\partial_u\eta_\delta|_{u=0}, \partial_u\alpha_\delta|_{u=0}\right)(t)\ . \end{aligned} \tag{4.48}$$

Since this equality holds for all $t\in[a,b]$ it follows immediately, that

$$db_{E_0}|_\eta(\partial_u\eta_\delta|_{u=0}) = (0,0) \quad\Rightarrow\quad \partial_u\eta_\delta|_{u=0}=0\ ,$$

which proves (by contraposition) that the bijection $b_{E_0}$ is a diffeomorphism.

*Step 2:*
We show that the critical points of the length functional $s_{\ell_h}(\gamma)$ defined in Definition 4.2 are in bijection with the critical points of the action integral

$$I:\Gamma(x_1,x_2,[a,b],E_0)\to\mathbb{R}\,,\quad I(\gamma,\alpha):=\int_{\alpha(a)}^{\alpha(b)} A_h(\gamma(s),\dot\gamma(s))\,ds\ , \tag{4.49}$$

where $A_h$ denotes the action with respect to $h$ defined in (4.24). By use of the substitution $s=\alpha(t)$ and with the notation $\xi_h(x,v)=(\mathcal{D}_F h)^{-1}(x,v)$, we get

$$\begin{aligned} \int_{\alpha(a)}^{\alpha(b)} A_h(\gamma(s),\dot\gamma(s))\,ds &= \int_{\alpha(a)}^{\alpha(b)} \xi_h(\gamma(s),\dot\gamma(s))\cdot\dot\gamma(s)\,ds \\ &= \int_a^b \xi_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t)))\cdot\dot\gamma(\alpha(t))\dot\alpha(t)\,dt\ . \end{aligned} \tag{4.50}$$

By (4.43) and the definition of $\ell_h$ given in Proposition 4.15, the right hand side of (4.50) is by the substitution $\eta(t)=\gamma(\alpha(t))$ equal to

$$\int_a^b \xi_h(\eta(t),\dot\eta(t)(\dot\alpha(t))^{-1})\cdot\dot\eta(t)\,dt = \int_a^b \xi_h\circ\tilde\tau_{E_0}(\eta(t),\dot\eta(t))\cdot\dot\eta(t)\,dt = \int_a^b \ell_{h,E_0}(\eta(t),\dot\eta(t))\,dt = s_{\ell_h}(\eta)\ ,$$

and thus $I(\gamma,\alpha)=s_{\ell_h}(\gamma\circ\alpha)$ for $\dot\alpha=\lambda^{-1}$. Since $\gamma\circ\alpha=b_{E_0}^{-1}(\gamma,\alpha)$, it follows that

$$s_{\ell_h}=I\circ b_{E_0} \quad\text{and thus}\quad ds_{\ell_h}|_\eta = dI|_{b_{E_0}(\eta)}\circ db_{E_0}|_\eta \tag{4.51}$$

(the last equation follows from the fact that the chain rule is valid on Banach manifolds). Since $b_{E_0}$ is a diffeomorphism (and thus $db_{E_0}|_\eta\neq 0$ for all $\eta\in\Gamma_{a,b}(x_1,x_2)$), it follows at once from (4.51) that the critical points of the length functional $s_{\ell_h}$ (i.e. the geodesics with respect to the Finsler function $\ell_h$) are mapped by $b_{E_0}$ bijectively to the critical points of the action integral $I$,

$$ds_{\ell_h}|_\eta=0 \qquad\Longleftrightarrow\qquad dI|_{b_{E_0}(\eta)}=0\ . \tag{4.52}$$

*Step 3:*
If $\gamma_0$ is a base integral curve of the hamiltonian vector field $X_h$ with energy $E_0$, then $E_h(\gamma_0(t),\dot\gamma_0(t)) = E_0$ for all $t\in[a,b]$ and thus it follows immediately, that $b_{E_0}(\gamma_0)=(\gamma_0,\mathbf{1})$, where $\mathbf{1}:[a,b]\to[a,b]$ is defined by $\mathbf{1}(t)=t$.

Thus by (4.52) it remains to show, that for any base integral curve $\gamma_0\in\Gamma_{a,b}(x_1,x_2)$ of the hamiltonian vector field $X_h$ with energy $E_0$, the pair $(\gamma_0,\mathbf{1})\in\Gamma(x_1,x_2,[a,b],E_0)$ is a critical point of the action integral $I$ (and thus a geodesic). If on the other hand $(\gamma_0,\mathbf{1})\in\Gamma(x_1,x_2,[a,b],E_0)$ (which implies $E_h(\gamma_0(t),\dot\gamma_0(t))=E_0$) is a critical point of $I$, then $(\gamma_0,\dot\gamma_0)$ solves Langrange's equation and thus $\gamma_0$ is a base integral curve of $X_h$.

We start analyzing the tangential of the action integral $dI|_{(\gamma,\alpha)}$ at a point $(\gamma,\alpha)$ in the manifold $\Gamma(x_1,x_2,[a,b],E_0)$.

Since $A_h=L_h+E_h$ by the definition (4.25) of the Lagrange function $L_h$, it follows from the definition (4.41) of $\Gamma(x_1,x_2,[a,b],E_0)$, that

$$A_h(\gamma_\delta(\alpha_\delta(t,u),u),\dot\gamma_\delta(\alpha_\delta(t,u),u)) = L_h(\gamma_\delta(\alpha_\delta(t,u),u),\dot\gamma_\delta(\alpha_\delta(t,u),u))+E_0\ , \tag{4.53}$$

thus the definition (4.49) of $I$ and (4.53) yield

$$dI|_{(\gamma,\alpha)}\left(\partial_u(\gamma,\alpha)_\delta|_{u=0}\right) = \partial_u I\left((\gamma_\delta,\alpha_\delta)\right)|_{u=0} = \frac{d}{du}\int_{\alpha_\delta(a,u)}^{\alpha_\delta(b,u)} \left(L_h(\gamma_\delta(s,u),\dot\gamma_\delta(s,u)) + E_0\right) ds\Big|_{u=0} . \quad (4.54)$$

Since both the integrand and the interval, over which we integrate, depend on the variational parameter $u$, we get using $\gamma_\delta(t,0)=\gamma(t)$ and $\alpha_\delta(t,0)=\alpha(t)$

$$\frac{d}{du}\int_{\alpha_\delta(a,u)}^{\alpha_\delta(b,u)} \left(L_h(\gamma_\delta(s,u),\dot\gamma_\delta(s,u)) + E_0\right) ds\Big|_{u=0} = \left[(L_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t))) + E_0)\cdot\partial_u\alpha_\delta|_{u=0}(t)\right]_a^b + \int_{\alpha(a)}^{\alpha(b)} \frac{d}{du}L_h(\gamma_\delta(s,u),\dot\gamma_\delta(s,u))\Big|_{u=0} ds . \quad (4.55)$$

For the remaining integrand on the right hand side of (4.55) we get

$$\frac{d}{du}L_h(\gamma_\delta(s,u),\dot\gamma_\delta(s,u))\Big|_{u=0} = D_\gamma L_h(\gamma(s),\dot\gamma(s))\cdot\partial_u\gamma_\delta|_{u=0}(s) + D_{\dot\gamma}L_h(\gamma(s),\dot\gamma(s))\partial_u\dot\gamma_\delta|_{u=0}(s) , \quad (4.56)$$

where we used again $\gamma_\delta(t,0)=\gamma(t)$. Since

$$\partial_u\dot\gamma_\delta|_{u=0}(s) = \partial_s\partial_u\gamma_\delta|_{u=0}(s) ,$$

we get by partial integration with respect to the second summand on the right hand side of (4.56) and since $\alpha(a)=0$

$$\int_{\alpha(a)}^{\alpha(b)} \frac{d}{du}L_h(\gamma_\delta(s,u),\dot\gamma_\delta(s,u))\Big|_{u=0} ds = \left[D_{\dot\gamma}L_h(\gamma(s),\dot\gamma(s))\cdot\partial_u\gamma_\delta(s,u)|_{u=0}\right]_0^{\alpha(b)} - \int_0^{\alpha(b)}\left(D_\gamma L_h(\gamma(s),\dot\gamma(s)) + \frac{d}{ds}D_{\dot\gamma}L_h(\gamma(s),\dot\gamma(s))\right)\cdot\partial_u\gamma_\delta|_{u=0}(s)\,ds . \quad (4.57)$$

It follows from (4.46) that

$$\left[D_{\dot\gamma}L_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t)))\partial_u\gamma_\delta(\alpha(t),u)|_{u=0}\right]_a^b = -\left[D_{\dot\gamma}L_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t)))\cdot\dot\gamma(\alpha(t))\partial_u\alpha_\delta|_{u=0}(t)\right]_a^b . \quad (4.58)$$

Since by (4.27) we have $A_h(\gamma,\dot\gamma) = D_{\dot\gamma}L_h(\gamma,\dot\gamma)\cdot\dot\gamma$, we get by (4.53)

$$-\left[D_{\dot\gamma}L_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t)))\cdot\dot\gamma(\alpha(t))\partial_u\alpha_\delta|_{u=0}(t)\right]_a^b = -\left[(L_h(\gamma(\alpha(t)),\dot\gamma(\alpha(t))) + E_0)\cdot\partial_u\alpha_\delta|_{u=0}(t)\right]_a^b . \quad (4.59)$$

Thus the first summand on the right hand side of (4.55) and the first summand on the right hand side of (4.56) (i.e. the boundary terms) cancel and we get by inserting (4.58) in (4.57) and the resulting terms in (4.54)

$$dI|_{(\gamma,\alpha)}\left(\partial_u(\gamma,\alpha)_\delta|_{u=0}\right) = \int_0^{\alpha(b)}\left(D_\gamma L_h(\gamma(s),\dot\gamma(s)) - \frac{d}{ds}D_{\dot\gamma}L_h(\gamma(s),\dot\gamma(s))\right)\cdot\partial_u\gamma_\delta|_{u=0}(s)\,ds . \quad (4.60)$$

For $(\gamma,\alpha)=(\gamma_0,\mathbf{1})$, the integrand is zero since $(\gamma_0,\dot\gamma_0)$ solves Lagrange´s equation and thus

$$dI|_{(\gamma_0,\mathbf{1})} = 0 \qquad \text{and} \qquad ds_{\ell_h}|_{\gamma_0} = 0 .$$

Therefore a base integral curve of $X_h$ with energy $E_0$ is a geodesic with respect to $\ell_h$.

On the other hand, if $\gamma_0$ is a Finslerian geodesic with energy $E_0$, the integral (4.60) is by definition zero for each tangent vector $\partial_u\gamma_{0,\delta}|_{u=0}$. As described in Remark 4.3, each tangent vector $\partial_u\gamma_{0,\delta}|_{u=0}\in T_{\gamma_0}\Gamma_{a,b}(x_1,x_2)$ can be considered as a mapping $\partial_u\gamma_{0,\delta}|_{u=0}:[a,b]\to TM$ such that $\partial_u\gamma_{0,\delta}|_{u=0}(t)\in T_{\gamma_0(t)}M$ and $\partial_u\gamma_{0,\delta}|_{u=0}(a) = \partial_u\gamma_{0,\delta}|_{u=0}(b) = 0$.

Thus we are in the situation, that for a given continuous function $f$, the integral $\int_a^b f(t)g(t)\,dt = 0$ for all $\mathscr{C}^2$-functions $g$ with $g(a)=g(b)=0$. Then by standard arguments (for example contraposition) it follows that $f=0$.

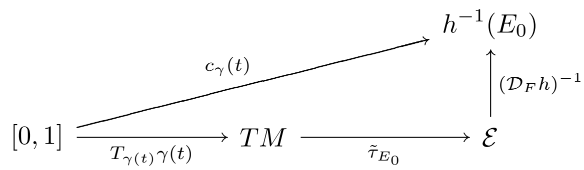
Thus it follows from the fact, that the integral on the right hand side of (4.60) is equal to zero for all choices of the function $\partial_u \gamma_{0,\delta}|_{u=0}$, that the other factor in the integral must vanish and thus $(\gamma_0, \dot\gamma_0)$ solves Lagrange´s equation.

□

Remark 4.19. *In the setting of Proposition 4.15, we use for a curve* $\gamma : [0,T] \to M$ *the following notations for the associated curves in the tangent and cotangent bundle:*

$$\begin{aligned} \check\gamma(t) &:= T_{\gamma(t)}\gamma(t) = (\gamma(t), \dot\gamma(t)) \in TM \\ \check c_\gamma(t) &:= \tilde\tau_{E_0}\check\gamma(t) \in \mathcal{E} \subset TM \\ \widehat\gamma(t) &:= (\mathcal{D}_F h)^{-1}\,\check\gamma(t) \in T^*M \\ c_\gamma(t) &:= (\mathcal{D}_F h)^{-1}\,\check c_\gamma(t) \in h^{-1}(E_0) \subset T^*M \end{aligned}$$

*The construction of the phase space curve* $c_\gamma$ *lying in the energy shell* $h^{-1}(E_0) \subset T^*M$ *is schematically shown in the following diagram.*




$$t \longrightarrow \check\gamma(t) := (\gamma(t), \dot\gamma(t)) \longrightarrow \check c_\gamma(t)$$

*In particular, for fixed* $E_0$ *each parameterized curve* $\gamma$ *on the manifold* $M$ *determines a unique curve* $c_\gamma$ *in the energy shell* $h^{-1}(E_0) \subset T^*M$*. Thus the lift* $c_\gamma$ *is uniquely determined by the base curve and the assumption of energy conservation . By Remark 4.16 the Finsler function* $\ell_{h,E_0}$ *can be written as* $\ell_{h,E_0}(x,v) = \xi_h(x,\tilde v)\cdot v$*, thus*

$$\int_0^1 \ell_{h,E_0}(\check\gamma(t))\,dt = \int_{c_\gamma} \xi\,dx\,.$$

## 4.4. Application to $H_\varepsilon$ and the Eikonal (in)-equality

Now we are going to use the general constructions and definitions given up to this point for the special case of a discrete Hamilton operator $H_\varepsilon$ satisfying Hypothesis 4.20.

In particular Definition 4.1, Lemma 4.8 and Proposition 4.15 allow to define a metric adapted to the Hamilton operator $H_\varepsilon$ as follows.

Hypothesis 4.20. *Let* $H_\varepsilon = T_\varepsilon + V_\varepsilon$ *be a self adjoint operator on* $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ *with associated phase space symbol* $h_\varepsilon(x,\xi;\varepsilon) := t(x,\xi) + \widehat V_\varepsilon$ *with the following properties:*

(a) $t \in S^0_0(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ *is a periodic kinetic energy function in the sense of Definition 2.4. Regarding* $t$ *as a function on* $\mathbb{R}^d \times \mathbb{R}^d$*, which is periodic with respect to* $\xi$*, we assume furthermore that the function* $\mathbb{R}^d \ni \xi \mapsto t(x,\xi)$ *is even and has an analytic continuation to* $\mathbb{C}^d$*. In addition we assume that for all* $x \in \mathbb{R}^d$ *the Fourier coefficients* $a_\gamma(x)$ *defined in* (2.20) *satisfy the condition*

$$a_\gamma(x) \begin{cases} \leq 0 & \text{for} \quad \gamma \neq 0 \\ \geq 0 & \text{for} \quad \gamma = 0 \end{cases} \qquad \text{and} \quad \operatorname{span}\{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, a_\gamma(x) < 0\} = \mathbb{R}^d\,. \tag{4.61}$$

(b) *The potential energy* $V_\varepsilon$ *is the lattice restriction of a function* $\widehat V_\varepsilon \in \mathscr{C}^\infty(\mathbb{R}^d)$*, which has an expansion*

$$\widehat V_\varepsilon(x) = \sum_{l=0}^N \varepsilon^l V_l(x) + R_{N+1}(x;\varepsilon)\,,$$

*where* $V_\ell \in \mathscr{C}^\infty(\mathbb{R}^d)$*. Furthermore* $R_{N+1} \in \mathscr{C}^\infty(\mathbb{R}^d \times (0,\varepsilon_0])$ *and for any compact set* $K \subset \mathbb{R}^d$ *there exists a constant* $C_K$ *such that* $\sup_{x\in K} |R_{N+1}(x;\varepsilon)| \leq C_K \varepsilon^{N+1}$.

(c) *We assume that there exist constants $R, C > 0$ such that $V_\varepsilon(x) > C$ for all $|x| \geq R$ and $\varepsilon \in (0, \varepsilon_0]$. In addition $V_0(x)$ has exactly one, strictly non-degenerate, minimum at $x_1 = 0$ with the value $V_0(0) = 0$.*

*We denote by $\tilde{h}_0(x,\xi) := \tilde{t}(x,\xi) - V_0(x) : \mathbb{R}^{2d} \to \mathbb{R}$ the phase function of order zero in $\varepsilon$, corresponding to the kinetic energy*

$$\tilde{t}(x,\xi) := -t(x,i\xi) = -\sum_\gamma a_\gamma(x)\cosh\left(\frac{1}{\varepsilon}\gamma\cdot\xi\right)$$

*occurring in the eikonal equation (3.10).*

Remark 4.21. (a) *The assumption on the analytic continuation on $\mathbb{R}^d \times (\mathbb{T}^d + i\mathbb{R}^d)$ implies that the Fourier transforms $a_\gamma$ decay exponentially with respect to $\gamma$; more precisely it follows from Proposition A.3 in Appendix A.1, that there exists a constant $C$ such that $\| e^{-\frac{c|.|}{\varepsilon}} a_.(x)\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq C$ for any $c > 0$ uniformly with respect to $x \in (\varepsilon\mathbb{Z})^d$.*

(b) *By the assumption (4.61), the kinetic energy $\tilde{t}_x := \tilde{t}(x, \,.\,) : \mathbb{R}^d_\xi \to \mathbb{R}$ is strictly convex with respect to $\xi$. This can be seen as follows.*

*In order to be strictly convex, the Hessian $\mathcal{D}$ of $\tilde{t}_x$, which is given by*

$$\mathcal{D} := (\mathcal{D}_{ik}) := \left(\partial_{\xi_i}\partial_{\xi_k}\tilde{t}(x,\xi)\right) = -\varepsilon^{-2}\left(\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\frac{\gamma}{\varepsilon}\cdot\xi\right)(\gamma_i\gamma_k)\right),$$

*has to be positive definite. The strict convexity therefore requires*

$$\langle v\,,\,\mathcal{D}v\rangle = -\varepsilon^{-2}\sum_\gamma a_\gamma(x)\cosh\left(\frac{\gamma\cdot\xi}{\varepsilon}\right)(\gamma\cdot v)^2 > 0\,, \qquad \text{for all} \quad v \in (\varepsilon\mathbb{Z})^d,\, v \neq 0, \tag{4.62}$$

*what is surely fulfilled by (4.61) (see the proof of Proposition 4.22 for details) .*

*This corresponds for $\xi = 0$ to the positive definiteness of the matrix $B(x)$ introduced in the Definition 2.4 of a periodic kinetic energy (see (2.23)).*

*Since $\tilde{t}_x$ is strictly convex and even, it follows at once that it has its absolute minimum at the point $\xi = 0$ and $\tilde{t}_x(\xi) > \tilde{t}_x(0) = 0$ for all $\xi \neq 0$ and $x \in \mathbb{R}^d$. In fact for all $x \in \mathbb{R}^d$*

$$\tilde{t}_x(0) = \tilde{t}_x\left(\frac{1}{2}\xi + \frac{1}{2}(-\xi)\right) \leq \frac{1}{2}\tilde{t}_x(\xi) + \frac{1}{2}\tilde{t}_x(-\xi) = \tilde{t}_x(\xi)\,.$$

*By the strict convexity, the point $\xi = 0$ is the only minimum of $\tilde{t}_x$.*

(c) *For the wide class of probabilistic operators introduced in Section 2.3, the assumption (4.61) on the sign of $a_\gamma$ is always fulfilled. In this context, the assumption on the span of the $\gamma$ with $a_\gamma < 0$ is an additional requirement on the transition matrix.*

Proposition 4.22. *The Hamilton function $\tilde{h}_0 : \mathbb{R}^{2d} \to \mathbb{R}$ defined in Hypothesis 4.20 is hyperregular.*

Proof:

By Proposition 4.12, it is enough to show that $\tilde{h}_0$ is hyperconvex in each fibre (i.e. with respect to $\xi$ for each fixed $x \in \mathbb{R}^d$). Thus we have to show that there exists a constant $\alpha > 0$ such that

$$\left\langle v\,,\, D^2_\xi\tilde{h}_0(x,\xi)v\right\rangle \geq \alpha\|v\|^2 \quad \text{for all} \quad x,\xi,v \in \mathbb{R}^d\,. \tag{4.63}$$

In the following considerations, we will skip the $x$-dependence of $\tilde{h}_0$, since we use only properties of $\tilde{h}_0$ holding for all $x \in \mathbb{R}^d$.

By Remark 4.21 we have

$$\left\langle v\,,\, D^2_\xi\tilde{h}_0(\xi)v\right\rangle = -\varepsilon^{-2}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma\cosh\left(\frac{\gamma\cdot\xi}{\varepsilon}\right)(\gamma\cdot v)^2\,, \qquad \xi, v \in \mathbb{R}^d\,. \tag{4.64}$$

By Hypothesis 4.20, for each $x \in \mathbb{R}^d$, the set of $\gamma \in (\varepsilon\mathbb{Z})^d$ with $a_\gamma(x) < 0$ span $\mathbb{R}^d$, thus we can choose a basis $\{\tilde{\gamma}^1, \ldots, \tilde{\gamma}^d\}$ of $\mathbb{R}^d$ with $a_{\tilde{\gamma}^i} < 0$. Since by assumption $-a_\gamma \geq 0$ for all $\gamma \neq 0$, each summand in (4.64) has positive sign and therefore

$$\left\langle v\,,\, D^2_\xi \tilde{h}_0(\xi) v\right\rangle \geq -\sum_{k=1}^d a_{\tilde{\gamma}^k} \cosh\left(\frac{\tilde{\gamma}^k}{\varepsilon}\cdot\xi\right)\left(\frac{\tilde{\gamma}^k}{\varepsilon}\cdot v\right)^2\,, \qquad \xi, v \in \mathbb{R}^d\,. \tag{4.65}$$

We use the notion of $\tilde{a}_{\frac{\gamma}{\varepsilon}}$ defined in (2.18) and set $\eta^i := \frac{1}{\varepsilon}\tilde{\gamma}^i$ (thus $\eta^i \in \mathbb{Z}^d$) and $C = \min_k \left(-\tilde{a}_{\eta^k}\right)$ (then $C > 0$ by the above considerations). Since $\cosh\left(\eta^k\cdot\xi\right) \geq 1$ for all $\xi \in \mathbb{R}^d$, equation (4.65) yields

$$\left\langle v\,,\, D^2_\xi \tilde{h}_0(\xi) v\right\rangle \geq C\sum_{k=1}^d (\eta^k\cdot v)^2 \geq 0\,.$$

The sum can take the value 0 only if $v$ is orthogonal to $\eta^k$ for all $k = 1,\dots d$. Since the vectors $\eta^i$, $i = 1,\dots d$ are a basis, this is only the case for $v = 0$ (the matrix $M = \left(C\sum_k \eta^k_i\eta^k_j\right)$ has maximal rank). Thus there exists a constant $\alpha > 0$ (the lowest eigenvalue of $M$), such that

$$\left\langle v\,,\, D^2_\xi \tilde{h}_0(\xi) v\right\rangle \geq \alpha\|v\|^2\,.$$

□

Definition 4.23. *In the setting of Proposition 4.15, we choose $M = \mathbb{R}^d$, $E_0 = 0$ and $h = \tilde{h}_0 = \tilde{t} - V_0$ (the energy phase function given in Hypothesis 4.20), which by Proposition 4.22 is hyperregular.*

*Recall that by Hypothesis 4.20, the set of singular points with respect to the energy $E_0 = 0$ is given by $S(0) = \{0\}$. We define*

$$\ell(x,v) := \begin{cases} \ell_{\tilde{h}_0,0}(x,v)\,, & x \in \widetilde{M} := \mathbb{R}^d\setminus\{0\}\\ 0 & x = 0\,.\end{cases}$$

*Then $\ell : \mathbb{R}^{2d} \to \mathbb{R}$ is continuous, since $\lim_{x\to 0}\tilde{\tau}_0(x,v) = (0,0)$.*

*The associated Finsler metric $d_\ell : \mathbb{R}^d\times\mathbb{R}^d \to [0,\infty)$ is given by*

$$d_\ell(x_0,x_1) = \inf_{\gamma\in\Gamma_{0,1}(x_0,x_1)} \int_0^1 \ell(\gamma(t),\dot{\gamma}(t))\,dt\,. \tag{4.66}$$

The following proposition permits to extend the solution $\varphi$ of the eikonal equation (3.10) constructed in Section 3.2 by the distance $d_\ell(0,x)$, satisfying the eikonal inequality

$$t(x, i\nabla\varphi(x)) + V_0(x) \geq 0\,. \tag{4.67}$$

outside of $\Omega$. To this end, we first notice that if $d_\ell$ is locally Lipschitz continuous, it is differentiable almost everywhere in both arguments. This follows from the Rademacher Theorem (see [**20**]). In fact restricted to a bounded domain $\Sigma$, the gradient $\nabla d_\ell$ is well defined in $\mathscr{L}^\infty(\Sigma)$ as almost everywhere limit of $\nabla(\zeta_\varepsilon * d_\ell)$ when $\varepsilon\to\infty$, where $\zeta_\varepsilon(x) = \varepsilon^{-d}\zeta(\frac{x}{\varepsilon}) \in \mathscr{C}^\infty_0(B(0,\varepsilon))$ is a standard mollifier. This construction is described for example in Helffer-Sjöstrand [**33**].

Proposition 4.24. *Let $\varphi$ denote the solution of the eikonal equation (3.10) in a neighborhood $\Omega$ of 0 constructed in Section 3.2. Then in the setting of Definition 4.23*

$$d^0(x) := d_\ell(0,x) = \varphi(x)\,, \qquad x\in\Omega\,. \tag{4.68}$$

*In addition for all $x\in\mathbb{R}^d$ and $R > 0$ there exists a $C > 0$ such that for all $\gamma\in(\varepsilon\mathbb{Z})^d$ with $|\gamma| < R$ and for all $\varepsilon\in(0,\varepsilon_0]$*

$$|d_\ell(x,x+\gamma)| \leq |\gamma| C\,. \tag{4.69}$$

*Thus $d_\ell$ is locally Lipschitz continuous. At the points $x\in\mathbb{R}^d$, where $d^0$ is differentiable, the eikonal inequality*

$$\tilde{h}_0(x,\nabla d^0(x)) \leq 0 \tag{4.70}$$

*holds.*

Proof:

Proof of (4.69) and (4.70) (eikonal inequality):
By the triangle inequality and the definition of $d_\ell(x,y)$, we have for any $v \in \mathbb{R}^d$ with $|v| = 1$ and $\delta > 0$

$$\begin{aligned} d^0(x+\delta v) - d^0(x) &\leq d^0(x) + d_\ell(x, x+\delta v) - d^0(x) = d_\ell(x, x+\delta v) \\ &= \inf_{\gamma \in \Gamma(x, x+\delta v)} \int_0^1 \ell(\tilde\gamma(t))\, dt \leq \int_0^1 \ell(\tilde\gamma_0(t))\, dt\,, \end{aligned} \tag{4.71}$$

where $\gamma_0(t) = x + t\delta v$. For this special curve we get by the homogeneity of the Finsler function $\ell$ the estimate

$$\int_0^1 \ell(\tilde\gamma_0(t))\, dt \leq \sup_{t\in[0,1]} \ell(x+t\delta v, \delta v) = \delta \sup_{t\in[0,1]} \ell(x+t\delta v, v)\,. \tag{4.72}$$

Thus (4.71) together with (4.72) prove (4.69) and $d_\ell$ is locally Lipschitz continuous.

By (4.71) and (4.72)

$$\partial_v d^0(x) = \lim_{\delta\to 0} \frac{d^0(x+\delta v) - d^0(x)}{\delta} \leq \lim_{\delta\to 0} \sup_{t\in[0,1]} \ell(x+t\delta v, v)$$

and thus we get for all $v \in \mathbb{R}^d$ with $|v| = 1$ the inequality $\partial_v d^0(x) = \nabla d^0(x)\cdot v \leq \ell(x,v)$. Since both sides are positive homogeneous of order one with respect to $v$, we can extend the inequality to all $v \in \mathbb{R}^d$ by multiplication of both sides with $|v|$, thus

$$\nabla d^0(x)\cdot v \leq \ell(x,v)\,, \qquad v\in\mathbb{R}^d\,. \tag{4.73}$$

As described in Remark 4.16, the Finsler function $\ell$ can be written as $\ell(x,v) = \xi_{\tilde h_0}(x,\tilde v)\cdot v$, where we used the notation $\xi_{\tilde h_0}(x,\tilde v) = \left(\mathcal{D}_f \tilde h_0\right)^{-1}(x,\tilde v)$ and $(x,\tilde v) = \tilde\tau_0(x,v)$ (i.e. $(x,\tilde v)\in\mathcal{E}$). It follows from (4.73), that

$$\nabla d^0(x)\cdot v \leq \xi_{\tilde h_0}(x,\tilde v)\cdot v\,, \qquad \text{for all} \quad (x,v)\in TM\,,$$

yielding

$$\left(\xi_{\tilde h_0}(x,\tilde v) - \nabla d^0(x)\right)\cdot v \geq 0\,, \qquad (x,v)\in TM\,. \tag{4.74}$$

Since $\tilde h_0(x,\xi)$ is differentiable, real valued and convex in each fibre (i.e. with respect to $\xi$ for fixed $x$), by (4.13) the inequality

$$\tilde h_0(x,\xi) \geq \tilde h_0(x,\eta) + D_\eta \tilde h_0(x,\eta)\cdot(\xi-\eta)$$

holds for all $x,\xi,\eta\in\mathbb{R}^d$. Thus by setting $\xi = \xi_{\tilde h_0}(x,\tilde v)$ and $\eta = \nabla d^0(x)$, we get for all $(x,v)\in TM$ the estimate

$$\tilde h_0(x,\xi_{\tilde h_0}(x,\tilde v)) \geq \tilde h_0(x,\nabla d^0(x)) + D_\xi \tilde h_0(x,\nabla d^0(x))\cdot(\xi_{\tilde h_0}(x,\tilde v) - \nabla d^0(x))\,. \tag{4.75}$$

The left hand side of (4.75) is by the definition of $\tilde v$ equal to zero. From the definition of the fibre derivative and with the notation introduced in Remark 4.10, it follows that

$$D_\xi \tilde h_0(x,\nabla d^0(x)) = \mathcal{D}_F \tilde h_0(x,\nabla d^0(x)) = v_{\tilde h_0}(x,\nabla d^0(x)) \in\mathbb{R}^d\,.$$

Choosing $(x,v) := (x, v_{\tilde h_0}(x,\nabla d^0(x))$ in equation (4.75) yields

$$0 \geq \tilde h_0(x,\nabla d^0(x)) + v\cdot(\xi_{\tilde h_0}(x,\tilde v) - \nabla d^0(x))$$

Thus from (4.74) the eikonal inequality (4.70) follows.

Proof of (4.68) (eikonal equality):
By the construction of $\varphi$ in Section 3.2, the outgoing manifold can be parameterized as $\Lambda_+ = \{(x,\nabla\varphi(x))\,|\, x\in\Omega\}$. Thus for a given $x\in\Omega$ there exists a bicharacteristic curve $\widehat\gamma_0 = (\gamma_0,\nabla\varphi(\gamma_0))\subset\Lambda_+$ of the hamiltonian vector field $X_{\tilde h_0}$, parameterized by $[-\infty,0]$, such that $\widehat\gamma_0(0) = (x,\nabla\varphi(x))$ and $\lim_{t\to-\infty}\widehat\gamma_0(t) = (0,0)$. Since $\widehat\gamma_0$ is an integral curve of $X_{\tilde h_0}$, it follows from Hamilton's equations (4.28) that

$$\dot\gamma_0 = D_\xi \tilde h_0\left(\gamma_0,\nabla\varphi(\gamma_0)\right) = \mathcal{D}_F\tilde h_0\left(\gamma_0,\nabla\varphi(\gamma_0)\right)$$

and therefore

$$\xi_{\tilde h_0}\left(\gamma_0,\dot\gamma_0\right) = \left(\mathcal{D}_F\tilde h_0\right)^{-1}\left(\gamma_0,\dot\gamma_0\right) = \nabla\varphi(\gamma_0)\,.$$

Thus

$$\frac{d}{dt}\varphi(\gamma_0) = \nabla\varphi \cdot \dot\gamma_0 = \left(\mathcal{D}_F \tilde h_0\right)^{-1}(\gamma_0, \dot\gamma_0)\cdot\dot\gamma_0 \ . \tag{4.76}$$

Since $\widehat\gamma_0$ is an integral curve, $(\gamma_0(t), \dot\gamma_0(t))$ lies on the energy shell $\mathcal{E}$. Therefore $\tilde\tau_0(\gamma_0, \dot\gamma_0) = (\gamma_0, \dot\gamma_0)$ and it follows at once from (4.76) and the definition of the Finsler function $\ell$ (see Definition 4.23 and Proposition 4.15) that

$$\frac{d}{dt}\varphi(\gamma_0) = \ell(\gamma_0, \dot{\gamma_0}) \tag{4.77}$$

The point $x = 0$ is a singular point of the Finsler manifold $(\mathbb{R}^d, \ell)$ (since $\tilde h_0(0,0) = 0$), thus the base integral curve $\gamma_0 : [-\infty, 0] \to \Omega \ni 0$ of $X_{\tilde h_0}$ is not a regular curve on a Finsler manifold in the sense of Definition 4.2. To avoid this difficulty, we restrict the curve $\gamma_0$ to $[-T, 0]$ and set $y_T := \gamma_0(-T)$. Then for each $T \in \mathbb{R}_+$ the points $y_T$ and $x$ can be joined by the integral curve $\gamma_0|_{[-T,0]}$ of $X_{\tilde h_0}$ and therefore by (4.77)

$$\varphi(x) - \varphi(y_T) = \int_{-T}^0 \ell(\gamma_0(t), \dot\gamma_0(t))\, dt \tag{4.78}$$

By Proposition 4.18 the integral curve $\gamma_0$ of $X_{\tilde h_0}$ is a geodesic with respect to the associated Finsler function $\ell$ (i.e., the integral $\int_{-T}^0 \ell(\gamma, \dot\gamma)\, dt$ is extremal for $\gamma = \gamma_0$). Thus it remains to show, that $\gamma_0$ is minimal geodesic with respect to $\ell$, i.e., the right hand side of (4.78) is minimal for variations over all curves in $\Gamma_{-T,0}(y_T, x)$. Then the length of $\gamma_0$ is by Definition equal to the distance $d_\ell(y_t, x)$.

To show that the geodesic $\gamma_0$ is minimal, we use Abate-Patrizio [**1**], Theorem 1.6.6 (see also Bao-Chern-Shen [**6**], Thm. 6.3.1). One of the conclusions of this Theorem is, that geodesics, which are short enough, actually minimize the curve length among all $\mathscr{C}^\infty$-curves with the same endpoints. Thus the length of any short geodesic joining $x$ and $y$ is equal to the Finsler distance $d_\ell(x, y)$.

The main ingredients of the proof of this theorem are the Euler equations (4.6), the Fundamental inequality (4.8) and the Gauss-Lemma on the orthogonality of radial geodesics and geodesic spheres with respect to the metric $g$.

For Ø small enough (with respect to $d^0$ and thus by Lemma 4.8 with respect to Euclidean distance) it follows from [**1**], Thm.1.6.6, that

$$\varphi(x) - \varphi(y_T) = \int_T^0 \ell(\gamma_0(t), \dot{\gamma_0}(t)) = \inf_{\gamma\in\Gamma_{-T,0}(y_T,x)} \int_{-T}^0 \ell(\gamma(t), \dot\gamma(t))\, dt = d_\ell(y_T, x) \ . \tag{4.79}$$

Since $\ell$ and $\varphi$ can be continuously extended to the point 0, it follows that

$$\lim_{T\to\infty} (\varphi(x) - \varphi(y_T)) = \lim_{T\to\infty} d_\ell(y_T, x) \ ,$$

leading to the result

$$\varphi(x) = d_\ell(0, x) = d^0(x) \ .$$

□

Remark 4.25. *The eikonal inequality* (4.70) *is valid not only for* $d_\ell(x, 0)$*, but in general for* $d_\ell(x, y)$*, where* $y$ *is fixed. In fact we have*

$$d_\ell(x + \delta v, y) - d_\ell(x, y) \le d_\ell(x, y) + d_\ell(x, x + \delta v) - d_\ell(x, y) \le d_\ell(x, x + \delta v) \ ,$$

*which can be inserted in* (4.71) *to give by the same considerations as above* $\nabla_x d_\ell(x, y)\cdot v \le \ell(x, v)$*. This leads to the inequality* $(\xi_{\tilde h_0}(x, \tilde v - \nabla_x d_\ell(x, y))\cdot v \ge 0$ *and thus almost everywhere for any fixed* $y \in \mathbb{R}^d$ *to the eikonal inequality*

$$\tilde h_0(x, \nabla_x d_\ell(x, y)) \le 0 \ . \tag{4.80}$$

CHAPTER 5

# Weighted estimates for Dirichlet eigenfunctions

The aim of this chapter is to find estimates for the weighted $\ell^2$-norm of eigenfunctions of the Dirichlet operator associated to $H_\varepsilon$ with respect to a neighborhood of one potential well.

These estimates show the exponential decay of the eigenfunctions of the low lying spectrum of $H_\varepsilon$ with a rate controlled by the Finsler distance constructed in Chapter 4. To analyze eigenfunctions concentrated at the potential minimum $x_1 = 0$, we introduce a bounded region $\Sigma \subset \mathbb{R}^d$ including $x_1$ and its lattice restriction $\Sigma_\varepsilon := \Sigma \cap (\varepsilon\mathbb{Z})^d$.

Definition 5.1. *Any function $u \in \ell^2(\Sigma_\varepsilon)$ can by zero extension, i.e. via $u(x) = 0$ for $x \notin \Sigma_\varepsilon$, be embedded in $\ell^2((\varepsilon\mathbb{Z})^d)$. If we denote this embedding by $i_{\Sigma_\varepsilon}$, we can define the space $\ell^2_{\Sigma_\varepsilon} := i_{\Sigma_\varepsilon}\left(\ell^2(\Sigma_\varepsilon)\right) \subset \ell^2((\varepsilon\mathbb{Z})^d)$ and the Dirichlet operator*

$$H_\varepsilon^\Sigma := \mathbf{1}_{\Sigma_\varepsilon} H_\varepsilon|_{\ell^2_{\Sigma_\varepsilon}} \;:\; \ell^2_{\Sigma_\varepsilon} \to \ell^2_{\Sigma_\varepsilon}\,. \tag{5.1}$$

We think of $H_\varepsilon^\Sigma$ as having Dirichlet boundary conditions on the boundary $\partial\Sigma$.

## 5.1. Preliminary Results

The first step to weighted estimates for eigenfunctions of $H_\varepsilon^\Sigma$ is contained in the following lemma, which gives a useful expression for the scalar product of $H_\varepsilon$ conjugated with an exponential weight $e^{\frac{\varphi}{\varepsilon}}$.

Lemma 5.2. *Let $H_\varepsilon$ be an operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ satisfying Hypothesis 4.20. and let $\varphi$ be a real valued function on $(\varepsilon\mathbb{Z})^d$, which is constant outside some bounded set. Then for any real valued $v \in \mathscr{D}(H_\varepsilon)$*

$$\begin{aligned}\left\langle\left(e^{\frac{\varphi}{\varepsilon}} H_\varepsilon e^{-\frac{\varphi}{\varepsilon}}\right) v\,,\, v\right\rangle_{\ell^2} &= \left\langle(V_\varepsilon + V_\varepsilon^\varphi)\, v\,,\, v\right\rangle_{\ell^2} \\ &\quad -\frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\frac{\varphi(x)-\varphi(x+\gamma)}{\varepsilon}\right)(v(x)-v(x+\gamma))^2\,,\end{aligned}$$

*where*

$$V_\varepsilon^\varphi(x) := \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right)\quad . \tag{5.2}$$

Proof:
By use of the symmetry of $T_\varepsilon$ and since $v$ and $\varphi$ are assumed to be real valued and $e^{\pm\frac{\varphi}{\varepsilon}} v \in \mathscr{D}(H_\varepsilon)$, we have

$$\begin{aligned}\left\langle\left(e^{\frac{\varphi}{\varepsilon}} T_\varepsilon e^{-\frac{\varphi}{\varepsilon}}\right) v\,,\, v\right\rangle_{\ell^2} &= \frac{1}{2}\left[\left\langle T_\varepsilon e^{-\frac{\varphi}{\varepsilon}}\, v\,,\, e^{\frac{\varphi}{\varepsilon}}\, v\right\rangle_{\ell^2} + \left\langle e^{-\frac{\varphi}{\varepsilon}}\, v\,,\, T_\varepsilon e^{\frac{\varphi}{\varepsilon}}\, v\right\rangle_{\ell^2}\right] \\ &= \frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\left(e^{\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))} + e^{-\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))}\right) v(x+\gamma)v(x) \\ &= \sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right) v(x+\gamma)v(x)\,.\end{aligned}$$

Since $v(x+\gamma)v(x) = v(x)(v(x+\gamma)-v(x)) + v^2(x)$ it follows from the definition and symmetry of $V_\varepsilon^\varphi$ that

$$\begin{aligned}\left\langle \left(e^{\frac{\varphi}{\varepsilon}} T_\varepsilon e^{-\frac{\varphi}{\varepsilon}}\right) v \,,\, v\right\rangle_{\ell^2} &= \sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x) \cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right) v(x)(v(x+\gamma)-v(x)) \\ &\quad + \sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right) v(x)^2 \qquad (5.3)\\ &= -\frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right)(2v(x)^2 - 2v(x)v(x+\gamma)) + \langle V_\varepsilon^\varphi v\,,\, v\rangle_{\ell^2}\end{aligned}$$

Again by the symmetry of $T_\varepsilon$, which yields $a_\gamma(x) = a_{-\gamma}(x+\gamma)$, together with the fact that cosh is even, we have by use of the substitutions $x' = x+\gamma$ and $\gamma' = -\gamma$

$$\begin{aligned}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} & a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right) v(x)^2 \\ &= \sum_{x',\gamma'\in(\varepsilon\mathbb{Z})^d} a_{-\gamma'}(x'+\gamma')\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x'+\gamma')-\varphi(x'))\right) v(x'+\gamma')^2 \\ &= \sum_{x',\gamma'\in(\varepsilon\mathbb{Z})^d} a_{\gamma'}(x')\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x')-\varphi(x'+\gamma'))\right) v(x'+\gamma')^2\end{aligned}$$

Thus by use of this transformation for one of the two terms multiplied with $v(x)^2$ on the right hand side of (5.3) we get

$$\begin{aligned}&\left\langle \left(e^{\frac{\varphi}{\varepsilon}} T_\varepsilon e^{-\frac{\varphi}{\varepsilon}}\right) v \,,\, v\right\rangle_{\ell^2} = \\ &-\frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right)\left(v(x)^2 - 2v(x)v(x+\gamma) + v(x+\gamma)^2\right) + \langle V_\varepsilon^\varphi v\,,\, v\rangle_{\ell^2} \\ &= -\frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\tfrac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right)(v(x)-v(x+\gamma))^2 + \langle V_\varepsilon^\varphi v\,,\, v\rangle_{\ell^2}\,.\end{aligned}$$

Since $V_\varepsilon$ commutes with $e^{-\frac{\varphi}{\varepsilon}}$, the lemma follows.

□

For the Dirichlet operator $H_\varepsilon^\Sigma$ conjugated with the weight function $e^{\frac{\varphi}{\varepsilon}}$, where $\varphi$ denotes a real valued phase function, Lemma 5.2 leads to the following norm estimate, which will be used later on to prove the main theorem.

LEMMA 5.3. *Let $\Sigma\subset\mathbb{R}^d$ denote a bounded region (or $\Sigma=\mathbb{R}^d$ respectively) and let for any fixed $\varepsilon\in(0,\varepsilon_0]$ denote by $\Sigma_\varepsilon = \Sigma\cap(\varepsilon\mathbb{Z})^d$ the restriction of $\Sigma$ to the $\varepsilon$-lattice. Let $H_\varepsilon^\Sigma$ be the associated Dirichlet operator on $\ell^2_{\Sigma_\varepsilon}$ as defined in (5.1), where $H_\varepsilon$ satisfies Hypothesis 4.20. Denote by $V_\varepsilon^\varphi$ the multiplication operator on $\ell^2((\varepsilon\mathbb{Z})^d)$ defined by (5.2) and, for $E\geq 0$ fixed, let $F_\pm:\Sigma\to[0,\infty)$ be a pair of functions such that $F(x) := F_+(x)+F_-(x) > 0$ and*

$$F_+^2(x) - F_-^2(x) = \widehat{V}_\varepsilon(x) + V_\varepsilon^\varphi(x) - E\,,\qquad x\in\Sigma\,. \tag{5.4}$$

*Then for a function $\varphi$ on $\Sigma$ and $v\in\ell^2_{\Sigma_\varepsilon}$ (or $v\in\mathscr{D}(H_\varepsilon)$ and $\varphi$ constant outside some bounded set respectively), both real valued, the estimate*

$$\|Fv\|^2_{\ell^2} \leq 4\left\|\tfrac{1}{F}\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\right\|^2_{\ell^2} + 8\|F_-v\|^2_{\ell^2}\,, \tag{5.5}$$

*holds.*

Proof:
First we state the algebraic inequality

$$\|Fv\|^2_{\ell^2} \leq 2\left(\|F_+v\|^2_{\ell^2} + \|F_-v\|^2_{\ell^2}\right) = 2\left(\|F_+v\|^2_{\ell^2} - \|F_-v\|^2_{\ell^2}\right) + 4\|F_-v\|^2_{\ell^2} \tag{5.6}$$

and that by the construction of $F_+$ and $F_-$

$$\|F_+v\|^2_{\ell^2} - \|F_-v\|^2_{\ell^2} = \langle (V_\varepsilon + V^\varphi - E)v\,,\, v\rangle_{\ell^2}\,. \tag{5.7}$$

Since the non-positivity of the coefficients $a_\gamma$ for $\gamma \neq 0$ assumed in Hypothesis 4.20 yields

$$-\frac{1}{2}\sum_{x,\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))\right)(v(x)-v(x+\gamma))^2 \geq 0 \tag{5.8}$$

and $\left\langle\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\,,\,v\right\rangle_{\ell^2} = \left\langle\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\,,\,v\right\rangle_{\ell^2}$ for $v \in \ell^2_{\Sigma_\varepsilon}$ (or for $v \in \mathscr{D}(H_\varepsilon)$ respectively), it follows from Lemma 5.2 that

$$\langle (V_\varepsilon + V_\varepsilon^\varphi - E)v\,,\,v\rangle_{\ell^2} \leq \left\langle\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\,,\,v\right\rangle_{\ell^2}\,, \tag{5.9}$$

(5.7) together with (5.9) yield by use of the Cauchy-Schwarz inequality

$$\begin{aligned} 2\left(\|F_+v\|^2_{\ell^2} - \|F_-v\|^2_{\ell^2}\right) &\leq 2\left\langle\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\,,\,v\right\rangle_{\ell^2} \\ &\leq 2\sqrt{2}\left\|\tfrac{1}{F}\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\right\|_{\ell^2}\frac{1}{\sqrt{2}}\|Fv\|_{\ell^2} \\ &\leq 2\left\|\tfrac{1}{F}\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\right\|^2_{\ell^2} + \frac{1}{2}\|Fv\|^2_{\ell^2}\,. \end{aligned} \tag{5.10}$$

By inserting (5.10) in (5.6) we get

$$\|Fv\|^2_{\ell^2} \leq 2\left\|\tfrac{1}{F}\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\right\|^2_{\ell^2} + \frac{1}{2}\|Fv\|^2_{\ell^2} + 4\|F_-v\|^2_{\ell^2}$$

and therefore

$$\|Fv\|^2_{\ell^2} \leq 4\left\|\tfrac{1}{F}\left(e^{\frac{\varphi}{\varepsilon}}(H_\varepsilon^\Sigma - E)e^{-\frac{\varphi}{\varepsilon}}\right)v\right\|^2_{\ell^2} + 8\|F_-v\|^2_{\ell^2}\,.$$

□

## 5.2. Weighted Estimates

We are now in a position to give estimates for the $\ell^2$-norm of weighted eigenfunctions of the Dirichlet operator $H_\varepsilon^\Sigma$. We will show, that semiclassically they decay exponentially at a rate controlled by the Finsler distance $d^0(x)$ of $x$ to the well at the origin.

THEOREM 5.4. *Let $\Sigma \subset \mathbb{R}^d$ be a bounded region including the point 0 such that $d^0 \in \mathscr{C}^2(\Sigma)$, where $d^0(x) := d_\ell(0,x)$ denotes the Finsler distance to the origin defined by (4.66) and denote for any $\varepsilon \in (0,\varepsilon_0]$ by $\Sigma_\varepsilon = \Sigma \cap (\varepsilon\mathbb{Z})^d$ the restriction of $\Sigma$ to the lattice.*

*Let $E \in [0, \varepsilon R_0]$ for $R_0$ fixed, assume Hypothesis 4.20 and let $H_\varepsilon^\Sigma$ denote a Dirichlet operator as introduced in (5.1).*

*Then there exist constants $\varepsilon_0, B, C > 0$, such that for all $\varepsilon \in (0,\varepsilon_0]$ and $u \in \ell^2_{\Sigma_\varepsilon}$ real valued*

$$\left\|\left(1+\tfrac{d^0}{\varepsilon}\right)^{-B} e^{\frac{d^0}{\varepsilon}} u\right\|_{\ell^2} \leq C\left[\varepsilon^{-1}\left\|\left(1+\tfrac{d^0}{\varepsilon}\right)^{-B} e^{\frac{d^0}{\varepsilon}}\left(H_\varepsilon^\Sigma - E\right)u\right\|_{\ell^2} + \|u\|_{\ell^2}\right]\,. \tag{5.11}$$

Proof:

We partly follow the ideas in the proof of Proposition 5.5 in Helffer-Sjöstrand [**33**].

First we notice that the symbol $t^\Sigma$ defined by

$$\Sigma \times \mathbb{T}^d \ni (x,\xi) \mapsto t^\Sigma(x,\xi) = \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in\Sigma}} a_\gamma(x) e^{-\frac{i}{\varepsilon}\gamma\xi} \tag{5.12}$$

is associated to the kinetic part $T_\varepsilon^\Sigma$ of the Dirichlet operator $H_\varepsilon^\Sigma$ in the sense that

$$T_\varepsilon^\Sigma u(x) = \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(t^\Sigma)u(x) \qquad \text{for any} \quad u \in \ell^2_{\Sigma_\varepsilon}\,.$$

In the following we write for simplicity $d(x) := d^0(x)$.

Let $\chi \in \mathscr{C}^\infty(\mathbb{R}_+,[0,1])$, such that $\chi(r) = 0$ for $r \leq \frac{1}{2}$ and $\chi(r) = 1$ for $r \geq 1$. In addition we assume that $0 \leq \chi'(r) < 2,3$ (this is possible, because by construction $\chi'(r) \geq 2 + \delta$ for $\delta > 0$ arbitrary small).

We define $g$ on $\Sigma$ by:

$$g(x) := \chi\left(\frac{d(x)}{B\varepsilon}\right)\,, \qquad x \in \Sigma\,, \tag{5.13}$$

where $B$ will be chosen later. Then $g(x) = 1$ for $d(x) \geq B\varepsilon$ and $g(x) = 0$ for $d(x) \leq \frac{B\varepsilon}{2}$. Let

$$\Phi(x) := d(x) - \frac{B\varepsilon}{2} \log\left(\frac{B}{2}\right) - g(x)\frac{B\varepsilon}{2} \log\left(\frac{2d(x)}{B\varepsilon}\right) . \tag{5.14}$$

For any $B$ we choose $\varepsilon < \varepsilon_B$ small enough, such that

$$V_0(x) + t(x, i\nabla d(x)) = 0 , \qquad x \in \Sigma \cap d^{-1}([0, B\varepsilon)) = \{y \in \Sigma \,|\, d(y) < B\varepsilon\} , \tag{5.15}$$

i.e. $\{y \in \Sigma \,|\, d(y) < B\varepsilon\} \subset \Omega$, where $\emptyset$ denotes the region, where the eikonal equation (3.10) holds.

By the definition of $g$

$$\nabla\Phi(x) = \nabla d(x) \left\{1 - \frac{B\varepsilon}{2d(x)}\chi\left(\frac{d(x)}{B\varepsilon}\right) - \frac{1}{2}\chi'\left(\frac{d(x)}{B\varepsilon}\right) \log\left(\frac{2d(x)}{B\varepsilon}\right)\right\} . \tag{5.16}$$

*Step 1:*

We will analyze the term $V_0(x) + t(x, i\nabla\Phi)$ in the different regions.

*Case 1:* $d(x) \leq \frac{B\varepsilon}{2}$

Since $\chi(x) = \chi'(x) = 0$ and the eikonal equation (3.10) holds, we get

$$V_0(x) + t(x, i\nabla\Phi(x)) = V_0(x) + t(x, i\nabla d(x)) = 0 , \qquad x \in \Sigma \cap d^{-1}([0, \tfrac{B\varepsilon}{2}]) . \tag{5.17}$$

*Case 2:* $d(x) \geq B\varepsilon$

Since $\chi'(x) = 0$ in this region, we have by (5.16)

$$\nabla\Phi(x) = \nabla d(x) \left(1 - \frac{B\varepsilon}{2d(x)}\right)$$

and thus

$$V_0(x) + t(x, i\nabla\Phi(x)) = V_0(x) + t\left(x, i\nabla d(x)\left(1 - \frac{B\varepsilon}{2d(x)}\right)\right) . \tag{5.18}$$

From the convexity of $\tilde{t}$ with respect to $\xi$ for fixed $x$ it follows that $t(x, i\xi) = -\tilde{t}(x, \xi)$ is concave and therefore for all $\xi, \eta \in \mathbb{R}^d$

$$t(x, \lambda i\xi + (1-\lambda)i\eta) \geq \lambda t(x, i\xi) + (1-\lambda)t(x, i\eta) \quad \text{for} \quad 0 \leq \lambda \leq 1 . \tag{5.19}$$

In the mentioned region, $0 \leq (1 - \frac{B\varepsilon}{2d(x)}) \leq 1$, thus with the choice $\lambda = (1 - \frac{B\varepsilon}{2d(x)})$ and $\eta = 0$ in (5.19) and since $t(x, 0) = 0$ for all $x \in (\varepsilon\mathbb{Z})^d$ we get by (5.18) the estimate

$$\begin{aligned} V_0(x) + t(x, i\nabla\Phi(x)) &\geq V_0(x) + \left(1 - \frac{B\varepsilon}{2d(x)}\right) t(x, i\nabla d(x)) \geq \\ &\geq V_0(x)\left(1 - \left(1 - \frac{B\varepsilon}{2d(x)}\right)\right) = \\ &= V_0(x)\frac{B\varepsilon}{2d(x)} , \end{aligned}$$

where for the second estimate we used that by Proposition 4.24 the eikonal inequality $t(x, i\nabla d(x)) \geq -V_0(x)$ holds. It follows from the expansions (3.2) of $V_0$ and (3.12) of $\varphi$ at zero (which equals $d$ in a neighborhood of zero), that $d(x) = O(|x|^2)$ and $V_0(x) = O(|x|^2)$ for $|x| \to 0$. Since the region $\Sigma$ was assumed to be bounded, it thus follows that there exists a constant $C_0 > 0$ such that

$$C_0^{-1} \leq \frac{V_0(x)}{2d(x)} \leq C_0 , \qquad x \in \Sigma \cap d^{-1}([B\varepsilon, \infty))$$

and we finally get

$$V_0(x) + t(x, i\nabla\Phi(x)) \geq \frac{B}{C_0}\varepsilon , \qquad x \in \Sigma \cap d^{-1}([B\varepsilon, \infty)) . \tag{5.20}$$

*Case 3:* $\frac{B\varepsilon}{2} < d(x) < B\varepsilon$

We define

$$f_1(x) := \frac{B\varepsilon}{2d(x)}\chi\left(\frac{d(x)}{B\varepsilon}\right) \quad \text{and} \quad f_2(x) := \frac{1}{2}\chi'\left(\frac{d(x)}{B\varepsilon}\right) \log\left(\frac{2d(x)}{B\varepsilon}\right) ,$$

such that by (5.16)

$$\nabla\Phi(x) = \nabla d(x)(1 - f_1(x) - f_2(x)) . \tag{5.21}$$

Since $1 < \frac{2d(x)}{B\varepsilon} < 2$, both functions are non-negative and therefore $1 - f_1(x) - f_2(x) \leq 1$. In addition it follows that $0 \leq f_1(x) \leq 1$ and by the assumption $\chi'(r) \leq 2,3$ we get $0 \leq f_2(x) \leq 1,15 \log 2$. Therefore $0 \leq f_1(x) + f_2(x) \leq 1,15 \log 2 + 1 \leq 2$ and thus the estimate

$$|1 - f_1(x) - f_2(x)| \leq 1 \tag{5.22}$$

holds. Setting

$$\lambda(x) := 1 - f_1(x) - f_2(x) = \left\{1 - \frac{B\varepsilon}{2d(x)}\left(\chi\left(\frac{d(x)}{B\varepsilon}\right)\right) - \frac{1}{2}\left(\chi'\left(\frac{d(x)}{B\varepsilon}\right)\right)\log\left(\frac{2d(x)}{B\varepsilon}\right)\right\},$$

it follows from (5.21) and (5.22), that

$$\nabla\Phi(x) = \lambda(x)\nabla d(x) \qquad \text{with} \quad |\lambda(x)| \leq 1 \quad x \in \mathbb{R}^d\,. \tag{5.23}$$

Thus again from (5.19) (the concavity of $t$) together with (5.23) and the fact that $t$ is even with respect to $i\xi$ it follows that

$$V_0(x) + t(x, i\nabla\Phi(x)) = V_0(x) + t(x, i\lambda(x)\nabla d(x)) \geq V_0(x) + |\lambda(x)| t(x, i\nabla d(x))\,. \tag{5.24}$$

Since by assumption the eikonal equation (5.15) holds for $d(x) < B\varepsilon$, the positivity of $V_0$ and (5.24) yield

$$V_0(x) + t(x, i\nabla\Phi(x)) \geq V_0(1 - |\lambda(x)|) \geq 0\,, \qquad x \in \Sigma \cap d^{-1}((\tfrac{B\varepsilon}{2}, B\varepsilon)\,. \tag{5.25}$$

*Step 2:*

In the second step, we analyze the operator $\widehat{V}_\varepsilon + V_\varepsilon^\Phi$, where $V^\Phi := V_\varepsilon^\Phi$ denotes the multiplication operator defined in Lemma 5.2.

To use Lemma 5.3, we have to find estimates not only for the zero order term $V_0 + t(x, i\nabla\Phi)$, that we analyzed up to this point, but for the complete sum $\widehat{V}_\varepsilon + V^\Phi$. The idea is, to write

$$\widehat{V}_\varepsilon(x) + V^\Phi(x) = \left(\widehat{V}_\varepsilon(x) - V_0(x)\right) + \left(V^\Phi(x) - t(x, i\nabla\Phi(x))\right) + \left(V_0(x) + t(x, i\nabla\Phi(x))\right) \tag{5.26}$$

and to find estimates for the differences in the first two brackets on the right hand side. By Hypothesis 4.20 and since $\Sigma$ is bounded, there exists a constant $C_1 > 0$ such that

$$\widehat{V}_\varepsilon(x) - V_0(x) \geq -C_1\varepsilon\,, \qquad x \in \Sigma\,. \tag{5.27}$$

The aim is now to show, that the difference between $t(x, i\nabla\Phi(x))$ and $V^\Phi$ is at least of order $\varepsilon$.

In the following considerations, we will use

LEMMA 5.5. *Let $g : \Sigma \to [0, 1]$ be defined by (5.13). Let $k \in \mathbb{N}$ and $d \in \mathscr{C}^k$. Then there exists a constant $C > 0$, such that for all $\varepsilon \in (0, \varepsilon_0)$ and for any $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d, |\alpha| \leq k$*

$$|\partial^\alpha g(x)| \leq C\varepsilon^{-\frac{|\alpha|}{2}}\,, \qquad x \in \Sigma\,.$$

Proof:

For $|\alpha| = 0$, this follows directly from the definition. Thus we assume $|\alpha| \geq 1$. Then the derivative is by the definition of the cut-off function supported in the region $\frac{B\varepsilon}{2} < d(x) < B\varepsilon$ and by the Leibnitz and chain rule

$$\partial^\alpha g(x) = \sum_{\substack{\beta,\gamma\in\mathbb{N}^d\\ |\beta|\geq 1, \beta+\gamma=\alpha}} C_{\gamma\beta}\frac{1}{(B\varepsilon)^{|\beta|}}\chi^{(|\beta|)}\left(\frac{d(x)}{B\varepsilon}\right)\partial^\gamma\left(\nabla d(x)\right)^\beta\,. \tag{5.28}$$

Since on the support of $\nabla g$ the eikonal equation holds, it follows from Proposition 4.24 that $d(x) = \varphi(x)$. Therefore by the expansion (3.12) of $\varphi$ it follows that $d(x) = \langle x\,,\, Ax\rangle + O(|x|^3)$ for some $d \times d$-matrix $A$ and $x \to 0$ and therefore $\nabla d(x) = O(|x|)$. Thus in the region with $\frac{B\varepsilon}{2} < d(x) < B\varepsilon$ (on the support of $\nabla g$), we have $|x| = O(\sqrt{\varepsilon})$, yielding $\nabla d(x) = O(\sqrt{\varepsilon})$. The higher derivatives of $d$ are by (3.12) bounded by a constant. Therefore the summands on the right hand side of (5.28) are of order $\varepsilon^k$ with $k = -|\beta| + \frac{1}{2}\max\{0, |\beta| - |\gamma|\}$. Thus for $|\beta| \geq |\gamma|$ it follows that $k = -|\beta| + \frac{|\beta| - (|\alpha| - |\beta|)}{2} = -\frac{|\alpha|}{2}$ and for $|\beta < |\gamma|$ we have $k = -|\beta| > -\frac{|\alpha|}{2}$. Thus the leading terms are of order $\varepsilon^{-\frac{|\alpha|}{2}}$. □

In the next step, we estimate the difference between $V^\Phi$ and $t^\Sigma(x, i\nabla\Phi)$ defined by (5.12). Since $t$ is an even function with respect to $\xi$, we analyze the modulus

$$\left|V^\Phi(x) - t^\Sigma(x, -i\nabla\Phi)\right| = \left| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in\Sigma_\varepsilon}} a_\gamma(x) \left\{ \cosh\left(\frac{1}{\varepsilon}(\Phi(x) - \Phi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Phi(x)\right)\right\}\right|$$
$$\leq \sum_{\gamma\in\Sigma'_\varepsilon(x)} |a_\gamma(x)| \left|\cosh\left(\frac{1}{\varepsilon}(\Phi(x) - \Phi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Phi(x)\right)\right| , \qquad x\in\Sigma\,, \quad (5.29)$$

where $\Sigma'_\varepsilon(x) := \{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, x+\gamma\in\Sigma\}$. By the mean value theorem for the function $\cosh z$ with $z_0 = -\frac{1}{\varepsilon}\gamma\nabla\Phi(x)$ and $z_1 = \frac{1}{\varepsilon}(\Phi(x) - \Phi(x+\gamma))$, we get from $|\sinh x| \leq e^{|x|}$

$$\left|\cosh\left(\frac{1}{\varepsilon}(\Phi(x) - \Phi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Phi(x)\right)\right|$$
$$\leq \sup_{t\in[0,1]} e^{\left|\frac{1}{\varepsilon}\{(\Phi(x)-\Phi(x+\gamma))t - \gamma\nabla\Phi(x)(1-t)\}\right|} \left|\frac{1}{\varepsilon}\{(\Phi(x) - \Phi(x+\gamma)) + \gamma\nabla\Phi(x)\}\right| . \quad (5.30)$$

By Proposition 4.24, (4.69) and the definition (5.14) of $\Phi$ there exist constants $c_1, c_2 > 0$ such that

$$|\Phi(x) - \Phi(x+\gamma)| \leq c_1|\gamma| \quad \text{and} \quad |\gamma\nabla\Phi(x)| \leq c_2|\gamma|\,, \qquad x\in\Sigma,\ \gamma\in\Sigma'_\varepsilon(x)\,.$$

Since $t\in[0,1]$ in (5.30), there exists therefore a constant $D > 0$, such that the exponential term on the right hand side of (5.30) can be estimated as

$$\left|e^{\frac{1}{\varepsilon}\{(\Phi(x)-\Phi(x+\gamma))t + \gamma\nabla\Phi(x)(1-t)\}}\right| \leq e^{\frac{D}{\varepsilon}|\gamma|}\,. \quad (5.31)$$

By second order Taylor-expansion, the remaining factor on the right hand side of (5.30) can be estimated as

$$\frac{1}{\varepsilon}\left|(\Phi(x) - \Phi(x+\gamma)) + \gamma\nabla\Phi(x)\right| \leq \sup_{t\in[0,1]} \frac{1}{\varepsilon} \sum_{\nu,\mu=1}^d |\gamma_\nu\gamma_\mu\partial_\nu\partial_\mu\Phi(x+t\gamma)|\,. \quad (5.32)$$

By the definition (5.14) of $\Phi$ we have

$$\partial_\nu\partial_\mu\Phi(x) = \partial_\nu\partial_\mu d(x) - \partial_\nu\partial_\mu\left(g(x)\frac{B\varepsilon}{2}\log\left(\frac{2d(x)}{B\varepsilon}\right)\right) = \partial_\nu\partial_\mu d(x) \quad (5.33)$$
$$-\left\{(\partial_\nu\partial_\mu g)(x)\frac{B\varepsilon}{2}\log\left(\frac{2d(x)}{B\varepsilon}\right) + (\partial_\nu g)(x)\frac{B\varepsilon}{2d(x)}(\partial_\mu d)(x) + (\partial_\mu g)(x)\frac{B\varepsilon}{2d(x)}(\partial_\nu d)(x)\right.$$
$$\left. -g(x)\frac{B\varepsilon}{2d(x)}\left(\frac{(\partial_\nu d)(x)(\partial_\mu d)(x)}{d(x)} + (\partial_\nu\partial_\mu d)(x)\right)\right\}$$

We will show, that this term is bounded uniformly in $\varepsilon$. To analyze the different summands, we introduce a constant $\delta > 0$ such that $\{x\in\Sigma \,|\, d(x) < \delta\} \subset \Omega$ and $\delta \geq \varepsilon_0 B$.

Since $\Sigma$ is bounded, all derivatives of $d$ are at least bounded by a constant independent of $\varepsilon$, thus the first summand is bounded.

The next three summands include a derivative of $g$ and are therefore supported in the region $\frac{B\varepsilon}{2} < d(x) < B\varepsilon$. Thus $1 < \frac{2d(x)}{B\varepsilon} < 2$ and from the expansion (3.12) of the solution of the eikonal equation $\varphi$, it follows that $\partial_\nu d(x) = O(\sqrt{\varepsilon})$ as described in the proof of Lemma 5.5. Together with Lemma 5.5, this yields the boundedness of these three terms.

For the last term, we analyze the regions $d(x) < \delta$ and $d(x) \geq \delta$ separately.

*Case 1:* $d(x) < \delta$:

By Proposition 4.24, $d$ coincides with the solution $\varphi$ of the eikonal equation, thus by the expansion (3.12) of $\varphi$, we have $d(x) = \langle x\,,\, Ax\rangle + O(|x|^3)$ for some $d\times d$-matrix $A$ and $x\to 0$ and thus $\partial_\nu d(x) = O(|x|)$ and $\partial_\nu\partial_\mu d(x) = O(1)$. Thus that there exists a constant $M > 0$ such that

$$\sum_{\nu,\mu}\left|\frac{(\partial_\nu d)(x)(\partial_\mu d)(x)}{d(x)}\right| + |(\partial_\nu\partial_\mu d)(x)| < M \qquad \text{for} \quad \delta \quad \text{small enough.}$$

Since in addition the for $d(x) > \frac{B\varepsilon}{2}$ (on the support of $g$), the term $\frac{B\varepsilon}{2d}$ is bounded by 1, the summand is bounded by a constant independent of $\varepsilon$.

*Case 2:* $d(x) \geq \delta$:
In this region, we use that the derivatives of $d$ are bounded on $\Sigma$ and that $d^{-1}(x) \leq \delta^{-1}$.

Thus we have shown, that there exists a constant $C > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$

$$|\partial_\nu \partial_\mu \Phi(x)| \leq C \, .$$

Therefore by (5.32) there exists a constant $C_3 > 0$ independent of the choice of $B$ such that for all $\varepsilon \in (0, \varepsilon_0]$

$$\frac{1}{\varepsilon} \left| (\Phi(x) - \Phi(x+\gamma)) + \gamma \nabla \Phi(x) \right| \leq \frac{C_3}{\varepsilon} |\gamma|^2 \, . \tag{5.34}$$

By Hypothesis 4.20, the coefficients $a_\gamma$ decay exponentially fast in $\gamma$, i.e. $e^{\frac{|\gamma| A}{\varepsilon}} a_\gamma(x) \in \ell^2\left((\varepsilon\mathbb{Z})^d_\gamma\right)$ for any $A < \infty$ with respect to summation over $\gamma$. We therefore can conclude by (5.29),(5.31) and (5.34)

$$\left| V^\Phi(x) - t(x, -i\nabla\Phi) \right| \leq \sum_{\gamma \in \Sigma'_\varepsilon(x)} e^{-\frac{A}{\varepsilon}|\gamma|} e^{\frac{D}{\varepsilon}|\gamma|} \frac{C_3}{\varepsilon} |\gamma|^2 \, .$$

Thus for $A$ big enough $A - D = D' > 0$ and we get with $y = \frac{\gamma}{\varepsilon} \in \mathbb{Z}^d$ the estimate

$$\left| V^\Phi(x) - t(x, -i\nabla\Phi(x)) \right| \leq \sum_{\gamma \in \Sigma'_\varepsilon(x)} e^{-\frac{D'}{\varepsilon}|\gamma|} \frac{C_3}{\varepsilon} |\gamma|^2 \leq \varepsilon \sum_{y \in \mathbb{Z}^d} e^{-|y| D'} C_3 |y|^2 \leq \varepsilon C_4 \, . \tag{5.35}$$

By (5.27) and (5.35) we get for all $x \in \Sigma$

$$\widehat{V}_\varepsilon(x) - V_0(x) + V^\Phi(x) - t(x, i\nabla\Phi(x)) \geq -C_1\varepsilon - C_4\varepsilon = -C_5\varepsilon \tag{5.36}$$

with $C_5$ independent of $B$.

Inserting (5.36) in (5.26), we get by (5.17) and (5.25)

$$\widehat{V}_\varepsilon(x) + V^\Phi(x) \geq -C_5\, \varepsilon \qquad \text{for} \quad d(x) < B\varepsilon \tag{5.37}$$

and by (5.20)

$$\widehat{V}_\varepsilon(x) + V^\Phi(x) \geq \left( \frac{B}{C_0} - C_5 \right) \varepsilon \qquad \text{for} \quad d(x) \geq B\varepsilon \, . \tag{5.38}$$

*Step 3:*

Now we are in the position to use Lemma 5.3 to get the stated estimates.

We require

$$\left( \frac{B}{C_0} - C_5 \right) \varepsilon - E \geq \varepsilon \, , \qquad E \in [0, \varepsilon R_0] \, , \tag{5.39}$$

thus we set $B$ such that it fulfills the condition $B \geq C_0(1 + R_0 + C_5)$, i.e. $B$ depends on the choice of the upper bound for $E$ (in particular $B$ increases with increasing $R_0$).

Let

$$\emptyset_- := \{ x \in \Sigma \,|\, \widehat{V}_\varepsilon(x) + V^\Phi(x) - E < 0 \} \qquad \text{and} \qquad \emptyset_+ := \Sigma \setminus \emptyset_- \, , \tag{5.40}$$

then from (5.39) it follows that $\emptyset_- \subset \{d(x) < \varepsilon B\}$ and by (5.37) together with the definition of $\emptyset_-$

$$|\widehat{V}_\varepsilon(x) + V^\Phi(x)| \leq \varepsilon \max\{C_5, R_0\} \qquad \text{for all} \quad x \in \emptyset_- \, . \tag{5.41}$$

We define the functions $F_\pm : \Sigma \to [0, \infty)$ by

$$F_+(x) := \sqrt{\varepsilon \, \mathbf{1}_{\{d(x) < B\varepsilon\}}(x) + (\widehat{V}_\varepsilon(x) + V^\Phi(x) - E) \, \mathbf{1}_{\emptyset_+}(x)} \tag{5.42}$$

and

$$F_-(x) := \sqrt{\varepsilon \, \mathbf{1}_{\{d(x) < B\varepsilon\}}(x) + (E - \widehat{V}_\varepsilon(x) - V^\Phi(x)) \, \mathbf{1}_{\emptyset_-}(x)} \, . \tag{5.43}$$

Then $F_\pm$ are well defined and furthermore there exists a constant $C > 0$ such that

$$F := F_+ + F_- \geq C\sqrt{\varepsilon} > 0 \, , \qquad F_- = O(\sqrt{\varepsilon}) \qquad \text{and} \qquad F_+^2 - F_-^2 = \widehat{V}_\varepsilon + V^\Phi - E \, . \tag{5.44}$$

With the choice $v = e^{\frac{\Phi}{\varepsilon}} u$, Lemma 5.3 thus yields the estimate

$$\left\| F e^{\frac{\Phi}{\varepsilon}} u \right\|^2_{\ell^2} \leq 4 \left\| \tfrac{1}{F} e^{\frac{\Phi}{\varepsilon}} \left( H^\Sigma_\varepsilon - E \right) u \right\|^2_{\ell^2} + 8 \left\| F_- e^{\frac{\Phi}{\varepsilon}} u \right\|^2_{\ell^2} \, . \tag{5.45}$$

The weight function $e^{\frac{\Phi}{\varepsilon}}$ is by definition given by

$$e^{\frac{\Phi(x)}{\varepsilon}} = e^{\frac{d(x)}{\varepsilon}} \left( \frac{B}{2} \right)^{-\frac{B}{2}} \left( \frac{2d(x)}{B\varepsilon} \right)^{-\frac{B}{2} g(x)} \, . \tag{5.46}$$

By the construction of the cut-off function $g$ there are constants $C, \tilde{C}, \tilde{C}', C' > 0$, such that

$$C\left(1+\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}} \le \left\{\begin{array}{ll} \left(\frac{B}{2}\right)^{-\frac{B}{2}}, & d(x) < B\varepsilon \\ \left(\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}}, & d(x) \ge B\varepsilon \end{array}\right\} \le \tilde{C}\left(\frac{B}{2}\right)^{-\frac{B}{2}}\left(\frac{2d(x)}{B\varepsilon}\right)^{-\frac{B}{2}g(x)}$$

and

$$\tilde{C}'\left(\frac{B}{2}\right)^{-\frac{B}{2}}\left(\frac{2d(x)}{B\varepsilon}\right)^{-\frac{B}{2}g(x)} \le \left\{\begin{array}{ll} \left(\frac{B}{2}\right)^{-\frac{B}{2}}, & d(x) \le \frac{B\varepsilon}{2} \\ \left(\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}}, & d(x) > \frac{B\varepsilon}{2} \end{array}\right\} \le C'\left(1+\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}} .$$

Thus by (5.46) we have the estimate

$$e^{\frac{d(x)}{\varepsilon}} C\left(1+\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}} \le e^{\frac{\Phi(x)}{\varepsilon}} \le e^{\frac{d(x)}{\varepsilon}} C'\left(1+\frac{d(x)}{\varepsilon}\right)^{-\frac{B}{2}} . \tag{5.47}$$

By (5.47) and (5.44) the left hand side of (5.45) is bounded from below by

$$\left\|F e^{\frac{\Phi}{\varepsilon}} u\right\|_{\ell^2}^2 \ge C\varepsilon \left\|\left(1+\tfrac{d}{\varepsilon}\right)^{-\frac{B}{2}} e^{\frac{d}{\varepsilon}} u\right\|_{\ell^2}^2 \tag{5.48}$$

and the first summand on the right hand side of (5.45) is bounded from above by

$$\left\|\tfrac{1}{F} e^{\frac{\Phi}{\varepsilon}}\left(H_\varepsilon^\Sigma - E\right) u\right\|_{\ell^2}^2 \le C\varepsilon^{-1}\left\|\left(1+\tfrac{d}{\varepsilon}\right)^{-\frac{B}{2}} e^{\frac{d}{\varepsilon}}\left(H_\varepsilon^\Sigma - E\right) u\right\|_{\ell^2}^2 . \tag{5.49}$$

Since $\emptyset_- \subset \{d(x) < B\varepsilon\}$ it follows from the definition of $F_-$ that $\frac{d(x)}{\varepsilon} \le C$ on its support. Therefore by (5.47) and (5.44) there exists a constant $C > 0$ such that the second summand on the right hand side of (5.45) is bounded from above by

$$\left\|F_- e^{\frac{\Phi}{\varepsilon}} u\right\|_{\ell^2}^2 \le C\varepsilon \left\|u\right\|_{\ell^2}^2 . \tag{5.50}$$

Inserting (5.48), (5.49) and (5.50) in equation (5.45), yields with $\tilde{B} := \frac{B}{2}$

$$\tilde{C}\varepsilon\left\|\left(1+\tfrac{d}{\varepsilon}\right)^{-\tilde{B}} e^{\frac{d}{\varepsilon}} u\right\|_{\ell^2}^2 \le \varepsilon^{-1}\left\|\left(1+\tfrac{d}{\varepsilon}\right)^{-\tilde{B}} e^{\frac{d}{\varepsilon}}\left(H_\varepsilon^\Sigma - E\right) u\right\|_{\ell^2}^2 + \varepsilon\left\|u\right\|_{\ell^2}^2 .$$

This proves the theorem. □

A direct consequence of Theorem 5.4 is the following result about the decay of the eigenfunctions of $H_\varepsilon^\Sigma$.

Theorem 5.6. *Let $u \in \ell^2_{\Sigma_\varepsilon}$ be a normalized eigenfunction of the Dirichlet operator $H_\varepsilon^\Sigma$ defined in (5.1) with respect to the eigenvalue $E \in [0, \varepsilon R_0]$. Then there exist constants $B, C > 0$, such that for all $\varepsilon \in (0, \varepsilon_0]$*

$$\left\|\left(1+\frac{d^0}{\varepsilon}\right)^{-B} e^{\frac{d^0}{\varepsilon}} u\right\|_{\ell^2} \le C .$$

Proof:

Using the normalization of $u$ for the second term on the right hand side of (5.11) and the fact that for the eigenfunction with eigenvalue $E$, the first term on the right hand side vanishes, the stated result follows at once from Theorem 5.4. □

It follows immediately that there exists a constant $M_0 \in \mathbb{N}$ which can be chosen depending only on the upper bound $R_0$ for the eigenvalue $E$ (see (5.39)), such that

$$\left\|e^{\frac{d^0}{\varepsilon}} u\right\|_{\ell^2} = O\left(\varepsilon^{-M_0}\right) . \tag{5.51}$$

This estimate will be used in Chapter 6 to compare the WKB-expansions computed in Chapter 3 with the exact eigenfunctions in the case of several wells.

CHAPTER 6

# Interaction between multiple wells

In the situation described in Chapter 2, where the potential energy is allowed to have a finite number of wells, we are now going to analyze the interaction between different wells and the tunnelling effect.

For a fixed spectral interval we will show that the difference between the exact spectrum and the spectra of Dirichlet realizations of the Hamilton operator at the different wells is exponentially small and determined by the Finsler distance between the two nearest neighboring wells.

## 6.1. Setting

In order to use the results given in the previous chapters, we have to combine the setting of Chapter 2, where the potential energy may have not only one but a finite number of wells, with some of the additional assumptions, which we made in Chapter 3 and 4.

For the WKB-expansion of the eigenfunctions and the weighted norm-estimates for the Dirichlet eigenfunctions, it was essential, that there was only one singular point of the potential $V_0$. Thus it will furthermore be necessary to define regions around the wells, which exclude all other wells. Then the associated Dirichlet operator fulfills the assumptions in the preceding chapters.

HYPOTHESIS 6.1. *Let $H_\varepsilon = T_\varepsilon + V_\varepsilon$ be a self adjoint operator on $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with associated phase space symbol $h_\varepsilon(x,\xi;\varepsilon) := t(x,\xi) + \widehat{V}_\varepsilon$ with the following properties:*

(a) *$t \in S_0^0(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ is a periodic kinetic energy function in the sense of Definition 2.4. Regarding $t$ as a function on $\mathbb{R}^d \times \mathbb{R}^d$, which is periodic with respect to $\xi$, we assume furthermore that the function $\mathbb{R}^d \ni \xi \mapsto t(x,\xi)$ is even and has an analytic continuation to $\mathbb{C}^d$. In addition we assume that for all $x \in \mathbb{R}^d$ the Fourier coefficients $a_\gamma(x)$ defined in (2.20) satisfy the condition*

$$a_\gamma(x)\begin{cases} \leq 0 & \text{for} \quad \gamma \neq 0 \\ \geq 0 & \text{for} \quad \gamma = 0 \end{cases} \qquad \text{and} \quad \operatorname{span}\{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, a_\gamma(x) < 0\} = \mathbb{R}^d \,. \tag{6.1}$$

(b) *The potential energy $V_\varepsilon$ is the lattice restriction of a function $\widehat{V}_\varepsilon \in \mathscr{C}^\infty(\mathbb{R}^d)$, which has an expansion*

$$\widehat{V}_\varepsilon(x) = \sum_{l=0}^{N} \varepsilon^l V_l(x) + R_{N+1}(x;\varepsilon)\,,$$

*where $V_\ell \in \mathscr{C}^\infty(\mathbb{R}^d)$. Furthermore $R_{N+1} \in \mathscr{C}^\infty(\mathbb{R}^d \times (0,\varepsilon_0])$ and for any compact set $K \subset \mathbb{R}^d$ there exists a constant $C_K$ such that $\sup_{x\in K}|R_{N+1}(x;\varepsilon)| \leq C_K\varepsilon^{N+1}$.*

(c) *We assume that there exist constants $R, C > 0$ such that $V_\varepsilon(x) > C$ for all $|x| \geq R$ and $\varepsilon \in (0,\varepsilon_0]$. In addition $V_0 \geq 0$ and it takes the value $V_0(x) = 0$ only at a finite number of strictly non-degenerate minima $\{x_k\}_{k=1}^m$.*

(d) *Let $d_\ell$ denote the Finsler distance associated to $\tilde{h}_0$ introduced in Chapter 4, Definition 4.23. Then we assume that there exists an $\eta > 0$ and a constant $C > 0$ such that for all $x \in (\varepsilon\mathbb{Z})^d$ we have $\|a_.(x)e^{\frac{d_\ell(x,x+\,.\,)}{\varepsilon}}|\,.\,|^{(d+\eta)/2}\|_{\ell^2\left((\varepsilon\mathbb{Z})^d_\gamma\right)} \leq C$.*

REMARK 6.2. (a) *As already discussed in the previous chapters, the analyticity of $t$ with respect to $\xi$ implies for its Fourier coefficients $a_\gamma$, that for all $B > 0$ there exists a constant $C$ such that for all $x \in \mathbb{R}^d$*

$$\|\, e^{-\frac{B|.|}{\varepsilon}} a_.(x)\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq C\,. \tag{6.2}$$

*This leads to an estimate of the sup-norm of $a_\gamma$, since we get that for all $B > 0$ there exists a constant $C > 0$ such that for all $x \in \mathbb{R}^d$*

$$\sum_\gamma |a_\gamma(x)|\, e^{\frac{B|\gamma|}{\varepsilon}} \leq C\ .$$

*This yields in particular*

$$\sup_{x\in\mathbb{R}^d} |a_\gamma(x)| \leq Ce^{-\frac{B|\gamma|}{\varepsilon}} \tag{6.3}$$

*and by use of* (4.69) *it follows that for any $B > 0$ and any bounded region $\Sigma \subset \mathbb{R}^d$ there exists a constant $C > 0$ such that*

$$\sum_{|\gamma|<B} \|a_\gamma(.)e^{\frac{d(.,.+\gamma)}{\varepsilon}}\|_{l^\infty(\Sigma)} \leq C\ . \tag{6.4}$$

**6.1.1. Definitions and Notations.** In order to analyze the problem of multiple wells and tunneling, we have to introduce several notations and some further hypotheses.

We denote by

$$\tilde{h}_0(x,\xi) := \tilde{t}(x,\xi) - V_0(x)\ :\ \mathbb{R}^{2d} \to \mathbb{R} \tag{6.5}$$

the phase function of order zero in $\varepsilon$, corresponding to the kinetic energy

$$\tilde{t}(x,\xi) := -t(x,i\xi) = -\sum_\gamma a_\gamma(x)\cosh\left(\frac{1}{\varepsilon}\gamma\cdot\xi\right) \tag{6.6}$$

occurring in the eikonal equation (3.10).

Let $\mathcal{C} := \{1, 2, \dots m\}$ denote the set of numbers of the wells of $V_0$. For each critical point $x_j$, $j \in \mathcal{C}$, we denote by $p_j(\varepsilon)$ a lattice point such that $V_0(p_j) \leq V_0(p)$ for all lattice points $p$ in a small neighborhood of $x_j$. Then $|x_j - p_j(\varepsilon)| \leq \frac{\sqrt{d}}{2}\varepsilon$.

We suppose $\varepsilon_0$ to be small enough to ensure, that $p_j(\varepsilon) \neq p_k(\varepsilon)$ for $k, j \in \mathcal{C}, k \neq j$ and for all $\varepsilon \in (0, \varepsilon_0]$. By Hypothesis 6.1 it is clear that $V_0(p_j) \geq 0$ and since the minima were assumed to be non-degenerate, it follows that $|V_0(p_j)| = O(\varepsilon^2)$.

We write $d_\ell =: d$, where $d_\ell$ is the Finsler distance defined in Chapter 4, Definition 4.23 and for each well $x_j \in \mathbb{R}^d$, $j \in \mathcal{C}$, we define $d^j(x) := d(x, x_j)$.

Let $S_0 := \min_{j\neq k} d_\ell(x_j, x_k)$ denote the minimum over all Finsler distances between two different wells and let $\eta > 0$ be small. Then for a fixed $S \in ]0, S_0 - \eta[$, for each $j \in \mathcal{C}$ the $S$-spheres at $x_j$

$$B(x_j, S) := \{x \in \mathbb{R}^d \mid d_\ell(x, x_j) < S\} \tag{6.7}$$

satisfy $x_k \neq B(x_j, S)$ for $k \neq j$.

In the following we give additional assumptions on the choice of $M_j$ and $I_\varepsilon$.

Hypothesis 6.3. (a) *For $B(x_j, S)$ defined in* (6.7), *we choose a compact manifold $M_j \subset \mathbb{R}^d$ with $\mathscr{C}^2$-boundary such that $\overline{B(x_j,S)} \subset \overset{\circ}{M_j}$ and $x_k \notin M_j$ for $k \neq j$. Furthermore we assume $S$ to be chosen such that $d^j \in \mathscr{C}^2(M_j)$.*

*We denote by $H_\varepsilon^{M_j}$ the Dirichlet realization of $H_\varepsilon$ on $M_{j,\varepsilon}$ as defined in Chapter 5,* (5.1).

(b) *Let $I_\varepsilon = [\alpha(\varepsilon), \beta(\varepsilon)]$ be an interval, such that $\alpha(\varepsilon), \beta(\varepsilon) \to 0$ for $\varepsilon \to 0$. Furthermore there exists a function $a(\varepsilon) > 0$ with the property $|\log a(\varepsilon)| = o\left(\frac{1}{\varepsilon}\right)$, $\varepsilon \to 0$, such that none of the operators $H_\varepsilon, H_\varepsilon^{M_1}, \dots H_\varepsilon^{M_m}$ has spectrum in $[\alpha(\varepsilon) - 2a(\varepsilon), \alpha(\varepsilon)[$ or $]\beta(\varepsilon), \beta(\varepsilon) + 2a(\varepsilon)]$.*

Thus there should be no spectrum exponentially close to the spectral interval $I_\varepsilon$. It will be seen later, that this assumption on the spectral interval can always be fulfilled by a small shift of the ends of $I_\varepsilon$.

The lattice subset associated to $M_j$ is denoted by $M_{j,\varepsilon} := M_j \cap (\varepsilon\mathbb{Z})^d$. For $\varepsilon$ sufficiently small we can assume that $p_k(\varepsilon) \notin M_{j,\varepsilon}$ for $k \neq j$.

Let

$$\begin{aligned}
\operatorname{spec}(H_\varepsilon)\cap I_\varepsilon &= \{\lambda_1,\dots,\lambda_N\}\,, & u_1,\dots,u_N &\in \ell^2\left((\varepsilon\mathbb{Z})^d\right) \\
\mathcal{F} &:= \operatorname{span}\{u_1,\dots u_N\} & & \\
\operatorname{spec}\left(H_\varepsilon^{M_j}\right)\cap I_\varepsilon &= \{\mu_{j,1},\dots,\mu_{j,n_j}\}\,, & v_{j,1},\dots,v_{j,n_j} &\in \ell^2\left(M_{j,\varepsilon}\right),\ j\in\mathcal{C} \\
\mathcal{E}_j &:= \operatorname{span}\{v_{j,1},\dots,v_{j,n_j}\}\,, & \mathcal{E} &:= \bigoplus \mathcal{E}_j
\end{aligned} \tag{6.8}$$

denote the eigenvalues of $H_\varepsilon$ and of the Dirichlet operators $H_\varepsilon^{M_j}$ in $I_\varepsilon$ and the corresponding orthonormal systems of eigenfunctions. $\mathcal{F}$ denotes the eigenspace spanned by the $u_k$ and $\mathcal{E}_j$ the eigenspaces spanned by $v_{j,k}$.

We denote by $\mathcal{V} := \left(\langle v_{i,k}\,,\, v_{j,l}\rangle_{\ell^2}\right)$ the matrix given by the scalar products of the Dirichlet-eigenfunctions.

**6.1.2. Decay estimates for the Dirichlet eigenfunctions.** Theorem 5.6 yields for $\Sigma = M_j$ and $d^j$ instead of $d^0$

COROLLARY 6.4. *Under the assumptions of Hypothesis 6.1 and 6.3 there exists a number $N_0\in\mathbb{N}$, such that for all $j\in\mathcal{C}$ and $1\le k\le n_j$ and for all $\varepsilon\in(0,\varepsilon_0]$*

$$\|e^{\frac{d^j}{\varepsilon}} v_{j,k}\|_{\ell^2} = O\left(\varepsilon^{-N_0}\right)\,.$$

In the following we will in addition need an estimate for the $\ell^2$-norm of weighted eigenfunctions $u_k$ of $H_\varepsilon$ on the whole lattice $(\varepsilon\mathbb{Z})^d$ instead estimates only for the Dirichlet eigenfunctions as in Theorem 5.6. Therefore we introduce a new distance function $\tilde d$ by replacing the Finsler distance $d$ in a $\mathscr{C}^1$ way by a constant outside of some balls around the several wells.

Define for $j\in\mathcal{C}$ and $C_0>0$

$$B_j := \left\{x\in\mathbb{R}^d \mid d^j(x)\le \tfrac{\pi}{4}C_0\right\} \tag{6.9}$$

$$R_j := \left\{x\in\mathbb{R}^d \mid \tfrac{\pi}{4}C_0 < d^j(x)\le \tfrac{\pi}{2}C_0\right\}$$

$$B_0 := \mathbb{R}^d\setminus\bigcup_{j\in\mathcal{C}}\left(B_j\cup R_j\right)\,. \tag{6.10}$$

where $C_0$ is chosen such that $d^j\in\mathscr{C}^2(B_j\cup R_j)$ and $d^j(x)=\min_{k\in\mathcal{C}} d^k(x)$ for $x\in B_j\cup R_j$.

We define

$$\tilde d(x) := \begin{cases} d^j(x) & ,\ x\in B_j,\ j\in\mathcal{C} \\ C_0\left[\frac{\pi}{4}-\frac12\cos\left(\frac{2d^j(x)}{C_0}\right)\right] & ,\ x\in R_j,\ j\in\mathcal{C} \\ C_0\left(\frac{\pi}{4}+\frac12\right) & ,\ x\in B_0\end{cases}\,. \tag{6.11}$$

Then $\tilde d\in\mathscr{C}^1(\mathbb{R}^d)$,

$$\tilde d(x)\le d^j(x)\qquad\text{for all}\quad x\in\mathbb{R}^d, j\in\mathcal{C} \tag{6.12}$$

and

$$\nabla\tilde d(x) = \begin{cases}\nabla d^j(x) & ,\ x\in B_j,\ j\in\mathcal{C} \\ \nabla d^j(x)\sin\left(\frac{2d^j}{C_0}\right) & ,\ x\in R_j,\ j\in\mathcal{C} \\ 0 & ,\ x\in B_0\end{cases}\,.$$

Thus $\nabla\tilde d$ is Lipschitz continuous and for all $x\in\mathbb{R}^d$ and $j\in\mathcal{C}$, there is a $\lambda_x\in[0,1]$ such that

$$\nabla\tilde d(x) = \lambda_x\,\nabla d^j(x)\,. \tag{6.13}$$

Furthermore we can define the second derivative of $\tilde d$ almost everywhere by use of the Rademacher Theorem (see Evans-Gariepy [**20**]) and it is bounded. Thus we can show the following result about the decay of the eigenfunctions of $H_\varepsilon$.

PROPOSITION 6.5. *Let $u\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ be a normalized eigenfunction of an operator $H_\varepsilon$ satisfying Hypothesis 6.1 with corresponding eigenvalue $E\in[0,\varepsilon R_0]$ and let $\tilde d$ be defined by (6.11).*

*Then for any $0<\delta\le 1$ there exists an $\varepsilon_0>0$ such that for all $\varepsilon\in(0,\varepsilon_0]$*

$$\|e^{\frac{\tilde d}{\varepsilon}} u\|_{\ell^2} = O\left(e^{\frac{\delta}{\varepsilon}}\right)\,. \tag{6.14}$$

Proof:

Since Lemma 5.3 is also valid in the case $\Sigma = \mathbb{R}^d$, we may follow the proof of Theorem 5.4. Fix $\delta > 0$ and let $\Phi := (1-\delta)\tilde{d}$, then by (6.13)

$$|\nabla_x \Phi(x)| \leq (1-\delta) \left| \nabla \left( \min_{k\in\mathcal{C}} d^k \right)(x) \right| , \qquad \text{a.e.}, \tag{6.15}$$

where the gradient of $\min_{k\in\mathcal{C}} d^k(x)$ is understood in the sense of the Rademacher Theorem for Lipschitz-continuous functions.

Since $t(x, i\xi)$ is concave and even with respect to $\xi$ with absolute maximum zero at $\xi = 0$ and $0 \leq (1-\delta) \leq 1$, it follows from (6.15) that

$$t(x, i\nabla\Phi(x)) \geq (1-\delta) t(x, i\nabla \min_{k\in\mathcal{C}} d^k(x)) .$$

Since the eikonal inequality (Lemma 4.24) is valid for each $d^j$, $j \in \mathcal{C}$, we therefore get

$$\begin{aligned} V_0(x) + t(x, i\nabla\Phi(x)) &\geq V_0(x) + (1-\delta) t \left( x, i\nabla \left( \min_{k\in\mathcal{C}} d^k \right)(x) \right) \\ &\geq V_0(x) - (1-\delta) V_0(x) = \delta V_0(x) . \end{aligned} \tag{6.16}$$

Thus with

$$B_\delta := \{ x \in \mathbb{R}^d \mid \tilde{d}(x) \leq \delta \} . \tag{6.17}$$

it follows from (6.16) and Hypothesis 6.1, that there exists a constant $C > 0$ such that

$$V_0(x) + t(x, i\nabla\Phi(x)) \geq \delta C , \qquad x \notin B_\delta . \tag{6.18}$$

To use Lemma 5.3, we have to analyze the term $\widehat{V}_\varepsilon + V^\Phi - E$.

We analyze separately the regions $|x| < R$ and $|x| \geq R$, where $R$ is chosen such that $\widehat{V}_\varepsilon(x) > C$ for some $C > 0$ and $|x| \geq R$. Furthermore we assume that $\{x \in \mathbb{R}^d \,|\, |x| \geq R\} \subset B_0$.

*Case 1:* $|x| < R$:
We write

$$\widehat{V}_\varepsilon(x) + V^\Phi(x) = \left( \widehat{V}_\varepsilon(x) - V_0(x) \right) + \left( V^\Phi(x) - t(x, i\nabla\Phi(x)) \right) + \left( V_0(x) + t(x, i\nabla\Phi(x)) \right) \tag{6.19}$$

and give estimates for the differences in the first two brackets on the right hand side of (6.19). To show positivity of $\widehat{V}_\varepsilon + V^\Phi$ outside of $B_\delta$, it is by (6.18) sufficient to show, that their negative part is at least of order $\varepsilon$.

This is obvious for the potential term (the first brackets), since by Hypothesis 6.1,(a4) there exists a constant $C_1$ such that

$$\widehat{V}_\varepsilon(x) - V_0(x) \geq -C_1 \varepsilon , \qquad x \in \mathbb{R}^d, |x| < R . \tag{6.20}$$

The modulus of the difference inside the second brackets on the right hand side of (6.19) (the term generated by the translation operator) is given by

$$\begin{aligned} \left| V^\Phi(x) - t(x, -i\nabla\Phi) \right| &= \left| \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x) \left\{ \cosh\left( \frac{1}{\varepsilon} (\Phi(x) - \Phi(x+\gamma)) \right) - \cosh\left( \frac{1}{\varepsilon} \gamma \nabla\Phi(x) \right) \right\} \right| \\ &\leq \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} |a_\gamma(x)| \left| \cosh\left( \frac{1}{\varepsilon} (\Phi(x) - \Phi(x+\gamma)) \right) - \cosh\left( \frac{1}{\varepsilon} \gamma \nabla\Phi(x) \right) \right| , \end{aligned} \tag{6.21}$$

As in the proof of Theorem 5.4, we use the Mean Value Theorem to get that for all $x$ and $\gamma$

$$\begin{aligned} &\left| \cosh\left( \frac{1}{\varepsilon} (\Phi(x) - \Phi(x+\gamma)) \right) - \cosh\left( -\frac{1}{\varepsilon} \gamma \nabla\Phi(x) \right) \right| \\ &\qquad \leq \sup_{t\in[0,1]} e^{\left| \frac{1}{\varepsilon} \{ (\Phi(x) - \Phi(x+\gamma)) t - \gamma\nabla\Phi(x)(1-t) \} \right|} \left| \frac{1}{\varepsilon} \{ (\Phi(x) - \Phi(x+\gamma)) + \gamma \nabla\Phi(x) \} \right| . \end{aligned} \tag{6.22}$$

By the definition of $\tilde{d}$ it is clear that there exist $C_1, C_2 > 0$, such that

$$|\tilde{d}(x) - \tilde{d}(x+\gamma)| \leq |\gamma| C_1 \quad \text{and} \quad |\gamma \nabla \tilde{d}(x)| \leq |\gamma| C_2 \qquad x \in \mathbb{R}^d, \gamma \in (\varepsilon\mathbb{Z})^d . \tag{6.23}$$

Since on the other hand by (6.2) we can deduce that for all $x \in \mathbb{R}^d$ and for any $B > 0$

$$|a_\gamma(x)|\; e^{\frac{1}{\varepsilon}\{(\Phi(x)-\Phi(x+\gamma))t+\gamma\nabla\Phi(x)(1-t)\}} \le e^{-\frac{B}{\varepsilon}|\gamma|}\;. \tag{6.24}$$

Second order Taylor-expansion yields for some $s_1 \in [0,1]$

$$\frac{1}{\varepsilon}\{(\Phi(x)-\Phi(x+\gamma))+\gamma\nabla\Phi(x)\} = \frac{1-\delta}{\varepsilon}\sum_{\nu,\mu=1}^{d}\gamma_\nu\gamma_\mu\partial_\nu\partial_\mu\tilde{d}(x+s_1\gamma)\;, \tag{6.25}$$

where $\partial_\mu\partial_\nu\tilde{d}$ is understood in the sense of Rademacher.

The second derivative of $\tilde{d}$ is bounded on $B_j \cup R_j$ for all $j \in \mathcal{C}$ and is zero for $x \in B_0$. By rescaling with $y = \frac{\gamma}{\varepsilon}$, we therefore can conclude by inserting (6.24) and (6.25) into (6.21) that for all $\varepsilon \in (0, \varepsilon_0]$

$$\left|V^\Phi(x) - t(x, -i\nabla\Phi)\right| \le \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{-\frac{B}{\varepsilon}|\gamma|}\frac{C_3}{\varepsilon}|\gamma|^2 \le \varepsilon\sum_{y\in\mathbb{Z}^d} e^{-|y|B}C_3|y|^2 \le \varepsilon C_4 \quad x\in\mathbb{R}^d, |x|<R\;. \tag{6.26}$$

*Case 2:* $|x| \ge R$:
In this region we have $\nabla\Phi(x) = 0$ and $\widehat{V}_\varepsilon(x) \ge C$. Thus to show that $\widehat{V}_\varepsilon + V^\Phi$ is positive, it is enough to show that $|V^\Phi(x)| = O(\varepsilon)$. Since $\Phi$ is constant in $B_0$, the difference $\Phi(x) - \Phi(x+\gamma)$ vanishes if $|\gamma| \le r$ for some $r > 0$, thus we have

$$|V^\Phi(x)| = \left|\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x)\cosh\left(\frac{1}{\varepsilon}(\Phi(x)-\Phi(x+\gamma))\right)\right| \le \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\|\gamma|>r}} |a_\gamma(x)|e^{\frac{1}{\varepsilon}|\Phi(x)-\Phi(x+\gamma)|}\;.$$

Since $\Phi$ is bounded and $|\gamma| > r$ implies $|a_\gamma(x)| \le e^{-\frac{B}{\varepsilon}}$ for any $B > 0$ and for all $x \in \mathbb{R}^d$ (see (6.3)), we have for some $C > 0$

$$|V^\Phi(x)| = O\left(e^{-\frac{C}{\varepsilon}}\right)\;, \qquad x\in\mathbb{R}^d, |x|\ge R\;.$$

Thus by the positivity of $V_\varepsilon$, this yields

$$\widehat{V}_\varepsilon(x) + V_\Phi(x) > C\;, \qquad x\in\mathbb{R}^d, |x|\ge R\;. \tag{6.27}$$

Thus by (6.16), (6.20), (6.26) and (6.27), there exist constants $C_1, C_2 > 0$ such that

$$\widehat{V}_\varepsilon + V^\Phi - E \ge \delta V_0 - C_1\varepsilon - E\;. \tag{6.28}$$

and thus for $\varepsilon$ small enough it follows from (6.18) that

$$\widehat{V}_\varepsilon + V^\Phi - E \ge C_2\delta\;, \qquad x \notin B_\delta\;. \tag{6.29}$$

We define functions $F_\pm : \mathbb{R}^d \to \mathbb{R}$ by

$$F_+(x) := \sqrt{\mathbf{1}_{B_\delta}(x) + \mathbf{1}_{\{\widehat{V}_\varepsilon+V^\Phi-E\ge 0\}}(x)(\widehat{V}_\varepsilon(x)+V^\Phi(x)-E)}$$

and

$$F_-(x) := \sqrt{\mathbf{1}_{B_\delta}(x) + \mathbf{1}_{\{\widehat{V}_\varepsilon+V^\Phi-E< 0\}}(x)(-\widehat{V}_\varepsilon-V^\Phi+E)}\;.$$

Then $F_+$ is strictly positive for $\varepsilon$ small enough, $F := F_+ + F_- > 0$ and $F_+^2 - F_-^2 = \widehat{V}_\varepsilon + V^\Phi - E$. Thus it follows from (6.29) that there exist constants $C, \tilde{C} > 0$ such that for $B_{\delta,\varepsilon} := B_\delta \cap (\varepsilon\mathbb{Z})^d$

$$\begin{aligned}\|Fe^{\frac{\Phi}{\varepsilon}}u\|^2_{\ell^2} &\ge \|F_+e^{\frac{\Phi}{\varepsilon}}u\|^2_{\ell^2} \ge \sum_{x\in B_{\delta,\varepsilon}} e^{\frac{2\Phi(x)}{\varepsilon}}|u(x)|^2 + \sum_{x\notin B_{\delta,\varepsilon}}[V_\varepsilon(x)+V^\Phi(x)-E]e^{\frac{2\Phi(x)}{\varepsilon}}|u(x)|^2 \ge \\ &\ge \|e^{\frac{\Phi}{\varepsilon}}u\|^2_{\ell^2(B_{\delta,\varepsilon})} + \delta C\|e^{\frac{\Phi}{\varepsilon}}u\|^2_{\ell^2(\Sigma\setminus B_{\delta,\varepsilon})} \ge \tilde{C}\|e^{\frac{\Phi}{\varepsilon}}u\|^2\;.\end{aligned} \tag{6.30}$$

Since $F_-$ is by (6.29) supported in $B_\delta$

$$\begin{aligned}\|F_-e^{\frac{\Phi}{\varepsilon}}u\|^2_{\ell^2} &= \|F_-e^{\frac{(1-\delta)\tilde{d}}{\varepsilon}}u\|^2_{\ell^2(B_{\delta,\varepsilon})} \le \\ &\le e^{\frac{2(\delta-\delta^2)}{\varepsilon}}\|F_-u\|^2_{\ell^2(B_{\delta,\varepsilon})} \le Ce^{\frac{2\delta}{\varepsilon}}\;.\end{aligned} \tag{6.31}$$

By Lemma 5.3, we get by (6.30) and (6.31) with $v = e^{\frac{\Phi}{\varepsilon}}u$, that, for any $\delta \in (0,1]$

$$\|e^{\frac{(1-\delta)\tilde{d}}{\varepsilon}}u\|_{\ell^2} = O\left(e^{\frac{\delta}{\varepsilon}}\right)$$

for eigenfunctions $u$ of $H_\varepsilon$.

Since $\tilde{d}(x) \leq C_0 \frac{\pi+2}{4} := \tilde{C}$, we get for some $C > 0$

$$Ce^{\frac{\delta}{\varepsilon}} \geq \|e^{\frac{(1-\delta)\tilde{d}}{\varepsilon}} u\|_{\ell^2} \geq e^{-\frac{\tilde{C}\delta}{\varepsilon}} \|e^{\frac{\tilde{d}}{\varepsilon}} u\|_{\ell^2} ,$$

proving (6.14) for $\tilde{\delta} := \delta(1 + \tilde{C})$.

□

## 6.2. Distance of the Eigenspaces

To analyze the difference between the eigenfunctions of the operator $H_\varepsilon$ acting on the whole lattice and those of the several Dirichlet operators (with respect to a given spectral interval $I_\varepsilon$), we have to compare $\mathcal{F}$ and $\mathcal{E}$ introduced in equation (6.8). For this reason, we introduce a distance function $\vec{\mathrm{dist}}$ between closed subspaces of a Hilbert space $\mathscr{H}$.

DEFINITION 6.6. *Let $\mathscr{H}$ be a Hilbert space with closed subspaces $\mathcal{E}$ and $\mathcal{F}$ and denote by $\Pi_\mathcal{E}$ and $\Pi_\mathcal{F}$ the orthogonal projections on $\mathcal{E}$ and $\mathcal{F}$ respectively. Then we define the nonsymmetric distance $\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F})$ between $\mathcal{E}$ and $\mathcal{F}$ by*

$$\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) := \|\Pi_\mathcal{E} - \Pi_\mathcal{F}\Pi_\mathcal{E}\| .$$

Then $\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) = 0$ if and only if $\mathcal{E} \subseteq \mathcal{F}$. In order to get estimates on the distance of the eigenspace of $H_\varepsilon$ and the direct sum of the eigenspaces of $H_\varepsilon^{M_j}$, $j \in \mathcal{C}$, we use the following two propositions, which are proven in Helffer-Sjöstrand [**33**] (Prop. 1.4. and Thm 2.4).

PROPOSITION 6.7. *Let $\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F})$ be the distance between closed subspaces $\mathcal{E}$ and $\mathcal{F}$ of a Hilbert space $\mathscr{H}$ as introduced in Definition 6.6. If $\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) < 1$ and $\vec{\mathrm{dist}}(\mathcal{F}, \mathcal{E}) < 1$, then the projections $\Pi_\mathcal{E}|_\mathcal{F} : \mathcal{F} \to \mathcal{E}$ and $\Pi_\mathcal{F}|_\mathcal{E} : \mathcal{E} \to \mathcal{F}$ are bijective with bounded inverse and $\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) = \vec{\mathrm{dist}}(\mathcal{F}, \mathcal{E})$.*

PROPOSITION 6.8. *Let $A$ be a self adjoint operator in a Hilbert space $\mathscr{H}$ and $I \subseteq \mathbb{R}$ denote a compact interval. Let $\mu_1, \ldots, \mu_N \in I$ and $\psi_1, \ldots \psi_N \in \mathscr{H}$ be linearly independent satisfying*

$$A\psi_j = \mu_j \psi_j + r_j$$

*where $\|r_j\| \leq \delta$.*

*Let $a > 0$ and assume that $\mathrm{spec}(A) \cap ((I + B(0, 2a)) \setminus I) = \emptyset$. Denoting by $\mathcal{E}$ the space spanned by $\psi_1, \ldots \psi_N$ and by $\mathcal{F}$ the eigenspace of $A$ associated to $\mathrm{spec}(A) \cap I$, then we have*

$$\vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) \leq \frac{\sqrt{N}\delta}{a\sqrt{\lambda_\Psi^{\min}}} , \tag{6.32}$$

*where $\lambda_\Psi^{\min}$ denotes the minimal eigenvalue of the Gram-matrix $\Psi = (\langle \psi_j, \psi_k \rangle_\mathscr{H})$.*

Thus if the spectrum of $A$ in $I$ is discrete of finite multiplicity and the right hand side of (6.32) is strictly smaller than 1, the operator $A$ has at least $N$ eigenvalues in $I$.

Based on these rather general facts, we now return to the special case of $\mathcal{E}$ and $\mathcal{F}$ given in (6.8).

THEOREM 6.9. *Let $H_\varepsilon$, $H_\varepsilon^{M_j}$, $\mathcal{F}$, $\mathcal{E}$ and $S$ be as described in Hypotheses 6.1 and 6.3 and in equation (6.8). Let $\vec{\mathrm{dist}}$ denote the distance between two subspaces of $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ introduced in Definition 6.6. Then for every $\sigma < S$ and for all $\varepsilon \in (0, \varepsilon_0]$*

$$\vec{\mathrm{dist}}(\mathcal{F}, \mathcal{E}) = \vec{\mathrm{dist}}(\mathcal{E}, \mathcal{F}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) .$$

*Moreover there is a bijection*

$$b : \mathrm{spec}(H_\varepsilon) \cap I_\varepsilon \to \bigcup_{j=1}^m \left(\mathrm{spec}(H_\varepsilon^{M_j}) \cap I_\varepsilon\right) ,$$

*such that*

$$b(\lambda) - \lambda = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) .$$

Proof:

*Step 1:*
We start proving the estimate

$$\vec{\operatorname{dist}}(\mathcal{E},\mathcal{F}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \ . \tag{6.33}$$

In order to use Proposition 6.8, we have to estimate the remainder $r_{j,k}$ for the approximate spectral problem

$$H_\varepsilon v_{j,k} = \mu_{j,k} v_{j,k} + r_{j,k} \ ,$$

where $v_{j,k}$ are the eigenfunctions of the Dirichlet operator $H_\varepsilon^{M_j}$ as defined (6.8). Therefore, we decompose the Hamilton operator $H_\varepsilon$ into its Dirichlet realization $H_\varepsilon^{M_j} = \mathbf{1}_{M_{j,\varepsilon}} H_\varepsilon \mathbf{1}_{M_{j,\varepsilon}}$ and a remaining part. Since $v_{j,k}$ is supported in $M_{j,\varepsilon}$

$$\begin{aligned} H_\varepsilon v_{j,k}(x) &= \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(x) v_{j,k}(x+\gamma) + V_\varepsilon(x) v_{j,k}(x) \\ &= \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon},\, x\in M_{j,\varepsilon}}} a_\gamma(x) v_{j,k}(x+\gamma) + \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon},\, x\notin M_{j,\varepsilon}}} a_\gamma(x) v_{j,k}(x+\gamma) + V_\varepsilon(x) v_{j,k}(x) \\ &= H_\varepsilon^{M_j} v_{j,k}(x) + \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon},\, x\notin M_{j,\varepsilon}}} a_\gamma(x) v_{j,k}(x+\gamma) \\ &=: \mu_{j,k} v_{j,k}(x) + r_{j,k}(x) \ . \end{aligned} \tag{6.34}$$

More general we can write

$$H_\varepsilon|_{\mathcal{E}} = H_\varepsilon \mathbf{1}_{M_{j,\varepsilon}}|_{\mathcal{E}} = \mathbf{1}_{M_{j,\varepsilon}} H_\varepsilon|_{\mathcal{E}} + [H_\varepsilon, \mathbf{1}_{M_{j,\varepsilon}}]|_{\mathcal{E}} \ . \tag{6.35}$$

Thus the remainder is given by

$$r_{j,k}(x) = [H_\varepsilon, \mathbf{1}_{M_{j,\varepsilon}}] v_{j,k}(x) = \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon},\, x\notin M_{j,\varepsilon}}} a_\gamma(x)\, v_{j,k}(x+\gamma)\,, \tag{6.36}$$

with the $\ell^2$-norm

$$\|r_{j,k}\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)} = \sum_{x\notin M_{j,\varepsilon}} \left| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} a_\gamma(x) v_{j,k}(x+\gamma) \right|^2 \leq \sum_{x\notin M_{j,\varepsilon}} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} |a_\gamma(x) v_{j,k}(x+\gamma)| \right)^2 \ .$$

To estimate this term, we use the fact, that by the definition of $M_{j,\varepsilon}$ there exists a constant $S_1 \in (S, S_0)$ such that for all $x \notin M_{j,\varepsilon}$ we have $d^j(x) \geq S_1$. Therefore for $x \notin M_{j,\varepsilon}$

$$\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} |a_\gamma(x) v_{j,k}(x+\gamma)| = \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| a_\gamma(x) e^{-\frac{d^j(x)}{\varepsilon}} e^{\frac{d^j(x)}{\varepsilon}} v_{j,k}(x+\gamma) \right| \leq e^{-\frac{S_1}{\varepsilon}} A(x) \ , \tag{6.37}$$

where

$$A(x) := \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| a_\gamma(x) e^{\frac{d^j(x)}{\varepsilon}} v_{j,k}(x+\gamma) \right| \ , \qquad x \notin M_{j,\varepsilon} \ .$$

By the triangle inequality $d^j(x) \leq d^j(x+\gamma) + d(x, x+\gamma)$, thus using the notation

$$\langle\gamma\rangle_\varepsilon := \sqrt{\varepsilon^2 + |\gamma|^2} \tag{6.38}$$

we get for all $x \notin M_{j,\varepsilon}$

$$A(x) \leq \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} \langle\gamma\rangle^{\frac{d+\eta}{2}} \langle\gamma\rangle^{-\frac{d+\eta}{2}} e^{\frac{d^j(x+\gamma)}{\varepsilon}} v_{j,k}(x+\gamma) \right|$$

for any $\eta > 0$. The last sum can be understood as $\ell^1$-norm with respect to $\gamma$, thus by the Cauchy-Schwarz inequality

$$\begin{aligned} A(x) &\leq \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} \langle\gamma\rangle^{\frac{d+\eta}{2}} \right|^2 \right)^{\frac12} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| \langle\gamma\rangle^{-\frac{d+\eta}{2}} e^{\frac{d^j(x+\gamma)}{\varepsilon}} v_{j,k}(x+\gamma) \right|^2 \right)^{\frac12} \\ &\leq C \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \left| \langle\gamma\rangle^{-\frac{d+\eta}{2}} e^{\frac{d^j(x+\gamma)}{\varepsilon}} v_{j,k}(x+\gamma) \right|^2 \right)^{\frac12}, \qquad x \notin M_{j,\varepsilon} \end{aligned} \tag{6.39}$$

where in the second step we choose $\eta$ according to Hypothesis 6.1,(d), such that the $\ell^2$-norm of $a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} \langle\gamma\rangle^{(d+\eta)/2}$ with respect to $\gamma$ is bounded by a constant $C$ uniformly with respect to $x$. Combining (6.37) and (6.39) and changing the order of summation yields for the $\ell^2$-norm of $r_{j,k}$

$$\begin{aligned} \|r_{j,k}\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)} &\leq e^{-\frac{2S_1}{\varepsilon}} \tilde C \sum_{x\notin M_{j,\varepsilon}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j,\varepsilon}}} \langle\gamma\rangle^{-(d+\eta)} \left| e^{\frac{d^j(x+\gamma)}{\varepsilon}} v_{j,k}(x+\gamma) \right|^2 \\ &\leq e^{-\frac{2S_1}{\varepsilon}} \tilde C \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} \langle\gamma\rangle^{-(d+\eta)} \sum_{x+\gamma\in M_{j,\varepsilon}} \left| e^{\frac{d^j(x+\gamma)}{\varepsilon}} v_{j,k}(x+\gamma) \right|^2 \\ &\leq e^{-\frac{2S_1}{\varepsilon}} \tilde C \| e^{\frac{d^j}{\varepsilon}} v_{j,k}\|_{\ell^2_{M^j_\varepsilon}} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} \langle\gamma\rangle^{-(d+\eta)} . \end{aligned}$$

Calculating the last sum explicitly, we get by Corollary 6.4 for some $\tilde N \in \mathbb{N}$ and all $\sigma \leq S < S_1$

$$\|r_{j,k}\|_{\ell^2((\varepsilon\mathbb{Z})^d)} = \|[H_\varepsilon, \mathbf{1}_{M_{j,\varepsilon}}] v_{j,k}\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq e^{-\frac{S_1}{\varepsilon}} C \varepsilon^{-(\tilde N + d)} = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) . \tag{6.40}$$

Proposition 6.8 therefore yields

$$\vec{\operatorname{dist}}(\mathcal{E}, \mathcal{F}) \leq \frac{\sqrt{N}}{a(\varepsilon)\sqrt{\lambda^{\min}_{\mathcal{V}}}} C e^{-\frac{\sigma}{\varepsilon}} , \tag{6.41}$$

where $a(\varepsilon)$ has the properties described in Hypothesis 6.3. Furthermore $\lambda^{\min}_{\mathcal{V}}$ denotes the smallest eigenvalue of the matrix $\mathcal{V} = \left(\langle v_\alpha , v_\beta\rangle_{\ell^2}\right)$ with $\alpha, \beta \in \mathcal{J} := \{(j,k) \,|\, j \in \mathcal{C},\, 1 \leq k \leq n_j\}$ and

$$N := \sum_{j=1}^m n_j \quad \text{with} \quad n_j := \#\{\mu_{j1}, \dots, \mu_{jn_j}\} . \tag{6.42}$$

Using the notation $j(\alpha) = j$ for $\alpha = (j,k)$, we get $\langle v_\alpha , v_\beta\rangle_{\ell^2} = \delta_{\alpha,\beta}$ if $j(\alpha) = j(\beta)$, because the systems of Dirichlet eigenfunctions associated to a single well were supposed to be orthonormal.

If the eigenfunctions $v_\alpha$ and $v_\beta$ belong to different wells, i.e. if $j(\alpha) \neq j(\beta)$, then at each point $x \in (\varepsilon\mathbb{Z})^d$ at least one of the functions $v_\alpha, v_\beta$ is exponential small, because they decrease exponentially (Corollary 6.4).

In fact we use the triangle inequality for the Finsler distance (Lemma 4.8) to get

$$d^{j(\alpha)}(x) + d^{j(\beta)}(x) = d(x_{j(\alpha)}, x) + d(x, x_{j(\beta)}) \geq d(x_{j(\alpha)}, x_{j(\beta)}) \geq S_0$$

and therefore

$$\begin{aligned} \left|\langle v_\alpha , v_\beta\rangle_{\ell^2}\right| &= \left| \sum_{x\in(\varepsilon\mathbb{Z})^d} v_\alpha(x) v_\beta(x) \right| = \left| \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{-\frac{d^{j(\alpha)}(x)}{\varepsilon}} e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x) e^{-\frac{d^{j(\beta)}(x)}{\varepsilon}} e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x) \right| \\ &\leq e^{-\frac{S_0}{\varepsilon}} \sum_{x\in(\varepsilon\mathbb{Z})^d} \left| e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x) e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x) \right| . \end{aligned}$$

By the Schwarz inequality and Corollary 6.4 this yields for general $\alpha, \beta \in \mathcal{J}$ and any $S_1 < S_0$

$$\langle v_\alpha , v_\beta\rangle_{\ell^2} = \delta_{\alpha,\beta} + O\left(e^{-\frac{S_1}{\varepsilon}}\right) . \tag{6.43}$$

We now claim that there exists a $N_0 \in \mathbb{N}$ such that for all $j \in \mathcal{C}$

$$n_j := \#\{\mu_{j1}, \ldots, \mu_{jn_j}\} = O\left(\varepsilon^{-N_0}\right) \ . \tag{6.44}$$

Then (6.43) implies that for each $\sigma < S$

$$\|\mathcal{V} - \mathbf{1}\,\| = O\left(n_j e^{-\frac{S_1}{\varepsilon}}\right) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right)$$

and in particular

$$\lambda_{\mathcal{V}}^{\min} = 1 + O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \ . \tag{6.45}$$

We prove (6.44) by a comparison argument as described in Reed-Simon [**49**], vol.4 and Helffer [**29**]. We compare $H_\varepsilon^{M_j}$ for $j \in \mathcal{C}$ with the associated cut translation operator $T_\varepsilon^K$ on a cube $K_\varepsilon = [-N, N]^d \cap (\varepsilon\mathbb{Z})^d$, which is chosen such that $M_{j,\varepsilon} \subset K_\varepsilon$. Then $K$ includes $\left(\frac{N}{\varepsilon}\right)^d$ lattice points and any translation operator on $K_\varepsilon$ can be written as a $\left(\frac{N}{\varepsilon}\right)^d \times \left(\frac{N}{\varepsilon}\right)^d$-matrix. Thus $T_\varepsilon^K$ can have at most $\left(\frac{N}{\varepsilon}\right)^d$ eigenvalues. Since $T_\varepsilon^K \leq H_\varepsilon^{M_j}$, the number of eigenvalues of $H_\varepsilon^{M_j}$ must be smaller or equal to that of $T_\varepsilon^K$. Thus for a suitable number $N_0 \in \mathbb{N}$, the number of eigenvalues $\mu_j$ is of order $\varepsilon^{-N_0}$.

Inserting (6.45) and (6.44) in (6.41) and taking into account the assumption on $a(\varepsilon)$ given in Hypothesis 6.3 yields (6.33) for each $\sigma \leq S$.

It follows from this estimate, that $H_\varepsilon$ has at least as many eigenvalues in $I_\varepsilon$ as the Dirichlet operators $H_\varepsilon^{M_j}$ for $j \in \mathcal{C}$, i.e.

$$\#\{\lambda_1, \ldots, \lambda_n\} := n \geq \sum_{j \in \mathcal{C}} n_j \ . \tag{6.46}$$

*Step 2:*
In the second step we prove the estimate

$$\vec{\operatorname{dist}}(\mathcal{F}, \mathcal{E}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \ . \tag{6.47}$$

By Proposition 6.7 and (6.33) shown in step 1 it suffices to show $\vec{\operatorname{dist}}(\mathcal{F}, \mathcal{E}) < 1$.

Let $B_0^+ := B_0 \cup \bigcup_{j \in \mathcal{C}} R_j$ with $B_j$, $R_j$ and $B_0$ defined in (6.9) and (6.10) and $u \in \mathcal{F}$ with $\|u\| \leq 1$. Then there exists a constant $C > 0$, such that

$$\mathbf{1}_{B_0^+}\, u = O\left(e^{-\frac{C}{\varepsilon}}\right) \qquad \text{in} \quad \ell^2\left((\varepsilon\mathbb{Z})^d\right) \tag{6.48}$$

and for all $j \in \mathcal{C}$

$$H_\varepsilon\, \mathbf{1}_{B_j}\, u = \lambda\, \mathbf{1}_{B_j}\, u + O\left(e^{-\frac{C}{\varepsilon}}\right) \qquad \text{in} \quad \ell^2\left((\varepsilon\mathbb{Z})^d\right) \ , \tag{6.49}$$

where $\lambda$ denotes the eigenvalue of $u$.

In fact it follows from Proposition 6.5 and the definition of $B_0^+$, that

$$\begin{aligned}
\|\,\mathbf{1}_{B_0^+}\, u\|_{\ell^2}^2 &= \sum_{x \in B_{0,\varepsilon}^+} |u(x)|^2 = \sum_{x \in B_{0,\varepsilon}^+} |e^{-\frac{\tilde{d}(x)}{\varepsilon}} e^{\frac{\tilde{d}(x)}{\varepsilon}} u(x)|^2 \\
&\leq e^{-\frac{\pi C_0}{2\varepsilon}} \|e^{\frac{\tilde{d}}{\varepsilon}} u\|_{\ell^2}^2 \\
&\leq e^{-\frac{C_1}{\varepsilon}} \ ,
\end{aligned}$$

proving (6.48) for any $C \leq C_1$.

To see equation (6.49), we write

$$H_\varepsilon\, \mathbf{1}_{B_j}\, u = \mathbf{1}_{B_j}\, H_\varepsilon u + [H_\varepsilon, \mathbf{1}_{B_j}]u = \lambda\, \mathbf{1}_{B_j}\, u + [H_\varepsilon, \mathbf{1}_{B_j}]u$$

where

$$[H_\varepsilon, \mathbf{1}_{B_j}]u(x) = [T_\varepsilon, \mathbf{1}_{B_j}]u(x) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_\gamma(x) \left[\mathbf{1}_{B_j}(x+\gamma) - \mathbf{1}_{B_j}(x)\right] u(x+\gamma) \ , \tag{6.50}$$

vanishing for $x$ and $x + \gamma$ both inside or outside of $B_j$. We divide the space into the regions $B_j$, $R_j$ and $\mathbb{R}^d \setminus (B_j \cup R_j)$ to get

$$\|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2} = \|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2(R_{j,\varepsilon})} + \|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2(B_{j,\varepsilon})} + \|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2((\varepsilon\mathbb{Z})^d \setminus (B_{j,\varepsilon} \cup R_{j,\varepsilon}))} \tag{6.51}$$

and analyze the three summands separately. For $x \in (\varepsilon\mathbb{Z})^d \setminus (B_j \cup R_j)$, the commutator is non-vanishing only if $x + \gamma \in B_j$ and thus if the modulus of $\gamma$ in (6.50) is at least $C_0\pi/4 (= C_2)$, yielding

$$\begin{aligned}\left\|[H_\varepsilon, \mathbf{1}_{B_j}]u\right\|_{\ell^2((\varepsilon\mathbb{Z})^d\setminus(B_{j,\varepsilon}\cup R_{j,\varepsilon}))} &= \left\| \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(\,.\,)\left[\mathbf{1}_{B_j}(\,.+\gamma) - \mathbf{1}_{B_j}(\,.\,)\right] u(\,.+\gamma)\right\|_{\ell^2((\varepsilon\mathbb{Z})^d\setminus(B_{j,\varepsilon}\cup R_{j,\varepsilon}))} \\ &\leq \left\{ \sum_{|\gamma|\geq C_2} \|a_\gamma(\,.\,)\|_{l^\infty((\varepsilon\mathbb{Z})^d\setminus(B_{j,\varepsilon}\cup R_{j,\varepsilon}))}\right\} \|u\|_{\ell^2}\ .\end{aligned}$$

Thus by (6.3) and since $u$ was assumed to be bounded

$$\|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2((\varepsilon\mathbb{Z})^d\setminus(B_{j,\varepsilon}\cup R_{j,\varepsilon}))} = O\left(e^{\frac{-C_3}{\varepsilon}}\right) \tag{6.52}$$

for any $C_3 > 0$. To estimate the $\ell^2$-norm inside the region $R_j$ (the first summand on the right hand side of (6.51)), we use that $d^j(x) \geq \frac{\pi C_0}{4}$ for $x \in R_j$. In addition $|\gamma| \leq B$ for some $B > 0$, since for $x \in R_j$, the difference of the characteristic functions (see (6.50)) vanishes, if $x + \gamma \notin B_j$. Thus

$$\begin{aligned}\|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2(R_{j,\varepsilon})} &= \left\| \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(\,.\,)\left[\mathbf{1}_{B_j}(\,.+\gamma) - \mathbf{1}_{B_j}(\,.\,)\right] u(\,.+\gamma)\right\|_{\ell^2(R_{j,\varepsilon})} \\ &\leq \left\{ \sum_{\substack{\gamma \\ |\gamma|\leq B}} \left\| a_\gamma(\,.\,) e^{-\frac{d^j(.)}{\varepsilon}} e^{\frac{d(x,x+\gamma)}{\varepsilon}}\right\|_{l^\infty(R_{j,\varepsilon})}\right\} \left\| e^{\frac{d^j}{\varepsilon}} u\right\|_{\ell^2(B_{j,\varepsilon})} \\ &\leq e^{-\frac{\pi C_0}{4\varepsilon}} \sum_{\gamma\leq B} \|a_\gamma(\,.\,)e^{\frac{d(x,x+\gamma)}{\varepsilon}}\|_{l^\infty(R_{j,\varepsilon})} C e^{-\frac{\delta}{\varepsilon}} \leq C e^{-\frac{C_4}{\varepsilon}}\ ,\end{aligned} \tag{6.53}$$

where we used (6.4) and Proposition 6.5. To analyze the $\ell^2$-norm inside of $B_j$ (the second summand on the right hand side of (6.51)), we divide the sum over $\gamma$ to get

$$\begin{aligned}\|[H_\varepsilon, \mathbf{1}_{B_j}]u\|_{\ell^2(B_{j,\varepsilon})} &\leq \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in R_j}} a_\gamma(\,.\,)u(\,.+\gamma)\right\|_{\ell^2(B_{j,\varepsilon})} + \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in(\varepsilon\mathbb{Z})^d\setminus(B_j\cup R_j)}} a_\gamma(\,.\,)u(\,.+\gamma)\right\|_{\ell^2(B_{j,\varepsilon})} \\ &=: A_1 + A_2\end{aligned}$$

Then by Proposition 6.5 and since $R_j$ is a bounded region

$$\begin{aligned} A_1 &= \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in R_j}} a_\gamma(\,.\,) e^{\frac{\tilde{d}(x+\gamma)}{\varepsilon}} e^{-\frac{\tilde{d}(x+\gamma)}{\varepsilon}} u(\,.+\gamma)\right\|_{\ell^2(B_{j,\varepsilon})} \\ &\leq e^{-\frac{\pi C_0}{2\varepsilon}} \sum_{|\gamma|<C} \|a_\gamma(.)\|_{\ell^\infty(R_{j,\varepsilon})} \|e^{\frac{\tilde{d}}{\varepsilon}} u\|_{\ell^2} \\ &\leq e^{-\frac{\pi C_0}{2\varepsilon}} C e^{\frac{\delta}{\varepsilon}} \leq e^{-\frac{C_4}{\varepsilon}}\ .\end{aligned} \tag{6.54}$$

By the same arguments which lead to (6.52), we get

$$A_2 \leq \sum_{|\gamma|\geq C_2} \|a_\gamma\|_{l^\infty(B_{j,\varepsilon})} \|u\|_{\ell^2} = O\left(e^{\frac{-C_5}{\varepsilon}}\right)\ . \tag{6.55}$$

Thus inserting (6.52), (6.53), (6.54) and (6.55) into (6.51) shows (6.49) for all $C < \tilde{C}$, choose for example $C = \min\{C_1, C_4, C_5\}$.

Now the idea is to estimate the distance between multiples of $\mathbf{1}_{B_j}\, u$ and the eigenspace $\mathcal{E}_j$ of $H_\varepsilon^{M_j}$ by use of Proposition 6.8. By (6.49) and since $B_{j,\varepsilon} \subset M_{j,\varepsilon}$, we have

$$H_\varepsilon^{M_j}\, \mathbf{1}_{B_j}\, u = \mathbf{1}_{M_{j,\varepsilon}}\, H_\varepsilon\, \mathbf{1}_{B_{j,\varepsilon}}\, u = \lambda\, \mathbf{1}_{B_{j,\varepsilon}}\, u + O\left(e^{-\frac{C}{\varepsilon}}\right)\ .$$

In the notation of Proposition 6.8 the remaining term is $r_j = O\left(e^{-\frac{C}{\varepsilon}}\right)$ and thus

$$\vec{\text{dist}}(\mathbb{R}\,\mathbf{1}_{B_j}\,u, \mathcal{E}_j) = \frac{1}{a\|\,\mathbf{1}_{B_j}\,u\|} O\left(e^{-\frac{C}{\varepsilon}}\right)\ . \tag{6.56}$$

We now claim that for some $\tilde{C}$

$$\left(\mathbf{1} - \Pi_{\mathcal{E}_j}\right)\mathbf{1}_{B_j}\,u = O\left(e^{-\frac{\tilde{C}}{\varepsilon}}\right)\ . \tag{6.57}$$

(6.57) can be shown as follows:

If $\|\,\mathbf{1}_{B_j}\,u\| \leq e^{-\frac{C}{2\varepsilon}}$, then (6.57) is trivially fulfilled. If on the other hand $\|\,\mathbf{1}_{B_j}\,u\| > e^{-\frac{C}{2\varepsilon}}$, the estimate (6.56) yields

$$\vec{\text{dist}}(\mathbb{R}\,\mathbf{1}_{B_j}\,u, \mathcal{E}_j) \leq \frac{1}{a} e^{-\frac{C}{\varepsilon}} e^{\frac{C}{2\varepsilon}} = O\left(e^{-\frac{\tilde{C}}{\varepsilon}}\right)\ ,$$

where in the last step we used Hypothesis 6.3.

Thus (6.57) follows by the definition of the distance.

Since $\Pi_{\mathcal{E}} = \sum_{k=1}^m \Pi_{\mathcal{E}_k}$ we have

$$\|\Pi_{\mathcal{E}}\,\mathbf{1}_{B_j}\,u\|_{\ell^2} \leq \|\Pi_{\mathcal{E}_j}\,\mathbf{1}_{B_j}\,u\|_{\ell^2} + \sum_{k\neq j} \|\Pi_{\mathcal{E}_k}\,\mathbf{1}_{B_j}\,u\|_{\ell^2}\ . \tag{6.58}$$

By the construction of $B_j$ it follows that $d^k(x) \geq \frac{C_0\pi}{2}$ for $x \in B_j \cup R_j$ and $k \neq j$, thus by Corollary 6.4 for some $N_0 \in \mathbb{N}$ and $\tilde{C} > 0$

$$\begin{aligned} \|\Pi_{\mathcal{E}_k}\,\mathbf{1}_{B_j}\,u\|_{\ell^2} &= \|\sum_l c_l v_{kl} e^{-\frac{d^k}{\varepsilon}} e^{\frac{d^k}{\varepsilon}}\,\mathbf{1}_{B_j}\,u\|_{\ell^2} \\ &\leq e^{-\frac{C_0\pi}{2\varepsilon}} \|e^{\frac{d^k}{\varepsilon}} v\|_{\ell^2_{M_{k,\varepsilon}}} \|u\|_{\ell^2} \leq C e^{-\frac{C_0\pi}{2\varepsilon}} \varepsilon^{N_0} = O\left(e^{\frac{-\tilde{C}}{\varepsilon}}\right)\ . \end{aligned} \tag{6.59}$$

Thus inserting (6.59) into (6.58) yields

$$\Pi_{\mathcal{E}}\,\mathbf{1}_{B_j}\,u = \Pi_{\mathcal{E}_j}\,\mathbf{1}_{B_j}\,u + O\left(e^{\frac{-\tilde{C}}{\varepsilon}}\right) \tag{6.60}$$

with respect to $\ell^2$-norm. Therefore we get by (6.57), (6.48) and (6.60)

$$\begin{aligned} \Pi_{\mathcal{E}} u &= \Pi_{\mathcal{E}}\left(\mathbf{1}_{B_0^+}\,u + \sum_{j=1}^m \mathbf{1}_{B_j}\,u\right) = \sum_{j=1}^m \Pi_{\mathcal{E}_j}\,\mathbf{1}_{B_j}\,u + O\left(e^{-\frac{C}{\varepsilon}}\right) \\ &= \mathbf{1}_{B_0^+}\,u + \sum_{j=1}^m \mathbf{1}_{B_j}\,u + O\left(e^{-\frac{\tilde{C}}{\varepsilon}}\right) = u + O\left(e^{-\frac{\tilde{C}}{\varepsilon}}\right)\ , \end{aligned} \tag{6.61}$$

thus $(\mathbf{1} - \Pi_{\mathcal{E}})u = 0$ modulo $O\left(e^{\frac{-\tilde{C}}{\varepsilon}}\right)$ and by choosing $u = \Pi_{\mathcal{F}} v$ for $\|v\| = 1$, we get by (6.61)

$$\begin{aligned} \vec{\text{dist}}(\mathcal{F}, \mathcal{E}) &= \|\Pi_{\mathcal{F}} - \Pi_{\mathcal{E}}\Pi_{\mathcal{F}}\|_\infty = \sup_{v\in\mathscr{H}, \|v\|=1} \|(\mathbf{1} - \Pi_{\mathcal{E}})\Pi_{\mathcal{F}} v\| \\ &\leq \sup_{u\in\mathcal{F}, \|u\|\leq 1} \|(\mathbf{1} - \Pi_{\mathcal{E}})u\| = O\left(e^{-\frac{\tilde{C}}{2\varepsilon}}\right)\ , \end{aligned}$$

because $u$ was an arbitrary element of $\mathcal{F}$. Therefore $\vec{\text{dist}}(\mathcal{F}, \mathcal{E}) < 1$ for $\varepsilon$ small enough and by Proposition 6.7

$$\vec{\text{dist}}(\mathcal{E}, \mathcal{F}) = \vec{\text{dist}}(\mathcal{F}, \mathcal{E}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \tag{6.62}$$

and

$$\#\{\lambda_1, \ldots, \lambda_n\} =: n = \sum_{j\in\mathcal{C}} n_j\ , \tag{6.63}$$

i.e. the number of eigenvalues of $H_\varepsilon$ with respect to $I_\varepsilon$ equals the number of eigenvalues of the several Dirichlet operators with respect to this spectral interval.

*Step 3:*

In the last step we show the existence of a bijection $b$ between both spectra such that

$$b(\lambda) - \lambda = O\left(e^{\frac{\sigma}{\varepsilon}}\right)\ .$$

For $\sigma < \sigma' < S$ we set $\tilde{a} := e^{-\frac{\sigma'}{\varepsilon}}$ and consider disjoint intervals $K_l$, such that $I_\varepsilon \subset \bigcup_{l\in L} K_l$, where $K_l = ]\alpha_l, \beta_l]$ with $\beta_l - \alpha_l = 2\tilde{a}$. Let $\tilde{L} \subseteq L$ be such that $l \in \tilde{L}$ implies that $K_l$ includes at least one eigenvalue of $H_\varepsilon$ or $H_\varepsilon^{M_j}$, $\quad j \in \mathcal{C}$.

Then by combining intervals $K_l, K_{l+1}$ with $l, l+1 \in \tilde{L}$, there are intervals $I_1, \dots I_{\tilde{N}} \subseteq I_\varepsilon$ covering the eigenvalues $\lambda_1, \dots \lambda_N, \mu_{1,1}, \dots, \mu_{m,n_m}$, such that the distance between two different intervals is at least $2\tilde{a}$ and by (6.44) and (6.63) there exists a constant $M_0$ such that $|I_k| = O\left(\varepsilon^{-M_0} a\right)$. By Proposition 6.7 and an adapted version of (6.62) with $I_\varepsilon$ replaced by $I_l$ it follows that in each interval $I_l$, the number of $\lambda$´s and $\mu$´s is equal.

Let $b : \mathrm{spec}(H_\varepsilon) \cap I_\varepsilon \to \bigcup_{j=1}^m \left(\mathrm{spec}(H_\varepsilon^{M_j}) \cap I_\varepsilon\right)$ be a bijection, such that $\lambda \in I_j \mapsto b(\lambda) \in I_j$, then

$$b(\lambda) - \lambda = O\left(\varepsilon^{-M_0} e^{-\frac{\sigma'}{\varepsilon}}\right) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) .$$

□

## 6.3. The Interaction Matrix

In the next two sections, we are going to improve the result given in Theorem 6.8 by explicitly analyzing the error term up to order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ for any $\sigma < S$, where $S < S_0$ as introduced in Hypothesis 6.3. To this end we will analyze the Hamilton operator $H_\varepsilon$, restricted to its eigenspace $\mathcal{F}$ associated to a spectral interval $I_\varepsilon$.

**6.3.1. Construction of the Interaction Matrix.** Modulo terms of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$, we will determine the diagonal and non-diagonal part of the matrix representing $H_\varepsilon|_\mathcal{F}$ with respect to a fixed basis in $\mathcal{F}$. The non-diagonal part describes the interaction between the different wells.

Definition 6.10. *For $\mathcal{E}$ and $\mathcal{F}$ defined in* (6.8)*, let $\Pi_0$ denote the projection onto $\mathcal{E}$ along $\mathcal{F}^\perp$ in $\ell^2((\varepsilon\mathbb{Z})^d)$.*

Then

$$\|\Pi_0 - \Pi_\mathcal{E}\| = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \tag{6.64}$$

for every $\sigma < S$ and $\varepsilon$ small enough, where $S < S_0$ as introduced in Hypothesis 6.3. This can be shown along the lines of Helffer-Sjöstrand [**33**], Lemma 2.8:

For $\varepsilon$ small enough, we can write $\mathcal{F} = \{x + Ax \,|\, x \in \mathcal{E}\}$ where $A : \mathcal{E} \to \mathcal{E}^\perp$ and by Theorem 6.9 it is clear that $\|A\| = O\left(e^{\frac{-\sigma}{\varepsilon}}\right)$ for all $\sigma < S$. Then $A^* : \mathcal{E}^\perp \to \mathcal{E}$ and $\mathcal{F}^\perp = \{y - A^*y \,|\, y \in \mathcal{E}^\perp\}$, because for all $x \in \mathcal{E}$ and $y \in \mathcal{E}^\perp$ we have $Ax \in \mathcal{E}^\perp$ and $A^*y \in \mathcal{E}$ and thus we get

$$\langle (1+A)x\,,\,(1-A^*)y\rangle_{\ell^2} = \langle x\,,\,y\rangle_{\ell^2} + \langle Ax\,,\,y\rangle_{\ell^2} - \langle x\,,\,A^*y\rangle_{\ell^2} - \langle Ax\,,\,A^*y\rangle_{\ell^2} = 0 .$$

Let $z = x + y$ for $x \in \mathcal{E}$, $y \in \mathcal{E}^\perp$, then $\Pi_\mathcal{E} z = x$ and $\Pi_0 z = \tilde{x}$ with $\tilde{x} \in \mathcal{E}$ such that $\tilde{x} - z \in \mathcal{F}^\perp$ by the definition of $\Pi_0$. Thus for some $\tilde{y} \in \mathcal{E}^\perp$ we can write $\tilde{x} - z = \tilde{x} - (x + y) = -\tilde{y} + A^*\tilde{y}$, giving the two equations $\tilde{x} - x = A^*\tilde{y}$ and $y = \tilde{y}$. Thus it follows from the estimate on the norm of $A$ that $\|\tilde{x} - x\| = O\left(e^{-\frac{\sigma}{\varepsilon}}\|y\|\right)$, which shows (6.64).

Moreover $\Pi_0 = \Pi_0\Pi_\mathcal{F}$ and the inverse of $\Pi_0|_\mathcal{F} : \mathcal{F} \to \mathcal{E}$ is given by $\Pi_\mathcal{F}|_\mathcal{E} : \mathcal{E} \to \mathcal{F}$. Since $\mathcal{F}$ and $\mathcal{F}^\perp$ are stable under the action of $H_\varepsilon$, we have

$$\Pi_0 H_\varepsilon \Pi_\mathcal{F} v = \Pi_0 H_\varepsilon v \qquad \text{for all} \quad v \in E . \tag{6.65}$$

By the identification of $\mathcal{E}$ and $\mathcal{F}$ via $\Pi_0|_\mathcal{F}$ and $\Pi_\mathcal{F}|_\mathcal{E}$ respectively, the operator $H_\varepsilon|_\mathcal{F}$ corresponds to the operator $\Pi_0 H_\varepsilon|_\mathcal{E}$.

Proposition 6.11. *Let $H_\varepsilon$, $\mathcal{E}$, $S$ and $v_{j,k}$, $j \in \mathcal{C}$, $k = 1, \dots n_j$ be as in the setting of Hypotheses 6.1 and 6.3 and in* (6.8)*. Let $\Pi_0$ denote the projection introduced in Definition 6.10. We write $\alpha := (j,k)$ and $j(\alpha) = j$.*

*Then the matrix of* $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ *in the basis* $\{v_{1,1}, \dots, v_{m,n_m}\}$ *of* $\mathcal{E}$ *is for every* $\sigma < S$ *and for all* $\varepsilon \in (0, \varepsilon_0]$ *given by*

$$\begin{pmatrix} \mu_{1,1} & & 0 \\ & \cdot & \\ 0 & & \cdot \\ & & \mu_{m,n_m} \end{pmatrix} + (w_{\alpha,\beta}) + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) ,$$

*where*

$$w_{\alpha,\beta} = \langle v_\alpha \,,\, r_\beta \rangle_{\ell^2} = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) \tag{6.66}$$

*with* $r_\beta$ *defined as in* (6.36) *by*

$$r_\beta(x) = [H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}] v_\beta(x) = (\mathbf{1} - \mathbf{1}_{M_{j(\beta)}}) T_\varepsilon v_\beta = \sum_{\substack{\gamma \in (\varepsilon \mathbb{Z})^d \\ x+\gamma \in M_{j(\beta)},\, x \notin M_{j(\beta)}}} a_\gamma(x)\, v_\beta(x+\gamma) \,. \tag{6.67}$$

*Furthermore* $w_{\alpha,\beta} = 0$ *for* $j(\alpha) = j(\beta)$.

Proof:

The eigenfunctions $v_\alpha$ are a basis of $\mathcal{E}$, which is not orthonormal for different wells (i.e. for $j(\alpha) \neq j(\beta)$), thus for any function $u \in \ell^2((\varepsilon\mathbb{Z})^d)$,we have a representation

$$\Pi_{\mathcal{E}} u = \sum_{\alpha,\beta} c_{\alpha,\beta} \langle v_\beta \,,\, u \rangle_{\ell^2} v_\alpha \,, \tag{6.68}$$

where

$$\sum_{\alpha,\beta} c_{\alpha,\beta} \langle v_\beta \,,\, v_\gamma \rangle_{\ell^2} v_\alpha = v_\gamma \,, \qquad \text{i.e.} \quad \sum_\beta c_{\alpha,\beta} \langle v_\gamma \,,\, v_\beta \rangle_{\ell^2} = \delta_{\alpha\gamma} \,.$$

For $\mathcal{V} = \left(\langle v_\alpha \,,\, v_\beta \rangle_{\ell^2}\right)$ we thus have $C := (c_{\alpha,\beta}) = (\mathcal{V}^{-1})^T$. It was shown in (6.43) that $\mathcal{V} = \mathbf{1} + O\left(e^{\frac{-S}{\varepsilon}}\right)$ for any $S < S_0$ and therefore

$$C = \mathbf{1} + O\left(e^{\frac{-S}{\varepsilon}}\right) \,. \tag{6.69}$$

Defining

$$\tau u := \sum_\alpha \langle u \,,\, v_\alpha \rangle_{\ell^2} v_\alpha \tag{6.70}$$

we get by straightforward calculation, using (6.69) and $\dim \mathcal{E} = O(\varepsilon^{-N_0})$ for some $N_0$ (see (6.44))

$$\|\tau - \Pi_{\mathcal{E}}\| = O\left(e^{\frac{-S}{\varepsilon}}\right) , \qquad \|\tau - \Pi_0\| = O\left(e^{\frac{-\sigma}{\varepsilon}}\right) , \tag{6.71}$$

where $\sigma < S$ and we used (6.64) for the second estimate.
By (6.34) and (6.40) we have for $\sigma < S$ and $r_\beta$ as in (6.67)

$$H_\varepsilon v_\beta(x) = \mu_\beta v_\beta(x) + r_\beta \,, \qquad \|r_\beta\|_{\ell^2((\varepsilon\mathbb{Z})^d)} = O\left(e^{\frac{-\sigma}{\varepsilon}}\right) \,. \tag{6.72}$$

Thus

$$\Pi_0 H_\varepsilon v_\beta = \Pi_0(\mu_\beta v_\beta) + \Pi_0 r_\beta = \mu_\beta v_\beta + \tau r_\beta + (\Pi_0 - \tau) r_\beta \,. \tag{6.73}$$

and by (6.71) and (6.72) this yields in $\ell^2$-norm

$$\Pi_0 H_\varepsilon v_\beta = \mu_\beta v_\beta + \tau r_\beta + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \,.$$

By the definition of $\tau$ in (6.70) and of $w_{\alpha\beta}$ in (6.66) we get

$$\begin{aligned} \Pi_0 H_\varepsilon v_\beta &= \mu_\beta v_\beta + \sum_\alpha \langle v_\alpha \,,\, r_\beta \rangle_{\ell^2} v_\alpha + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \\ &= \mu_\beta v_\beta + \sum_\alpha w_{\alpha\beta} v_\alpha + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \,. \end{aligned}$$

This shows the matrix representation of $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ with respect to the basis of Dirichlet eigenfunctions $v_\alpha$ modulo terms of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$, where the interaction matrix is defined by (6.66). The fact that $w_{\alpha\beta} = 0$, if the eigenfunctions $v_\alpha$ and $v_\beta$ are supported near the same well, follows directly from the representation of $r_\beta$ by use of sums as given in (6.67), since in this case $x \notin M_{j(\beta)} = M_{j(\alpha)}$ and thus $v_\alpha(x) = 0$.

□

Defining the matrix

$$M = (m_{\alpha\beta}) := (\mu_\alpha \delta_{\alpha\beta} + w_{\alpha\beta}) \tag{6.74}$$

it follows from Proposition 6.11, that modulo $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ (which we will denote by $\equiv$)

$$\langle v_\alpha \,,\, \Pi_0 H_\varepsilon v_\beta \rangle_{\ell^2} \equiv \left\langle v_\alpha \,,\, \textstyle\sum_\gamma m_{\gamma\beta} v_\gamma \right\rangle_{\ell^2} = (\mathcal{V}M)_{\alpha\beta} \tag{6.75}$$

Comparing the operator $\Pi_0 H_\varepsilon|_\mathcal{E}$ with the self adjoint operator $\Pi_\mathcal{E} H_\varepsilon|_\mathcal{E}$, we get

$$\Pi_0 H_\varepsilon|_\mathcal{E} - \Pi_\mathcal{E} H_\varepsilon|_\mathcal{E} = O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \tag{6.76}$$

for $\sigma < S_1$, since by (6.72) and (6.64)

$$(\Pi_0 - \Pi_\mathcal{E}) H_\varepsilon v_\alpha = (\Pi_0 - \Pi_\mathcal{E}) \mu_\alpha v_\alpha + (\Pi_0 - \Pi_\mathcal{E}) r_\alpha = 0 + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \;. \tag{6.77}$$

Although this shows that $\Pi_0 H_\varepsilon|_\mathcal{E}$ is nearly self adjoint (i.e. self adjoint modulo terms of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$), its matrix representation modulo $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ is not symmetric, since the basis of Dirichlet eigenfunctions is not orthonormal (only the Dirichlet eigenfunctions belonging to the same well were assumed to be orthogonal).

We will now replace the basis of eigenfunctions by its orthonormalization and expect the matrix representing the "nearly self adjoint" operator $\Pi_0 H_\varepsilon|_\mathcal{E}$ to be "nearly symmetric" with respect to the new basis ("nearly" means modulo terms of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$).

If we denote the basis of eigenfunctions in $\mathcal{E}$ by $\vec{v} := (v_{1,1}, \ldots, v_{m,n_m})$, its orthonormalization is given by $\vec{e} := \vec{v}\mathcal{V}^{-\frac{1}{2}}$, where $\mathcal{V} = (\langle v_\alpha \,,\, v_\beta \rangle_{\ell^2}) =: \mathbf{1} + L$ with $L = (l_{\alpha\beta}) = O\left(e^{\frac{-\sigma}{\varepsilon}}\right)$. Thus $\vec{e}$ forms an orthonormal basis in $\mathcal{E}$.

Since by (6.72) $r_\beta = (H_\varepsilon - \mu_\beta) v_\beta$, the "lack of symmetry" $w_{\alpha\beta} - w_{\beta\alpha}$ can by (6.66) and (6.67) be computed as

$$\begin{aligned} w_{\alpha\beta} - w_{\beta\alpha} &= \langle r_\beta \,,\, v_\alpha \rangle_{\ell^2} - \langle r_\alpha \,,\, v_\beta \rangle_{\ell^2} \\ &= \langle H_\varepsilon v_\beta \,,\, v_\alpha \rangle_{\ell^2} - \langle \mu_\beta v_\beta \,,\, v_\alpha \rangle_{\ell^2} - \langle H_\varepsilon v_\alpha \,,\, v_\alpha \rangle_{\ell^2} + \langle \mu_\alpha v_\alpha \,,\, v_\beta \rangle_{\ell^2} \\ &= (\mu_\alpha - \mu_\beta) \langle v_\alpha \,,\, v_\beta \rangle_{\ell^2} = (\mu_\alpha - \mu_\beta)\, l_{\alpha\beta} \;, \end{aligned} \tag{6.78}$$

since the eigenfunctions $v_\gamma$ where chosen to be real and $H_\varepsilon$ is self adjoint. Since by (6.74) and (6.75) we have

$$\vec{v}^T \Pi_0 H_\varepsilon|_\mathcal{E} \vec{v} = \mathcal{V}M \;,$$

the matrix of $\Pi_0 H_\varepsilon|_\mathcal{E}$ in the basis $\vec{e}$ is modulo $e^{-\frac{2\sigma}{\varepsilon}}$ given by

$$\begin{aligned} \left(\langle e_\alpha \,,\, \Pi_0 H_\varepsilon|_\mathcal{E} e_\beta \rangle_{\ell^2}\right) &= \left(\vec{e}^T \Pi_0 H_\varepsilon|_\mathcal{E} \vec{e}\right) = \left(\mathcal{V}^{-\frac{1}{2}} \vec{v}^T \Pi_0 H_\varepsilon|_\mathcal{E} \vec{v} \mathcal{V}^{-\frac{1}{2}}\right) \\ &\equiv \mathcal{V}^{-\frac{1}{2}} \mathcal{V} M \mathcal{V}^{-\frac{1}{2}} = (\mathbf{1} + L)^{\frac{1}{2}} M (\mathbf{1} + L)^{-\frac{1}{2}} \\ &\equiv (\mathbf{1} + \frac{1}{2} L) M (\mathbf{1} - \frac{1}{2} L) \equiv ((\mu_\alpha \delta_{\alpha\beta}) + (w_{\alpha\beta})) + \frac{1}{2} [L, (\mu_\alpha \delta_{\alpha\beta})] \\ &\equiv (\mu_\alpha \delta_{\alpha\beta}) + \left(w_{\alpha\beta} + \frac{1}{2}\, l_{\alpha\beta} (\mu_\beta - \mu_\alpha)\right) \;. \end{aligned}$$

By (6.78) we can write

$$\tilde{w}_{\alpha\beta} := w_{\alpha\beta} + \frac{1}{2}\, l_{\alpha\beta} (\mu_\alpha - \mu_\beta) = w_{\alpha\beta} + \frac{1}{2} (w_{\alpha\beta} - w_{\beta\alpha}) = \frac{1}{2} (w_{\alpha\beta} + w_{\beta\alpha}) \;. \tag{6.79}$$

Since $T$ is symmetric, the same is true for $(\tilde{w}_{\alpha\beta})$ and we have

Proposition 6.12. *In the setting of Proposition 6.11 let* $\mathcal{V} := (\langle v_\alpha \,,\, v_\beta \rangle_{\ell^2})$ *and denote by* $\vec{e} := \vec{v}\mathcal{V}^{-\frac{1}{2}}$ *the orthonormalization of* $\vec{v}$.

*Then for $\sigma < S$ and for $\varepsilon \in (0, \varepsilon_0]$, the matrix of $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ with respect to $\vec{e}$ is given by*

$$\begin{pmatrix} \mu_{1,1} & & 0 \\ & \ddots & \\ 0 & & \mu_{m,n_m} \end{pmatrix} + (\tilde{w}_{\alpha,\beta}) + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) ,$$

*where*

$$\tilde{w}_{\alpha,\beta} = \frac{1}{2}(w_{\alpha\beta} + w_{\beta\alpha}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right) .$$

*and $\tilde{w}_{\alpha,\beta} = 0$ for $j(\alpha) = j(\beta)$.*

Thus in the orthonormal basis, the nearly symmetric operator corresponds to a nearly symmetric matrix. The next theorem concerns the matrix representation of $H_\varepsilon$ restricted to the space $\mathcal{F}$, spanned by the eigenfunctions $\{u_1, \ldots, u_N\}$, with respect to an orthonormal basis of $\mathcal{F}$. We will see, that it is identical to the matrix of $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ with respect to $\vec{e}$ modulo terms of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$. We denote by $\vec{f}$ the orthogonal projection of $\vec{e}$ to $\mathcal{F}$, i.e. $f_\alpha = \Pi_{\mathcal{F}} e_\alpha$. Then the orthonormalization $\vec{g}$ of $\vec{f}$ is given by $\vec{g} := \vec{f} F^{-\frac{1}{2}}$ where $F := \left(\langle f_\alpha \, , \, f_\beta \rangle_{\ell^2}\right)$ denotes the Gram-matrix of $\vec{f}$. With respect to the basis $\vec{g}$, the self adjoint operator $H_\varepsilon|_{\mathcal{F}}$ is represented by a symmetric matrix.

THEOREM 6.13. *In the setting of Hypotheses 6.1 and 6.3, let $\{v_{1,1}, \ldots, v_{m,n_m}\}$ denote the Dirichlet eigenvectors of $H_\varepsilon$ with respect to the spectral interval $I_\varepsilon$ and denote by $\mathcal{V} = \left(\langle v_\alpha \, , \, v_\beta \rangle_{\ell^2}\right)$ its Gram-matrix. Let $\vec{e} = \vec{v}\mathcal{V}^{-\frac{1}{2}}$ be its orthonormalization and $f_\alpha = \Pi_{\mathcal{F}} e_\alpha$ the orthogonal projection of $\vec{e}$ to the space $\mathcal{F}$ spanned by the eigenfunctions of $H_\varepsilon$ with respect to $I_\varepsilon$. Denoting by $F = \left(\langle f_\alpha \, , \, f_\beta \rangle_{\ell^2}\right)$ its Gram-matrix, we choose $\vec{g} := \vec{f} F^{-\frac{1}{2}}$ as orthonormal basis of $\mathcal{F}$.*

*Then the following statements hold for all $\varepsilon \in (0, \varepsilon_0]$.*

(a) *The matrix of $H_\varepsilon|_{\mathcal{F}}$ with respect to $\vec{g}$ is for all $\sigma < S$ given by*

$$\begin{pmatrix} \mu_{1,1} & & 0 \\ & \ddots & \\ 0 & & \mu_{m,n_m} \end{pmatrix} + (\tilde{w}_{\alpha,\beta}) + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) ,$$

*where*

$$\tilde{w}_{\alpha,\beta} = \frac{1}{2}(w_{\alpha\beta} + w_{\beta\alpha}) = O\left(e^{-\frac{\sigma}{\varepsilon}}\right)$$

*with*

$$w_{\alpha,\beta} = \left\langle v_\alpha \, , \, (\mathbf{1} - \mathbf{1}_{M_{j(\beta)}}) T_\varepsilon v_\beta \right\rangle_{\ell^2} = \sum_{\substack{x \in (\varepsilon\mathbb{Z})^d \\ x \notin M_{j(\beta)}}} \sum_{\substack{\gamma \in (\varepsilon\mathbb{Z})^d \\ x+\gamma \in M_{j(\beta)}}} a_\gamma(x) \bar{v}_\beta(x+\gamma) v_\alpha(x)$$

*and $\tilde{w}_{\alpha,\beta} = 0$ for $j(\alpha) = j(\beta)$.*

(b) *There exists a bijection $b : \operatorname{spec}(H_\varepsilon|_{\mathcal{F}}) \to \operatorname{spec}\left((\mu_\alpha \delta_{\alpha\beta} + \tilde{w}_{\alpha\beta})\right)$ such that $|b(\lambda) - \lambda| = O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ for all $\sigma < S$.*

Proof:

(a) Let

$$\tilde{M} = (\tilde{m}_{\alpha\beta}) := (\mu_\alpha \delta_{\alpha\beta} + \tilde{w}_{\alpha\beta}) . \tag{6.80}$$

We will proceed in two steps. First we show, that the matrix representation of $H_\varepsilon|_{\mathcal{F}}$ with respect to $\vec{f}$ is modulo $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ equal to the matrix representing $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ with respect to $\vec{e}$, i.e. equal to $\tilde{M}$. Then we show that the difference between the matrix representations of $H_\varepsilon|_{\mathcal{F}}$ with respect to $\vec{f}$ and to $\vec{g}$ is again of the same order.

As mentioned below Definition 6.10, the eigenspaces $\mathcal{E}$ and $\mathcal{F}$ can be identified by the projections $\Pi_{\mathcal{F}}|_{\mathcal{E}}$ and $\Pi_0|_{\mathcal{F}}$. Furthermore $\Pi_{\mathcal{F}}\Pi_0 = \Pi_{\mathcal{F}}$, because both projections are along $\mathcal{F}^\perp$ (i.e. $\ker \Pi_0 = \ker \Pi_{\mathcal{F}} = \mathcal{F}^\perp$). The invariance of $\mathcal{F}$ under the action of $H_\varepsilon$ yields $\Pi_{\mathcal{F}} H_\varepsilon = H_\varepsilon \Pi_{\mathcal{F}}$, we therefore get for any $v \in \mathcal{E}$

$$H_\varepsilon \Pi_{\mathcal{F}} v = \Pi_{\mathcal{F}} H_\varepsilon v = \Pi_{\mathcal{F}} \Pi_0 H_\varepsilon v$$

and thus by Proposition 6.12

$$\begin{aligned} H_\varepsilon f_\beta &= H_\varepsilon \Pi_{\mathcal{F}} e_\beta = \Pi_{\mathcal{F}} \Pi_0 H_\varepsilon e_\beta = \\ &= \Pi_{\mathcal{F}} \left( \sum_\alpha \tilde{m}_{\alpha\beta} e_\alpha + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) \right) = \\ &= \sum_\alpha \tilde{m}_{\alpha\beta} f_\alpha + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) . \end{aligned}$$

In the last step we used, that the projection is bounded and therefore does not change the order of the perturbation term.

To see that replacing the basis $\vec{f}$ by $\vec{g} = \vec{f} F^{-\frac{1}{2}}$ changes the matrix representation of $H_\varepsilon|_{\mathcal{F}}$ only by terms $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$, we write $e_\alpha = f_\alpha + r_\alpha$ where $f_\alpha \in \mathcal{F}$ and $r_\alpha \in \mathcal{F}^\perp$. From the representation

$$r_\alpha = e_\alpha - f_\alpha = (\Pi_{\mathcal{E}} - \Pi_{\mathcal{F}} \Pi_{\mathcal{E}}) e_\alpha \, ,$$

together with Theorem 6.9 and $\|e_\alpha\| = 1$, it follows that

$$\|r_\alpha\| = \|(\Pi_{\mathcal{E}} - \Pi_{\mathcal{F}}\Pi_{\mathcal{E}}) e_\alpha\| \le \|\Pi_{\mathcal{E}} - \Pi_{\mathcal{F}}\Pi_{\mathcal{E}}\| = \vec{\operatorname{dist}}(\mathcal{E}, \mathcal{F}) = O\left(e^{\frac{-\sigma}{\varepsilon}}\right) . \tag{6.81}$$

Moreover since $f_\alpha$ and $r_\beta$ are orthogonal for all $\alpha, \beta$ by construction, we get

$$\delta_{\alpha\beta} = \langle e_\alpha \, , \, e_\beta \rangle_{\ell^2} = \langle f_\alpha + r_\alpha \, , \, f_\beta + r_\beta \rangle_{\ell^2} = \langle f_\alpha \, , \, f_\beta \rangle_{\ell^2} + \langle r_\alpha \, , \, r_\beta \rangle_{\ell^2} \, .$$

Therefore by (6.65) and the Cauchy-Schwarz-inequality

$$F_{\alpha\beta} = \langle f_\alpha \, , \, f_\beta \rangle_{\ell^2} = \delta_{\alpha\beta} + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) .$$

and thus

$$\vec{g} = \vec{f} F^{-\frac{1}{2}} = \vec{f} \left( \mathbf{1} + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) \right)^{-\frac{1}{2}} = \vec{f} + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) .$$

Since $H_\varepsilon$ is bounded on $\mathcal{F}$, this yields for $f_\alpha = g_\alpha + l_\alpha$ with $\|l_\alpha\| = O(e^{-\frac{2\sigma}{\varepsilon}})$ the estimate

$$H_\varepsilon f_\alpha = H_\varepsilon (g_\alpha + l_\alpha) = \sum_\beta \widehat{m}_{\beta\alpha} g_\alpha + H_\varepsilon l_\alpha + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) = \sum_\beta \widehat{m}_{\beta\alpha} g_\alpha + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right) , \tag{6.82}$$

where $\widehat{M} = (\widehat{m}_{\alpha\beta})$ denotes the matrix representing $H_\varepsilon|_{\mathcal{F}}$ in the basis $\vec{g}$. On the other hand

$$H_\varepsilon|_{\mathcal{F}} f_\alpha = \sum_\beta \tilde{m}_{\beta\alpha} f_\beta = \sum_\beta \tilde{m}_{\beta\alpha} (g_\beta + l_\beta) = \sum_\beta \tilde{m}_{\beta\alpha} g_\beta + R \, , \tag{6.83}$$

where by the boundedness of the matrix elements $\tilde{m}_{\beta\alpha}$ and by the norm of $l_\beta$ the norm of the remaining term $R$ is of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$. Combining (6.82) and (6.83) and multiplying with $g_\gamma$ yields the postulated result, namely $M_{\beta\alpha} = \tilde{M}_{\beta\alpha} + O\left(e^{-\frac{2\sigma}{\varepsilon}}\right)$.

(b) To show the second statement of the theorem concerning the spectra of $H_\varepsilon|_{\mathcal{F}}$ and $M$, we have to estimate the relation between the eigenvalues of two symmetric operators on a finite dimensional space in terms of their difference. The assertion thus follows from the subsequent Theorem of Lidskii proven in Kato [**44**] (Thm 6.11, chapter 2).

THEOREM 6.14. *Let $A, B$ symmetric operators on a finite dimensional vector space and denote by $C := A - B$ their difference, which is assumed to be finite. Denote by $\alpha_i, \beta_i, \gamma_i$ for $i = 1, \ldots, N$ the repeated eigenvalues of $A, B$ and $C$ respectively in ascending order. Then for any convex function $\Phi : \mathbb{R} \to \mathbb{R}$, the following inequality holds:*

$$\sum_n \Phi(\beta_n - \alpha_n) \le \sum_n \Phi(\gamma_n) \, . \tag{6.84}$$

Thus choosing the convex function $\Phi(x) = x^2$, Theorem 6.14 shows, that the difference between the eigenvalues of $H_\varepsilon|_{\mathcal{F}}$ and $M$ is again of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$, showing the last statement of Theorem 6.13.

□

Idea of the Proof of Theorem 6.14:

The idea of the proof of this theorem is to define a family of operators $T(s) = A + sC$ for $0 \le s \le 1$. Then it can be shown, that the repeated eigenvalues $\mu_n(s)$ are continuous and piecewise holomorphic functions of $s$ with $\mu_n(0) = \alpha_n$ and $\mu_n(1) = \beta_n$ and that in the interval $[0, 1]$ are only a finite number of points, where the derivative of $\mu_n$ may be discontinuous. For each value $s$, a complete orthonormal system of eigenvectors $\phi_n(s)$ can be chosen, such that the $\phi_n$ are piecewise holomorphic in $s$. Differentiation of the spectral equation for $T(s)$ gives

$$(C - \mu_n'(s))\,\phi_n(s) + (T(s) - \mu_n(s))\,\phi'(s) = 0\;.$$

Taking the inner product with $\phi_n(s)$ and using the symmetry of $T(s)$ yields $\mu_n'(s) = \langle \phi_n(s)\,,\, C\phi_n(s)\rangle$. This can be integrated to give

$$\beta_n - \alpha_n = \mu_n(1) - \mu_n(0) = \int_0^1 \langle \phi_n(s)\,,\, C\phi_n(s)\rangle\, ds\;.$$

If $\{x_j\}$ denotes an orthonormal basis of eigenvectors of $C$, then

$$\langle \phi_n(s)\,,\, C\phi_n(s)\rangle = \sum_j \gamma_j |\langle \phi_n(s)\,,\, x_j\rangle|^2$$

and thus

$$\beta_i - \alpha_i = \sum \sigma_{ij}\gamma_j\;,$$

where $\sum_j \sigma_{ij} = \sum_i \sigma_{ij} = 1$ and $\sigma_{ij} \ge 0$.

A square matrix $(\sigma_{ij})$ with these properties lies in the convex hull of the set of all permutation matrices.

□

COROLLARY 6.15. *If there is only one well $x_0$ and $S_0$ denotes the distance of the well to the boundary of a bounded region $M \subset \mathbb{R}^d$, then with $S < S_0$ there exists a bijection $b : \mathrm{spec}\,(H_\varepsilon|_{\mathcal{F}}) \cap I_\varepsilon \to \mathrm{spec}\,\big(H_\varepsilon^M\big) \cap I_\varepsilon$ such that for all $\sigma < S$ and $\varepsilon \in (0, \varepsilon_0]$ we have $|b(\lambda) - \lambda| = O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$.*

REMARK 6.16. *In the case of one well, the interaction matrix is of order $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$, as follows directly from Theorem 6.13. Furthermore the discussions up to now are also valid in the case, that the operator $H_\varepsilon$ on $(\varepsilon\mathbb{Z})^d$ is replaced for some compact subset $M$ of $\mathbb{R}^d$, by a Dirichlet operator on $M_\varepsilon = M \cap (\varepsilon\mathbb{Z})^d$.*

**6.3.2. Examples and Interpretation.** Let us consider the case of two wells $x_1$ and $x_2$ each having only one Dirichlet eigenvalue $\mu_1$ and $\mu_2$ respectively inside of the given interval $I_\varepsilon$ for fixed $\varepsilon$. Then $d(x_1, x_2) = S_0$ and by Proposition 6.12 and Theorem 6.13, the eigenvalues of $H_\varepsilon$ with respect to $I_\varepsilon$ are for all $\sigma < S \in [0, S_0 - \eta]$ given by

$$\lambda_\pm = \frac{\mu_1 + \mu_2}{2} \pm \sqrt{\frac{1}{4}(\mu_1 - \mu_2)^2 + \tilde{w}_{12}^2} + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)\;.$$

The difference between these eigenvalues is thus

$$|\lambda_+ - \lambda_-| = \sqrt{(\mu_1 - \mu_2)^2 + 4\tilde{w}_{12}^2} + O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)\;.$$

If the difference between $\mu_1$ and $\mu_2$ is larger than $e^{-\frac{\delta_0}{\varepsilon}}$ for some $0 < \delta_0 < S_0$, then $H_\varepsilon$ admits two eigenvalues $\lambda_+ = \tilde{\mu}_1$ and $\lambda_- = \tilde{\mu}_2$ and the difference between them is at least of the order $e^{-\frac{\delta_0}{\varepsilon}}$. Computing formally the coordinates of the eigenfunctions $b_+$ and $b_-$ of $\Pi_0 H_\varepsilon|_{\mathcal{E}}$ associated to $\lambda_+$ and $\lambda_-$ with respect to the basis $\{e_1, e_2\}$ yields

$$\left(\frac{\mu_1 - \mu_2}{2} \pm \sqrt{\tfrac{1}{4}(\mu_1 - \mu_2)^2 + \tilde{w}_{12}^2}\right) b_{\pm,1} = \tilde{w}_{12} b_{\pm,2}\;.$$

Thus by setting $w_{12}' := \frac{4\tilde{w}_{12}^2}{(\mu_1 - \mu_2)^2} = O\left(e^{\frac{-2(\sigma - \delta_0)}{\varepsilon}}\right)$ and expanding the square root we get

$$|b_{+,1}| \le Ce^{-\frac{\sigma - \delta_0}{\varepsilon}}\,|b_{+,2}| \quad \text{and} \quad |b_{-,2}| \le Ce^{-\frac{\sigma - \delta_0}{\varepsilon}}\,|b_{-,1}|\;.$$

Thus the corresponding eigenfunctions $b_+$ and $b_-$ are located modulo exponentially small error at the wells $x_2$ and $x_1$ respectively. Thus the tunnelling effect does not change the basic properties of the eigenfunctions and the wells are almost independent (or non resonant). The concept of non resonant wells will be introduced later in more detail for the general case.

These considerations lead us later on to the assumption, that the difference between two eigenvalues attached to different wells is exponentially small, such that the effect of tunnelling is not negligible.

The tunnelling effect is relevant in the case of a symmetric double well, where $\mu_1 = \mu_2 = \mu$. Then

$$\lambda_\pm = \mu \pm \tilde{w}_{12}$$

and thus the splitting is of the same order of magnitude as the interaction term $\tilde{w}_{12}$. In the basis $\{e_1, e_2\}$ defined in Theorem 6.12, the normalized eigenfunctions of $H_\varepsilon$ are modulo $O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$ given by

$$u_1 = \frac{1}{\sqrt{2}}(e_1 + e_2) \quad \text{and} \quad u_2 = \frac{1}{\sqrt{2}}(e_1 - e_2)\ .$$

Therefore $u_1 + u_2$ is localized near $x_1$ and $u_1 - u_2$ is localized near $x_2$.

$V_0$ was defined as restriction of a function on $\mathbb{R}^d$ independent of the scaling parameter $\varepsilon$. Thus the position of the wells $x_j$ for $j = 1, \dots m$ is fixed with respect to the underlaying space $\mathbb{R}^d$. Nevertheless the change of the $\varepsilon$ will change the interaction of the wells. So it might occur that two wells are resonant for some values of $\varepsilon$ and non-resonant for others or that they become more and more resonant for $\varepsilon \to 0$. This behavior can be traced back to three different effects. The first lies in the change of the higher order terms $\sum_{k=1}^\infty \varepsilon^k V_k$ in the expansion of the potential energy, giving rise to a change of the whole scenery of the potential energy and in particular of the depth of the wells and thus of the low spectrum. The second effect is produced by the change of the position of the lattice points with respect to the underlying space $\mathbb{R}^d$ and thus to the potential wells. Therefore the minimal potential energy at the wells is different from the minimal potential energy at a neighboring lattice point. This fact does not change the WKB-expansions for the eigenfunctions and eigenvalues at one fixed well as noticed in Chapter 3, but since the difference between the eigenvalues must be exponentially small, this effect might change the resonance property. A third point lies in the fact, that the spectral interval itself depends on the value of $\varepsilon$.

Now we come to a slightly more general case, where there might be more than two wells, but for fixed $\varepsilon$ only two of them have an eigenvalue (and exactly one) in the spectral interval $I_\varepsilon$. Again the tunnelling effect is relevant only, if the difference between these eigenvalues is exponentially small.

Let $0 < a < S_0$, $S_0 + a < 2S$ and assume that for all $\delta > 0$

$$\mu_\alpha - \mu_\beta = O\left(e^{\frac{-(a-\delta)}{\varepsilon}}\right)\ .$$

Since by (6.43) we have $\langle v_\alpha\, ,\, v_\beta\rangle_{\ell^2} = O\left(e^{\frac{-S}{\varepsilon}}\right)$ for $S < S_0$ suitable, it follows from (6.78) that

$$w_{\alpha\beta} = w_{\beta\alpha} \mod O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right)\ .$$

If $d(x_{j(\alpha)}, x_{j(\beta)}) \geq S_0 + a$ or if $j(\alpha) = j(\beta)$, then

$$w_{\alpha\beta} = 0 \mod O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right)\ . \tag{6.85}$$

For $j(\alpha) = j(\beta)$ this is a direct consequence of Theorem 6.13. In the case $d(x_{j(\alpha)}, x_{j(\beta)}) \geq S_0 + a$, the estimate (6.85) can be seen as follows. By the triangle inequality for the distance function $d$

$$\begin{aligned}
|w_{\alpha\beta}| &= \left| \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} a_\gamma(x) v_\beta(x+\gamma) v_\alpha(x)\right| \\
&= \left| \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} a_\gamma(x) e^{-\frac{d^{j(\beta)}(x)}{\varepsilon}} e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x+\gamma) e^{-\frac{d^{j(\alpha)}(x)}{\varepsilon}} e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| \\
&\leq \left| \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} a_\gamma(x) e^{-\frac{d(x_{j(\beta)},x_{j(\alpha)})}{\varepsilon}} e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x+\gamma) e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| .
\end{aligned}$$

By the assumption on $d(x_{j(\alpha)}, x_{j(\beta)})$, this yields

$$\begin{aligned}
|w_{\alpha\beta}| &\leq e^{-\frac{(S_0+a)}{\varepsilon}} \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| a_\gamma(x) e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x+\gamma) e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| \qquad (6.86)\\
&\leq e^{-\frac{(S_0+a)}{\varepsilon}} \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| a_\gamma(x) e^{\frac{d^{j(\beta)}(x)}{\varepsilon}} v_\beta(x+\gamma)\right| \\
&=: e^{-\frac{(S_0+a)}{\varepsilon}} \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| A(x)
\end{aligned}$$

Again by the triangle inequality $d^{j(\beta)}(x) \leq d(x, x+\gamma) + d^{j(\beta)}(x+\gamma)$, thus for all $x \notin M_{j,\varepsilon}$

$$\begin{aligned}
A(x) &\leq \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right| \\
&\leq \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} \langle\gamma\rangle^{\frac{d+2}{2}}\right| \left| \langle\gamma\rangle^{-\frac{d+2}{2}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right| .
\end{aligned}$$

By the Cauchy-Schwarz inequality, we get

$$\begin{aligned}
A(x) &\leq \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| a_\gamma(x) e^{\frac{d(x,x+\gamma)}{\varepsilon}} \langle\gamma\rangle^{\frac{d+2}{2}}\right|^2\right)^{(1/2)} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| \langle\gamma\rangle^{-\frac{d+2}{2}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2\right)^{(1/2)} \\
&\leq C \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| \langle\gamma\rangle^{-\frac{d+2}{2}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2\right)^{(1/2)} , \qquad x\notin M_{j,\varepsilon}\,, \qquad (6.87)
\end{aligned}$$

where by Hypothesis 6.1,(d) the last estimate is uniform with respect to $x$. Inserting (6.87) into (6.86) and using the Cauchy-Schwarz inequality again for the summation over $x$, we get

$$\begin{aligned}
|w_{\alpha\beta}| &\leq e^{-\frac{(S_0+a)}{\varepsilon}} C \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right| \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| \langle\gamma\rangle^{-\frac{d+2}{2}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2\right)^{(1/2)} \\
&\leq e^{-\frac{(S_0+a)}{\varepsilon}} C \left( \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\alpha)}(x)}{\varepsilon}} v_\alpha(x)\right|^2\right)^{\frac{1}{2}} \left( \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d\\ x\notin M_{j(\beta)}}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in M_{j(\beta)}}} \left| \langle\gamma\rangle^{-\frac{d+2}{2}} e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2\right)^{\frac{1}{2}}
\end{aligned}$$

By Theorem 5.6 there exists $N_0 \in \mathbb{N}$, such that the first sum is of order $\varepsilon^{-N_0}$ and by inverting the order of summation in the second sum, this yields

$$|w_{\alpha\beta}| \leq e^{-\frac{(S_0+a)}{\varepsilon}} C\varepsilon^{-N_0} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j(\beta)}}} \langle\gamma\rangle^{-(d+2)} \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d \\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2 \right)^{(1/2)} .$$

Again by Theorem 5.6, we get

$$\begin{aligned} |w_{\alpha\beta}| &\leq e^{-\frac{(S_0+a)}{\varepsilon}} C\varepsilon^{-N_0} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j(\beta)}}} \langle\gamma\rangle^{-(d+2)} \sum_{\substack{x\in(\varepsilon\mathbb{Z})^d \\ x\notin M_{j(\beta)}}} \left| e^{\frac{d^{j(\beta)}(x+\gamma)}{\varepsilon}} v_\beta(x+\gamma)\right|^2 \right)^{(1/2)} \\ &\leq e^{-\frac{(S_0+a)}{\varepsilon}} C\varepsilon^{-N_0} \left( \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in M_{j(\beta)}}} \langle\gamma\rangle^{-(d+2)} \varepsilon^{-2N_0} \right)^{(1/2)} \leq e^{-\frac{(S_0+a)}{\varepsilon}} \tilde{C}\varepsilon^{-2N_1} \\ &= O\left(e^{-\frac{(S_0+a-\delta)}{\varepsilon}}\right) \end{aligned}$$

for some $N_1 \in \mathbb{N}$ and any $\delta > 0$. This proves (6.85).
The estimate (6.85) leads us to the assumption, that $d(x_{j(\alpha)}, x_{j(\beta)}) < S_0 + a$.

HYPOTHESIS 6.17. *Assume that only two wells have an eigenvalue (and exactly one) in the spectral interval $I_\varepsilon$. We denote the eigenvalues by $\mu_\alpha$, $\mu_\beta$ and the corresponding wells by $x_{j(\alpha)}$, $x_{j(\beta)}$. Let $0 < a < S_0$, $S_0 + a < 2S$ and assume that $d(x_{j(\alpha)}, x_{j(\beta)}) < S_0 + a$ and that for all $\delta > 0$*

$$\mu_\alpha - \mu_\beta = O\left(e^{\frac{-(a-\delta)}{\varepsilon}}\right) . \tag{6.88}$$

*Consider the closed "ellipse" defined by*

$$E_{\alpha\beta} := \{x \in \mathbb{R}^d \,|\, d^{j(\alpha)}(x) + d^{j(\beta)}(x) \leq S_0 + a\} , \tag{6.89}$$

*such that $E_{\alpha\beta} \subset \mathring{M}_{j(\alpha)} \cup \mathring{M}_{j(\beta)}$. We choose $\Omega \subset \mathbb{R}^d$ such that $x_{j(\alpha)} \in \Omega, x_{j(\beta)} \notin \Omega$ and furthermore $E \cap \Omega \subset \mathring{M}_{j(\alpha)}$ and $E \cap \Omega^c \subset \mathring{M}_{j(\beta)}$.*

The next lemma concerns the support of the commutator of $H_\varepsilon$ with the characteristic function with respect to a fixed set.

LEMMA 6.18. *Let $A \subset \mathbb{R}^d$ and denote by $\partial A$ its boundary. For any $\delta > 0$ we define $\delta A := \{x \in \mathbb{R}^d \,|\, \exists y \in \partial A : \; |x - y| \leq \delta\}$, thus $\delta A$ is an arbitrary small neighborhood of $\partial A$. Let $\delta > 0$ be fixed, then in operator norm for any $C > 0$ and for all $\varepsilon \in (0, \varepsilon_0]$*

$$[H_\varepsilon, \mathbf{1}_A] = \mathbf{1}_{\delta A}[H_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A} + O\left(e^{\frac{-C}{\varepsilon}}\right) . \tag{6.90}$$

Thus the commutator of $H_\varepsilon$ with the characteristic function of a set $A$ is supported modulo exponentially small error near the boundary of $A$.

Proof:

The potential energy $V_\varepsilon$ commutes with the characteristic function $\mathbf{1}_A$, we therefore can write by use of a partition of unity

$$\begin{aligned} [H_\varepsilon, \mathbf{1}_A] &= \mathbf{1}_{\delta A}[T_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A} + (1 - \mathbf{1}_{\delta A})\,[T_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A} + + \mathbf{1}_{\delta A}[T_\varepsilon, \mathbf{1}_A]\,(1 - \mathbf{1}_{\delta A}) + \\ &\quad (1 - \mathbf{1}_{\delta A})\,[T_\varepsilon, \mathbf{1}_A]\,(1 - \mathbf{1}_{\delta A}) =: K_1 + K_2 + K_3 + K_4 . \end{aligned} \tag{6.91}$$

For any $u \in \ell^2((\varepsilon\mathbb{Z})^d)$ we have by the definition of $T_\varepsilon$

$$[T_\varepsilon, \mathbf{1}_A]u(x) = \sum_\gamma a_\gamma(x)\,(\mathbf{1}_A(x+\gamma) - \mathbf{1}_A(x))\,u(x+\gamma) .$$

The difference between the characteristic functions in each summand is given by

$$(\mathbf{1}_A(x+\gamma) - \mathbf{1}_A(x)) = \begin{cases} -1 \quad , & x \in A,\ (x+\gamma) \notin A \\ \ \ 1 \quad , & x \notin A,\ (x+\gamma) \in A \\ \ \ 0 \quad , & \text{sonst} \end{cases} . \tag{6.92}$$

Thus $K_2$, $K_3$ and $K_4$ defined in (6.91) are nonzero only in the following cases:

$$K_2 \neq 0 \quad \Longrightarrow \quad (x \in (\delta A)^c \text{ and } (x+\gamma) \in \delta A) \quad \text{and} \quad \begin{cases} x+\gamma \in A^c \cap \delta A & \text{if} \quad x \in A \setminus \delta A \\ x+\gamma \in A \cap \delta A & \text{if} \quad x \in A^c \setminus \delta A \end{cases}$$

$$K_3 \neq 0 \quad \Longrightarrow \quad (x \in \delta A \text{ and } (x+\gamma) \in (\delta A)^c) \quad \text{and} \quad \begin{cases} x \in A^c \cap \delta A & \text{if} \quad x+\gamma \in A \setminus \delta A \\ x \in A \cap \delta A & \text{if} \quad x+\gamma \in A^c \setminus \delta A \end{cases}$$

$$K_4 \neq 0 \quad \Longrightarrow \quad x, (x+\gamma) \in (\delta A)^c \quad \text{and} \quad \begin{cases} x \in A^c \setminus \delta A & \text{if} \quad x+\gamma \in A \setminus \delta A \\ x \in A \setminus \delta A & \text{if} \quad x+\gamma \in A \setminus \delta A \end{cases}$$

Thus for all these terms the sum over $\gamma$ is reduced to the terms with $|\gamma| > \delta$ and we have the estimate

$$\|([H_\varepsilon, \mathbf{1}_A] - \mathbf{1}_{\delta A}[H_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A})u\|_{\ell^2} \leq 3 \left\| \sum_{|\gamma|>\delta} a_\gamma(x) u(x+\gamma) \right\|_{\ell^2} . \tag{6.93}$$

By the exponential decrease of $a_\gamma$ discussed in Remark 6.2, we get for any $\tilde{C} > 0$

$$\left\| \sum_{|\gamma|>\delta} a_\gamma(x) u(x+\gamma) \right\|_{\ell^2} \leq C \sum_{|\gamma|>\delta} e^{-\frac{\tilde{C}|\gamma|}{\varepsilon}} \|u\|_{\ell^2} \tag{6.94}$$

and therefore we can conclude by (6.93) for any $C > 0$

$$\|([H_\varepsilon, \mathbf{1}_A] - \mathbf{1}_{\delta A}[H_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A})\|_\infty = O\left(e^{-\frac{C}{\varepsilon}}\right) . \tag{6.95}$$

□

By use of Lemma 6.18, we can now show the following proposition.

PROPOSITION 6.19. *Under the assumptions of Hypothesis 6.17 and with the notation* $\widehat{\delta\Gamma}^{(c)} := \delta\Omega \cap \Omega^{(c)} \cap E$, *the elements* $w_{\alpha\beta}$ *of the interaction matrix are for all* $\delta > 0$ *and* $\varepsilon \in (0, \varepsilon_0]$ *given by*

$$\begin{aligned} w_{\alpha\beta} &= \langle [T_\varepsilon, \mathbf{1}_\Omega]\,\mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \rangle_{\ell^2} + O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right) \\ &= \left\langle \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\alpha\,,\, T_\varepsilon\, \mathbf{1}_{\widehat{\delta\Gamma}^c}\, v_\beta \right\rangle_{\ell^2} - \left\langle T_\varepsilon\, \mathbf{1}_{\widehat{\delta\Gamma}^c}\, v_\alpha\,,\, \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\beta \right\rangle_{\ell^2} + O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right) . \end{aligned}$$

Proof:

The interaction matrix can by (6.66) and (6.67) be written as $w_{\alpha\beta} = \left\langle v_\alpha\,,\, [H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}] v_\beta \right\rangle_{\ell^2}$, thus in the setting of Hypothesis 6.17 by considerations similar to those leading to (6.85), it follows that

$$w_{\alpha\beta} = \left\langle \mathbf{1}_E\, v_\alpha\,,\, [H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}]\,\mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} + O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right) .$$

In the following we write $\equiv$ for equality modulo $O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right)$. Lemma 6.18 shows, that modulo $O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right)$ the commutator $[H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}]$ is supported near the boundary of $M_{j(\beta)}$, which by construction is included in $\Omega$, thus

$$\left\langle \mathbf{1}_E\, \mathbf{1}_{\Omega^c}\, v_\alpha\,,\, [H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}]\,\mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} \equiv 0$$

and

$$\left\langle \mathbf{1}_E\, v_\alpha\,,\, [H_\varepsilon, \mathbf{1}_{M_{j(\beta)}}\,\mathbf{1}_E] v_\beta \right\rangle_{\ell^2} \equiv \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \left(H_\varepsilon\, \mathbf{1}_{M_{j(\beta)}} - \mathbf{1}_{M_{j(\beta)}}\, H_\varepsilon\right) \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} .$$

Similar to the proof of (6.85) it follows, that all contributions from $E^c$ to the scalar product are zero modulo $O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right)$, thus modulo terms of the same order, it is possible to commute $H_\varepsilon$

and $\mathbf{1}_E$ within the scalar product. Since $v_\eta \subset M_{j(\eta)}$ we get

$$\begin{aligned}
&\left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \left(H_\varepsilon\, \mathbf{1}_{M_{j(\beta)}} - \mathbf{1}_{M_{j(\beta)}}\, H_\varepsilon\right) \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} \\
&\qquad\equiv \left\langle \mathbf{1}_{M_{j(\beta)}}\, \mathbf{1}_E\, H_\varepsilon\, \mathbf{1}_\Omega\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} - \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \mu_\beta\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} \\
&\qquad\equiv \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, H_\varepsilon v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} + \left\langle \mathbf{1}_E [H_\varepsilon, \mathbf{1}_\Omega] v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} - \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \mu_\beta\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} .
\end{aligned}$$

Now we use $\Omega \subset M_{j(\alpha)}$ and the assumption (6.88) on $\mu_\alpha - \mu_\beta$ together with (6.43) and the fact that we can commute $H_\varepsilon$ and $\mathbf{1}_E$ to proceed as

$$\begin{aligned}
&\left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, H_\varepsilon v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} + \left\langle \mathbf{1}_E [H_\varepsilon, \mathbf{1}_\Omega] v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} - \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \mu_\beta\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} \equiv \\
&\quad \equiv \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, \mathbf{1}_{M_{j(\alpha)}}\, H_\varepsilon v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} + \left\langle [H_\varepsilon, \mathbf{1}_\Omega]\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} - \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, \mu_\beta\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} \equiv \\
&\qquad \equiv \left\langle [H_\varepsilon, \mathbf{1}_\Omega]\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} + \left\langle \mathbf{1}_E\, \mathbf{1}_\Omega\, v_\alpha\,,\, v_\beta \right\rangle_{\ell^2} (\mu_\alpha - \mu_\beta) \equiv \left\langle [H_\varepsilon, \mathbf{1}_\Omega]\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} .
\end{aligned}$$

This shows the first equality of Proposition 6.19, since the potential energy commutes with the characteristic function $\mathbf{1}_\Omega$.

To get the symmetric term claimed in the second equation, we use again Lemma 6.18 to get with $\widehat{\delta\Gamma} = \delta\Omega \cap \Omega \cap E$

$$\begin{aligned}
\left\langle [H_\varepsilon, \mathbf{1}_\Omega]\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} &\equiv \left\langle \mathbf{1}_{\delta\Omega} [H_\varepsilon, \mathbf{1}_\Omega]\, \mathbf{1}_{\delta\Omega}\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} = \\
&\left\langle T_\varepsilon\, \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\alpha\,,\, \mathbf{1}_{\delta\Omega}\, \mathbf{1}_E\, v_\beta \right\rangle_{\ell^2} - \left\langle T_\varepsilon\, \mathbf{1}_{\delta\Omega}\, \mathbf{1}_E\, v_\alpha\,,\, \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\beta \right\rangle_{\ell^2} .
\end{aligned} \tag{6.96}$$

Substituting $\mathbf{1}_{\delta\Omega}\, \mathbf{1}_E = \mathbf{1}_{\widehat{\delta\Gamma}} + \mathbf{1}_{\widehat{\delta\Gamma^c}}$, which holds by definition, the terms with $\mathbf{1}_{\widehat{\delta\Gamma}}$ on both sides of the scalar product cancel and we can conclude

$$w_{\alpha\beta} \equiv \left\langle T_\varepsilon\, \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\alpha\,,\, \mathbf{1}_{\widehat{\delta\Gamma^c}}\, v_\beta \right\rangle_{\ell^2} - \left\langle T_\varepsilon\, \mathbf{1}_{\widehat{\delta\Gamma^c}}\, v_\alpha\,,\, \mathbf{1}_{\widehat{\delta\Gamma}}\, v_\beta \right\rangle_{\ell^2}$$

and thus by the symmetry of $T_\varepsilon$, the second equation in the proposition is shown.

□

The symmetric version of the interaction matrix given in Proposition 6.19 is quite similar to the case of a Schrödinger operator on $\mathbb{R}^d$, where under analogue assumptions, one gets for $\Gamma := E \cap \partial\Omega$

$$w_{\alpha\beta} \equiv h^2 \int_\Gamma \left( v_\alpha \frac{\partial v_\beta}{\partial n} - v_\beta \frac{\partial v_\alpha}{\partial n} \right) dS .$$

The normal derivative in the integral is replaced by the translation term, where the translation passes the boundary $\partial\Omega$. The reduction to a surface integral over the boundary of $\Omega$ in $E$ has its analogue in the reduction of the sum to an arbitrary small (but $\varepsilon$-independent) neighborhood of this boundary.

As last example we consider the case, that the difference of the eigenvalues is only polynomially small, i.e. that for all $N \in \mathbb{N}$ we have $\mu_\alpha - \mu_\beta = O\left(\varepsilon^N\right)$. Then along the same lines as in the last example it can be shown that if $d(x_{j(\alpha)}, x_{j(\beta)}) > S_0$, then for all $N \in \mathbb{N}$

$$w_{\alpha\beta} = 0 \mod \varepsilon^N O\left(e^{\frac{-S_0}{\varepsilon}}\right)$$

Heuristically we can use the symbolic calculus introduced in Appendix B to see directly, that the commutator of $H_\varepsilon$ and $\mathbf{1}_\Omega$ and thus the interaction matrix is supported in a arbitrary small neighborhood of the hyperplane $\Gamma$. By Lemma B.6 and Lemma B.7, the symbol of the commutator (which can be defined only in the sense of distributions, because $\mathbf{1}_\Omega$ is not differentiable at $\Gamma$) is given by

$$\begin{aligned}
[t(x,\xi), \mathbf{1}_\Omega(x)] \quad &\sim \quad t(x,\xi)\, \mathbf{1}_\Omega(x) + \sum_{\substack{\alpha\in\mathbb{N}^d \\ |\alpha|>0}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!} \left(\partial_\xi^\alpha t(x,\xi)\right) \left(\partial_x^\alpha\, \mathbf{1}_\Omega(x)\right) - \mathbf{1}_\Omega(x) t(x,\xi) - 0 \sim \\
&\sim \quad i\varepsilon \sum_{\nu=1}^d \left(\partial_{\xi_\nu} t\right)(x,\xi) \left(\partial_{x_\nu}\, \mathbf{1}_\Omega\right)(x) + \frac{(i\varepsilon)^2}{2} \sum_{\nu,\eta=1}^d \left(\partial^2_{\xi_\nu \xi_\eta} t\right)(x,\xi) \left(\partial^2_{x_\nu x_\eta}\, \mathbf{1}_\Omega\right)(x) + \dots
\end{aligned}$$

Thus all summands include derivatives of $\mathbf{1}_\Omega$, i.e. $\delta$-distributions at the hyperplane $\Gamma$. Furthermore the first order term is the expectation value of the derivative of the kinetic energy at $\Gamma$. The choice of $\Omega$ (and thus of $\Gamma$) was quite arbitrary (except from the assumption that it should include one of the wells and exclude the other).

This together with the form of $w_{\alpha\beta}$ given in Proposition 6.19 suggests the interpretation of a physical current between the two wells, flowing through any separating hyperplane. This leads to the conclusion, that the proximity of eigenvalues (in this case $\mu_\alpha$ and $\mu_\beta$) causes a probability for the tunnelling from one well to the other.

## 6.4. The "Spectrum" of one well

In Hypothesis 6.3, $M_j$ was not defined directly, but described by some properties. Thus there is still some freedom in the choice of $M_j$. We show, that the results of the preceding sections are independent of this special choice.

Then we compare the spectrum at one well with a fixed eigenvalue of $H_\varepsilon$. For this point, we have to introduce a sphere of influence for the given well with respect to the eigenvalue and its eigenfunction. Then in a ball around the well, the eigenfunction is determined by the well.

PROPOSITION 6.20. *Let $M_1, M_1'$ denote compact sub-manifolds with $\mathscr{C}^2$-boundary at the well $x_1$ as described in Hypothesis 6.3 and $M_{1,\varepsilon}, M_{1,\varepsilon}'$ their restrictions to the lattice. Let $S_1 < S_{(1)} := \min_{k\neq 1} d(x_1, x_k)$ and $a(\varepsilon)$, $I_\varepsilon$ be as defined in Hypothesis 6.3. Choose $c(\varepsilon) \in ]0, a(\varepsilon)]$ such that $\log c(\varepsilon) = o\left(\frac{1}{\varepsilon}\right)$ and let $B(0, c(\varepsilon))$ denote the ball of radius $c(\varepsilon)$ at zero.*

*Then for $\varepsilon$ sufficiently small there exists a bijection*

$$b : \operatorname{spec}\left(H_\varepsilon^{M_1}\right) \cap I_\varepsilon \to \operatorname{spec}\left(H_\varepsilon^{M_1'}\right) \cap \left(I_\varepsilon + \overline{B(0, c(\varepsilon))}\right) ,$$

*such that for all $\sigma < S_1$*

$$|b(\lambda) - \lambda| = O\left(e^{\frac{-2\sigma}{\varepsilon}}\right) .$$

Proof:
This proof follows directly Helffer,Sjöstrand [**33**], Proposition 2.15.

Without loss of generality, we can assume that $M_1 \subseteq M_1'$ (by introduction of a third domain $\widehat{M_1}$). Let $J_\varepsilon$ be an interval with the properties described in Hypothesis 6.3 for $H_\varepsilon$, $H_\varepsilon^{M_1}$ and $H_\varepsilon^{M_1'}$ and such that $I_\varepsilon + B(0, 2a(\varepsilon)) \subseteq J_\varepsilon$. Then it follows from Remark 6.16 that $H_\varepsilon^{M_1'}$ can be interpreted as the full operator for a one well problem and by Corollary 6.15 there exists a bijection $b : \operatorname{spec}(H_\varepsilon^{M_1'}) \cap J_\varepsilon \to \operatorname{spec}(H_\varepsilon^{M_1}) \cap J_\varepsilon$ with $|b(\lambda) - \lambda| = O\left(e^{\frac{-2\sigma}{\varepsilon}}\right)$. The proposition follows from restricting $b$ to $\operatorname{spec}(H_\varepsilon^{M_1}) \cap I_\varepsilon$.

□

By Proposition 6.20 we are now able to define the "spectrum" of one well.

DEFINITION 6.21. *Let $\operatorname{spec}(x_1)$, the spectrum of the well $x_1$, be defined by the collection of the spectra $\operatorname{spec}(H_\varepsilon^{M_1}) \cap (I_\varepsilon + \overline{B(0, c(\varepsilon))})$ for any $M_1$ fulfilling Hypothesis 6.3*

Proposition 6.20 and Definition 6.21 are valid and chosen respectively in the same way for the other wells.

DEFINITION 6.22. *For $\varepsilon \in (0, \varepsilon_0]$, let $u_\varepsilon \in \ell^2((\varepsilon\mathbb{Z})^d)$ denote a normalized eigenfunction of $H_\varepsilon$ to the eigenvalue $\lambda_\varepsilon$.*

(a) *Let $\psi$ denote the maximum of all functions $\phi$ on $\mathbb{R}^d$, such that for all $\varepsilon \in (0, \varepsilon_0]$*
  i) *$|\phi(x) - \phi(y)| \leq d(x, y)$ for all $x, y \in \mathbb{R}^d$.*
  ii) *$\|e^{\frac{\phi}{\varepsilon}} u_\varepsilon\|_{\ell^2(K_\varepsilon)} = O\left(e^{\frac{\delta}{\varepsilon}}\right)$ for all $\delta > 0$ and $K \subset \mathbb{R}^d$ compact, where $K_\varepsilon = K \cap (\varepsilon\mathbb{Z})^d$.*

(b) *For $j \in \mathcal{C}$ we define $a_j := \psi(x_j) \geq 0$ and $S_{(j)} := \min_{k \in \mathcal{C}, k \neq j} d^j(x_k)$.*
*Then for $B(x_j, r) := \{x \in \mathbb{R}^d \,|\, |x - x_j| < r\}$ we set*

$$r_j := \max\{r \in [0, S_{(j)}] \,|\, x \in B(x_j, r) \Rightarrow \psi(x) = a_j + d^j(x)\} . \tag{6.97}$$

REMARK 6.23. (a) *In Definition 6.22(a), the function $\psi$ is well defined. This follows from the fact that for two functions satisfying (a)i) and (a)ii), the pointwise maximum of them also does. Furthermore at each point $x \in (\varepsilon\mathbb{Z})^d$, the family of the values of functions $\phi(x)$ satisfying (a)i) and (a)ii) is bounded, since by (a)ii) each $\phi$ must be bounded for* *some points (because $u$ is localized by Proposition 6.5 and normalized) and thus by i) it is bounded for all $x \in \mathbb{R}^d$.*

(b) *The positivity of $a_j$ defined in Definition 6.22(b) follows from the fact that the distance function $\tilde{d}$ defined in* (6.11) *has the properties (a)i) and ii) (as will be shown later on) and thus $\psi(x_j) \geq \tilde{d}(x_j) = 0$.*

*The fact that $\tilde{d}$ satisfies (a)ii) follows directly from Proposition 6.5.*

*To see the inequality (a)i), we have to analyze the different regions defined in* (6.9) *separately. In all cases we use* (6.12) *together with the fact that the inequality is by use of the triangle inequality valid for each distance function $d^j$.*

1) $x, y \in B_0 \quad \Rightarrow \quad |\tilde{d}(x) - \tilde{d}(y)| = 0 \leq d(x,y)$
2) $y \in B_j$ *for some* $j \in \mathcal{C} \quad \Rightarrow \quad \tilde{d}(x) \leq d^j(x) \leq d^j(y) + d(x,y) = \tilde{d}(y) + d(x,y)$.
3) $y, x \in R_j$ *for some* $j \in \mathcal{C}$ *and assume without loss of generality* $d^j(x) \geq d^j(y)$*:* *Setting* $z_1 := \frac{2d^j(y)}{C_0}$ *and* $z_2 := \frac{2d^j(x)}{C_0}$ *it follows from the definition of* $R_j$ *that* $\frac{\pi}{2} < z_i \leq \pi$ *and we have*

$$d^j(x) - d^j(y) - \tilde{d}(x) + \tilde{d}(y) = \frac{C_0}{2}(z_2 + \cos z_2 - (z_1 + \cos z_1)) =: g(z_2) - g(z_1) \,,$$

*where we set* $g(z) = \frac{C_0}{2}(z + \cos z)$*. Then in the considered interval* $g'(z) = \frac{C_0}{2}(1 - \sin z) > 0$ *and therefore* $g(z_2) - g(z_1) \geq 0$ *and therefore*

$$\tilde{d}(x) - \tilde{d}(y) \leq d^j(x) - d^j(y) \leq d(x,y) \,. \tag{6.98}$$

4) $y \in R_j$ *and* $x \in R_k$ *for* $j \neq k$ *and we assume without loss of generality* $\tilde{d}(x) \geq \tilde{d}(y)$*:* *We set* $z = \frac{2d^j(y)}{C_0}$ *(then* $\frac{\pi}{2} < z \leq \pi$*) and we notice that* $d^j(x) > \frac{C_0\pi}{2}$ *and* $\tilde{d}(x) \leq \frac{C_0\pi}{4} + \frac{C_0}{2}$ *to get*

$$d^j(x) - d^j(y) - \tilde{d}(x) + \tilde{d}(y) > \frac{C_0}{2}(\pi - 1 - z - \cos z) =: f(z) \,.$$

*Then* $f(\pi) = 0$ *and* $f'(z) = -1 + \sin z < 0$ *and therefore* $f(z) \geq 0$ *for* $\frac{\pi}{2} < z \leq \pi$*, yielding* (6.98).
5) $y \in R_j$ *for some* $j \in \mathcal{C}$ *and* $x \in B_0$*:* *Then* $d^j(x) \geq d^j(y)$ *and* $\tilde{d}(x) = \frac{C_0}{2}(\frac{\pi}{2} + 1) \geq \tilde{d}(y)$*. Furthermore* $d^j(x) > \frac{C_0\pi}{2}$ *and setting* $z := \frac{2d^j(y)}{C_0}$ *gives* $\frac{\pi}{2} < z \leq \pi$*. Thus*

$$d^j(x) - d^j(y) - \tilde{d}(x) + \tilde{d}(y) = d^j(x) - \frac{C_0}{2}(z + 1 + \cos z) > \frac{C_0}{2}(\pi - z - 1 - \cos z) = f(z)$$

*and by the same considerations as for the previous case we get* (6.98).

By (a)i) it follows at once that $|a_j - a_k| \leq d(x_j, x_k)$.

Since by Proposition 6.5 the eigenfunction $u_\varepsilon$ is localized at some of the wells and it is assumed to be normalized, there is by (a)ii) at least one well $x_j$ with $a_j = 0$ and the eigenfunction $u_\varepsilon$ is localized at those wells $x_k$, for which $a_k = 0$. At all the other wells, it is exponentially small.

Since the number $r_j$ is defined with respect to $\psi$, it depends by (a)ii) on the eigenfunction $u_\varepsilon$ (and thus on the eigenvalue $\lambda_\varepsilon$). It describes radius of the sphere of influence of the well $x_j$ with respect to $u$. For $a_j = 0$ we have $r_j \geq \frac{1}{2}S_0$ with equality if for the well $x_k$ with $d_l(x_j, x_k) = S_0$ we also have $a_k = 0$. If $r_j > 0$, then inside of the ball around $x_j$ with radius $r_j$ the eigenfunction $u$ decreases exponentially with a rate controlled by the distance $d^j$ to the well [1]. Take $j \in \mathcal{C}$ such that $r_j > 0$. Then for $k \neq j$ and $x \in \partial B(x_j, r_j)$ we have by (a)i) the estimate $a_j + r_j - a_k = \psi(x) - \psi(x_k) \leq d_l(x, x_k) = d^k(x)$ and thus $a_j + r_j \leq a_k + d_k(x)$ and $a_j + 2r_j \leq a_k + d_j(x) + d_k(x)$. By a variation over $x \in \partial B(x_j, r_j)$, we get

$$a_j + 2r_j \leq a_k + d(x_j, x_k) \qquad \text{for all} \quad k \neq j, k \in \mathcal{C} \,.$$

To show the estimates on $e^{\frac{a_j}{\varepsilon}} \|u_\varepsilon\|_{\ell^2(B(x_j, r_j))}$ given in Lemma 6.25, we need the following hypothesis on the function $\psi$.

[1]In this sense one might say that for $r_j > 0$ the eigenfunction $u_\varepsilon$ "feels" the well $x_j$, having at $x_j$ a little bump. For $a_j > 0$ this bump is on an exponentially small level

HYPOTHESIS 6.24. *We assume that the function $\psi$ given in Definition 6.22 remains the maximal function satisfying (a)i) and (a)ii), if we replace the interval $(0,\varepsilon_0]$ by any subset $J\subset(0,\varepsilon_0]$ with accumulation point zero.*

LEMMA 6.25. *In the setting of Definition 6.22 choose $x_j$ such that $r_j>0$ and assume that Hypothesis 6.24 holds. Let $B_\varepsilon(x_j,r_j):=B(x_j,r_j)\cap(\varepsilon\mathbb{Z})^d$.*

*Then for any $\delta>0$ there exists a constant $C_\delta>0$ and $\varepsilon_0>0$ such that for all $\varepsilon\in(0,\varepsilon_0]$*

$$\frac{1}{C_\delta}e^{-\frac{\delta}{\varepsilon}}\leq e^{\frac{a_j}{\varepsilon}}\|u_\varepsilon\|_{\ell^2(B_\varepsilon(x_j,r_j))}\leq C_\delta e^{\frac{\delta}{\varepsilon}}\ . \tag{6.99}$$

Proof:

For simplicity we supress the $\varepsilon$-dependance of $u$, writing $u=u_\varepsilon$.
The second inequality in (6.99) follows directly from property (a)ii) in the definition of $\psi$ and $r_j$, since

$$e^{\frac{a_j}{\varepsilon}}\|u\|_{\ell^2(B_\varepsilon(x_j,r_j))}\leq\left\|e^{\frac{a_j+d^j}{\varepsilon}}u\right\|_{\ell^2(B_\varepsilon(x_j,r_j))}=\left\|e^{\frac{\psi}{\varepsilon}}u\right\|_{\ell^2(B_\varepsilon(x_j,r_j))}=O\left(e^{\frac{\delta}{\varepsilon}}\right)\ .$$

The first inequality in (6.99) is valid, since $\psi$ was chosen to be the maximal function with the properties given in Definition 6.22(a)i),ii) even for a subset of $(0,\varepsilon_0)$ with accumulation point 0. This can be seen by contradiction. The formal contradiction of the statement leads to statement holding for all $C$ and $\varepsilon_0$. Thus we assume that there exists a $\tilde\delta_0>0$ such that for all $n\in\mathbb{N}^*$ there exists a $\varepsilon_n<\frac{\varepsilon_0}{n}$ such that

$$e^{\frac{a_j}{\varepsilon_n}}\|u\|_{\ell^2(B_\varepsilon(x_j,r_j))}<\frac{1}{n}e^{-\frac{\delta_0}{\varepsilon_n}}\ . \tag{6.100}$$

It follows from the definition of $\varepsilon_n$, that (6.100) holds for all $\varepsilon\in J:=\{\varepsilon_n\,|\,n\in\mathbb{N}^*\}$, where $J\subset[0,\varepsilon_0)$ with accumulation point zero.

Setting for $\delta_0:=\min\{\tilde\delta_0,r_j\}$ and $B_{\delta_0}:=B(x_j,\frac{\delta_0}{2})$

$$\tilde\psi(x):=\begin{cases}a_j+\frac{\delta_0}{2}\,, & x\in B_{\delta_0}\\ \psi(x)\,, & x\in(\varepsilon\mathbb{Z})^d\setminus B_{\delta_0}\end{cases}$$

we have $\tilde\psi(x)\geq\psi(x)$ for all $x\in\mathbb{R}^d$ and $\tilde\psi(x)>\psi(x)$ for $x\in B_{\delta_0}$. We get by (6.100) and the fact that $\psi(x)=a_j+d^j(x)$ for $x\in B_{\delta_0}$ that for all $n\in\mathbb{N}^*$ there exists $\varepsilon_n<\frac{\varepsilon_0}{n}$ such that

$$\left\|e^{\frac{\tilde\psi}{\varepsilon_n}}u\right\|_{\ell^2(B_{\delta_0,\varepsilon})}=e^{\frac{\delta_0}{2\varepsilon_n}}e^{\frac{a_j}{\varepsilon_n}}\|u\|_{\ell^2(B_{\delta_0,\varepsilon})}\leq\frac{1}{n}e^{-\frac{\delta_0}{2\varepsilon_n}}\ .$$

This yields for any compact set $K\subset\mathbb{R}^d$ for any $\delta>0$

$$\left\|e^{\frac{\tilde\psi}{\varepsilon_n}}u\right\|_{\ell^2(K_\varepsilon)}\leq\left\|e^{\frac{\psi}{\varepsilon_n}}u\right\|_{\ell^2(K_\varepsilon\setminus B_{\delta_0,\varepsilon})}+\left\|e^{\frac{\tilde\psi}{\varepsilon_n}}u\right\|_{\ell^2(B_{\delta_0,\varepsilon})}\leq C_1e^{\frac{\delta}{\varepsilon_n}}+C_2e^{-\frac{\delta_0}{2\varepsilon_n}}\leq Ce^{\frac{\delta}{\varepsilon_n}}\ .$$

showing property (a)ii) in Definition 6.22 for $\tilde\psi$, if $[0,\varepsilon_0)$ is replaced by the subset $J$. To see (a)i), we have to analyze the different regions separately.

(a) $x,y\in B_{\delta_0}\quad\Rightarrow\quad|\tilde\psi(x)-\tilde\psi(y)|=0\leq d(x,y)$.
(b) $x,y\notin B_{\delta_0}\quad\Rightarrow\quad|\tilde\psi(x)-\tilde\psi(y)|=|\psi(x)-\psi(y)|\leq d(x,y)$ by the definition of $\psi$.
(c) $x\in B_{\delta_0},y\notin B_{\delta_0}$: We use the fact that for all $z\in\partial B_{\delta_0}$ we have $d(x,y)\leq d(x,z)+d(z,y)$ and there exists a constant $r>0$ such that $d(x,z)\geq r$. The distance $d(x,y)=d_l(x,y)$ was defined in Definition 4.23 as the infimum of the curve length $s_l$ of all regular curves joining $x$ and $y$ with respect to the Finsler function $l$, thus there exists a regular curve $\gamma$, such that $s_l(\gamma)\leq d(x,y)+\frac{r}{2}$. Denoting by $\gamma(t_0):=z_0\in\partial B_{\delta_0}$ the point of intersection of $\gamma$ with the boundary of $B_{\delta_0}$, it follows that

$$d(x,y)+\frac{r}{2}\geq d(x,z_0)+d(z_0,y)\geq r+d(z_0,y)$$

and therefore we have $d(x,y)\geq d(z_0,y)$. Since by definition $\tilde\psi(x)=\psi(z_0)$ it follows

$$|\tilde\psi(x)-\tilde\psi(y)|=|\psi(z_0)-\psi(y)|\leq d(z_0,y)\leq d(x,y)\ .$$

Thus the function $\tilde\psi$ has the properties (a)i) and ii) at least on a subset $J\subset[0,\varepsilon_0)$ with accumulation point zero and is larger than $\psi$, which is a contradiction to the definition of $\psi$ as maximal function with these properties satisfying Hypothesis 6.24. This shows the first estimate in (6.99).

□

The next proposition concerns the difference of the spectrum at a given well to the fixed eigenvalue $\lambda$ of $H_\varepsilon$ subject to the value of $r_j$.

PROPOSITION 6.26. *For $\varepsilon \in (0, \varepsilon_0]$ let $u_\varepsilon$ denote a normalized eigenfunction of $H_\varepsilon$ with associated eigenvalue $\lambda_\varepsilon$ satisfying Hypothesis 6.24 and choose $j \in \mathcal{C}$ such that $r_j > 0$, where $r_j$ is the radius of the sphere of influence of $x_j$ as given in Definition 6.22.*

*For $a(\varepsilon)$ and $I_\varepsilon$ as defined in Hypothesis 6.3, let $c(\varepsilon) \in ]0, a(\varepsilon)]$ such that $\log c(\varepsilon) = o\left(\frac{1}{\varepsilon}\right)$ and $B(0, c(\varepsilon))$ denote the ball of radius $c(\varepsilon)$ at zero.*

*Then for any $\delta > 0$*

$$A(\lambda_\varepsilon, \mathrm{spec}(x_j)) := \min\left\{ |\lambda_\varepsilon - x| \,|\, x \in \mathrm{spec}\left(H_\varepsilon^{M_j}\right) \cap \left(I_\varepsilon + \overline{B(0, c(\varepsilon))}\right)\right\} = O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right) ,$$

*where $M^j$ is chosen such that $\overline{B(x_j, r_j - \delta)} \subset M_j$.*

Proof:

For the sake of simplicity, we set $u = u_\varepsilon$ and for a set $\Omega \subset \mathbb{R}^d$ we write $\ell^2(\Omega)$ instead of $\ell^2(\Omega_\varepsilon)$, where $\Omega_\varepsilon = \Omega \cap (\varepsilon\mathbb{Z})^d$.

Let $\delta > 0$ be fixed and set

$$B_{r_j} := B\left(x_j, r_j - \frac{\delta}{2}\right) \quad \text{and} \quad \tilde{u} := \frac{u}{\|u\|_{\ell^2(B_{r_j})}} , \tag{6.101}$$

such that $\|\tilde{u}\|_{\ell^2(B_{r_j})} = 1$. By (6.99) we have $\|u\|_{\ell^2(B_{r_j})} \geq Ce^{-\frac{a_j+\tilde{\delta}}{\varepsilon}}$ for any $\tilde{\delta} > 0$ and therefore

$$\|\tilde{u}\|_{\ell^2((\varepsilon\mathbb{Z})^d)} = \frac{\|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}}{\|u\|_{\ell^2(B_{r_j})}} \leq Ce^{\frac{a_j+\tilde{\delta}}{\varepsilon}} . \tag{6.102}$$

Since by (6.97) (the definition of $r_j$) we have $\psi(x) = d^j(x) + a_j$ for $x \in B(x_j, r_j)$, it follows by the properties of $\psi$ given in Definition 6.22 together with (6.101) and (6.102) with $\tilde{\delta} = \frac{\delta}{4}$ that

$$\|e^{\frac{d^j}{\varepsilon}}\tilde{u}\|_{\ell^2(B(x_j,r_j))} = \frac{e^{-\frac{a_j}{\varepsilon}}}{\|u\|_{\ell^2(B_{r_j})}}\|e^{\frac{\psi}{\varepsilon}}u\|_{\ell^2(B(x_j,r_j))} = O\left(e^{\frac{\delta}{2\varepsilon}}\right) . \tag{6.103}$$

Let $v := \mathbf{1}_{B_{r_j}}\,\tilde{u}$, then

$$H_\varepsilon v = \lambda v + O\left(e^{\frac{-(r_j-\delta)}{\varepsilon}}\right) \quad \text{in} \quad \ell^2(B_{r_j}) . \tag{6.104}$$

This can be seen as follows. Since

$$H_\varepsilon\,\mathbf{1}_{B_{r_j}}\,\tilde{u} = \mathbf{1}_{B_{r_j}}\,H_\varepsilon\tilde{u} + [H_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u} = \lambda v + [H_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u} ,$$

we have to analyze the $\ell^2$-norm of the commutator, which is given by

$$\begin{aligned}\left\|[H_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}\right\|_{\ell^2(B_{r_j})} &= \left\|\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma\left(\tau_\gamma\,\mathbf{1}_{B_{r_j}} - \mathbf{1}_{B_{r_j}}\,\tau_\gamma\right)\tilde{u}\right\|_{\ell^2(B_{r_j})}\\ &= \left\|\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(.)\left(\mathbf{1}_{B_{r_j}}(.+\gamma) - \mathbf{1}_{B_{r_j}}(.)\right)\tilde{u}(.+\gamma)\right\|_{\ell^2(B_{r_j})}\end{aligned}$$

Since for $x \in B_{r_j}$ we have

$$\mathbf{1}_{B_{r_j}}(.+\gamma) - \mathbf{1}_{B_{r_j}}(.) = \begin{cases} 0 & \text{for} \quad x+\gamma \in B_{r_j} \\ -1 & \text{for} \quad x+\gamma \notin B_{r_j} \end{cases} ,$$

it follows by the triangle inequality that

$$
\begin{aligned}
\left\|[H_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}\right\|_{\ell^2(B_{r_j})} &= \left\| - \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\notin B_{r_j}}} a_\gamma(.)\tilde{u}(.+\gamma)\right\|_{\ell^2(B_{r_j})} \\
&\leq \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in B(x_j,r_j)\setminus B_{r_j}}} a_\gamma(.)\tilde{u}(.+\gamma)\right\|_{\ell^2(B_{r_j})} + \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\notin B(x_j,r_j)}} a_\gamma(.)\tilde{u}(.+\gamma)\right\|_{\ell^2(B_{r_j})} \\
&=: S_1 + S_2\,. \qquad (6.105)
\end{aligned}
$$

We will analyze $S_1$ and $S_2$ separately.

For $x \in B_{r_j}$ and $x+\gamma \in B(x_j, r_j)\setminus B_{r_j}$ it is clear that $|\gamma| < B$ for some $B > 0$, thus by (6.103) and the Hölder inequality we have

$$
\begin{aligned}
S_1 &= \left\| \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ x+\gamma\in B(x_j,r_j)\setminus B_{r_j}}} a_\gamma(.)e^{-\frac{d^j(.+\gamma)}{\varepsilon}} e^{\frac{d^j(.+\gamma)}{\varepsilon}}\tilde{u}(.+\gamma)\right\|_{\ell^2(B_{r_j})} \\
&\leq e^{-\frac{(2r_j-\delta)}{2\varepsilon}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d \\ |\gamma|<B}} \|a_\gamma\|_{\ell^\infty(B_{r_j})} \left\| e^{\frac{d^j}{\varepsilon}}\tilde{u}\right\|_{\ell^2(B(x_j,r_j))} \\
&\leq Ce^{-\frac{(r_j-\delta)}{\varepsilon}} \qquad (6.106)
\end{aligned}
$$

To estimate $S_2$ we use the exponential decay of the coefficients $a_\gamma$ as assumed in Hypothesis 6.1 (see Remark 6.2) together with (6.102). Since $B_{r_j}$ is bounded and $|\gamma| > \frac{\delta}{2}$ for $x \in B_{r_j}$ and $x+\gamma \notin B(x_j, r_j)$, we get for any $A > 0$ by the Hölder inequality

$$
S_2 \leq \sum_{|\gamma|>\frac{\delta}{2}} \|a_\gamma\|_{l^\infty(B_{r_j})} \|\tilde{u}\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq Ce^{-\frac{A\delta}{2\varepsilon}} e^{\frac{a_j+\delta}{\varepsilon}}
$$

and thus, choosing $A$ big enough,

$$
S_2 \leq Ce^{-\frac{r_j}{\varepsilon}}\,. \qquad (6.107)
$$

Thus inserting (6.106) and (6.107) in (6.105), the statement (6.104) is proven.

Let $\mathcal{E}_j$ denote the eigenspace to $\operatorname{spec}(H_\varepsilon^{M_j}) \cap I_\varepsilon$ as introduced in Hypothesis 6.1. Then by (6.104) we can use Proposition 6.8 to get

$$
\vec{\operatorname{dist}}(v, \mathcal{E}_j) = O\left(e^{\frac{-(r_j-\delta)}{\varepsilon}}\right)
$$

and thus

$$
\|\Pi_{\mathcal{E}_j} v\|_{\ell^2(B_{r_j})} \equiv \|v\|_{\ell^2(B_{r_j})} \equiv 1 \qquad \text{modulo} \quad O\left(e^{\frac{-(r_j-\delta)}{\varepsilon}}\right)\,. \qquad (6.108)
$$

In addition we have

$$
H_\varepsilon \Pi_{\mathcal{E}_j} v = \Pi_{\mathcal{E}_j} \mathbf{1}_{B_{r_j}} H_\varepsilon\tilde{u} + \Pi_{\mathcal{E}_j}[H_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u} = \Pi_{\mathcal{E}_j}\lambda v + \Pi_{\mathcal{E}_j}[T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}\,. \qquad (6.109)
$$

But since

$$
\Pi_{\mathcal{E}_j} u(x) = \sum_k \langle u\,,\, v_{j,k}\rangle_{\ell^2} v_{j,k}(x)\,,
$$

where $\{v_{j,k}\}$ is an orthonormal basis for $\mathcal{E}_j$ as described in Hypothesis 6.1, we get

$$
\Pi_{\mathcal{E}_j}[T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}(x) = \sum_k \left\langle [T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}\,,\, v_{j,k}\right\rangle_{\ell^2} v_{j,k}(x) \qquad (6.110)
$$

where

$$
\left\langle [T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde{u}\,,\, v_{j,k}\right\rangle_{\ell^2} = \sum_{y\in(\varepsilon\mathbb{Z})^d}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} a_\gamma(y)v_{j,k}(y)\left[\mathbf{1}_{B_{r_j}}(y+\gamma) - \mathbf{1}_{B_{r_j}}(y)\right]\tilde{u}(y+\gamma)\,. \qquad (6.111)
$$

The following considerations are similar to the proof of Proposition 6.5 and (6.104). We notice that the summands vanish if $y$ and $y+\gamma$ are both inside or outside of $B_{r_j}$, more precisely

$$\mathbf{1}_{B_{r_j}}(y+\gamma)-\mathbf{1}_{B_{r_j}}(y)=\begin{cases}0 & \text{for}\quad y,y+\gamma\in B_{r_j}\quad\text{or}\quad y,y+\gamma\notin B_{r_j}\\ 1 & \text{for}\quad y\notin B_{r_j},\ y+\gamma\in B_{r_j}\\ -1 & \text{for}\quad y\in B_{r_j},\ y+\gamma\notin B_{r_j}\ .\end{cases}$$

Thus by (6.111)

$$\left\langle [T_\varepsilon,\mathbf{1}_{B_{r_j}}]\tilde u\,,\,v_{j,k}\right\rangle_{\ell^2}=-\sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\notin B_{r_j}}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)+\sum_{y\notin B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)\ .$$

By use of $B(x_j,r_j)$, we can split both sums again to get

$$\begin{aligned}\left\langle [T_\varepsilon,\mathbf{1}_{B_{r_j}}]\tilde u\,,\,v_{j,k}\right\rangle_{\ell^2}=&\ -\sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B(x_j,r_j)\setminus B_{r_j}}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)\\ &-\sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\notin B(x_j,r_j)}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)\\ &+\sum_{y\in B(x_j,r_j)\setminus B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)\\ &+\sum_{y\notin B(x_j,r_j)}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}}a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)\\ =:&\ S_1+S_2+S_3+S_4\ .\end{aligned}\tag{6.112}$$

By the definition of $B_{r_j}$ and the triangle inequality, we get

$$\begin{aligned}|S_1|\ &=\ \sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B(x_j,r_j)\setminus B_{r_j}}}\left|a_\gamma(y)v_{j,k}(y)e^{-\frac{2d^j(y+\gamma)}{\varepsilon}}e^{\frac{2d^j(y+\gamma)}{\varepsilon}}\tilde u(y+\gamma)\right|\le\\ &\le\ e^{-\frac{(2r_j-\delta)}{\varepsilon}}\sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B(x_j,r_j)\setminus B_{r_j}}}\left|a_\gamma(y)e^{\frac{d(y,y+\gamma)}{\varepsilon}}v_{j,k}(y)e^{\frac{d^j(y)}{\varepsilon}}e^{\frac{d^j(y+\gamma)}{\varepsilon}}\tilde u(y+\gamma)\right|\ .\end{aligned}$$

Since for $y\in B_{r_j}$ and $y+\gamma\in B(x_j,r_j)\setminus B_{r_j}$ we get $|\gamma|<B$ for some $B>0$, the Hölder inequality yields

$$\begin{aligned}|S_1|\ &\le\ e^{-\frac{(2r_j-\delta)}{\varepsilon}}\left\{\sum_{|\gamma|<B}\left\|a_\gamma e^{\frac{d(.,.+\gamma)}{\varepsilon}}\right\|_{l^\infty(B_{r_j})}\right\}\left\|v_{j,k}e^{\frac{d^j}{\varepsilon}}\right\|_{\ell^2(B_{r_j})}\left\|e^{\frac{d^j}{\varepsilon}}\tilde u\right\|_{\ell^2(B(x_j,r_j))}\le\\ &\le\ Ce^{-\frac{(2r_j-\delta)}{\varepsilon}}\varepsilon^{-N_0}e^{\frac{\delta}{2\varepsilon}}=O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right)\ .\end{aligned}\tag{6.113}$$

The last estimate follows from Corollary 6.4, (6.103) and (6.4).

To estimate the norm of $S_2$, we use that for $x\in B_{r_j}$ and $x+\gamma\notin B(x_j,r_j)$ we have $|\gamma|\ge\frac{\delta}{2}$. Thus by use of the Hölder inequality

$$\begin{aligned}|S_2|\ &=\ \sum_{y\in B_{r_j}}\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\notin B(x_j,r_j)}}|a_\gamma(y)v_{j,k}(y)\tilde u(y+\gamma)|\le\\ &\le\ \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ |\gamma|\ge\frac{\delta}{2}}}\|a_\gamma\|_{l^\infty(B_{r_j})}\|v_{j,k}\|_{\ell^2(B_{r_j})}\ \|\tilde u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}=\\ &\le\ Ce^{-\frac{A\delta}{2\varepsilon}}e^{\frac{a_j+\delta}{\varepsilon}}=O\left(e^{\frac{-C}{\varepsilon}}\right)\end{aligned}\tag{6.114}$$

for any $C>0$, where in the last step we used the exponential decay of $a_\gamma$ described in (6.3) together with (6.102). To estimate the third sum $S_3$, we go along the same lines as for $S_1$. By the triangle inequality for $d^j$ and the Hölder inequality, we have for some $B$

$$\begin{aligned}
|S_3| &= \sum_{y\in B(x_j,r_j)\setminus B_{r_j}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}} \left| a_\gamma(y) e^{-\frac{2d^j(y)}{\varepsilon}} e^{\frac{d^j(y)}{\varepsilon}} v_{j,k}(y) e^{\frac{d^j(y)}{\varepsilon}} \tilde u(y+\gamma)\right| \leq \\
&\leq e^{-\frac{(2r_j-\delta)}{\varepsilon}} \sum_{y\in B(x_j,r_j)\setminus B_{r_j}} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}} \left| a_\gamma(y) e^{\frac{d(y,y+\gamma)}{\varepsilon}} e^{\frac{d^j(y)}{\varepsilon}} v_{j,k}(y) e^{\frac{d^j(y+\gamma)}{\varepsilon}} \tilde u(y+\gamma)\right| \leq \\
&\leq e^{-\frac{(2r_j-\delta)}{\varepsilon}} \left\{ \sum_{|\gamma|<B} \left\| a_\gamma(.) e^{\frac{d_l(.,.+\gamma)}{\varepsilon}} \right\|_{l^\infty(B(x_j,r_j)\setminus B_{r_j})} \right\} \left\| v_{j,k} e^{\frac{d^j}{\varepsilon}} \right\|_{\ell^2(B(x_j,r_j))} \left\| e^{\frac{d^j}{\varepsilon}} \tilde u \right\|_{\ell^2(B_{r_j})} .
\end{aligned}$$

Thus by use of Corollary 6.4, (6.103) and (6.4), we get

$$|S_3| \leq Ce^{-\frac{(2r_j-\delta)}{\varepsilon}} \varepsilon^{-N_0} e^{\frac{\delta}{2\varepsilon}} = O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right) . \tag{6.115}$$

With the same arguments as in the estimate of $S_2$ (i.e. in particular by the exponential decrease of $a_\gamma$), we get for $S_4$

$$\begin{aligned}
|S_4| &= \sum_{y\notin B(x_j,r_j)} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ y+\gamma\in B_{r_j}}} |a_\gamma(y) v_{j,k}(y)\tilde u(y+\gamma)| \leq \\
&\leq \|v_{j,k}\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ |\gamma|\geq\frac{\delta}{2}}} \|a_\gamma\|_{\ell^\infty((\varepsilon\mathbb{Z})^d\setminus B(x_j,r_j))} \|\tilde u\|_{\ell^2(B_{r_j})} = \\
&= O\left(e^{\frac{-C}{\varepsilon}}\right)
\end{aligned} \tag{6.116}$$

for any $C>0$. Inserting (6.113), (6.114), (6.115) and (6.116) into (6.112) gives

$$\left\langle [T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde u \,,\, v_{j,k}\right\rangle_{\ell^2} = O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right)$$

and thus we have by (6.110)

$$\Pi_{\mathcal{E}_j}[T_\varepsilon, \mathbf{1}_{B_{r_j}}]\tilde u = O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right) . \tag{6.117}$$

Inserting (6.117) into (6.109) gives in $\ell^2(B_{r_j})$

$$H_\varepsilon \Pi_{\mathcal{E}_j} v = \lambda \Pi_{\mathcal{E}_j} v + O\left(e^{\frac{-2r_j+\delta}{\varepsilon}}\right)$$

and thus

$$H_\varepsilon^{M_j}\Pi_{\mathcal{E}_j} v = \mathbf{1}_{M_j}\, H_\varepsilon \Pi_{\mathcal{E}_j} v = \lambda \Pi_{\mathcal{E}_j} v + O\left(e^{\frac{-2r_j+\delta}{\varepsilon}}\right) .$$

Since $\mathcal{E}_j$ is the eigenspace of $H_\varepsilon^{M_j}$ with respect to $I_\varepsilon$, we have on the other hand $H_\varepsilon^{M_j}\Pi_{\mathcal{E}_j} v = \mu \Pi_{\mathcal{E}_j} v$ for some $\mu \in \operatorname{spec}(x_j)$, therefore

$$(\lambda - \mu)\Pi_{\mathcal{E}_j} v = O\left(e^{\frac{-2(r_j-\delta)}{\varepsilon}}\right) .$$

Thus by (6.108) the proposition is shown.

□

It follows from Proposition 6.26 that if for a well $x_j$ one has for all $\delta > 0$

$$A(\lambda, \operatorname{spec}(x_j)) \geq \frac{1}{C_\delta} e^{-\frac{\delta}{\varepsilon}} ,$$

then $r_j = 0$. As described above Proposition 6.26 one might say that the eigenfunction $u$ does not "feel" the well $x_j$, or in other words the existence of the well at $x_j$ has no influence on the decay of $u$. Such a well is called non-resonant with respect to the eigenvalue $\lambda$.

### 6.5. Comparison of exact and asymptotic Dirichlet eigenfunctions

To relate the asymptotic sums constructed in Chapter 3 with the eigenfunctions of the Dirichlet operator, we fix one well $x_1$ and choose coordinates centered at $x_1$ (i.e. we set $x_1 = 0$). As discussed in Remark 3.2, this special choice can be done without loss of generality. We consider the normalized eigenfunctions $v_{1,k}$ associated to the eigenvalue $\mu_{1,k}$ for $1 \leq k \leq n_1$, where $\mu_{1,k} \in I_\varepsilon = [0, R_0\varepsilon]$ and $R_0$ is not an element of the spectrum of the harmonic oscillator $K$ as introduced in Chapter 2.

The analysis of the distance between the spectra of the operators $H_\varepsilon$ and $H_\varepsilon^{M_j}$ in the preceding subsections, especially Corollary 6.15 combined with Theorem 2.10 for the case of one well (i.e. if $m = 1$) lead to the following result, where $H^1$ is defined in (2.48).

COROLLARY 6.27. *There exists a bijection* $b : \operatorname{spec}(H_\varepsilon^{M_1}) \cap I_\varepsilon \to \operatorname{spec}(H^1) \cap I_\varepsilon$ *and a constant* $C_0 > 0$*, such that for all* $\varepsilon \in (0, \varepsilon_0]$

$$|b(\lambda) - \lambda| \leq C_0 \varepsilon^{\frac{6}{5}} \ .$$

HYPOTHESIS 6.28. *We denote by* $\mathcal{E}_{1,0}$ *the eigenspace of* $H_\varepsilon^{M_1}$ *for the interval* $I_\varepsilon(E_0) = \varepsilon E_0 + B(0, C_0\varepsilon^{\frac{6}{5}})$*, where* $E_0$ *is an eigenvalue of the harmonic oscillator* $K$ *defined in Theorem 2.10. Let* $N_0$ *denote the dimension of* $\mathcal{E}_{1,0}$*. Let* $\{v_{1,1}, \dots, v_{1,N_0}\}$ *be an orthonormal basis of eigenfunctions of* $\mathcal{E}_{1,0}$ *and* $\{\mu_{1,1}, \dots \mu_{1,N_0}\}$ *the associated eigenvalues.*

*Let* $\mathcal{O}' \subset M_1$ *be an open sufficiently small neighborhood of* $x_1$ *as described in Chapter 3 and* $\chi \in \mathscr{C}_0^\infty(\mathbb{R}^d)$ *a cut-off function, which is supported in* $\mathcal{O}'$ *and equal to 1 in* $\mathcal{O}$*. For the (realizations of) asymptotic sums* $a_{1,k}$ *and* $\tilde{E}_{1,k}$ *defined in* (3.92) *and* (3.93) *let*

$$\widehat{u}_{1,j} := \varepsilon^{\frac{d}{4}} a_{1,j} e^{-\frac{\varphi}{\varepsilon}} \chi \ , \quad 1 \leq k \leq N_0$$

*and denote by* $\tilde{\mathcal{E}}_{1,0}$ *the span of* $\{\widehat{u}_{1,1}, \dots, \widehat{u}_{1,N_0}\}$*.*

By use of Theorem 3.18 and Corollary 6.27 the next corollary follows from Proposition 6.8 (with $\delta = O(\varepsilon^\infty)$, $a^{-1} = O(\varepsilon^{-\frac{6}{5}})$ and $N = N_0$)).

COROLLARY 6.29. *For* $\mathcal{E}_{1,0}$ *and* $\tilde{\mathcal{E}}_{1,0}$ *defined in Hypothesis 6.28, we have*

$$\vec{\operatorname{dist}}(\mathcal{E}_{1,0}, \tilde{\mathcal{E}}_{1,0}) = O\left(\varepsilon^\infty\right) \ .$$

*The eigenvalues of* $H_\varepsilon^{M_1}$ *in* $I_\varepsilon(E_0)$ *are given by* $\varepsilon \tilde{E}_{1,k} + O\left(\varepsilon^\infty\right)$*.*

It follows from Corollary 6.29, that there is an orthogonal matrix $(c_{j,k}(\varepsilon))_{1 \leq j,k \leq N_0}$, such that

$$v_{1,j} = \sum_{k=1}^{N_0} c_{j,k} \widehat{u}_{1,k} + O\left(\varepsilon^\infty\right) \ , \tag{6.118}$$

where $(c_{j,k})$ can be chosen such that $c_{j,k} = 0$ if $\tilde{E}_{1,k}$ is not asymptotically equal to $\mu_{1,j}$. If all $\tilde{E}_{1,j}$ have different expansions, then $(c_{j,k})$ may be chosen as identity matrix.

In Bao-Chern-Shen [**6**] it is shown, that short geodesics minimize the distance and are unique up to reparameterization . We call a geodesic between two points minimal, if its length equals the metric distance between these points. By Lemma 4.24 together with the construction of $\phi$ in Section 3.2, we can choose a subset $\mathcal{O}$ of $M_1$, such that the following statements hold.

HYPOTHESIS 6.30. *Let* $\mathcal{O} \subset M_1$ *containing* $0 (= x_1)$*, such that the following holds.*

(a) *For* $d^1(x) := d(x_1, x)$ *let* $\Lambda_+ := \{(x, \nabla d^1(x)) \mid x \in \mathcal{O}\}$*, then we assume that* $e^{tX_q}(x, \xi) \subset \Lambda_+$ *for all* $t \leq 0$*,* $(x, \xi) \in \Lambda_+$ *and* $e^{tX_q}(x, \xi) \to (0, 0)$ *for* $t \to -\infty$*, i.e. that* $\Lambda_+$ *is equal to the outgoing manifold defined in Section 3.2.*

(b) *The base integral curves of the Hamiltonian vector field* $X_q$ *joining any two points in* $\Omega \setminus \{0\}$ *realize the minimal geodesics with respect to the Finsler distance* $d$ *as introduced in Definition 4.4.*

*The restriction of* $\mathcal{O}$ *to the lattice is denoted by* $\mathcal{O}_\varepsilon$*.*

By Proposition 4.18, the base integral curves on $\mathbb{R}^d \setminus \{x_1, \dots x_m\}$ are geodesics with respect to $d$. Since it is shown in Abate-Patricio [**1**], Thm. 1.6.6., that short geodesics are minimal, assumption (b) holds for $\Omega$ sufficiently small.
The same is true for assumption (a), since by Proposition 4.24 for $\emptyset$ small enough $d^0 = \varphi$ on $\emptyset$, where $\varphi$ denotes the solution of the eikonal equation (3.10). The fact that (a) holds for $d^1$ replaced by $\varphi$ follows from the construction of $\varphi$ in Section 3.2 for $\emptyset$ sufficiently small. Since $\varphi \in \mathscr{C}^\infty(\emptyset)$, the same is true for $d^1$.

LEMMA 6.31. *Let $X_q$ denote the Hamilton vector field defined in* (3.14) *and for $x_0 \in \Omega$ let $x_t(x_0)$ denote the base integral curve of $X_q$ given by*

$$]-\infty, 0[\ni t \mapsto \Pi_x e^{tX_q}(x_0, \nabla d^1(x_0)) =: x_t(x). \tag{6.119}$$

*Let $y_0 \in \emptyset$ such that $y_0 \notin \{0\} \cup \{x_t(x_0) \mid -\infty < t \leq 0\}$, then*

$$d^1(x_0) < d^1(y_0) + d(y_0, x_0)\ .$$

Proof:

By the triangle inequality the statement is true for $\leq$ instead of $<$. The idea of the proof is to show, that equality may only occur, if $y_0$ lays on the integral curve of $X_q$ with starting point $x_0$.
Let $\gamma_0 : [0,1] \to \emptyset$ be the curve along the segment $\{0\} \cup \{x_t(x_0) \mid -\infty < t \leq 0\}$, parameterized such that $\gamma_0(0) = x_0$ and $\gamma_0(1) = 0$. Thus $\gamma_0$ is by construction and Hypothesis 6.30 a minimal geodesic between 0 and $x_0$. In Bao-Chern-Shen [**6**], Thm. 6.3.1, it is shown that minimal geodesics are unique up to reparameterization. Equality in the lemma would contradict this uniqueness, because this would mean that there are two different curves from 0 to $x_0$, which minimize the curve length and are thus minimizing geodesics.

□

By a standard compactness argument, we have the following

COROLLARY 6.32. *Let $K_1$, $K_2 \subset \emptyset$ be compact and assume that $K_2$ is disjoint from $\widehat{K}_1$, the compact union of all minimal geodesics from all points of $K_1$ to 0.*
*Then there exists $\delta > 0$ such that for all $x \in \widehat{K}_1$, $y \in K_2$*

$$d^1(x) \leq (1-\delta)\left(d^1(y) + d_l(y,x)\right)\ .$$

The main purpose of this section is to compare for one fixed well, which we choose to be $x_1$, the asymptotic eigenfunctions derived via WKB-procedure with the exact eigenfunctions. To get approximate eigenfunctions, which are defined in $\emptyset$ , we replace the phase function $\varphi$ by the Finsler distance $d^1$ associated to the well and solve the transport equations globally. Then the functions $\widehat{u}_{ik}$ constructed in Section 3.5.2 satisfy (3.95) for $x \in \emptyset$. In consideration of the different normalization factors in $\mathscr{L}^2$ and $\ell^2$, we multiply the factor $\varepsilon^{\frac{d}{2}}$ to the original version of the approximate eigenfunctions constructed in Section 3.5.2.

THEOREM 6.33. *Let $\emptyset \subset\subset M_1$ satisfying Hypothesis 6.30. For $a_{1,k}$ given in Theorem 3.18 and $\chi \in \mathscr{C}_0^\infty(\mathbb{R}^d)$ with $\chi(x) = 1$ for $x \in \emptyset$, let*

$$\widehat{u}_{1,j} := \varepsilon^{\frac{d}{4}} a_{1,j} e^{-\frac{d^1}{\varepsilon}} \chi\ , \quad 1 \leq k \leq N_0 \tag{6.120}$$

*and define $v'_{1,j} := \sum_k c_{j,k} \widehat{u}_{1,k}$, where $(c_{j,k})$ is the matrix determined by (6.118).*
*Then for every compact set $K \subset \emptyset$, for every $N \in \mathbb{N}$ and for all $\varepsilon \in (0, \varepsilon_0]$*

$$\left\| e^{\frac{d^1}{\varepsilon}} \left(v_{1,k} - v'_{1,k}\right) \right\|_{\ell^2(K_\varepsilon)} = O\left(\varepsilon^N\right)\ ,$$

*where $K_\varepsilon := K \cap (\varepsilon\mathbb{Z})^d$.*

Proof:

For $w := v_{1,k} - v'_{1,k}$, we set

$$(H_\varepsilon^{M_1} - E_k)v_{1,k} - (H_\varepsilon^{M_1} - E_k)v'_{1,k} = (H_\varepsilon^{M_1} - E_k)w =: r\ .$$

Since the first term on the left hand side vanishes exactly on Ø and the second is by Theorem 3.18 of order $\varepsilon^N e^{-\frac{d^1}{\varepsilon}}$ for any $N \in \mathbb{N}$, we get for any compact $K \subset Ø$ the estimate

$$\left\| e^{\frac{d^1}{\varepsilon}} r \right\|_{\ell^2(K_\varepsilon)} = O\left(\varepsilon^N\right)\ . \tag{6.121}$$

In addition, from the definition of the functions $v'_{1,k}$ and Corollary 6.4, it follows that for some $N_0 \in \mathbb{N}$

$$\left\| e^{\frac{d^1}{\varepsilon}} w \right\|_{\ell^2(K_\varepsilon)} = O\left(\varepsilon^{-N_0}\right)\ . \tag{6.122}$$

By (6.118) we have $v_{1,k} = v'_{1,k} + O\left(\varepsilon^\infty\right)$, thus for any $N \in \mathbb{N}$ and $K \subset Ø$

$$\|w\|_{\ell^2(K_\varepsilon)} = O\left(\varepsilon^N\right)\ . \tag{6.123}$$

For a fixed compact set $K \subset Ø$, we denote by $\widehat{K}$ the union of all minimal geodesics from 0 to points in $K$. In order to use Lemma 5.3, we have to consider functions $u$, which are supported on the bounded region Ø. Therefore we choose a compact set $G$ such that $K \subset\subset G \subset \Omega$ and define $\tilde{w} := \mathbf{1}_G\, w$. Then by (6.121) and (6.122) we have for all $N \in \mathbb{N}$ and some $N_0 \in \mathbb{N}$

$$\begin{aligned} \left\| e^{\frac{d^1}{\varepsilon}} (H_\varepsilon^{M_1} - E_k)\tilde{w} \right\|_{\ell^2(Ø_\varepsilon)} &\leq \left\| e^{\frac{d^1}{\varepsilon}} \mathbf{1}_G (H_\varepsilon^{M_1} - E_k) w \right\|_{\ell^2(G_\varepsilon)} + \left\| e^{\frac{d^1}{\varepsilon}} [H_\varepsilon^{M_1}, \mathbf{1}_G] w \right\|_{\ell^2(\delta G_\varepsilon)} \\ &= O\left(\varepsilon^N\right) + O\left(\varepsilon^{-N_0}\right)\ , \end{aligned} \tag{6.124}$$

where for the estimate of the second summand we used in addition the boundedness of the commutator and Lemma 6.18. Here we choose $\delta$ such that $\delta G \cap \widehat{K} = \emptyset$. In order to take the estimates in the different regions into account, we define for $N \in \mathbb{N}$ the phase function

$$\Psi_N(x) := \min\{\Phi_N(x), \Psi(x)\}\,, \tag{6.125}$$

where for the phase function $\Phi$ defined in (5.14) in the proof of Theorem 5.4 and $\tilde{\delta} > 0$ as in Corollary 6.32 we set

$$\Phi_N(x) := \Phi(x) + N\varepsilon \log \frac{1}{\varepsilon} \qquad \text{and} \qquad \Psi(x) := \inf_{y \in \delta G} \Phi(y) + (1 - \tilde{\delta}) d(x, y)\ . \tag{6.126}$$

Then for some neighborhood $W$ of $\widehat{K}$ and for each $N$ there is an $\varepsilon_N$ such that for all $\varepsilon < \varepsilon_N$

$$\Psi_N(x) = \Phi_N(x)\,, \qquad x \in W\ . \tag{6.127}$$

This can be seen as follows. We have $B := \{d(x) < B\varepsilon\} \subset W$ for $\varepsilon$ small enough, $\Phi(x) \leq \Phi(y)$ for $x \in B, y \notin B$ and $\Phi$ is monotonically increasing with $d$ for $x \notin B$, i.e. $\Phi(x) \geq \Phi(y)$ if $d(x) \geq d(y)$. Therefore we can restrict the discussion to the case $d(x) \geq B\varepsilon$, where the function $g$ is equal to one. It follows from Corollary 6.32, that $\Phi(x) \leq (1 - \tilde{\delta})(\Phi(y) + d(x, y))$ for $x \in \widehat{K}$ and $y \in \delta G$, leading to the estimate

$$\Phi_N(x) \leq \inf_{y \in \delta G} -\tilde{\delta}\Phi(y) + N\varepsilon \log \frac{1}{\varepsilon} + \Phi(y) + (1 - \tilde{\delta}) d(x, y) \leq \Psi(x)\ ,$$

where the second estimate holds for $\varepsilon$ small enough to ensure that $N\varepsilon \log \frac{1}{\varepsilon} \leq \tilde{\delta}\Phi(y)$ for all $y \in \delta G$. This shows (6.127).

Furthermore for $x \in \delta G$ it is clear that $\Psi(x) \leq \Phi(x)$ and therefore

$$\Psi_N(x) = \Psi(x) \leq \Phi(x)\,, \qquad x \in \delta G\ . \tag{6.128}$$

Since $\Psi_N$ was defined as minimum, we have in addition

$$\Psi_N(x) \leq \Phi_N(x)\,, \qquad x \in Ø\ . \tag{6.129}$$

Now the proof goes along the lines of the proof of Theorem 5.4. Thus we start to give estimates for $V_\varepsilon + V^{\Psi_N}$, where $V^{\Psi_N}$ is defined by (5.2).

It follows at once by the definition of $V^{\Phi_N}$ and of $\Phi_N$, that $V^{\Phi_n} = V^\Phi$. Thus we have by (5.37) and (5.38) the estimates

$$V_\varepsilon(x) + V^{\Phi_N}(x) \geq -C_5\, \varepsilon \qquad \text{for} \quad d(x) < B\varepsilon \tag{6.130}$$

and

$$V_\varepsilon(x) + V^{\Phi_N}(x) \geq \left(\frac{B}{C_0} - C_5\right)\varepsilon \qquad \text{for} \quad d(x) \geq B\varepsilon\,. \tag{6.131}$$

To analyze $V_\varepsilon + V^\Psi$, we first notice that $\Psi$ is upper-$\mathscr{C}^2$ on $G$ in the sense of Rockafellar-Wets [**51**] and thus Lipschitz continuous. It follows at once from [**51**], Theorem 10.31, that

$$L\Psi(x) := \limsup_{x_1,x_2\to x} \frac{|\Psi(x_1)-\Psi(x_2)|}{|x_1-x_2|} = \max_{y\in Y_x}(1-\tilde\delta)|\nabla_x d(x,y)|\,, \qquad x\in G\,,$$

where $Y_x := \{y\in \delta G\,|\,\Psi(x) = \Phi(y) + (1-\tilde\delta)d(x,y)\}$. Furthermore is follows from [**51**], Theorem 10.31 and Theorem 9.7 that $\Psi$ is differentiable almost everywhere (Theorem of Rademacher) and that $|\nabla\Psi| = L\Psi$. Thus $\nabla\Psi = \max_{y\in Y_x}(1-\tilde\delta)|\nabla_x d(x,y)|$ almost everywhere and by the generalized eikonal inequality (4.80) it follows that for some $a>0$

$$V_0(x) + t(x,-i\nabla\Psi(x)) \geq V_0(x) - (1-\tilde\delta)V_0(x) = \tilde\delta V_0(x) \geq a\,, \quad x\notin W\,. \tag{6.132}$$

Similar to the proof of Theorem 5.4, it is necessary to estimate $V_\varepsilon + V^\Psi$, thus by use of (5.26) and (5.27) it remains to find an estimate for $V^\Psi(x) - t(x,-i\nabla\Psi(x))$. We have

$$\begin{aligned}\left|V^\Psi(x) - t^\Sigma(x,-i\nabla\Psi)\right| &= \left|\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in\Omega}} a_\gamma(x)\left\{\cosh\left(\frac{1}{\varepsilon}(\Psi(x)-\Psi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Psi(x)\right)\right\}\right|\\ &\leq \sum_{\gamma\in\Omega'_x}|a_\gamma(x)|\left|\cosh\left(\frac{1}{\varepsilon}(\Psi(x)-\Psi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Psi(x)\right)\right|\,, \qquad x\in\emptyset\,,\end{aligned} \tag{6.133}$$

where $\emptyset'_\varepsilon(x) := \{\gamma\in(\varepsilon\mathbb{Z})^d\,|\,x+\gamma\in\emptyset\}$. As in the proof of Theorem 5.4, we get by the Mean Value Theorem

$$\begin{aligned}&\left|\cosh\left(\frac{1}{\varepsilon}(\Psi(x)-\Psi(x+\gamma))\right) - \cosh\left(-\frac{1}{\varepsilon}\gamma\nabla\Psi(x)\right)\right|\\ &\qquad\leq \sup_{t\in[0,1]} e^{\left|\frac{1}{\varepsilon}\{(\Psi(x)-\Psi(x+\gamma))t-\gamma\nabla\Psi(x)(1-t)\}\right|}\left|\frac{1}{\varepsilon}\{(\Psi(x)-\Psi(x+\gamma))+\gamma\nabla\Psi(x)\}\right|\,.\end{aligned} \tag{6.134}$$

Since $\Psi$ is Lipschitz continuous and the region is bounded, we have for some $C,\tilde C$

$$|\gamma\nabla\Psi(x)| \leq C|\gamma| \quad \text{and} \quad |\Psi(x)-\Psi(x+\gamma)| \leq \tilde C \tag{6.135}$$

for all $x$, where $\Psi$ is differentiable and for all $\gamma\in\emptyset'_\varepsilon(x)$. Thus there exists a constant $D>0$, such that the exponential term on the right hand side of (6.134) can for almost all $x\in\emptyset$, for all $\gamma\in\emptyset'_\varepsilon(x)$ and for all $\varepsilon\in(0,\varepsilon_0]$ be estimated as

$$\left|e^{\frac{1}{\varepsilon}\{(\Psi(x)-\Psi(x+\gamma))t+\gamma\nabla\Phi(x)(1-t)\}}\right| \leq e^{\frac{D}{\varepsilon}|\gamma|}\,. \tag{6.136}$$

By second order Taylor-expansion, the remaining factor on the right hand side of (6.134) can be estimated as

$$\frac{1}{\varepsilon}\left|(\Psi(x)-\Psi(x+\gamma))+\gamma\nabla\Psi(x)\right| \leq \sup_{t\in[0,1]}\frac{1}{\varepsilon}\left|\sum_{\nu,\mu=1}^d \gamma_\nu\gamma_\mu\partial_\nu\partial_\mu\Psi(x+t\gamma)\right|\,. \tag{6.137}$$

Again by Rockafellar-Wets [**51**], Thm. 9.7 and Thm.10.31, the modulus of the second derivative of $\Psi$ at a point $x$ is equal to the the second derivative of $d(x,y)$ for some $y\in\delta G$, which is bounded for all $x\in\emptyset$. Therefore we get for some $C_3>0$

$$\frac{1}{\varepsilon}\left|(\Psi(x)-\Psi(x+\gamma))+\gamma\nabla\Psi(x)\right| \leq \frac{C_3}{\varepsilon}|\gamma|^2\,, \tag{6.138}$$

yielding to

$$\left|V^\Psi(x) - t(x,-i\nabla\Psi(x))\right| \leq \varepsilon C_4\,. \tag{6.139}$$

for some $C_4$ by the same arguments as in the proof of Theorem 5.4.
Thus we have by (6.130), (6.131), (6.132), (5.27) and (6.139)

$$V_\varepsilon(x) + V^{\Psi_N}(x) \geq -C_6\,\varepsilon \qquad \text{for} \quad d(x) < B\varepsilon \tag{6.140}$$

and

$$V_\varepsilon(x) + V^{\Psi_N}(x) \geq \left(\frac{B}{C_0} - C_6\right)\varepsilon \qquad \text{for} \quad d(x) \geq B\varepsilon\,. \tag{6.141}$$

We now choose $B$ such that

$$(\frac{B}{C_0} - C_6)\varepsilon - E_k \geq \varepsilon$$

and define for

$$\emptyset_- := \{x \in \emptyset \,|\, V_\varepsilon(x) + v^{\Psi_N}(x) - E_k < 0\} \quad \text{and} \quad \emptyset_+ := \emptyset \setminus \emptyset_l$$

the functions $F_\pm : \emptyset \to [0,\infty)$ by

$$F_+(x) := \sqrt{\varepsilon\,\mathbf{1}_{\{d(x)<B\varepsilon\}}(x) + (V_\varepsilon(x) + V^{\Psi_N}(x) - E_k)\,\mathbf{1}_{\emptyset_+}(x)} \tag{6.142}$$

$$F_-(x) := \sqrt{\varepsilon\,\mathbf{1}_{\{d(x)<B\varepsilon\}}(x) + (E_k - V_\varepsilon(x) - V^{\Psi_N}(x))\,\mathbf{1}_{\emptyset_-}(x)}\,. \tag{6.143}$$

Then $F_\pm$ are well defined and there exists a constant $C > 0$ such that

$$F := F_+ + F_- \geq C\sqrt{\varepsilon} > 0\,, \qquad F_- = O(\sqrt{\varepsilon}) \qquad \text{and} \qquad F_+^2 - F_-^2 = V_\varepsilon + V^{\Psi_N} - E_k\,. \tag{6.144}$$

Furthermore by (6.140) and (6.141)

$$\operatorname{supp} F_- \subset \{d(x) < B\varepsilon\}\,. \tag{6.145}$$

Now we are going to use Lemma 5.3, yielding for $v = e^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w$ the estimate

$$\left\|Fe^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)} \leq 4\left\|\tfrac{1}{F}e^{\frac{\Psi_N}{\varepsilon}}\left(H_\varepsilon^{M_1} - E_k\right)\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)} + 8\left\|F_-e^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)}\,. \tag{6.146}$$

Since $e^{\frac{\Phi_N}{\varepsilon}} = e^{\frac{\Phi}{\varepsilon}}\varepsilon^{-N}$, we have by (6.127), (6.144) and (5.47) for some $N_0 \in \mathbb{N}$

$$\left\|Fe^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)} \geq \left\|Fe^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w\right\|^2_{\ell^2(K_\varepsilon)} \geq C\varepsilon^{1+N_0-N}\|e^{\frac{d^1}{\varepsilon}}w\|_{\ell^2(K_\varepsilon)} \tag{6.147}$$

and by (6.145) and (6.123)

$$\left\|F_-e^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)} = \left\|F_-e^{\frac{\Psi_N}{\varepsilon}}w\right\|^2_{\ell^2(\{d(x)<B\varepsilon\}_\varepsilon)} \leq C\varepsilon^{1-N}\|w\|^2_{\ell^2(\{d(x)<B\varepsilon\}_\varepsilon)} = O(1)\,. \tag{6.148}$$

Furthermore by (6.128), (6.144) and (6.129)

$$\begin{aligned}\left\|\tfrac{1}{F}e^{\frac{\Psi_N}{\varepsilon}}\left(H_\varepsilon^{M_1} - E_k\right)\mathbf{1}_G\,w\right\|^2_{\ell^2(\emptyset_\varepsilon)} &\leq \left\|\tfrac{1}{F}e^{\frac{\Psi_N}{\varepsilon}}\,\mathbf{1}_G\left(H_\varepsilon^{M_1} - E_k\right)w\right\|^2_{\ell^2(G_\varepsilon)} + \left\|\tfrac{1}{F}e^{\frac{\Psi_N}{\varepsilon}}\left[H_\varepsilon^{M_1}, \mathbf{1}_G\right]w\right\|^2_{\ell^2(\delta G_\varepsilon)} \\ &\leq C\varepsilon^{1+N_0-N}\left\|e^{\frac{d^1}{\varepsilon}}\left(H_\varepsilon^{M_1} - E_k\right)w\right\|^2_{\ell^2(G_\varepsilon)} + \left\|\tfrac{1}{F}e^{\frac{\Phi}{\varepsilon}}\left[H_\varepsilon^{M_1}, \mathbf{1}_G\right]w\right\|^2_{\ell^2(\delta G_\varepsilon)} \\ &= O(1) + O\left(\varepsilon^{-N_0}\right)\,,\end{aligned} \tag{6.149}$$

where in the last step we used (6.124). Thus inserting (6.147), (6.148) and (6.149) in (6.146) yields

$$\|e^{\frac{d^1}{\varepsilon}}w\|_{\ell^2(K_\varepsilon)} = O\left(\varepsilon^N\right)$$

for all $N \in \mathbb{N}$, proving the theorem.

□

## 6.6. Asymptotic eigenfunctions and the interaction matrix

Theorem 6.33 enables us, to analyze the elements $w_{\alpha\beta}$ of the transition matrix by use of the approximate eigenfunctions $\widehat{u}_{1,j}$ in the case of two wells as introduced in Hypothesis 6.17.

Since in Chapter 3 the well was assumed to be at zero, we have to translate the asymptotic expansions $\widehat{u}_\alpha$ and $\widehat{u}_\beta$ to the wells $x_{j(\alpha)}$ and $x_{j(\beta)}$ respectively.

Hypothesis 6.34. *In the setting of Hypothesis 6.17 we simplify the notation by writing $x_j$ and $x_k$ for the wells, $\mu_j$, $\mu_k$ for the Dirichlet eigenvalues respectively and $E := E_{\alpha\beta}$ for the "ellipse". In addition we assume the following:*

(a) *There are neighborhoods $\Omega_j$ and $\Omega_k$ of the points $x_j$ and $x_k$ respectively, such that Hypothesis 6.30 is fulfilled for the distance functions $d^j$ and $d^k$ in $\Omega_j$ and $\Omega_k$ respectively.*

(b) *The assumptions on* $E$ *and* $\Omega$ *given in Hypothesis 6.17 hold for* $\overset{\circ}{M}_{j(\alpha)}$ *and* $\overset{\circ}{M}_{j(\beta)}$ *replaced by* $\Omega_j$ *and* $\Omega_k$.

(c) *The Finsler distance between the two wells is minimal, i.e.* $d_l(x_j, x_k) = S_0$ *and there is a unique geodesic* $\gamma_{jk}$ *of length* $S_0$ *joining them, which is included in* $\emptyset_j \cup \emptyset_k$.

(d) *For* $y_{jk} \in \gamma_{jk} \cap \emptyset_j \cap \emptyset_k$ *choose the neighborhood* $\Omega$ *defined in Hypothesis 6.17 such that* $\Gamma := \partial\emptyset \cap E \cap \emptyset_j \cap \emptyset_k$ *defines a smooth hypersurface intersecting* $\gamma_{jk}$ *transversally at* $y_{jk}$ *and having no other intersections with* $\gamma_{jk}$ *(here* $\partial\emptyset$ *denotes the boundary of* $\emptyset$*).*

(e) *For* $A \subset \mathbb{R}^d$ *and* $\delta > 0$ *we define* $\delta A := \{x \in \mathbb{R}^d \,|\, \exists y \in \partial A : \; |x - y| \leq \delta\}$. *Then we set* $\widehat{\delta\Gamma}^{(c)} := \delta\Omega \cap \Omega^{(c)} \cap E$ *and* $\widehat{\delta\Gamma}_\varepsilon^{(c)} := \widehat{\delta\Gamma}^{(c)} \cap (\varepsilon\mathbb{Z})^d$.

With the assumptions in Hypothesis 6.34, it is by Theorem 6.33 possible to replace modulo terms of order $e^{-\frac{S_0}{\varepsilon}}\varepsilon^\infty$ the Dirichlet eigenfunctions, which are needed to compute the interaction matrix $w_{jk}$, by their approximating WKB-expansions.

PROPOSITION 6.35. *If Hypothesis 6.34 holds, then for*

$$\widehat{u}_l := \varepsilon^{\frac{d}{4}} a_l e^{-\frac{d^l}{\varepsilon}} \chi\,, \quad l = j, k\,,$$

*where* $a_l$ *denotes the asymptotic expansion* (3.92) *at the well* $x_l$, *the elements of the interaction matrix are given by*

$$\begin{aligned} w_{jk} &= \left\langle \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon} \widehat{u}_j \,,\, T_\varepsilon \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c} \widehat{u}_k \right\rangle_{\ell^2} - \left\langle T_\varepsilon \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c} \widehat{u}_j \,,\, \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon} \widehat{u}_k \right\rangle_{\ell^2} + O\left(\varepsilon^\infty e^{-\frac{S_0}{\varepsilon}}\right) \\ &= \sum_{x \in \widehat{\delta\Gamma}_\varepsilon} \sum_{\substack{\gamma \in (\varepsilon\mathbb{Z})^d \\ x+\gamma \in \widehat{\delta\Gamma}_\varepsilon^c}} a_\gamma(x) \sum_{l \geq -N_j} \sum_{m \geq -N_k} \varepsilon^{l+m+\frac{d}{2}} \Big( \tilde{a}_{j,l}(x) e^{-\frac{d^j(x)}{\varepsilon}} \tilde{a}_{k,m}(x+\gamma) e^{-\frac{d^k(x+\gamma)}{\varepsilon}} \\ &\qquad - \tilde{a}_{j,l}(x+\gamma) e^{-\frac{d^j(x+\gamma)}{\varepsilon}} \tilde{a}_{k,m}(x) e^{-\frac{d^k(x)}{\varepsilon}} \Big) + O\left(e^{-\frac{S_0}{\varepsilon}} \varepsilon^\infty\right)\,. \end{aligned}$$

*The constants* $N_j$ *and* $N_k$ *depend on the energy* $\mu_j$ *and* $\mu_k$. *If* $\mu_j$ *and* $\mu_k$ *are both principle eigenvalues for the Dirichlet operators, then* $N_j = N_k = 0$.

Proof:

Since by Hypothesis 6.17 each of the two wells has exactly one eigenvalue within the spectral interval $I_\varepsilon$, we have $v_j' = \widehat{u}_j$ in the setting of Theorem 6.33. We denote by $\equiv$ equality modulo $O\left(e^{-\frac{S_0}{\varepsilon}}\varepsilon^\infty\right)$. Setting

$$A := \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon} T_\varepsilon \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c} - \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c} T_\varepsilon \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon}\,, \tag{6.150}$$

we have by Proposition 6.19 to estimate the difference

$$\begin{aligned} \left| w_{jk} - \langle \widehat{u}_j \,,\, A\widehat{u}_k \rangle_{\ell^2} \right| &= \left| \langle v_j \,,\, Av_k \rangle_{\ell^2} - \langle \widehat{u}_j \,,\, A\widehat{u}_k \rangle_{\ell^2} \right| + O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right) \\ &\leq \left| \langle v_j - \widehat{u}_j \,,\, Av_k \rangle_{\ell^2} \right| + \left| \langle \widehat{u}_j \,,\, A(v_k - \widehat{u}_k) \rangle_{\ell^2} \right| + O\left(e^{\frac{-(S_0+a-\delta)}{\varepsilon}}\right) \end{aligned} \tag{6.151}$$

where $v_j, v_k$ denote the exact Dirichlet eigenfunctions. We have by (6.150), the triangle inequality and since $d^j(x) + d^k(x) \geq S_0$ for all $x \in E$

$$\begin{aligned} \left| \langle v_j - \widehat{u}_j \,,\, Av_k \rangle_{\ell^2} \right| &= \Bigg| \sum_{x \in (\varepsilon\mathbb{Z})^d} \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} \Big[ \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon}(x) \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c}(x+\gamma) - \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon^c}(x) \mathbf{1}_{\widehat{\delta\Gamma}_\varepsilon}(x+\gamma) \Big] \times \\ &\qquad \times e^{\frac{d^j(x)}{\varepsilon}} e^{-\frac{d^j(x)}{\varepsilon}} (v_j(x) - \widehat{u}_j(x))\, a_\gamma(x) e^{\frac{d^k(x)}{\varepsilon}} e^{-\frac{d^k(x)}{\varepsilon}} v_k(x+\gamma) \Bigg| \\ &\leq e^{-\frac{S_0}{\varepsilon}} \left\| e^{\frac{d^j}{\varepsilon}} (v_j - v_j') \right\|_{\ell^2(\widehat{\delta\Gamma}_\varepsilon \cup \widehat{\delta\Gamma}_\varepsilon^c)} \left\| e^{\frac{d^k}{\varepsilon}} v_k \right\|_{\ell^2(\widehat{\delta\Gamma}_\varepsilon \cup \widehat{\delta\Gamma}_\varepsilon^c)} \sum_{|\gamma| < B} \left\| a_\gamma e^{\frac{d(.,.+\gamma)}{\varepsilon}} \right\|_{\ell^\infty(\widehat{\delta\Gamma} \cup \widehat{\delta\Gamma}^c)}\,. \end{aligned}$$

In the last step we used $\widehat{u}_j = v_j'$ and that for some $B > 0$ we have $|\gamma| < B$ if $x \in \widehat{\delta\Gamma}_\varepsilon$ and $x + \gamma \in \widehat{\delta\Gamma}_\varepsilon^c$ and vice versa. Therefore by Theorem 6.33, Theorem 5.6 and (6.4) we have

$$\left| \langle v_j - \widehat{u}_j \,,\, Av_k \rangle_{\ell^2} \right| = O\left(e^{-\frac{S_0}{\varepsilon}} \varepsilon^\infty\right)\,. \tag{6.152}$$

The second summand on the right hand side of (6.151) can be estimated similarly, which proves the first equation in Proposition 6.35. To get the second equation, we only use the definition of $\widehat{u}_j$ together with the asymptotic expansion of $a_j$ constructed in (3.92).

□

**6.6.1. Estimates for the interaction-matrix for finite step kinetic energy.** In the setting of Hypothesis (6.34), i.e. if we have only two wells inside a specified region with eigenvalues inside of an exponentially small interval, we are now going to estimate the interaction matrix in the case, that the step length of the translations caused by the the kinetic energy operator is finite and scaled by $\varepsilon$, i.e., $a_\gamma$ vanishes for $|\gamma| > N\varepsilon$ for some $N$. Furthermore we will restrict the discussion to energies, which belong to the ground state with respect to the two wells. In this case, the constants $N_j, N_k$ occurring in the expansion of the interaction matrix $w_{jk}$ in Proposition 6.35 are both equal to zero (see Remark 3.19).

Hypothesis 6.36. *We assume that there exists a $N \in \mathbb{N}$ such that $a_\gamma = 0$ if $|\gamma| > \varepsilon N$. We associate to each pair $(x, x+\gamma) \in \widehat{\delta\Gamma}_\varepsilon \times \widehat{\delta\Gamma}^c_\varepsilon$, which occurs in the formula for the interaction matrix element $w_{jk}$ in Proposition 6.35, a point $y_{x\gamma} \in \Gamma$ as the point of intersection of $\Gamma$ with the straight line between $x$ and $x+\gamma$. Then we set*

$$\Gamma^* := \{y \in \Gamma \,|\, y = y_{x\gamma},\ x \in \widehat{\delta\Gamma}_\varepsilon, x+\gamma \in \widehat{\delta\Gamma}^c_\varepsilon\}$$

*and*

$$\widehat{\delta\Gamma}'_\varepsilon(y) := \{\gamma \in (\varepsilon\mathbb{Z})^d \,|\, \exists x \in \widehat{\delta\Gamma}\ :\ y = y_{x\gamma}\}\ .$$

*Then we define for $y \in \Gamma^*$ and $\xi \in \mathbb{T}^d$*

$$\tilde{t}^\delta(y,\xi) := -\sum_{\gamma \in \widehat{\delta\Gamma}'_\varepsilon(y)} a_\gamma(y) e^{\frac{\gamma\cdot\xi}{\varepsilon}}\ .$$

*We denote by $\equiv$ equality modulo $O\left(e^{-\frac{S_0}{\varepsilon}}\varepsilon^\infty\right)$.*

By Hypothesis 6.1, the symbol $\tilde{t}^\delta$ is hyperconvex with respect to $\xi$ (see Remark 4.21).

Theorem 6.37. *Under the assumptions given in Hypotheses 6.36 and 6.34, and for $v'_j$ as defined in Theorem 6.33, the elements of the interaction matrix are for $\delta = N\varepsilon$ given by*

$$w_{jk} \equiv \sum_{x \in \widehat{\delta\Gamma}_\varepsilon} v'_j(x) v'_k(x) \left(\tilde{t}^\delta(x, \nabla d^j(x)) - \tilde{t}^\delta(x, \nabla d^k(x)) + O(\varepsilon)\right)\ . \tag{6.153}$$

*If $v'_j$ and $v'_k$ are both strictly positive in $\widehat{\delta\Gamma}_\varepsilon$, we have modulo $O\left(\varepsilon^\infty e^{-\frac{S_0}{\varepsilon}}\right)$*

$$\sum_{x \in \widehat{\delta\Gamma}_\varepsilon} v'_j(x) v'_k(x) \nabla_\xi \tilde{t}^\delta(x, \nabla d^k(x))(\nabla d^j(x)) - \nabla d^k(x))$$
$$\leq w_{jk} \leq \sum_{x \in \widehat{\delta\Gamma}_\varepsilon} v'_j(x) v'_k(x) \nabla_\xi \tilde{t}^\delta(x, \nabla d^j(x))(\nabla d^j(x)) - \nabla d^k(x))\ . \tag{6.154}$$

Proof:

We start proving that Proposition 6.35 holds for $\delta = N\varepsilon$ for some $N \in \mathbb{N}$. This is a direct consequence of the assumption $a_\gamma = 0$ for $|\gamma| > N\varepsilon$, since then right hand side of (6.94) is equal to zero for $\delta = \varepsilon N$ and therefore we get

$$\|([H_\varepsilon, \mathbf{1}_A] - \mathbf{1}_{\delta A}[H_\varepsilon, \mathbf{1}_A]\,\mathbf{1}_{\delta A})\|_\infty = 0\ , \tag{6.155}$$

leading at once to Proposition 6.19 and Proposition 6.35 for this choice of $\delta$.
By Proposition 6.35 we have

$$w_{jk} \equiv \sum_{x \in \widehat{\delta\Gamma}_\varepsilon} \sum_{\substack{\gamma \in (\varepsilon\mathbb{Z})^d \\ x+\gamma \in \widehat{\delta\Gamma}^c_\varepsilon}} a_\gamma(x) \varepsilon^{\frac{d}{2}} \left(a_j(x) e^{-\frac{d^j(x)}{\varepsilon}} a_k(x+\gamma) e^{-\frac{d^k(x+\gamma)}{\varepsilon}} - a_j(x+\gamma) e^{-\frac{d^j(x+\gamma)}{\varepsilon}} a_k(x) e^{-\frac{d^k(x)}{\varepsilon}}\right)\ . \tag{6.156}$$

By (3.9) and $\gamma = O(\varepsilon)$, Taylor expansion at the points $x \in \widehat{\delta\Gamma}_\varepsilon$ yields

$$\sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in\widehat{\delta\Gamma}^c_\varepsilon}} a_\gamma(x)a_j(x)e^{-\frac{d^j(x)}{\varepsilon}}a_k(x+\gamma)e^{-\frac{d^k(x+\gamma)}{\varepsilon}} = -a_j(x)a_k(x)e^{-\frac{1}{\varepsilon}(d^j(x)+d^k(x))}(\tilde{t}^\delta(x,\nabla d^k(x))+O(\varepsilon)) \,. \tag{6.157}$$

Inserting (6.157) in (6.156) yields

$$w_{jk} \equiv \sum_{x\in\widehat{\delta\Gamma}_\varepsilon} \varepsilon^{\frac{d}{2}}a_j(x)a_k(x)e^{-\frac{1}{\varepsilon}(d^j(x)+d^k(x))}\left(\tilde{t}^\delta(x,\nabla d^j(x)) - \tilde{t}^\delta(x,\nabla d^k(x)) + O(\varepsilon)\right) \,.$$

Since by the assumptions $v_l' = \widehat{u}_l$. where $\widehat{u}_l$ is defined in Proposition 6.35, equation (6.153) is shown.

To show (6.154), we use that for any convex function $f$ on $\mathbb{R}^d$

$$\nabla f(\eta)(\xi-\eta) \le f(\xi) - f(\eta) \le \nabla f(\xi)(\xi-\eta)\,, \qquad \eta,\xi\in\mathbb{R}^d \,.$$

Thus for $v_j'$ and $v_k'$ both positive in $\widehat{\delta\Gamma}$, (6.159) follows from the convexity of $\tilde{t}^\delta$.

□

Now we restrict ourselves to the case, that $E_0$ describes the ground state of the system with respect to $x_j$ and $x_k$. Then it is possible to give the leading order term with respect to $\varepsilon$.

THEOREM 6.38. *Under the assumptions given in Hypotheses 6.36 and 6.34, we assume that $E_0$ is the principal eigenvalue of the harmonic oscillators at $x_j$ and $x_k$. Then*

$$|w_{jk}| = O\left(\varepsilon^{\frac{1}{2}}e^{-\frac{S_0}{\varepsilon}}\right) \,. \tag{6.158}$$

*If $v_j'$ and $v_k'$ are both strictly positive on $\Gamma$ and $\Gamma$ is transversal to all geodesics from $x_j$ and $x_k$ to $y\in\Gamma$, we have for some $C>0$*

$$C\varepsilon^{\frac{1}{2}} \le -w_{jk}e^{\frac{S_0}{\varepsilon}} \le \frac{1}{C}\varepsilon^{1-\frac{d}{2}} \,. \tag{6.159}$$

*If furthermore there exists a constant $C>0$ such that*

$$d^j(y) + d^k(y) \ge S_0 + \frac{1}{C}d^2(y,y_{jk})\,, \tag{6.160}$$

*we get for some $C'>0$ the estimate*

$$C'\varepsilon^{\frac{1}{2}} \le -w_{jk}e^{\frac{S_0}{\varepsilon}} \le \frac{1}{C'}\varepsilon^{\frac{1}{2}} \,. \tag{6.161}$$

Proof:

To show (6.158), we analyze the Taylor expansion at the points $y_{x\gamma}\in\Gamma^*$ as introduced in Hypothesis 6.36. We get

$$\begin{aligned} w_{jk} \equiv \sum_{x\in\widehat{\delta\Gamma}_\varepsilon}\ \sum_{\substack{\gamma\in(\varepsilon\mathbb{Z})^d\\ x+\gamma\in\widehat{\delta\Gamma}^c_\varepsilon}} & a_\gamma(x)\varepsilon^{\frac{d}{2}}a_j(y_{x\gamma})a_k(y_{x\gamma})e^{-\frac{1}{\varepsilon}(d^j(y_{x\gamma})+d^k(y_{x\gamma}))} \\ & \times e^{-\frac{1}{\varepsilon}(\nabla d^j(y_{x\gamma})+\nabla d^k(y_{x\gamma}))(x-y_{x\gamma})}\left(e^{-\frac{1}{\varepsilon}\nabla d^k(y_{x\gamma})\gamma} - e^{-\frac{1}{\varepsilon}\nabla d^j(y_{x\gamma})\gamma} + O(\varepsilon)\right) \,. \end{aligned} \tag{6.162}$$

By the boundedness of the region $\widehat{\delta\Gamma}$, the fact that the product $a_ja_k(y_{x\gamma})$ is of order zero in $\varepsilon$ for the ground state and the estimate $(x-y) = O(\varepsilon) = \gamma$, which follows from the assumption that there are only finite steps allowed, it follows

$$|w_{jk}| \le C\varepsilon^{\frac{d}{2}}\sum_{y\in\Gamma^*} e^{-\frac{1}{\varepsilon}(d^j(y)+d^k(y))} \,.$$

This sum can be estimated via the integral over the hypersurface $\Gamma$. By the scaling of the sum with respect to $\varepsilon$, we get a factor $\varepsilon^{-(d-1)}$, since the codimension of $\Gamma$ is one. Thus we get

$$|w_{jk}| \le \tilde{C}\varepsilon^{1-\frac{d}{2}}\int_\Gamma e^{-\frac{1}{\varepsilon}(d^j(y)+d^k(y))}\,d\sigma(y)\,. \tag{6.163}$$

By Hypothesis 6.34 we have for some $C > 0$

$$S_0 \leq d^j(y) + d^k(y) \leq S_0 + Cd^2(y, y_{jk}), \qquad y \in \Gamma . \tag{6.164}$$

Inserting (6.164) in (6.163) we can use of the method of stationary phase (see for example Grigis-Sjöstrand [**24**]) to analyze the integral on the right hand side of (6.163). This leads to an additional factor $\varepsilon^{\frac{d-1}{2}}$ and thus to the estimate (6.158).
For (6.159), we have to analyze the terms in (6.162) more detailed. By assumption, $a_j(y)a_k(y) > 0$ for all $y \in \Gamma$. Since $\Gamma$ was assumed to be transversal to all geodesics from $x_j$ and $x_k$, it follows by the construction of $\emptyset$, including $x_j$ and excluding $x_k$, and from the definition of $\widehat{\delta\Gamma}$ and $\widehat{\delta\Gamma}^c$ in Hypothesis 6.34, that $\nabla d^k(y)\gamma < 0$ and $\nabla d^j(y)\gamma > 0$ for all $y \in \Gamma, \gamma \in \widehat{\delta\Gamma}'_\varepsilon(y)$. Thus there exists a constant $C > 0$ such that for all $y \in \Gamma, x \in \widehat{\delta\Gamma}, \gamma \in \widehat{\delta\Gamma}'_\varepsilon(y)$

$$\frac{1}{C} \leq a_j(y)a_k(y)e^{-\frac{1}{\varepsilon}(\nabla d^j(y)+\nabla d^k(y))(x-y)} \left(e^{-\frac{1}{\varepsilon}\nabla d^k(y)\gamma} - e^{-\frac{1}{\varepsilon}\nabla d^j(y)\gamma}\right) \leq C . \tag{6.165}$$

Since by Hypothesis 6.1 the coefficients $a_\gamma$ are negative and bounded, we get by inserting the first estimate in (6.164) and (6.165) in (6.163)

$$-w_{jk} \leq \frac{1}{C}e^{-\frac{S_0}{\varepsilon}}\varepsilon^{\frac{d}{2}} \sum_{y\in\Gamma^*} 1 . \tag{6.166}$$

and by inserting the second estimate in (6.164) and (6.165) in (6.163)

$$Ce^{-\frac{S_0}{\varepsilon}}\varepsilon^{\frac{d}{2}} \sum_{y\in\Gamma^*} e^{-C\frac{d_l^2(y,y_{jk})}{\varepsilon}} \leq -w_{jk} . \tag{6.167}$$

In both equations, the sum over $\Gamma^*$ can be estimated via the integral over $\Gamma$. By the scaling of the sum with respect to $\varepsilon$, we get a factor $\varepsilon^{-(d-1)}$, since the codimension of $\Gamma$ is one. Therefore (6.166) yields

$$-w_{jk} \leq \frac{1}{C}e^{-\frac{S_0}{\varepsilon}}\varepsilon^{1-\frac{d}{2}} . \tag{6.168}$$

The integral that we get in (6.167) can be estimated again by the method of stationary phase, yielding the additional factor $\varepsilon^{\frac{d-1}{2}}$. Thus we get by (6.167) together with (6.168) the equation (6.159). This statement can be improved by an additional assumption (6.160). Then we get instead of (6.166) the estimate

$$-w_{jk} \leq \frac{1}{C}e^{-\frac{S_0}{\varepsilon}}\varepsilon^{\frac{d}{2}} \sum_{y\in\Gamma^*} e^{-C\frac{d_l^2(y,y_{jk})}{\varepsilon}} ,$$

yielding (6.161) again by the method of stationary phase.

□

Thus at least for the principal eigenvalue and under quite strong assumptions it is possible to find the exact order of $w_{jk}$ with respect to $\varepsilon$. It coincides with the values in the case of Schrödinger operators on $\mathbb{R}^d$ as described in Helffer [**29**] and in Helffer-Sjöstrand [**33**].

APPENDIX A

# Technical details and supplementary computations

## A.1. The discrete Fourier transform

We show some properties of the discrete Fourier transform introduced in Chapter 3.

Equation (2.5):
We show this equation for $u \in l_c\left((\varepsilon\mathbb{Z})^d\right)$, the summable functions with compact support, in order to check the scaling factors. The generalization to $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ can be done by the usual density arguments, as described in Reed, Simon [**49**]. By definition

$$
\begin{aligned}
(\mathscr{F}_\varepsilon\mathscr{F}_\varepsilon^{-1}u)(x) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{[-\pi,\pi]^d} e^{-\frac{i}{\epsilon}x\xi}(\mathscr{F}_\varepsilon^{-1}u)(\xi)\,d\xi = \\
&= \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{[-\pi,\pi]^d} e^{-\frac{i}{\epsilon}x\xi}\left(\frac{1}{\sqrt{2\pi}}\right)^d \sum_{x'\in(\varepsilon\mathbb{Z})^d} e^{ix'\frac{\xi}{\epsilon}}u(x')\,d\xi = \\
&= \left(\frac{1}{2\pi}\right)^d \sum_{x'\in(\varepsilon\mathbb{Z})^d} u(x') \int_{[-\pi,\pi]^d} e^{\frac{i}{\epsilon}\xi(x'-x)}\,d\xi\,.
\end{aligned}
$$

Since $\frac{x}{\epsilon} \in \mathbb{Z}$, we have

$$
\left(\frac{1}{2\pi}\right)^d \int_{[-\pi,\pi]^d} e^{\frac{i}{\epsilon}\xi(x'-x)}\,d\xi = \begin{cases} 1 & \text{for} \quad x = x' \\ 0 & \text{for} \quad x \neq x' \end{cases}
$$

and therefore equation (2.5) is shown for $u \in l_c\left((\varepsilon\mathbb{Z})^d\right)$.
Equation (2.6):
Let $g(x) := e^{-x^2}$ and $f \in \mathscr{P}_t(\mathbb{T}^d)$, the polynomials of trigonometric functions. Then

$$
\begin{aligned}
\mathscr{F}_\varepsilon^{-1}\left(g\mathscr{F}_\varepsilon f\right)(\xi) &= (2\pi)^{-\frac{d}{2}} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\cdot\xi}g(x)(\mathscr{F}_\varepsilon f)(x) = \\
&= (2\pi)^{-\frac{d}{2}} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\cdot\xi}g(x)\,(2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} e^{-ix\frac{\xi'}{\varepsilon}}f(\xi')\,d\xi' = \\
&= (2\pi)^{-d} \int_{[-\pi,\pi]^d} f(\xi') \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x(\xi-\xi')}g(x)\,d\xi' = \\
&= (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} f(\xi')(\mathscr{F}_\varepsilon^{-1}g)(\xi-\xi')\,d\xi',
\end{aligned}
$$

where we used, that $g$ is a Schwartz function and $f \in \mathscr{P}_t$ to interchange integration an summation. If we now start with $g_a(x) := g(ax) = e^{a^2x^2}$, for which $\lim_{a\to 0} g(ax) = 1$ and with $\mathscr{F}_{\varepsilon,a}^{-1}f(\xi) := \frac{a}{\sqrt{2\pi}}^d \sum_{x'\in(a\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x'\xi}g(x')$, for which $\lim_{a\to 0}\mathscr{F}_{\varepsilon,a}^{-1}f(\xi) = F^{-1}f(\xi)$ in the sense of a Riemannian sum, we get with $\eta = \frac{\xi'-\xi}{a}$

$$
\begin{aligned}
\mathscr{F}_\varepsilon^{-1}\left(g_a\mathscr{F}_\varepsilon f\right)(\xi) &= (2\pi)^{-d} \int_{[-\pi,\pi]^d} f(\xi') \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x(\xi-\xi')}g(ax)\,d\xi' = \\
&= (2\pi)^{-d} \int_{[-\pi,\pi]^d} f(\xi') \sum_{x'\in(a\varepsilon\mathbb{Z})^d} e^{\frac{i}{a\varepsilon}x'(\xi-\xi')}g(x')\,d\xi' = \\
&= (2\pi)^{-\frac{d}{2}} \int_{[\frac{\xi-\pi}{a},\frac{\xi+\pi}{a}]^d} f(\xi+a\eta)(\mathscr{F}_{\varepsilon,a}^{-1}g)(-\eta)\,d\eta\,.
\end{aligned}
$$

In the limit $a \to 0$, the last integral is equal to

$$f(\xi)\,(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} F_\varepsilon^{-1} g(-\eta) d\eta = f(\xi) F_\varepsilon (F_\varepsilon^{-1} g)(0) = f(\xi)\,.$$

Since on the other hand

$$\lim_{a\to 0} (2\pi)^{-\frac{d}{2}} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\epsilon}x\xi} g(ax)(\mathscr{F}_\varepsilon f)(x) = g(0)\mathscr{F}_\varepsilon^{-1}(\mathscr{F}_\varepsilon f)(\xi)\,,$$

we are done. As in the previous assumption, we refer to Reed, Simon [**49**] for the generalization to $f \in \mathscr{L}^2(\mathbb{T}^d)$.

Equation (2.7):

For $u, v \in l_c\left((\varepsilon\mathbb{Z})^d\right)$, we have by the definitions (2.1) and (2.2)

$$\begin{aligned}
\langle v\,,\, u\rangle_{\ell^2} &= \sum_{x\in(\varepsilon\mathbb{Z})^d} \bar{v}(x) u(x) = \\
&= \sum_{x\in(\varepsilon\mathbb{Z})^d} \frac{1}{\sqrt{2\pi}^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}x\xi} (\overline{\mathscr{F}_\varepsilon^{-1} v})(\xi)\, d\xi\, u(x) = \\
&= \int_{[-\pi,\pi]^d} (\overline{\mathscr{F}_\varepsilon^{-1} v})(\xi) \frac{1}{\sqrt{2\pi}^d} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\xi} u(x)\, d\xi = \\
&= \int_{[-\pi,\pi]^d} (\overline{\mathscr{F}_\varepsilon^{-1} v})(\xi) (\mathscr{F}_\varepsilon^{-1} u)(\xi)\, d\xi = \\
&= \left\langle \mathscr{F}_\varepsilon^{-1} v\,,\, \mathscr{F}_\varepsilon^{-1} u\right\rangle_{\mathbb{T}}\,.
\end{aligned}$$

The change of integration and summation is possible, since the integral is taken over a compact range.

Lemma A.1. *For fixed $x \in (\varepsilon\mathbb{Z})^d$ let $f_x \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ not depending on the choice of $\varepsilon$, i.e. we assume that there exists a function $\tilde{f}_x : \mathbb{Z}^d \to \mathbb{R}$ such that $f_x(\gamma) = \tilde{f}_x(\frac{\gamma}{\varepsilon})$. Furthermore we assume $(\mathscr{F}_\varepsilon f_x) \in \mathscr{C}^\infty\left(\mathbb{T}^d\right)$.*
*Then there exists a constant $C_x > 0$, such that for all $N \in \mathbb{N}$ and for all $\varepsilon > 0$*

$$|f_x(\gamma)| \le \frac{C_x}{1 + \left(\frac{|\gamma|}{\varepsilon}\right)^{2N}}\,, \qquad x \in (\varepsilon\mathbb{Z})^d\,. \tag{A.1}$$

*If $\mathscr{F}_\varepsilon f_x$ is bounded with respect to $x$, then the estimate holds uniformly in $x$, i.e., there exists a constant $C > 0$ such that for all $N \in \mathbb{N}, \varepsilon > 0$*

$$\sup_{x\in(\varepsilon\mathbb{Z})^d} |f_x(\gamma)| \le \frac{C}{1 + \left(\frac{|\gamma|}{\varepsilon}\right)^{2N}}\,, \qquad x \in (\varepsilon\mathbb{Z})^d\,. \tag{A.2}$$

Proof:

By the Fourier inversion formula, we have for fixed $x \in (\varepsilon\mathbb{Z})^d$

$$f_x(\gamma) = (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}\gamma\xi} \left(\mathscr{F}_\varepsilon^{-1} f_x\right)(\xi)\, d\xi\,.$$

The operator $L := \frac{1-\Delta_\xi}{1+\left(\frac{|\gamma|}{\varepsilon}\right)^2}$ has the property $Le^{-\frac{i}{\varepsilon}\gamma\xi} = e^{-\frac{i}{\varepsilon}\gamma\xi}$. Thus we can introduce $L$ into the integral and get by partial integration

$$\begin{aligned}
f_x(\gamma) &= (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} \left(L^N e^{-\frac{i}{\varepsilon}\gamma\xi}\right) \left(\mathscr{F}_\varepsilon^{-1} f_x\right)(\xi)\, d\xi \\
&= (2\pi)^{-\frac{d}{2}} \left(1 + \frac{|\gamma|^2}{\varepsilon^2}\right)^{-N} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}\gamma\xi} (1-\Delta_\xi)^N \left(\mathscr{F}_\varepsilon^{-1} f_x\right)(\xi)\, d\xi\,.
\end{aligned} \tag{A.3}$$

Since the last integral is bounded by assumption, (A.1) follows from the triangle inequality.
If $\mathscr{F}_\varepsilon^{-1} f_x$ is bounded with respect to $x$, the same is true for $f_x$ by the compactness of the torus. Thus taking the supremum over all $x$ on both sides in (A.3) shows (A.2).

□

LEMMA A.2. *Let $g \in l_c\left((\varepsilon\mathbb{Z})^d\right)$ with $g(\gamma) = 0$ for $|\gamma| \geq A$ and such that $g$ does not depend on the value of $\varepsilon$ in the sense of Lemma A.1.*
*Then $\left(\mathscr{F}_\varepsilon^{-1} g\right)$ can be continued to an entire analytic function. Using the notation $\zeta = \xi + i\eta$, then for $\xi \in [-\pi,\pi]^d$ there exist a constant $C > 0$, such that for all $N \in \mathbb{N}$*

$$|\mathscr{F}_\varepsilon^{-1} g(\zeta)| \leq \frac{C e^{\frac{A}{\varepsilon}|\eta|}}{1 + \left(\frac{|\zeta|}{\varepsilon}\right)^{2N}} .$$

Proof:
Since $g \in l_c\left((\varepsilon\mathbb{Z})^d\right)$, the function

$$\mathscr{F}_\varepsilon^{-1} g(\zeta) = (2\pi)^{-\frac{d}{2}} \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon} x\zeta} g(\gamma)$$

is well defined and analytic for all values of $\eta$, because we can differentiate each summand of the finite sum. To use partial summation similar to the proof of Lemma 2.13 c, we introduce the operator

$$L_\varepsilon := \frac{1 - \varepsilon^2 \Delta_\varepsilon}{1 + \sum_{\nu=1}^d (2 - 2\cos\zeta_\nu)} ,$$

where $\Delta_\varepsilon$ is the discrete Laplacian defined in (2.60), which is symmetric with respect to the $\ell^2$ scalar product. Thus $L_\varepsilon$ obeys this symmetry property too and in addition $L_\varepsilon e^{\frac{i}{\varepsilon}\gamma\zeta} = e^{\frac{i}{\varepsilon}\gamma\zeta}$ by construction. Therefore

$$\begin{aligned}
\mathscr{F}_\varepsilon^{-1} g(\zeta) &= (2\pi)^{-\frac{d}{2}} \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} \left(L_\varepsilon^N e^{\frac{i}{\varepsilon}\gamma\zeta}\right) g(\gamma) = \\
&= (2\pi)^{-\frac{d}{2}} \left(1 + \sum_{\nu=1}^d (2 - 2\cos\zeta_\nu)\right)^{-N} \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}\gamma\zeta} (1 + \varepsilon^2 \Delta_\varepsilon)^N g(\gamma)
\end{aligned}$$

and from $g(\gamma) = 0$ for $|\gamma| \geq A$, it follows that

$$\left| \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}\gamma\zeta} (1 + \varepsilon^2\Delta_\varepsilon)^N g(\gamma) \right| \leq \left| e^{\frac{i}{\varepsilon} A(\xi + i\eta)} \right| \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} \left| (1 + \varepsilon^2\Delta_\varepsilon)^N g(\gamma) \right| \leq e^{\frac{A}{\varepsilon}|\eta|} C . \tag{A.4}$$

Furthermore

$$\begin{aligned}
|2 - 2\cos\zeta_\nu| &= |2 - 2\cos\xi_\nu \cosh\eta_\nu - i\sin\xi_\nu \sinh\eta_\nu| = \\
&= \left((2 - 2\cos\xi_\nu\cosh\eta_\nu)^2 + (2\sin\xi_\nu\sinh\eta_\nu)^2\right)^{\frac{1}{2}} = \\
&= 2\left(1 + \cos^2\xi_\nu\cosh^2\eta_\nu - 2\cos\xi_\nu\cosh\eta_\nu + \sin^2\xi_\nu(\cosh^2\eta_\nu - 1)\right)^{\frac{1}{2}} = \\
&= 2\left(1 + (\cos^2\xi_\nu + \sin^2\xi_\nu)\cosh^2\eta_\nu - 2\cos\xi_\nu\cosh\eta_\nu - \sin^2\xi_\nu\right)^{\frac{1}{2}} = \\
&= 2\left(\cos^2\xi_\nu - 2\cos\xi_\nu\cosh\eta_\nu + \cosh^2\eta_\nu\right)^{\frac{1}{2}} = \\
&= 2(\cosh\eta_\nu - \cos\xi_\nu) ,
\end{aligned}$$

where for the last equality we used that $\cosh\eta_\nu \geq \cos\xi_\nu$. With the estimates

$$\cosh\eta_\nu \geq 1 + \frac{\eta_\nu^2}{2} , \quad \pi^2(1 - \cos\xi_\nu) \geq \xi_\nu^2 \quad \text{for} \quad \eta_\nu \in \mathbb{R},\, |\xi_\nu| \leq \pi ,$$

we can conclude

$$2(\cosh\eta_\nu - \cos\xi_\nu) \geq 2\left(1 + \frac{\eta_\nu^2}{2} - \cos\xi_\nu\right) \geq 2\left(\frac{\eta_\nu^2}{2} + \frac{\xi_\nu^2}{\pi^2}\right) \geq 2\frac{1}{\pi^2}\left(\eta_\nu^2 + \xi_\nu^2\right) = \frac{|\zeta_\nu|^2}{\pi^2} .$$

We thus get for $|\xi_\nu| \leq \pi$ the estimate

$$|2 - 2\cos\zeta_\nu| \geq \frac{|\zeta_\nu|^2}{\pi^2} \qquad 1 \leq \nu \leq d . \tag{A.5}$$

Combining (A.4) and (A.5) yields

$$\begin{aligned} \left|\mathscr{F}_\varepsilon^{-1} g(\zeta)\right| &\leq (2\pi)^{-\frac{d}{2}} \left|1+\sum_{\nu=1}^{d}(2-2\cos\zeta_\nu)\right|^{-N} \left|\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}\gamma\zeta}(1+\varepsilon^2\Delta_\varepsilon)^N g(\gamma)\right| \leq \\ &\leq \frac{Ce^{\frac{A}{\varepsilon}|\eta|}}{\left(1+\sum_\nu \frac{|\zeta_\nu|^2}{\pi^2}\right)^N} \leq \frac{Ce^{\frac{A}{\varepsilon}|\eta|}}{1+\left(\frac{|\zeta_\nu|}{\pi}\right)^{2N}}\,, \end{aligned}$$

which proves the lemma.

□

Proposition A.3. *For $f\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ the Fourier-transform $\left(\mathscr{F}_\varepsilon^{-1}f\right)$ has an analytic continuation to the set $K_a:=\{\zeta\in\mathbb{C}^d\,|\,|\Im\zeta|<a\}$ with the property that $\left(\mathscr{F}_\varepsilon^{-1}f\right)(\,\cdot\,-i\eta)\in\mathscr{L}^2(\mathbb{T}^d)$ for each $\eta\in\mathbb{R}^d$ with $|\eta|<a$ and that for any $b<a$*

$$\sup_{|\eta|\leq b}\|\left(\mathscr{F}_\varepsilon^{-1}f\right)(\,\cdot\,-i\eta)\|_{\mathbb{T}^d}<\infty\,,$$

*if and only if $e^{\frac{b}{\varepsilon}\gamma}f\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$.*

Proof:

$\Longrightarrow$:
For any $g\in l_c\left((\varepsilon\mathbb{Z})^d\right)$ we have by (2.7)

$$\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}\overline{g(\gamma)}f(\gamma)=\int_{[-\pi,\pi]^d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\xi)}(\mathscr{F}_\varepsilon^{-1}f)(\xi)\,d\xi\,. \tag{A.6}$$

Since by Lemma A.2 and by assumption $\mathscr{F}^{-1}g$ and $\mathscr{F}_\varepsilon^{-1}f$ can be continued analytically to the set $K_a$, the Cauchy Integral Theorem gives for $|\eta|<a$

$$\begin{aligned} &\int_{[-\pi,\pi]^d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\zeta)}(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\zeta-\int_{-\pi-i\eta_1}^{\pi-i\eta_1}\dots\int_{-\pi-i\eta_d}^{\pi-i\eta_d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\zeta)}(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\zeta+ \\ &\quad+\int_{\pi}^{\pi-i\eta_1}\dots\int_{\pi}^{\pi-i\eta_d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\zeta)}(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\zeta-\int_{-\pi}^{-\pi-i\eta_1}\dots\int_{-\pi}^{-\pi-i\eta_d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\zeta)}(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\zeta=0\,. \end{aligned} \tag{A.7}$$

The Fourier transforms of lattice functions are $2\pi$-periodic in $\xi$ for each fixed value of $\eta$, since for $h\in\ell^2\left((\varepsilon\mathbb{Z})^d\right)$

$$\left(\mathscr{F}_\varepsilon^{-1}h\right)(\pi-i\eta)=(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}e^{\frac{i}{\varepsilon}|\gamma|\pi}e^{\frac{\gamma}{\varepsilon}\eta}h(\gamma)=(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}(-1)^{\frac{|\gamma|}{\varepsilon}}e^{\frac{\gamma}{\varepsilon}\eta}h(\gamma)$$

and

$$\left(\mathscr{F}_\varepsilon^{-1}h\right)(-\pi-i\eta)=(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}e^{-\frac{i}{\varepsilon}|\gamma|\pi}e^{\frac{\gamma}{\varepsilon}\eta}h(\gamma)=(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}(-1)^{\frac{|\gamma|}{\varepsilon}}e^{\frac{\gamma}{\varepsilon}\eta}h(\gamma)\,.$$

Therefore the last two integral terms in (A.7) cancel each other and

$$\begin{aligned} \int_{[-\pi,\pi]^d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\zeta)}(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\zeta &= \int_{[-\pi,\pi]^d}(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}e^{-\frac{i}{\varepsilon}\gamma\xi}\overline{g}(\gamma)(\mathscr{F}_\varepsilon^{-1}f)(\zeta)\,d\xi= \\ &= \int_{[-\pi,\pi]^d}(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}e^{-\frac{i}{\varepsilon}\gamma(\xi-i\eta)}\overline{g}(\gamma)(\mathscr{F}_\varepsilon^{-1}f)(\xi-i\eta)\,d\xi= \\ &= \int_{[-\pi,\pi]^d}(2\pi)^{-\frac{d}{2}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}\overline{e^{\frac{i}{\varepsilon}\gamma(\xi+i\eta)}g(\gamma)}(\mathscr{F}_\varepsilon^{-1}f)(\xi-i\eta)\,d\xi= \\ &= \int_{[-\pi,\pi]^d}\overline{(\mathscr{F}_\varepsilon^{-1}g)(\xi+i\eta)}(\mathscr{F}_\varepsilon^{-1}f)(\xi-i\eta)\,d\xi \end{aligned} \tag{A.8}$$

Defining $h_\eta(\xi) := (\mathscr{F}_\varepsilon^{-1} f)(\xi - i\eta)$, we get by (A.6) and (A.8) and since $g \in l_c\left((\varepsilon\mathbb{Z})^d\right)$

$$\begin{aligned}
\sum_{\gamma\in(\varepsilon\mathbb{Z})^d} \overline{g(\gamma)} f(\gamma) &= \int_{[-\pi,\pi]^d} \overline{(\mathscr{F}_\varepsilon^{-1} g)(\xi + i\eta)} h_\eta(\xi)\, d\xi = \\
&= \int_{[-\pi,\pi]^d} (2\pi)^{-\frac{d}{2}} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{-\frac{i}{\varepsilon}\gamma\xi} e^{-\frac{\gamma}{\varepsilon}\eta} \overline{g}(\gamma) h_\eta(\xi)\, d\xi = \\
&= \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{-\frac{\gamma}{\varepsilon}\eta} \overline{g}(\gamma) (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}\gamma\xi} h_\eta(\xi)\, d\xi = \\
&= \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{-\frac{\gamma}{\varepsilon}\eta} \overline{g}(\gamma) (\mathscr{F}_\varepsilon h_\eta)(\gamma)\ .
\end{aligned}$$

The function $g$ was arbitrary, we therefore get almost everywhere

$$(\mathscr{F}_\varepsilon h_\eta)(\gamma) = e^{\frac{\gamma}{\varepsilon}\eta} f(\gamma)\ .$$

Since $h_\eta \in \mathscr{L}^2\left(\mathbb{T}^d\right)$ for each fixed $\eta$, this yields $e^{\frac{\gamma}{\varepsilon}\eta} f(\gamma) \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$.

$\Longleftarrow$: Since $e^{\frac{b}{\varepsilon}|\gamma|} f \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$, we can perform the Fourier-transform to get

$$\begin{aligned}
\mathscr{F}_\varepsilon^{-1}\left(e^{\frac{b}{\varepsilon}|\gamma|} f\right) &= \frac{1}{\sqrt{2\pi}^d} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}\gamma\cdot\xi} e^{\frac{b}{\varepsilon}|\gamma|} f(\gamma) = \\
&= \frac{1}{\sqrt{2\pi}^d} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}\gamma\cdot(\xi - ib)} f(\gamma) = \\
&= \mathscr{F}_\varepsilon^{-1} f(\xi - ib)
\end{aligned}$$

Thus $\mathscr{F}_\varepsilon^{-1} f$ has a continuation to $K_b$ and is bounded for each fixed $\xi \in \mathbb{T}^d$. □

## A.2. Simultaneous diagonalization of two quadratic forms

In Chapter 2 we need only the diagonalization of the kinetic energy for x fixed at a critical point $x_j$. Since each symmetric matrix $B(x_j)$ can by use of two orthogonal matrices $P$ and $P^t$ be diagonalized by $P^t B(x_j) P =: B_D$, where $B_D$ is diagonal, we have

$$\langle \xi\,,\, B(x_j)\xi\rangle = \langle \xi\,,\, B_D\xi\rangle = \left\langle B_D^{\frac{1}{2}}\xi\,,\, B_D^{\frac{1}{2}}\xi\right\rangle =: \langle \xi'\,,\, \xi'\rangle\ .$$

Then for $x' = B_D^{\frac{1}{2}} x$

$$\langle x'\,,\, Ax'\rangle = \left\langle B_D^{\frac{1}{2}} x\,,\, AB_D^{\frac{1}{2}} x\right\rangle = \left\langle x\,,\, B_D^{\frac{1}{2}} AB_D^{\frac{1}{2}} x\right\rangle =: \left\langle x\,,\, \tilde{A}x\right\rangle .$$

In Chapter 3, we assumed that the kinetic and potential energy are diagonalized simultaneously, if there is only one well $x_1 = 0$. This can be done as follows.
The symbol of the quadratic part of the kinetic energy at $x = 0$ is given by

$$t_{q0}(\xi) = \langle \xi\,,\, B\xi\rangle\ ,$$

where $B := B(0)$ is a symmetric positive definite matrix. The harmonic part of the potential $V_0^1$ takes the form

$$V_0^1 = \langle x\,,\, Ax\rangle\ ,$$

where the matrix $A$ is symmetric as well. This setting can be reduced to the case, where the quadratic term of both operators is diagonal, as treated in Chapter 3. Since $B$ is symmetric and positive definite, $\langle x\,,\, y\rangle_B := \langle x\,,\, By\rangle$ defines a scalar product for which $t_{q0}$ is already diagonal. Denoting by $C^T$ the matrix for which $\langle Cx\,,\, y\rangle_B = \left\langle x\,,\, C^T y\right\rangle_B$ and by $C^t$ the transposed matrix of $C$, we get $C^T = B^{-1}C^t B$. To be orthogonal with respect to the $B$-scalar product, C therefore has to satisfy the relation $C^{-1} = B^{-1}C^t B$. Since the harmonic part of the potential given above is a quadratic form with form matrix $A$, we can find another matrix $A_B$ representing this form, which is symmetric with respect to $\langle .\,,\, .\rangle_B$ and which therefore can be diagonalized by conjugation with a $B$-orthogonal matrix $C$. We thus have

$$\langle x\,,\, A_B x\rangle_B = \left\langle x\,,\, C^T A_d C x\right\rangle_B = \langle Cx\,,\, A_d Cx\rangle_B = \langle x'\,,\, A_d x'\rangle_B$$

where $A_d := C^T A_B C$ denotes the diagonalized matrix and $x' := Cx$ is an element of the transformed lattice $C(\varepsilon\mathbb{Z})^d$. By this transformation of the $x$-variable, we get the related transformation $\xi' = (C^T)^{-1}\xi = C\xi$ for the momentum variable, which preserves the $B$- scalar product. Expressed in the new variables, we therefore have

$$t_{q0}(\xi') = \langle \xi' \,,\, \xi' \rangle_B \quad \text{and} \quad V_h = \langle x' \,,\, A_d x' \rangle_B = \sum_{\nu=1}^{d} \lambda_\nu^2 x_\nu'^2 \,,$$

where $\lambda_j^2$, $j = 1, \dots d$, are the eigenvalues of $A_d$. Since $C$ does not depend on $\varepsilon$, the estimates given in these notes are not changed by these transformations. For $x \neq 0$, the kinetic energy is of course not diagonal with the chosen transformation.

## A.3. Kinetic Energy as translation operator

At first we determine the inverse Fourier transformed of the translation operator $\tau_{\varepsilon e_\nu}$ to a neighboring lattice point. We have

$$\begin{aligned}
(\mathscr{F}_\varepsilon^{-1}\tau_{\varepsilon e_\nu} u)(\xi) &= \frac{1}{\sqrt{2\pi}^d} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{ix\frac{\xi}{\varepsilon}} \tau_{\varepsilon e_\nu} u(x) = \\
&= \frac{1}{\sqrt{2\pi}^d} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{ix\frac{\xi}{\varepsilon}} u(x+\varepsilon e_\nu) = \frac{1}{\sqrt{2\pi}^d} \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{i(y-\varepsilon e_\nu)\frac{\xi}{\varepsilon}} u(y) = \\
&= \frac{1}{\sqrt{2\pi}^d} e^{-i\xi_\nu} \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{iy\frac{\xi}{\varepsilon}} u(y) = e^{-i\xi_\nu} (\mathscr{F}_\varepsilon^{-1} u)(\xi) \,,
\end{aligned}$$

from which the form of the symbol $t$ in subsection 2.3 follows. Any translation $\tau_\gamma$ can be written as linear combination of these elementary translations, i.e. $\gamma = \sum_{\nu=1}^d \varepsilon k_\nu e_\nu$ for $k_\nu \in \mathbb{Z}$, thus the form (2.20) of $T_\varepsilon$ as translation operator follows from the form (2.17) of the associated symbol. Since in particular

$$\begin{aligned}
T_\varepsilon v(x) = \mathscr{F}_\varepsilon t \mathscr{F}_\varepsilon^{-1} v(x) &= \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}x\xi} t(x,\xi) \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}y\xi} v(y)\, d\xi = \\
= \frac{1}{(2\pi)^d} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} v(x-\gamma) \int_{[-\pi,\pi]^d} &e^{-\frac{i}{\varepsilon}\gamma\xi} t(x,\xi)\, d\xi = \frac{1}{(2\pi)^d} \sum_{\gamma\in(\varepsilon\mathbb{Z})^d} \tau_{-\gamma} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}\gamma\xi} t(x,\xi)\, d\xi\; v(x) \,,
\end{aligned}$$

we have

$$a_{-\gamma}(x) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}\gamma\xi} t(x,\xi)\, d\xi \,. \tag{A.9}$$

Thus $a_{-\gamma} = \mathscr{F}_\varepsilon t$, i.e., $a_\gamma$ is the Fourier transform of the symbol $t \in \mathscr{C}^\infty(\mathbb{T}^d)$ and it follows by Lemma A.1, that $|\gamma|^{\frac{d+1}{2}} a_\gamma$ is square summable with respect to $\gamma$ for each fixed $x \in (\varepsilon\mathbb{Z})^d$. If we assume in addition that the symbol $t$ has an analytic continuation to $\mathbb{C}^d$ (as we do in Hypothesis 4.20) and is bounded in the region $\{z = (\xi + i\eta) \in \mathbb{C}^d \,|\, |\eta| \leq b\}$, then $a_\gamma$ decreases for $|\gamma| \to \infty$ exponentially, i.e. $e^{\frac{|\gamma| b}{\varepsilon}} a_\gamma \in \ell^2((\varepsilon\mathbb{Z})^d)$ as shown in Proposition A.3.

## A.4. Unitary Transformation

To show the unitary equivalence of $H^j$, given by (2.48), to $\varepsilon K_j$ as defined in Theorem 2.10, we define the unitary operators

$$(T(b)k)(x) := k(x-b) \,, \quad (D(\varepsilon)k)(x) := \varepsilon^{\frac{d}{2}} k(\varepsilon x) \,, \quad k \in \mathscr{L}^2(\mathbb{R}^d).$$

Then

$$\begin{aligned}
D\left(\varepsilon^{-\frac12}\right) T\left(\varepsilon^{-\frac12}x_j\right) \varepsilon\, K_j T\left(-\varepsilon^{-\frac12}x_j\right) D\left(\varepsilon^{\frac12}\right) k(x) &= D\left(\varepsilon^{-\frac12}\right) T\left(\varepsilon^{-\frac12}x_j\right) \varepsilon\, K_j \varepsilon^{\frac{d}{4}} k\left(\varepsilon^{-\frac12}x + x_j\right) = \\
= D\left(\varepsilon^{-\frac12}\right) \varepsilon \left(-\varepsilon\Delta + \sum_{kl} A^j_{kl}\left(x - \varepsilon^{-\frac12}x_j\right)_k \left(x - \varepsilon^{-\frac12}x_j\right)_l + V_1(x_j)\right) &\varepsilon^{\frac{d}{4}} k\left(\varepsilon^{-\frac12}x\right) = \\
= \left(-\varepsilon^2\,\Delta + \sum_{kl} A^j_{kl}\,(x-x_j)_k\,(x-x_j)_l + \varepsilon\, V_1(x_j)\right) &k(x) = H^j k(x)
\end{aligned}$$

and the assertion is shown.

.

## A.5. Direct computation of $w_{\alpha\beta} - w_{\beta\alpha}$

We compute directly the difference between the matrix elements $w_{\alpha\beta}$ and $w_{\beta\alpha}$ without using the microlocal calculus.

$$
\begin{aligned}
w_{\alpha\beta} - w_{\beta\alpha} = \frac{1}{2}\Bigg\{ & \sum_{x\in M_{j(\alpha)}\setminus M_{j(\beta)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\beta)}}} a_\gamma(x) v_\beta(x+\gamma) v_\alpha(x) + \\
& + \sum_{x\in M_{j(\beta)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\setminus M_{j(\beta)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) - \\
& - \sum_{x\in M_{j(\beta)}\setminus M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) - \\
& - \sum_{x\in M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\beta)}\setminus M_{j(\alpha)}}} a_\gamma(x) v_\beta(x+\gamma) v_\alpha(x) \Bigg\}
\end{aligned}
$$

The combination of the first with the fourth and the second with the third summand yields

$$
\begin{aligned}
w_{\alpha\beta} - w_{\beta\alpha} = \frac{1}{2}\Bigg\{ & \sum_{x\in M_{j(\alpha)}\setminus M_{j(\beta)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\beta)}\cap M_{j(\alpha)}}} a_\gamma(x) v_\alpha(x) v_\beta(x+\gamma) - \\
& - \sum_{x\in M_{j(\beta)}\cap M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\beta)}\setminus M_{j(\alpha)}}} a_\gamma(x) v_\alpha(x) v_\beta(x+\gamma) + \\
& + \sum_{x\in M_{j(\beta)}\cap M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\setminus M_{j(\beta)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) - \\
& + \sum_{x\in M_{j(\beta)}\setminus M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) \Bigg\}\,. \qquad \text{(A.10)}
\end{aligned}
$$

Since $v_\alpha$ is an eigenfunction of the associated Dirichlet operator, we have

$$
\langle (\mu_\alpha - V) v_\alpha\,,\, v_\beta \rangle_{\ell^2} = \sum_{x\in M_{j(\alpha)}\cap M_{j(\beta)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) \qquad \text{(A.11)}
$$

and therefore we can rewrite the first and third term in (A.10) to get

$$
\begin{aligned}
w_{\alpha\beta} - w_{\beta\alpha} \quad = \quad & \frac{1}{2}\Bigg\{ \sum_{x\in M_{j(\alpha)}\setminus M_{j(\beta)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x) v_\alpha(x) v_\beta(x+\gamma) - \langle (\mu_\beta - V) v_\beta\,,\, v_\alpha \rangle_{\ell^2} + \\
+ \quad & \sum_{x\in M_{j(\beta)}\cap M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x) v_\alpha(x) v_\beta(x+\gamma) + \langle (\mu_\alpha - V) v_\alpha\,,\, v_\beta \rangle_{\ell^2} - \\
- \quad & \sum_{x\in M_{j(\beta)}\cap M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) - \\
- \quad & \sum_{x\in M_{j(\beta)}\setminus M_{j(\alpha)}} \sum_{\substack{\gamma \\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x) v_\beta(x) v_\alpha(x+\gamma) \Bigg\}\,.
\end{aligned}
$$

Combining the first with the third and the fifth with the sixth term, this yields

$$\frac{1}{2}\left\{(\mu_\alpha-\mu_\beta)\langle v_\alpha\,,\,v_\beta\rangle_{\ell^2}+\sum_{x\in M_{j(\alpha)}}\sum_{\substack{\gamma\\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x)v_\alpha(x)v_\beta(x+\gamma)-\right.$$

$$\left.-\sum_{x\in M_{j(\beta)}}\sum_{\substack{\gamma\\ x+\gamma\in M_{j(\alpha)}\cap M_{j(\beta)}}} a_\gamma(x)v_\beta(x)v_\alpha(x+\gamma)\right\}\,. \tag{A.12}$$

By the substitution $\tilde{x}=x+\gamma$ and $\tilde{\gamma}=-\gamma$ in the last two terms and by using the symmetry relation $a_\gamma(x)=a_{-\gamma}(x+\gamma)$, the term (A.12) is equal to

$$\frac{1}{2}(\mu_\alpha-\mu_\beta)\langle v_\alpha\,,\,v_\beta\rangle_{\ell^2}\quad+\sum_{\tilde{x}\in M_{j(\alpha)}\cap M_{j(\beta)}}\sum_{\substack{\tilde{\gamma}\\ \tilde{x}+\tilde{\gamma}\in M_{j(\alpha)}}} a_{\tilde{\gamma}}(\tilde{x})v_\beta(\tilde{x})v_\alpha(\tilde{x}+\tilde{\gamma})-$$

$$-\sum_{\tilde{x}\in M_{j(\beta)}\cap M_{j(\alpha)}}\sum_{\substack{\tilde{\gamma}\\ \tilde{x}+\tilde{\gamma}\in M_{j(\beta)}}} a_{\tilde{\gamma}}(\tilde{x})v_\alpha(\tilde{x})v_\beta(\tilde{x}+\tilde{\gamma})\,.$$

Using again (A.11), we therefore can conclude

$$w_{\alpha\beta}-w_{\beta\alpha}=(\mu_\alpha-\mu_\beta)\langle v_\alpha\,,\,v_\beta\rangle_{\ell^2}\,.$$

## A.6. Direct proof of Lemma 2.12

Lemma 2.12 can also be proven without using the symbolic calculus introduced in Appendix B in the following way.

Proof:
(a):
Since by definition, $\sum_{j=0}^m \chi_j^2$ is a partition of $\mathbf{1}$, we can split $H_\varepsilon$ as

$$H_\varepsilon=\frac{1}{2}\sum_{j=0}^m\chi_j^2\,H_\varepsilon+\frac{1}{2}H_\varepsilon\sum_{j=0}^m\chi_j^2=\sum_{j=0}^m\chi_j\,H_\varepsilon\,\chi_j+\frac{1}{2}\sum_{j=0}^m[\chi_j,[\chi_j,H_\varepsilon]]\,. \tag{A.13}$$

To show the assertion, we thus have to estimate the double commutator. By the action of $T_\varepsilon$ as translation operator in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ as described in (2.20), we calculate

$$[\chi,[\chi,\tau_\gamma]]=\chi^2\tau_\gamma+\tau_\gamma\chi^2-2\chi\tau_\gamma\chi=(\chi-(\tau_\gamma\chi))^2\tau_\gamma\,.$$

Thus for $\psi\in\ell^2((\varepsilon\mathbb{Z})^d)$

$$\langle\psi\,,\,[\chi_j,[\chi_j,H_\varepsilon]]\,\psi\rangle_{\ell^2}=\left\langle\psi\,,\,\textstyle\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}a_\gamma(\chi_j-(\tau_\gamma\chi_j))^2\tau_\gamma\psi\right\rangle_{\ell^2}\leq$$

$$\leq\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}\|a_\gamma\|_\infty\,\|\chi_j-(\tau_\gamma\chi_j)\|_\infty^2\,\|\psi\|_{\ell^2}^2\,. \tag{A.14}$$

Using the Taylor expansion to first order with the notation $\chi_j(x)=\tilde{\chi}_j(\varepsilon^{-\frac{2}{5}}x)$ and the fact that $\frac{|\gamma|}{\varepsilon}$ is integer, we have with a suitable $\eta\in(0,1)$

$$\|\chi_j(x)-\chi_j(x+\gamma)\|^2=\varepsilon^{\frac{6}{5}}\left(\frac{|\gamma|}{\varepsilon}\right)^2\left\|\sum_{\nu=1}^d(\partial_\nu\tilde{\chi}_j)(x+\eta\gamma)\right\|^2\,.$$

The coefficient $\frac{|\gamma|}{\varepsilon}\in\mathbb{Z}$ is not bounded, because the transitions are allowed to be of any length. To estimate the right hand side of (A.14), we thus have to include the decrease of $a_\gamma(x)$ in $\gamma$. It follows from the smoothness of $t_\pi$ and the form (A.9), that $a_\gamma(x)$ decreases faster than $(1+\frac{|\gamma|}{\varepsilon})^{-N}$ for increasing $|\gamma|$ and for all $N\in\mathbb{N}$ (Lemma A.1). Thus the series $\sum_{|\gamma|}a_\gamma(x)\left(\frac{|\gamma|}{\varepsilon}\right)^2$ is convergent and

$$\sum_{\gamma\in(\varepsilon\mathbb{Z})^d}\|a_\gamma\|_\infty\,\|\chi_j-\tau_\gamma\chi_j\|_\infty^2\,\|\psi\|_{\ell^2}^2=O\left(\varepsilon^{\frac{6}{5}}\right)\|\psi\|_{\ell^2}^2\,.$$

Then

$$\|\,[\chi_j,[\chi_j,T_\varepsilon]]\,\|=O\left(\varepsilon^{\frac{6}{5}}\right)$$

and point (a) of the lemma is proven.
(b):
By a splitting similar to (A.13) we have

$$T_\varepsilon + \tilde{V}_\varepsilon^j = \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_0)(T_\varepsilon + \tilde{V}_\varepsilon^j)\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_0) + \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_1)(T_\varepsilon + \tilde{V}_\varepsilon^j)\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_1) + \\ + \frac{1}{2}\sum_{k=0}^{1}\left[\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_k), [\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde{\phi}_k), (T_\varepsilon + \tilde{V}_\varepsilon^j)]\right]\,. \quad \text{(A.15)}$$

We first consider the double commutator $\left[\tilde{\phi}_k, [\tilde{\phi}_k, \mathscr{F}_\varepsilon^{-1}\tilde{V}_\varepsilon^j\mathscr{F}_\varepsilon]\right]$. The constant term keeps constant under the conjugation and therefore commutes with $\tilde{\phi}_k$. By (2.4) we have

$$(\mathscr{F}_\varepsilon^{-1}\tilde{V}_\varepsilon^j\psi)(\xi) = \frac{1}{\sqrt{2\pi}^d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\left(e^{-\frac{i}{\varepsilon}\xi x}\sum_{\nu,\mu=1}^{d}\tilde{A}_{\nu\mu}^j x_\nu x_\mu \psi(x)\right)\,.$$

Using the identity $\partial_\xi e^{-\frac{i}{\varepsilon}\xi x} = -\frac{i}{\varepsilon}x e^{-\frac{i}{\varepsilon}\xi x}$ we can continue

$$\frac{1}{\sqrt{2\pi}^d}\sum_{x\in(\varepsilon\mathbb{Z})^d}\left(\sum_{\nu,\mu=1}^{d}\tilde{A}_{\nu\mu}^j(-\varepsilon^2)\left(\partial_{\xi_\nu}\partial_{\xi_\mu}e^{-\frac{i}{\varepsilon}\xi x}\right)\psi(x)\right) = -\varepsilon^2\sum_{\nu,\mu=1}^{d}\tilde{A}_{\nu\mu}^j\partial_\nu\partial_\mu(\mathscr{F}_\varepsilon^{-1}\psi)(\xi)\,,$$

where for the last equality we changed summation and differentiation. We have

$$[\tilde{\phi}(\xi), [\tilde{\phi}(\xi), \partial_\nu\partial_\mu]] = \tilde{\phi}^2(\xi)\partial_\nu\partial_\mu + \partial_\nu\partial_\mu\tilde{\phi}^2(\xi) - 2\tilde{\phi}(\xi)\partial_\nu\partial_\mu\tilde{\phi}(\xi) = \\ = 2\tilde{\phi}^2(\xi)\partial_\nu\partial_\mu + 2\tilde{\phi}(\xi)\partial_\nu\tilde{\phi}(\xi)\partial_\mu + 2\tilde{\phi}(\xi)\partial_\mu\tilde{\phi}(\xi)\partial_\nu + 2(\partial_\nu\tilde{\phi}(\xi))(\partial_\mu\tilde{\phi}(\xi)) + 2\tilde{\phi}(\xi)(\partial_\nu\partial_\mu\tilde{\phi}(\xi)) - \\ - 2(\partial_\nu\partial_\mu\tilde{\phi}(\xi)) - 2\tilde{\phi}(\xi)(\partial_\nu\tilde{\phi}(\xi))\partial_\mu - 2\tilde{\phi}(\xi)(\partial_\mu\tilde{\phi}(\xi))\partial_\nu - 2\tilde{\phi}^2(\xi)\partial_\nu\partial_\mu = 2(\partial_\nu\tilde{\phi}(\xi))(\partial_\mu\tilde{\phi}(\xi))\,,$$

With $\tilde{\phi}_k(\xi) =: \tilde{\tilde{\phi}}_k(\varepsilon^{-\frac{2}{5}}\xi)$ we thus can deduce for $\psi \in \ell^2((\varepsilon\mathbb{Z})^d)$ that

$$\left\langle \mathscr{F}_\varepsilon^{-1}\psi(\xi)\,,\,\left[\tilde{\phi}_k, [\tilde{\phi}_k, (\mathscr{F}_\varepsilon^{-1}\tilde{V}_\varepsilon^j\mathscr{F}_\varepsilon)]\right]\mathscr{F}_\varepsilon^{-1}\psi(\xi)\right\rangle_{\mathbb{T}} = \quad \text{(A.16)} \\ = 2\varepsilon^{\frac{6}{5}}\sum_{\nu,\mu=1}^{d}\tilde{A}_{\nu\mu}^j\left\langle \mathscr{F}_\varepsilon^{-1}\psi(\xi)\,,\,(\partial_\nu\tilde{\tilde{\phi}}_k)(\partial_\mu\tilde{\tilde{\phi}}_k)\mathscr{F}_\varepsilon^{-1}\psi(\xi)\right\rangle_{\mathbb{T}}\,.$$

Since the derivatives of $\tilde{\phi}_k$ are bounded by definition, it follows by (A.16) that

$$\left[\tilde{\phi}_k, [\tilde{\phi}_k, (\mathscr{F}_\varepsilon^{-1}\tilde{V}_\varepsilon^j\mathscr{F}_\varepsilon)]\right] = O\left(\varepsilon^{\frac{6}{5}}\right)\,.$$

To treat the double commutator $\left[\tilde{\phi}_k(\xi), [\tilde{\phi}_k(\xi), T_\varepsilon]\right]$, we have by Lemma B.10 to analyze the commutator with $a_\gamma(\varepsilon D_\xi)$. To this end, we write $a_\gamma(\varepsilon D_\xi) = a_{1\gamma}\varepsilon D_\xi + a_{2\gamma}\varepsilon^2 D_\xi^2 + O(D_\xi^3)$. For the first term

$$[\tilde{\phi}_k(\xi), [\tilde{\phi}_k(\xi), a_{1\gamma}\varepsilon D_\xi]] = \varepsilon\left(\tilde{\phi}_k^2(\xi)D_\xi - 2\tilde{\phi}_k(\xi)D_\xi\tilde{\phi}_k(\xi) + D_\xi\tilde{\phi}_k^2(\xi)\right) = 0\,.$$

For the second term, the estimates are the same as for $\tilde{V}_\varepsilon^j$ and for higher orders of derivatives they are even better. Therefore by (A.15) the assertion (b) of the lemma is shown. □

## A.7. Valuation on $\mathcal{K}_{\frac{1}{2}}$

Let $v_\varepsilon : \mathcal{K}_{\frac{1}{2}} \to \mathbb{R}_0^+$ be a real-valued function, defined by $v_\varepsilon(k) := \varepsilon^n$ for $k = \sum_{j\in\frac{\mathbb{N}^*}{2},\, j\geq n}\varepsilon^j k_j$ and $v_\varepsilon(0) := 0$. To be a valuation on $\mathcal{K}_{\frac{1}{2}}$, $v_\varepsilon$ must have the following properties for all $k, l \in \mathcal{K}_{\frac{1}{2}}$:

1) $v_\varepsilon(k) = 0$ if and only if $k = 0$,
2) $v_\varepsilon(k + l) \leq \max\{v_\varepsilon(k), v_\varepsilon(l)\}$,
3) $v_\varepsilon(kl) = v_\varepsilon(k)v_\varepsilon(l)$.

These properties of $v_\varepsilon$ can be verified by direct calculation.
We call $v_\varepsilon$ the $\varepsilon$-adic valuation on $\mathcal{K}_{\frac{1}{2}}$ and define the $\varepsilon$-norm on $\mathcal{V}$ by

$$\|p\|_{\mathcal{V}} := (v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}}))^{\frac{1}{2}}\,, \qquad p \in \mathcal{V}. \tag{A.17}$$

The $\varepsilon$-norm has the properties of a norm, i.e.

(a) $\|p\|_{\mathcal{V}} \geq 0$:
$v_\varepsilon(k) \geq 0$ for all $k \in \mathcal{K}_{\frac{1}{2}}$.
(b) $\|p\|_{\mathcal{V}} = 0$ if and only if $p = 0$:
1) and $(\langle p\,,\, p\rangle_{\mathcal{V}} = 0 \Leftrightarrow p = 0)$.
(c) $\|kp\|_{\mathcal{V}} = v_\varepsilon(k)\|p\|_{\mathcal{V}}$ for all $k \in \mathcal{K}_{\frac{1}{2}}, p \in \mathcal{V}$:
from the definition of the scalar product in $\mathcal{V}$ we get $\|kp\|_{\mathcal{V}} = (v_\varepsilon(k^2\langle p\,,\, p\rangle_{\mathcal{V}})^{\frac{1}{2}}$. By 3) this is equal to $(v_\varepsilon(k^2)v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}}))^{\frac{1}{2}} = v(k)\|p\|_{\mathcal{V}}$.
(d) $\|p+q\|_{\mathcal{V}} \leq \|p\|_{\mathcal{V}} + \|q\|_{\mathcal{V}}$ for all $p, q \in \mathcal{V}$.
By the linearity of the scalar product and 2)

$$\begin{aligned}\|p+q\|_{\mathcal{V}} &= (v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}} + \langle p\,,\, q\rangle_{\mathcal{V}} + \langle q\,,\, p\rangle_{\mathcal{V}} + \langle q\,,\, q\rangle_{\mathcal{V}}))^{\frac{1}{2}} \leq \\ &\leq (\max\{v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}}), v_\varepsilon(\langle p\,,\, q\rangle_{\mathcal{V}}), v_\varepsilon(\langle q\,,\, p\rangle_{\mathcal{V}}), v_\varepsilon(\langle q\,,\, q\rangle_{\mathcal{V}})\})^{\frac{1}{2}}. \end{aligned} \tag{A.18}$$

From the definition of the scalar product we get

$$\min\{v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}}), v_\varepsilon(\langle q\,,\, q\rangle_{\mathcal{V}})\} \leq v_\varepsilon(\langle p\,,\, q\rangle_{\mathcal{V}}), v_\varepsilon(\langle q\,,\, p\rangle_{\mathcal{V}}) \leq \max\{v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}}), v_\varepsilon(\langle q\,,\, q\rangle_{\mathcal{V}})\}.$$

Thus the last term in equation (A.18) is equal to

$$\max\{v_\varepsilon(\langle p\,,\, p\rangle_{\mathcal{V}})^{\frac{1}{2}}, v_\varepsilon(\langle q\,,\, q\rangle_{\mathcal{V}})^{\frac{1}{2}}\} = \max\{\|p\|_{\mathcal{V}}, \|q\|_{\mathcal{V}}\} \leq \|p\|_{\mathcal{V}} + \|q\|_{\mathcal{V}}.$$

For an operator $T$ on $\mathcal{V}$ we define the $\varepsilon$-norm by $\|T\|_{\mathcal{V}} := \sup_{p\in\mathcal{V}} \frac{\|Tp\|_{\mathcal{V}}}{\|p\|_{\mathcal{V}}}$. Because $\|\,.\,\|_{\mathcal{V}}$ obeys all the properties of a norm, we can deduce that $M : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$, defined by

$$M(u, v) := (v_\varepsilon(\langle u - v\,,\, u - v\rangle_{\mathcal{V}}))^{\frac{1}{2}}\ ,$$

is a metric on $\mathcal{V}$, which therefore is a metric space.

APPENDIX B

# Symbolic Calculus in the discrete setting

We introduce the notion of symbolic calculus including the small parameter $\varepsilon \in (0,1]$, where the symbols are allowed to include $\varepsilon$ not only directly but also as scaling parameter, as described in [**16**]. Since the phase space is given by $(\varepsilon\mathbb{Z})^d \times \mathbb{T}^d$, the relation between the operators and their symbols is given by use of the discrete Fourier transformation defined in (2.4),(2.3).
For the general theory of microlocal analysis, we refer to [**24**], [**50**] and [**41**], where symbol spaces and spaces of associated pseudo-differential operators are introduced.
The calculus introduced in the following sections allows, to given norm estimates of the difference between $T_\varepsilon$ and the approximating operator $T_{\varepsilon qj}$ defined in (2.29) for each fixed potential minimum $x_j$.

## B.1. Pseudo-differential operators on the lattice $(\varepsilon\mathbb{Z})^d$

DEFINITION B.1. (a) *A function $m : \mathbb{R}^d \times \mathbb{T}^d \to [0,\infty)$ is called an order function, if there exist constants $C_0, N_1 > 0$, such that*

$$m(x,\xi) \leq C_0 \langle x-y\rangle^{N_1} m(y,\eta)\,, \qquad x,y \in \mathbb{R}^d,\ \xi,\eta \in \mathbb{T}^d\,,$$

*where we used the notation $\langle x\rangle := \sqrt{1+|x|^2}$.*

(b) *For an order function $m$ on $\mathbb{R}^d \times \mathbb{T}^d$, the symbol space $S(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ consists of all $a \in \mathscr{C}^\infty(\mathbb{R}^d \times \mathbb{T}^d)$, for which for all $\alpha,\beta \in \mathbb{N}^d$ there is a constant $C_{\alpha,\beta}$ such that*

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \leq C_{\alpha,\beta} m(x,\xi)\,, \qquad x \in \mathbb{R}^d,\ \xi \in \mathbb{T}^d\,,$$

*where as usual $\partial_x^\alpha := \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d}$. We often write $S(m)$, if the underlying space is clear.*

(c) *The Fréchet-Semi-Norms of a symbol $a \in S(m)$ are defined as*

$$\|a\|_{\alpha,\beta} := \sup_{x,\xi} \frac{|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)|}{m(x,\xi)}\,.$$

(d) *If the symbol $a(x,\xi;\varepsilon)$ depends on a small parameter $\varepsilon \in (0,1]$, a is said to be in $S(m)$, if $a(\cdot\,;\varepsilon)$ is uniformly bounded in $S(m)$ for $\varepsilon$ varying in $(0,1]$. Let $S^k(m) := \varepsilon^k S(m)$ describe for $k \in \mathbb{R}$ the space of symbols of the form $\varepsilon^k a(x,\xi;\varepsilon)$ for $a \in S(m)$. For $\delta \in [0,1]$, the space $S^k_\delta(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ consists of functions $a(x,\xi;\varepsilon)$ on $\mathbb{R}^d \times \mathbb{T}^d \times (0,1]$, belonging to $S(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ for every fixed $\varepsilon$ and satisfying*

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi;\varepsilon)| \leq C_{\alpha,\beta} m(x,\xi)\varepsilon^{k-\delta(|\alpha|+|\beta|)}\,, \quad x \in \mathbb{R}^d,\ \xi \in \mathbb{T}^d\,.$$

(e) *Let $a_j \in S^{k_j}_\delta(m), k_j \nearrow \infty$, then we write $a \sim \sum_{j=0}^\infty a_j$ if $a - \sum_{j=0}^N a_j \in S^{k_{N+1}}_\delta(m)$ for every $N \in \mathbb{N}$.*

(f) *A pseudo-differential operator $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a) : \mathcal{K}\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow \mathcal{K}'\left((\varepsilon\mathbb{Z})^d\right)$ is defined by*

$$\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)v(x) := (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi} a(x,\xi;\varepsilon)v(y)\,d\xi\,, \tag{B.1}$$

*where $a \in S^k_\delta(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$,*

$$\mathcal{K}\left((\varepsilon\mathbb{Z})^d\right) := \{u : (\varepsilon\mathbb{Z})^d \to \mathbb{C} \mid u \text{ has compact support}\}$$

*and $\mathcal{K}'\left((\varepsilon\mathbb{Z})^d\right)$ denotes its dual with respect to $\langle\,.\,,\,.\,\rangle_{\ell^2}$.*

In the following, some properties of the symbols and operators of definition B.1 are collected.

LEMMA B.2. *Let $a \in S^0_\delta(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ and*

$$s\left((\varepsilon\mathbb{Z})^d\right) := \left\{ u : (\varepsilon\mathbb{Z})^d \to (\varepsilon\mathbb{Z})^d \;\middle|\; \|u\|_\alpha := \sup_{x\in(\varepsilon\mathbb{Z})^d} \sum_{j=1}^d \left|x_j^{\alpha_j} u(x)\right| < \infty,\, \alpha \in \mathbb{N}^d \right\}.$$

*We consider on $s$ the natural topology $\tau$ associated to the family of semi-norms $\|\cdot\|_\alpha$.*
*Then the operator $A$ associated to $a$ defined in* (B.1) *is continuous : $s\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow s\left((\varepsilon\mathbb{Z})^d\right)$ with respect to $\tau$.*

Proof:
We start proving, that $A : s\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow l^\infty\left((\varepsilon\mathbb{Z})^d\right)$, where $l^\infty\left((\varepsilon\mathbb{Z})^d\right)$ denotes the bounded functions on $(\varepsilon\mathbb{Z})^d$. By use of the operator

$$L_1(y-x,\xi) := \frac{1-\varepsilon^2\Delta_\xi}{1+|y-x|^2} = \frac{1-\varepsilon^2\Delta_\xi}{\langle y-x\rangle^2}\,, \tag{B.2}$$

for which $L_1(y-x,\xi)e^{\frac{i}{\varepsilon}(y-x)\xi} = e^{\frac{i}{\varepsilon}(y-x)\xi}$, we have for $u \in s\left((\varepsilon\mathbb{Z})^d\right)$ and $a \in \mathscr{S}\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ (the space of Schwartz-functions on $\mathbb{R}^d \times \mathbb{T}^d$), by repeated partial integration

$$\begin{aligned}
|Au(x)| &= \left|(2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} \left(L_1^k(y-x,\xi)e^{\frac{i}{\varepsilon}(y-x)\xi}\right) a(x,\xi;\varepsilon)u(y)\,d\xi\right| \\
&\le (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} \left|\frac{e^{\frac{i}{\varepsilon}(y-x)\xi}}{\langle y-x\rangle^{2k}} \left(1-\varepsilon^2\Delta_\xi\right)^k a(x,\xi;\varepsilon)u(y)\right| d\xi \\
&\le c_a(2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \frac{|u(y)|}{\langle y-x\rangle^{2k}} \int_{[-\pi,\pi]^d} |m(x,\xi)|\,d\xi\,.
\end{aligned}$$

In the second step, we used that the boundary terms vanish, since $a(x,\ .\ ;\varepsilon)$ is $2\pi$-periodic. By definition there exist $C, N_0 > 0$ such that

$$m(x,\xi) \le C\langle y-x\rangle^{N_0}\langle y\rangle^{N_0} m(0,0)\,.$$

We therefore can conclude with the substitution $y' = y - x$

$$\begin{aligned}
|Au(x)| &\le \frac{c_a}{2\pi^d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \frac{|u(y)|}{\langle y-x\rangle^{2k}} \int_{[-\pi,\pi]^d} |m(x,\xi)|\,d\xi \\
&\le \tilde{c}_a \sum_{y\in(\varepsilon\mathbb{Z})^d} \langle y\rangle^{N_0}|u(y)|\langle y-x\rangle^{N_0-2k} \\
&\le \tilde{\tilde{c}}_a \sup_{y\in(\varepsilon\mathbb{Z})^d} \left(\langle y\rangle^{N_0}|u(y)|\right) \sum_{y'\in(\varepsilon\mathbb{Z})^d} \langle y'\rangle^{N_0-2k} \int_{[-\pi,\pi]^d} \langle\xi\rangle^{N_0} d\xi \\
&\le C_{a,\varepsilon} \sup_{\substack{\alpha\in\mathbb{N}^d \\ |\alpha|\le N_0}} \|u\|_\alpha
\end{aligned}$$

for $k$ big enough. Therefore $\sup_{x\in(\varepsilon\mathbb{Z})^d} |Au(x)| < \infty$ and A is uniformly continuous $s\left((\varepsilon\mathbb{Z})^d\right) \to l^\infty\left((\varepsilon\mathbb{Z})^d\right)$ for $a$ varying in a bounded set in $S^0_\delta(m)$ and by a density argument for $a \in S^0_\delta(m)$.
To show that $A : s\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow s\left((\varepsilon\mathbb{Z})^d\right)$, we estimate for $u \in s\left((\varepsilon\mathbb{Z})^d\right)$

$$\left|\langle x\rangle^l Au(x)\right| = \sum_{y\in(\varepsilon\mathbb{Z})^d} (2\pi)^{-d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi}\langle x\rangle^l a(x,\xi;\varepsilon)u(y)\,d\xi\,.$$

If the supremum of this term is finite, we can deduce that $Au \in s\left((\varepsilon\mathbb{Z})^d\right)$. By definition we have for $a \in S^0_\delta(m)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$

$$\begin{aligned}\left|\partial^p_{x_\nu}\left(\langle x\rangle^l a(x,\xi;\varepsilon)\right)\right| &= \left|\sum_{m'+m''=p}\left(\partial^{m'}_{x_\nu}\langle x\rangle^l\right)\left(\partial^{m''}_{x_\nu}a(x,\xi;\varepsilon)\right)\right| \\ &\leq \left|\varepsilon^{-p\delta}m(x,\xi)c_l\langle x\rangle^l + \sum_{j<p}\varepsilon^{-j\delta}m(x,\xi)\sum_{k\leq l}c_k x^k\right| \\ &\leq C_p m(x,\xi)\varepsilon^{-p\delta}\langle x\rangle^l\,.\end{aligned}$$

With the new order function $m_l(x,\xi) := m(x,\xi)\langle x\rangle^l$, this yields $\langle x\rangle^l a(x,\xi;\varepsilon) \in S^0_\delta(m_l)\left(\mathbb{R}^d \times \mathbb{T}^d\right)$. Since the boundedness was shown for all order functions $m$, we can conclude by induction $Au(x) \in s\left((\varepsilon\mathbb{Z})^d\right)$. Furthermore for any $\alpha \in \mathbb{N}^d$, there exists $C_\alpha$, $N_\alpha$ such that

$$\|Au\|_\alpha \leq C_\alpha \sup_{|\beta|\leq N_\alpha}\|u\|_\beta\,,\quad u \in s\left((\varepsilon\mathbb{Z})^d\right)\,.$$

Thus the mapping is continuous.

□

In order to prove the subsequent lemmata, we introduce the convolution and $\delta$-distribution in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ and $\mathscr{L}^2\left(\mathbb{T}^d\right)$. We denote by

$$u *_\varepsilon v(x) := \sum_{y\in(\varepsilon\mathbb{Z})^d} u(y)v(x-y)\,,\qquad u,v \in \ell^2\left((\varepsilon\mathbb{Z})^d\right) \tag{B.3}$$

the convolution on $(\varepsilon\mathbb{Z})^d$ and by

$$f *_\pi g(\xi) := \int_{[-\pi,\pi]^d} f(\eta)g(\xi-\eta)\,d\eta\,,\qquad f,g \in \mathscr{L}^2\left(\mathbb{T}^d\right) \tag{B.4}$$

the convolution on the $d$-dimensional torus. In addition we introduce $\delta$-distributions adapted to the discrete calculus. Let

$$\delta_\varepsilon(x) := \begin{cases} 1 & \text{for } x=0 \\ 0 & \text{otherwise}\end{cases}\,. \tag{B.5}$$

Then $\sum_{x\in(\varepsilon\mathbb{Z})^d} u(x)\delta_\varepsilon(x) = u(0)$ and we can represent this distribution by

$$\delta_\varepsilon(x) = (2\pi)^{-d}\int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}x\xi}d\xi\,, \tag{B.6}$$

as can be seen by direct calculation. The distribution $\delta_\pi$ defined by the relation

$$(2\pi)^{-d}\int_{[-\pi,\pi]^d}\delta_\pi(\eta)f(\eta)\,d\eta := f(0)\,, \tag{B.7}$$

can be written as

$$\delta_\pi(\eta) = \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\eta} \tag{B.8}$$

by use of $\mathscr{F}_\varepsilon{\mathscr{F}_\varepsilon}^{-1} = \mathbf{1}$.

Lemma B.3. *Let $u,v \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ and $f,g \in \mathscr{L}^2\left(\mathbb{T}^d\right)$. Let $*_\varepsilon$ and $*_\pi$ as defined in (B.3) and (B.4). Then*

(a) $((\mathscr{F}_\varepsilon f) *_\varepsilon (\mathscr{F}_\varepsilon g))(x) = (2\pi)^{\frac{d}{2}}\left(\mathscr{F}_\varepsilon(f\cdot g)\right)(x)\,.$
(b) $\left(\mathscr{F}_\varepsilon(f *_\pi g)\right)(x) = (2\pi)^{\frac{d}{2}}\left((\mathscr{F}_\varepsilon f)\cdot(\mathscr{F}_\varepsilon g)\right)(x)\,.$
(c) $\left({\mathscr{F}_\varepsilon}^{-1}(u *_\varepsilon v)\right)(\xi) = (2\pi)^{\frac{d}{2}}\left(({\mathscr{F}_\varepsilon}^{-1}u)\cdot(\mathscr{F}^{-1}v)\right)(\xi)\,.$
(d) $\left(({\mathscr{F}_\varepsilon}^{-1}u) *_\pi ({\mathscr{F}_\varepsilon}^{-1}v)\right)(\xi) = (2\pi)^{\frac{d}{2}}\left({\mathscr{F}_\varepsilon}^{-1}(u\cdot v)\right)(\xi)\,.$

Proof:

(a)

$$\begin{aligned}
((\mathscr{F}_\varepsilon f) *_\varepsilon (\mathscr{F}_\varepsilon g))(x) &= \sum_{y\in(\varepsilon\mathbb{Z})^d} (\mathscr{F}_\varepsilon f)(y)(\mathscr{F}_\varepsilon g)(x-y) \\
&= \sum_{y\in(\varepsilon\mathbb{Z})^d} (2\pi)^{-d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}y\xi} f(\xi)\,d\xi \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}(x-y)\eta} g(\eta)\,d\eta \\
&= (2\pi)^{-d} \iint_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}x\eta} f(\xi) g(\eta) \delta_\pi(\eta-\xi)\,d\eta d\xi = \\
&= \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}x\xi} f(\xi) g(\xi)\,d\xi \\
&= (2\pi)^{\frac{d}{2}} \left(\mathscr{F}_\varepsilon(f\cdot g)\right)(x)
\end{aligned}$$

(b)

$$\begin{aligned}
\left(\mathscr{F}_\varepsilon(f *_\pi g)\right)(x) &= \left(\mathscr{F}_\varepsilon \int_{[-\pi,\pi,]^d} f(\eta) g(\xi-\eta)\,d\eta\right)(x) \\
&= (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}x\xi} \int_{[-\pi,\pi,]^d} f(\eta) g(\xi-\eta)\,d\eta\xi \\
&= (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} d\eta\, f(\eta) \int_{[-\pi,\pi,]^d} d\mu\, e^{-\frac{i}{\varepsilon}x(\mu+\eta)} g(\mu) \\
&= (2\pi)^{-\frac{d}{2}} \int_{[-\pi,\pi]^d} d\eta\, e^{-\frac{i}{\varepsilon}x\eta} f(\eta) \int_{[-\pi,\pi,]^d} d\mu\, e^{-\frac{i}{\varepsilon}x\mu} g(\mu) \\
&= (2\pi)^{\frac{d}{2}} \left((\mathscr{F}_\varepsilon f)\cdot(\mathscr{F}_\varepsilon g)\right)(x)\,.
\end{aligned}$$

(c)

$$\begin{aligned}
\left(\mathscr{F}_\varepsilon^{-1}(u *_\varepsilon v)\right)(\xi) &= \left(\mathscr{F}_\varepsilon^{-1} \sum_{y\in(\varepsilon\mathbb{Z})^d} u(y) v(x-y)\right)(\xi) \\
&= (2\pi)^{-\frac{d}{2}} \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\xi} \sum_{y\in(\varepsilon\mathbb{Z})^d} u(y) v(x-y) \\
&= (2\pi)^{-\frac{d}{2}} \sum_{y\in(\varepsilon\mathbb{Z})^d} u(y) \sum_{z\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}(z+y)\xi} v(z) \\
&= (2\pi)^{-\frac{d}{2}} \sum_{y\in(\varepsilon\mathbb{Z})^d} u(y) e^{\frac{i}{\varepsilon}y\xi} \sum_{z\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}z\xi} v(z) \\
&= (2\pi)^{\frac{d}{2}} \left((\mathscr{F}_\varepsilon^{-1} u)\cdot(\mathscr{F}_\varepsilon^{-1} v)\right)(\xi)
\end{aligned}$$

(d)

$$\begin{aligned}
\left((\mathscr{F}_\varepsilon^{-1} u) *_\pi (\mathscr{F}_\varepsilon^{-1} v)\right)(\xi) &= \int_{[-\pi,\pi]^d} d\eta (\mathscr{F}_\varepsilon^{-1} u)(\eta)(\mathscr{F}_\varepsilon^{-1} v)(\xi-\eta) \\
&= (2\pi)^{-d} \int_{[-\pi,\pi]^d} d\eta \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\eta} u(x) \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}y(\xi-\eta)} v(y) \\
&= (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \sum_{x\in(\varepsilon\mathbb{Z})^d} u(x) v(y) \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y\xi+(x-y)\eta)}\,d\eta \\
&= \sum_{x\in(\varepsilon\mathbb{Z})^d} u(x) \sum_{y\in(\varepsilon\mathbb{Z})^d} v(y) e^{\frac{i}{\varepsilon}y\xi}\,\delta_\varepsilon(y-x) \\
&= \sum_{x\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}x\xi} u(x) v(x) \\
&= (2\pi)^{\frac{d}{2}} \left(\mathscr{F}_\varepsilon^{-1}(u\cdot v)\right)(\xi)\,.
\end{aligned}$$

□

## B.2. Stationary phase and applications

The following lemma describes the method of stationary phase in a special case, which is an important tool in the subsequent proofs.

LEMMA B.4. *Denote $D_x = -i\partial_x(= -i\nabla_x)$, then for any $N \in \mathbb{N}$ there exists a constant $C_N$, such that, for any $\varepsilon \in (0, \varepsilon_0]$, $u \in \mathscr{C}_0^\infty\left(\mathbb{R}^d \times \mathbb{T}^d\right)$,*

$$\sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\eta\, e^{-\frac{i}{\varepsilon}z\eta} u(z,\eta) = (2\pi)^d \sum_{k=0}^{N-1} \frac{1}{k!} \left( (i\varepsilon D_z \cdot D_\eta)^k u \right)(z,\eta)|_{\substack{z=0\\ \eta=0}} + S_N(u,\varepsilon)$$

*with*

$$|S_N(u,\varepsilon)| \leq \frac{C}{N!}\, \varepsilon^N \sum_{|\alpha+\beta|\leq 2d+1} \|\partial_z^\alpha \partial_\eta^\beta (\partial_z \cdot \partial_\eta)^N u\|_1 \,,$$

*where* $\|\,.\,\|_1 := \|\,.\,\|_{l^1((\varepsilon\mathbb{Z})^d)\times\mathscr{L}^1(\mathbb{T})}$.

Proof:
For the function $f(\mu, y) := e^{-\frac{i}{\varepsilon}y\mu}$, the Fourier transform is given by

$$\left(\mathscr{F}_{\varepsilon\,\mu\to z} \mathscr{F}^{-1}_{\varepsilon\,y\to\eta} f\right)(z,\eta) = e^{-\frac{i}{\varepsilon}z\eta}\,, \tag{B.9}$$

since by definition

$$\begin{aligned} \left(\mathscr{F}_{\varepsilon\,\mu\to z} \mathscr{F}^{-1}_{\varepsilon\,y\to\eta} f\right)(z,\eta) &= (2\pi)^{-d} \int_{[-\pi,\pi]^d} d\mu\, e^{-\frac{i}{\varepsilon}z\mu} \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}y\eta} e^{-\frac{i}{\varepsilon}y\mu} \\ &= (2\pi)^{-d} \int_{[-\pi,\pi]^d} d\mu\, e^{-\frac{i}{\varepsilon}z\mu} \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}y(\eta-\mu)} = (2\pi)^{-d} \int_{[-\pi,\pi]^d} d\mu\, e^{-\frac{i}{\varepsilon}z\mu} \delta_\pi(\eta-\mu) = e^{-\frac{i}{\varepsilon}z\eta}\,. \end{aligned}$$

In addition for Schwartz-functions $u$ and $v$

$$\begin{aligned} &\sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\mu\, v(\mu,y) \left(\mathscr{F}^{-1}_{\varepsilon\,z\to\mu} \mathscr{F}_{\varepsilon\,\eta\to y} u\right)(\mu,y) \qquad \text{(B.10)} \\ &\quad = (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\mu\, v(\mu,y) \sum_{z\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}z\mu} \int_{[-\pi,\pi]^d} d\eta\, e^{-\frac{i}{\varepsilon}y\eta} u(z,\eta) \\ &\quad = (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\eta \sum_{z\in(\varepsilon\mathbb{Z})^d} u(z,\eta) e^{-\frac{i}{\varepsilon}y\eta} \int_{[-\pi,\pi]^d} d\mu\, e^{\frac{i}{\varepsilon}\mu z} v(\mu,y) \\ &\quad = (2\pi)^{-\frac{d}{2}} \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\eta\, u(z,\eta) \sum_{y\in(\varepsilon\mathbb{Z})^d} e^{-\frac{i}{\varepsilon}y\eta} \left(\mathscr{F}_{\varepsilon\,\mu\to(-z)} v\right)(-z,y) \\ &\quad = \int_{[-\pi,\pi]^d} d\eta \sum_{z\in(\varepsilon\mathbb{Z})^d} u(z,\eta) \left(\mathscr{F}^{-1}_{\varepsilon\,y\to(-\eta)} \mathscr{F}_{\varepsilon\,\mu\to z} v\right)(-z,-\eta)\,. \end{aligned}$$

Similarly to the usual Fourier transformation in $\mathbb{R}^d$ one can show

$$\mathscr{F}_{\varepsilon\,\eta\to y}(\eta\cdot u)(z,y) = -\varepsilon D_y(\mathscr{F}_{\varepsilon\,\eta\to y} u)(z,y) \quad \text{and} \tag{B.11}$$

$$\mathscr{F}^{-1}_{\varepsilon\,z\to\mu}(z\cdot u)(\mu,\eta) = \varepsilon D_\mu(\mathscr{F}^{-1}_{\varepsilon\,z\to\mu} u)(\mu,\eta)\,. \tag{B.12}$$

Using Lemma B.3, we can define and deduce for $f$ polynomially bounded

$$\begin{aligned} f((-\varepsilon D_x),(\varepsilon D_\xi))u(x,\xi) &:= \mathscr{F}^{-1}_{\varepsilon y\to\xi}\left(f((-\varepsilon D_x),y)\cdot\left(\mathscr{F}_{\varepsilon\xi\to y}u\right)(x,y)\right)(\xi) \qquad \text{(B.13)}\\ &= (2\pi)^{-\frac{d}{2}}\left(\left(\mathscr{F}^{-1}_{\varepsilon y\to\xi}f\right)((-\varepsilon D_x),\,.\,)*_\pi u(x,\,.\,)\right)(\xi)\\ &= (2\pi)^{-\frac{d}{2}}\int_{[-\pi,\pi]^d}d\eta\,\left(\mathscr{F}^{-1}_{\varepsilon y\to\eta}f\right)((-\varepsilon D_x),\eta)u(x,\xi-\eta)\\ &:= (2\pi)^{-\frac{d}{2}}\int_{[-\pi,\pi]^d}d\eta\,\mathscr{F}_{\varepsilon\mu\to x}\left(\left(\mathscr{F}^{-1}_{\varepsilon y\to\eta}f\right)(\mu,\eta)\cdot\left(\mathscr{F}^{-1}_{\varepsilon x\to\mu}u\right)(\mu,\xi-\eta)\right)(x)\\ &= (2\pi)^{-d}\int_{[-\pi,\pi]^d}d\eta\,\left(\left(\mathscr{F}_{\varepsilon\mu\to x}\mathscr{F}^{-1}_{\varepsilon y\to\eta}f\right)(\,.\,,\eta)*_\varepsilon u(\,.\,,\xi-\eta)\right)(x)\\ &= (2\pi)^{-d}\int_{[-\pi,\pi]^d}d\eta\sum_{z\in(\varepsilon\mathbb{Z})^d}\left(\mathscr{F}_{\varepsilon\mu\to z}\mathscr{F}^{-1}_{\varepsilon y\to\eta}f\right)(z,\eta)u(x-z,\xi-\eta) \end{aligned}$$

and therefore with (B.10)

$$\sum_{y\in(\varepsilon\mathbb{Z})^d}\int_{[-\pi,\pi]^d}d\mu\,(\mu\cdot y)^k\left(\mathscr{F}^{-1}_{\varepsilon z\to\mu}\mathscr{F}_{\varepsilon\eta\to y}u\right)(\mu,y) = (2\pi)^d(-\varepsilon^2 D_z D_\eta)^k u(z,\eta)|_{\substack{z=0\\ \eta=0}}\,. \qquad \text{(B.14)}$$

Together with the Taylor expansion for the exponential function, which gives for real $t$

$$|e^{it}-\sum_{k=0}^{N-1}\frac{(it)^k}{k!}|\le\frac{|t|^N}{N!}\ ,$$

it follows that

$$\sum_{z\in(\varepsilon\mathbb{Z})^d}\int_{[-\pi,\pi]^d}d\eta\,e^{-\frac{i}{\varepsilon}z\eta}u(z,\eta) = (2\pi)^d\sum_{k=0}^{N-1}\frac{1}{k!}(i\varepsilon D_z D_\eta)^k u(z,\eta)|_{\substack{z=0\\ \eta=0}} + S_N(u,\varepsilon)\,,$$

where

$$\begin{aligned} |S_N(u,\varepsilon)| &\le \frac{C}{N!}\varepsilon^N\sum_{y\in(\varepsilon\mathbb{Z})^d}\int_{[-\pi,\pi]^d}d\mu\,|(\mu\cdot y)^N\left(\mathscr{F}^{-1}_{\varepsilon z\to\mu}\mathscr{F}_{\varepsilon\eta\to y}u\right)(\mu,y)|\\ &\le \frac{C\varepsilon^N}{N!}\sum_{|\alpha+\beta|\le 2d+1}\|\partial_z^\alpha\partial_\eta^\beta(\partial_z\cdot\partial_\eta)^N u\|_1\,. \end{aligned}$$

□

By use of the method of stationary phase it is possible to prove the following lemma concerning the map $e^{i\varepsilon D_x D_\xi}$. This will be used later to define the symbol associated to the composition of two operators as a special product between the symbols of the single operators.

LEMMA B.5. *Let $0\le\delta\le\frac{1}{2}$ and $m$ be an order function. Then $e^{i\varepsilon D_x D_\xi}: S^r_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)\to S^r_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ is continuous. If $\delta<\frac{1}{2}$, then*

$$e^{i\varepsilon D_x D_\xi}b(x,\xi)\sim\sum_{j=0}^{\infty}\frac{1}{j!}\left((i\varepsilon D_x\cdot D_\xi)^j\,b\right)(x,\xi)$$

*in $S^r_\delta(m)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$. If we write $e^{i\varepsilon D_x D_\xi}b=\sum_{j=0}^{N-1}\frac{(i\varepsilon D_x\cdot D_\xi)^j}{j!}\,b+R_N(b,\varepsilon)$, the remainder $R_N$ is an element of the symbol class $S_\delta^{N(1-2\delta)}(m)$ and it depends linearly on the derivatives of $b$ with respect to $x$ and $\xi$ of order $j$ for $N\le j\le N+2d+1$.*

Proof:

*Step 1:* We start with the asymptotic sum in the case $\delta<\frac{1}{2}$.
We restrict the proof to $r=0$, the case $r\neq 0$ is then obvious.

Using equation (B.13) with $f((-\varepsilon D_x),(\varepsilon D_\xi))=e^{i\varepsilon D_x\cdot D_\xi}$ and (B.9), we have

$$(2\pi)^d e^{i\varepsilon D_x\cdot D_\xi}b(x,\xi;\varepsilon)=\int_{[-\pi,\pi]^d}\sum_{z\in(\varepsilon\mathbb{Z})^d}e^{-\frac{i}{\varepsilon}z\cdot\eta}b(x-z,\xi-\eta;\varepsilon)\,d\eta\,. \qquad \text{(B.15)}$$

To analyze the integral given by (B.15), we introduce a cut-off-function $\zeta \in \mathcal{K}\left((\varepsilon\mathbb{Z})^d\right)$ localized in a neighborhood of 0. This allows to split the symbol into the two summands $b_1$ and $b_2$ by multiplication with $\mathbf{1} - \zeta(z)$ and $\zeta(z)$ respectively. The aim is now to show $b_1 \in S^\infty(m)$ and $b_2 \in S^0_\delta(m)$ having the required asymptotic expansion. We start by analyzing $b_1$. By use of the operator

$$L_2(z, \eta) := \frac{-\varepsilon^2 \Delta_\eta}{|z|^2}\,, \tag{B.16}$$

which is well defined on the support of $1 - \zeta(z)$ and has the property $L_2(z,\eta)e^{-\frac{i}{\varepsilon}z\eta} = e^{-\frac{i}{\varepsilon}z\eta}$, we have by partial integration

$$\begin{aligned} b_1(x,\xi;\varepsilon) &= \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} \left(L_2^k(z,\eta)e^{-\frac{i}{\varepsilon}z\cdot\eta}\right)(\mathbf{1} - \zeta(z))b(x-z,\xi-\eta;\varepsilon)\,d\eta \\ &= \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}z\cdot\eta}\frac{(\mathbf{1} - \zeta(z))}{|z|^{2k}}(-\varepsilon^2\Delta_\eta)^k b(x-z,\xi-\eta;\varepsilon)\,d\eta\,. \end{aligned}$$

Since $b \in S^0_\delta(m)$, the integrand is for some $C > 0$ bounded from above

$$C\varepsilon^{2k(1-\delta)}\frac{m(x-z,\xi-\eta)}{\langle z\rangle^{2k}} \le C\varepsilon^{2k(1-\delta)}\frac{m(x,\xi)}{\langle z\rangle^{2k}}\langle z\rangle^{N_0}\,.$$

This term is integrable and summable for $k$ big enough yielding

$$b_1(x,\xi;\varepsilon) = \varepsilon^{2k(1-\delta)-d}O(m(x,\xi))\,.$$

The derivatives can be estimated similarly, because

$$\partial_x^\alpha e^{i\varepsilon D_x\cdot D_\xi}b(x,\xi;\varepsilon) = e^{i\varepsilon D_x\cdot D_\xi}\partial_x^\alpha b(x,\xi;\varepsilon)\,.$$

Since this holds for every $k \in \mathbb{N}$, we have $b_1 \in S^\infty(m)$.
For $b_2$ the method of stationary phase described in Lemma B.4 leads to

$$\begin{aligned} b_2(x,\xi;\varepsilon) &= \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon}z\cdot\eta}\zeta(z)b(x-z,\xi-\eta;\varepsilon)\,d\eta \\ &= (2\pi)^d\sum_{j=0}^{N-1}\frac{(i\varepsilon D_x\cdot D_\xi)^j}{j!}b(x,\xi;\varepsilon) + R_N(b,\zeta,\varepsilon) \end{aligned} \tag{B.17}$$

with

$$\begin{aligned} |R_N(b,\zeta,\varepsilon)| &\le C_N\varepsilon^N\sum_{|\alpha+\beta|\le 2d+1}\|\partial_z^\alpha\partial_\eta^\beta(\partial_z\cdot\partial_\eta)^N\zeta(z)b(x-z,\xi-\eta;\varepsilon)\|_1 \\ &\le C_N' m(x,\xi)\varepsilon^{(1-2\delta)N-\delta(2d+1)-d}\,. \end{aligned} \tag{B.18}$$

Derivatives of this term are of the same order multiplied by $\varepsilon^{-\delta l}$. Therefore $R_N \in S_\delta^{(1-2\delta)N-\delta(2d+1)-d}(m)$. Furthermore it follows directly by the formula (B.18), that only derivatives of order between $N$ and $N + 2d + 1$ contribute to the remainder and the dependance of the derivatives of $b$ is linear.
Splitting the remaining term $R_N$ into an explicit sum, in which the summands are elements of $S_\delta^{N(1-2\delta)}(m)$, and a second remaining term $R_M$ with $M = (1-2\delta)(N+k) - \delta(2d+1) - d \ge N(1-2\delta)$ for $k \in \mathbb{N}$ big enough, it follows that $R_N \in S_\delta^{N(1-2\delta)}(m)$. Since the Fréchet norms of $e^{i\varepsilon D_x D_\xi}a(x,\xi;\varepsilon)$ in $S^0_\delta(m)$ depend only on a finite number of Fréchet norms of $a(x,\xi;\varepsilon)$, the mapping is continuous.

*Step 2:* The continuity for $\delta = \frac{1}{2}$.
We choose a cut-off function in $z$ and in $\eta$, which is $\varepsilon$-scaled, i.e. we split the integral (B.15) by multiplying with $\zeta\left(\frac{z}{\sqrt{\varepsilon}}, \frac{\eta}{\sqrt{\varepsilon}}\right)$ and $\mathbf{1} - \zeta\left(\frac{z}{\sqrt{\varepsilon}}, \frac{\eta}{\sqrt{\varepsilon}}\right)$. The first integral is thus by the substitution

$\tilde{z} = \frac{z}{\sqrt{\varepsilon}}$ and $\tilde{\eta} = \frac{\eta}{\sqrt{\varepsilon}}$

$$\begin{aligned} b_1(x,\xi) &= \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{-\frac{i}{\varepsilon} z\cdot\eta} \left(\mathbf{1} - \zeta\left(\frac{z}{\sqrt{\varepsilon}}, \frac{\eta}{\sqrt{\varepsilon}}\right)\right) b(x-z,\xi-\eta;\varepsilon)\, d\eta \\ &= \sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} e^{-i\tilde{z}\cdot\tilde{\eta}} \left(\mathbf{1} - \zeta(\tilde{z},\tilde{\eta})\right) b(x-\sqrt{\varepsilon}\tilde{z}, \xi - \sqrt{\varepsilon}\tilde{\eta};\varepsilon)\, d\tilde{\eta}\,. \end{aligned}$$

To analyze this integral, we use the differential operators

$$L_3(\tilde{z},\tilde{\eta}) := \frac{-\Delta_{\tilde{\eta}}}{|\tilde{z}|^2} \quad \text{and}$$

$$L_4(\tilde{z},\tilde{\eta}) := \frac{-\varepsilon\Delta_{\tilde{z}}^{\sqrt{\varepsilon}}}{2d - 2\sum_{\nu=1}^d \cos(\sqrt{\varepsilon}\tilde{\eta}_\nu)}\,,$$

where

$$-\Delta_{\tilde{z}}^{\sqrt{\varepsilon}} := \frac{1}{\varepsilon}\left(2d - \sum_{\nu=1}^d (\tau_{\sqrt{\varepsilon}e_\nu} + \tau_{-\sqrt{\varepsilon}e_\nu})\right) \tag{B.19}$$

denotes the discrete Laplacian on the $\sqrt{\varepsilon}$-lattice (compare the definitions and arguments in the proof of Lemma 2.13,(c)). Then

$$\begin{aligned} b_1(x,\xi) = &\sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} \left(L_4^k(\tilde{z},\tilde{\eta}) L_3^l(\tilde{z},\tilde{\eta}) e^{-i\tilde{z}\cdot\tilde{\eta}}\right)\left(\mathbf{1} - \zeta(\tilde{z},\tilde{\eta})\right) \times \\ &\qquad \times b(x-\sqrt{\varepsilon}\tilde{z},\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon)\, d\tilde{\eta} \\ = &\sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} \left(L_4^{k-1}(\tilde{z},\tilde{\eta}) L_3^l(\tilde{z},\tilde{\eta}) e^{-i\tilde{z}\cdot\tilde{\eta}}\right)\left(2d - \sum_\nu 2\cos(\sqrt{\varepsilon}\tilde{\eta}_\nu)\right)^{-1} \times \\ &\qquad \times \Big\{\big(2d\left(\mathbf{1} - \zeta(\tilde{z},\tilde{\eta})\right) b(x-\sqrt{\varepsilon}\tilde{z},\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon) - \\ &\quad - \sum_{\nu=1}^d \Big\{\big(\mathbf{1} - \zeta(\tilde{z}+\sqrt{\varepsilon}e_\nu,\tilde{\eta})\big) b(x-\sqrt{\varepsilon}(\tilde{z}+\sqrt{\varepsilon}e_\nu),\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon) + \\ &\qquad + \big(\mathbf{1} - \zeta(\tilde{z}-\sqrt{\varepsilon}e_\nu,\tilde{\eta})\big) b(x-\sqrt{\varepsilon}(\tilde{z}-\sqrt{\varepsilon}e_\nu),\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon)\Big\}\Big)\Big\}\, d\tilde{\eta}\,. \end{aligned} \tag{B.20}$$

By Taylor expansion, the last term is equal to

$$\begin{aligned} &\sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} \left(L_4^{k-1}(\tilde{z},\tilde{\eta}) L_3^l(\tilde{z},\tilde{\eta}) e^{-i\tilde{z}\cdot\tilde{\eta}}\right)\left(2d - \sum_\nu 2\cos(\sqrt{\varepsilon}\tilde{\eta}_\nu)\right)^{-1} \\ &\quad \sum_{\nu=1}^d \int_0^{\sqrt{\varepsilon}} (t-\sqrt{\varepsilon})\partial_{\tilde{z}_\nu}^2 \left\{\left(\mathbf{1} - \zeta(\tilde{z}+te_\nu,\tilde{\eta})\right) b(x-\sqrt{\varepsilon}(\tilde{z}+te_\nu),\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon) + \right. \\ &\qquad \left. + \left(\mathbf{1} - \zeta(\tilde{z}-te_\nu,\tilde{\eta})\right) b(x-\sqrt{\varepsilon}(\tilde{z}-te_\nu),\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon)\right\}\, dt\, d\tilde{\eta}\,. \end{aligned}$$

Iterating this argument $k$ times gives with the notation $(f(a+b,c))^S := f(a+b,c) + f(a-b,c)$

$$\begin{aligned} b_1(x,\xi) = &\sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} \left(L_3^l(\tilde{z},\tilde{\eta}) e^{-i\tilde{z}\cdot\tilde{\eta}}\right)\left(2d - \sum_\nu 2\cos(\sqrt{\varepsilon}\tilde{\eta}_\nu)\right)^{-k} \\ &\sum_{\nu_1,\ldots,\nu_k=1}^d \int_0^{\sqrt{\varepsilon}} dt_1 \ldots \int_0^{\sqrt{\varepsilon}} dt_k \partial_{\tilde{z}_{\nu_1}}^2 \ldots \partial_{\tilde{z}_{\nu_k}}^2 \left\{\left(\mathbf{1} - \zeta(\tilde{z}+t_1e_{\nu_1}+\ldots+t_ke_{\nu_k},\tilde{\eta})\right) \times \right. \\ &\qquad \left. \times b(x-\sqrt{\varepsilon}(\tilde{z}+t_1e_{\nu_1}+\ldots+t_ke_{\nu_k}),\xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon)\right\}^S \prod_{i=1}^k (t_i - \sqrt{\varepsilon})\, d\tilde{\eta}\,. \end{aligned}$$

Integrating by parts with $L_3$ similar to the first part of the proof and taking the norm, the integrand can be estimated by

$$\varepsilon^{\frac{d}{2}} O(1)|\tilde{z}|^{-2l} \sum_{|\alpha|\leq l} \left| Q_\alpha(-D_{\tilde{\eta}}) \left\{ \frac{(\mathbf{1} - \zeta(\tilde{z},\tilde{\eta}))}{(2d - \sum_\nu 2\cos(\sqrt{\varepsilon}\tilde{\eta}_\nu))^k} \right\} \right| \times$$
$$\times \sum_{\nu_1,\dots,\nu_k=1}^{d} \int_0^{\sqrt{\varepsilon}} dt_1 \dots \int_0^{\sqrt{\varepsilon}} dt_k \prod_{i=1}^{k} |t_i - \sqrt{\varepsilon}| \left\{ m(x - \sqrt{\varepsilon}(\tilde{z} + t_1 e_{\nu_1} + \dots + t_k e_{\nu_k}), \xi - \sqrt{\varepsilon}\tilde{\eta}) \right\}^S \tag{B.21}$$

To estimate the derivatives of $(2\sum_\nu(1 - \cos(\sqrt{\varepsilon}\tilde{\eta}_\nu)))^{-k}$, we introduce the notation

$$P_{k,l}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right) := a_{kl}\cos^k(\sqrt{\varepsilon}t)\sin^l(\sqrt{\varepsilon}t)$$

with $k, l \geq 0$ and $a_{kl} \geq 0$. Then

$$\begin{aligned}\partial_t P_{k,l}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right) &= \sqrt{\varepsilon} a_{kl}\left(-k\cos^{k-1}(\sqrt{\varepsilon}t)\sin^{l+1}(\sqrt{\varepsilon}t) + \right.\\ &\quad \left. + l\cos^{k+1}(\sqrt{\varepsilon}t)\sin^{l-1}(\sqrt{\varepsilon}t)\right)\\ &= \sqrt{\varepsilon}\left\{P_{(k-1),(l+1)}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right) + P_{(k+1),(l-1)}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right)\right\}\end{aligned}$$

and for the function

$$f(t) := \frac{P_{kl}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right)}{(1 - \cos(\sqrt{\varepsilon}t))^m},$$

we therefore get

$$\begin{aligned}\partial_t f(t) \quad = \quad & \sqrt{\varepsilon}\left\{\frac{P_{(k-1),(l+1)}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right) + P_{(k+1),(l-1)}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right)}{(1 - \cos(\sqrt{\varepsilon}t))^m} - \right.\\ & \left. - \frac{P_{k,(l+1)}\left(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t)\right)}{(1 - \cos(\sqrt{\varepsilon}t))^{m+1}}\right\}.\end{aligned}$$

Using the estimates $\pi^2(1 - \cos(\sqrt{\varepsilon}t)) \geq \varepsilon t^2$ and $|P_{k,l}(\cos(\sqrt{\varepsilon}t), \sin(\sqrt{\varepsilon}t))| \leq P_{k,l}(1, |\sqrt{\varepsilon}t|)$ for $|\sqrt{\varepsilon}t| \leq \pi$, we get

$$|f(t)| \leq \frac{a_{kl}|\sqrt{\varepsilon}t|^l}{(\sqrt{\varepsilon}t)^{2m}} = O\left(\varepsilon^{\frac{l}{2}-m}\right) Q_{l-2m}(|t|),$$

where $Q_s(t)$ denotes a Polynomial in t of order $s$ and

$$\begin{aligned}|\partial_t f(t)| \quad \leq \quad & \sqrt{\varepsilon}\left\{\frac{a_{(k-1),(l+1)}|\sqrt{\varepsilon}t|^{l+1} + a_{(k+1),(l-1)}|\sqrt{\varepsilon}t|^{l-1}}{(\sqrt{\varepsilon}t)^{2m}} - \frac{a_{k,(l+1)}|\sqrt{\varepsilon}t|^{l+1}}{(\sqrt{\varepsilon}t)^{2(m+1)}}\right\}\\ = \quad & O\left(\varepsilon^{\frac{l}{2}-m+1}\right) Q_{l+1-2m}(|t|) + O\left(\varepsilon^{\frac{l}{2}-m}\right) Q_{l-1-2m}(|t|).\end{aligned}$$

Derivatives of functions of the form $f(t)$ lead therefore to sums of the same form and leave the order in $\varepsilon$ unchanged. Since $(1 - \cos(\sqrt{\varepsilon}t))^{-m}$ is of the form of $f(t)$ with $k = l = 0$ and the order in $|t|$ increases with each derivative at most by one, (B.21) can be estimated by

$$\begin{aligned}&\varepsilon^{\frac{d}{2}-k} O(1) \frac{m(x,\xi)}{\langle\tilde{z}\rangle^{2l}} \frac{Q_l(|\tilde{\eta}|)}{\langle\tilde{\eta}\rangle^{2k}} \langle\sqrt{\varepsilon}\tilde{z}\rangle^{N_1} 2^k \sum_{\nu_1,\dots,\nu_k} \prod_{i=1}^{k} \int_0^{\sqrt{\varepsilon}} |t_i - \sqrt{\varepsilon}| \langle\sqrt{\varepsilon}t_i e_{\nu_i}\rangle^{N_1} dt_i\\ &\qquad \leq \varepsilon^{\frac{d}{2}} O(1) \frac{m(x,\xi) Q_l(|\tilde{\eta}|)}{\langle\tilde{z}\rangle^{2l}\langle\tilde{\eta}\rangle^{2k}} \langle\sqrt{\varepsilon}\tilde{z}\rangle^{N_1},\end{aligned}$$

since each integral with respect to $t_i$ is smaller or equal to $c\varepsilon$. We thus finally get

$$|b_1(x,\xi)| \leq Cm(x,\xi) \sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}}, \frac{\pi}{\sqrt{\varepsilon}}]^d} \langle\tilde{z}\rangle^{-2l} Q_l(|\tilde{\eta}|) \langle\tilde{\eta}\rangle^{-2k} \langle\sqrt{\varepsilon}\tilde{z}\rangle^{N_1} d\tilde{\eta}, \tag{B.22}$$

which is $O(m(x,\xi))$ for $k, l$ big enough. By arguments analogue to the case $\delta < \frac{1}{2}$ for derivatives, $b_1 \in S^0_\delta(m)$.

The second integral can be estimated directly, using again the substitution $\tilde{z} = \frac{z}{\sqrt{\varepsilon}}$ and $\tilde{\eta} = \frac{\eta}{\sqrt{\varepsilon}}$, by

$$\begin{aligned} |b_2(x,\xi)| &= \left| \sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} e^{-i\tilde{z}\cdot\tilde{\eta}} \zeta(\tilde{z},\tilde{\eta}) b(x-\sqrt{\varepsilon}\tilde{z}, \xi-\sqrt{\varepsilon}\tilde{\eta};\varepsilon)\, d\tilde{\eta} \right| \leq \\ &\leq Cm(x,\xi) \sum_{\tilde{z}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \varepsilon^{\frac{d}{2}} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} \zeta(\tilde{z},\tilde{\eta}) \langle \sqrt{\varepsilon}\tilde{z}\rangle^{N_1} \langle\sqrt{\varepsilon}\tilde{\eta}\rangle^{N_2}\, d\tilde{\eta}\,. \end{aligned}$$

Therefore $b_2$ is also $O(m(x,\xi))$ and by the same arguments as above is an element of $S^0_\delta(m)$ and the mapping is continuous. □

The following corollary concerns the composition of symbols.

Corollary B.6. *The map*

$$\mathscr{C}^\infty\left(\mathbb{R}^d\times\mathbb{T}^d\right) \times \mathscr{C}^\infty\left(\mathbb{R}^d\times\mathbb{T}^d\right) \ni (a,b) \longmapsto a\#b \in \mathscr{C}^\infty\left(\mathbb{R}^d\times\mathbb{T}^d\right)$$

*with*

$$(a\#b)(x,\xi;\varepsilon) := \left(e^{-i\varepsilon D_y\cdot D_\xi} a(x,\xi;\varepsilon) b(y,\eta;\varepsilon)\right)|_{\substack{y=x\\ \eta=\xi}} \tag{B.23}$$

*has a bilinear continuous extension :*

$$S^{r_1}_{\delta_1}(m_1)\left(\mathbb{R}^d\times\mathbb{T}^d\right) \times S^{r_2}_{\delta_2}(m_2)\left(\mathbb{R}^d\times\mathbb{T}^d\right) \to S^{r_1+r_2}_{\delta}(m_1 m_2)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$$

*for all $\delta_k\in[0,\frac{1}{2}], k=1,2$ and all order functions $m_1,m_2$, where $\delta := \max\{\delta_1,\delta_2\}$. For $\delta_j<\frac{1}{2}$, $j=1,2$*

$$(a\#b)(x,\xi;\varepsilon) \sim \sum_{\alpha\in\mathbb{N}^d} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!} \left(\partial^\alpha_\xi a(x,\xi;\varepsilon)\right)\left(\partial^\alpha_x b(x,\xi;\varepsilon)\right) \tag{B.24}$$

*in $S^{r_1+r_2}_\delta(m_1m_2)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ for all $a,b\in S^{r_j}_{\delta_j}(m_j)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$, $j=1,2$. Writing $a\#b(x,\xi;\varepsilon) = \sum_{|\alpha|=0}^{N-1}\frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\left(\partial^\alpha_\xi a(x,\xi;\varepsilon)\right)\left(\partial^\alpha_x b(x,\xi;\varepsilon)\right) + R_N(a,b,\varepsilon)$, the remainder $R_N$ is an element of the symbol class $S^{N(1-\delta_1-\delta_2)}_\delta(m_1m_2)$ and it depends linearly on a finite number of derivatives of the single symbols $a$ and $b$. Furthermore it depends only on derivatives of $a$ and $b$ with respect to $\xi$ and $x$ respectively which are at least of order $N$.*

Proof:
By the Leibnitz rule, the map

$$S^{r_1}_{\delta_1}(m_1)\times S^{r_2}_{\delta_2}(m_2) \ni (a,b)\mapsto a\cdot b \in S^{r_1+r_2}_\delta(m_1m_2)$$

is continuous, since each Fréchet-norm of the product depends only on a finite number of Fréchet-norms of $a$ and $b$. The same is true for the restriction map. The main part follows by Lemma B.5 by doubling the dimension of the space.

□

The next lemma relates the #-product of symbols with the composition of the associated operators.

Lemma B.7. *Let $a\in S^{r_1}_{\delta_1}(m_1)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$, $b\in S^{r_2}_{\delta_2}(m_2)\left(\mathbb{R}^d\times\mathbb{T}^d\right)$ with $0\leq\delta_k\leq\frac{1}{2}, k=1,2$ and $u\in s\left((\varepsilon\mathbb{Z})^d\right)$. For $a\#b$ given by (B.23),*

$$\left(\mathrm{Op}^{\mathbb{T}^d}_\varepsilon(a)\right)\circ\left(\mathrm{Op}^{\mathbb{T}^d}_\varepsilon(b)\right) = \mathrm{Op}^{\mathbb{T}^d}_\varepsilon(a\#b)$$

*in $\mathcal{L}\left(s\left((\varepsilon\mathbb{Z})^d\right)\right)$.*

Proof:
Denoting by $K_A(x,y)$ the kernel of the operator $\mathrm{Op}^{\mathbb{T}^d}_\varepsilon(a)$, i.e.

$$\left\langle v\,,\,\mathrm{Op}^{\mathbb{T}^d}_\varepsilon(a)u\right\rangle_{\ell^2} =: \langle v\times u\,,\,K_A\rangle_{\ell^2\times\ell^2}\,, \tag{B.25}$$

(B.1) gives

$$\left\langle v\,,\,\mathrm{Op}^{\mathbb{T}^d}_\varepsilon(a)u\right\rangle_{\ell^2} = \sum_{x\in(\varepsilon\mathbb{Z})^d}\sum_{y\in(\varepsilon\mathbb{Z})^d} u(y)\bar{v}(x)(2\pi)^{-d}\int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi} a(x,\xi;\varepsilon)\,d\xi$$

and therefore

$$K_A(x,y;\varepsilon) = (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi} a(x,\xi;\varepsilon)\, d\xi = (2\pi)^{-\frac{d}{2}} \left(\mathscr{F}_{\varepsilon\xi\to(x-y)} a\right)(x, x-y;\varepsilon)\,. \tag{B.26}$$

Since by definition

$$\begin{aligned} Cu(x) &:= \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a) \circ \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(b) u(x) = \mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a) \circ (2\pi)^{-d} \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-z)\xi} b(z,\xi;\varepsilon) u(y)\, d\xi \\ &= (2\pi)^{-2d} \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(z-x)\eta} a(x,\eta;\varepsilon) \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-z)\xi} b(z,\xi;\varepsilon) u(y)\, d\xi d\eta\,, \end{aligned}$$

the kernel $K_C$ associated to the operator $C$ as defined in (B.25) takes the form

$$K_C(x,y;\varepsilon) = (2\pi)^{-2d} \sum_{z\in(\varepsilon\mathbb{Z})^d} \iint_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}((z-x)\eta + (y-z)\xi)} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\, d\xi d\eta\,.$$

Thus by (B.26) the symbol associated to the operator $C$ is given by

$$\begin{aligned} c(x,\nu;\varepsilon) &= (2\pi)^{\frac{d}{2}} \left(\mathscr{F}^{-1}_{\varepsilon(x-y)\to\nu} K_C\right)(x,\nu;\varepsilon) = \sum_{(x-y)\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}(x-y)\nu} K_C(x,(x-y);\varepsilon) \qquad \text{(B.27)} \\ &= \sum_{(x-y)\in(\varepsilon\mathbb{Z})^d} e^{\frac{i}{\varepsilon}(x-y)\nu} (2\pi)^{-2d} \sum_{z\in(\varepsilon\mathbb{Z})^d} \int\int\limits_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}((z-x)\eta+(y-z)\xi)} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\, d\xi d\eta\,. \end{aligned}$$

With the substitution $x-y=r$, this leads to

$$\begin{aligned} &(2\pi)^{-2d} \sum_{r\in(\varepsilon\mathbb{Z})^d} \sum_{z\in(\varepsilon\mathbb{Z})^d} \iint_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(r\nu + (z-x)\eta + (x-r-z)\xi)} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\, d\xi d\eta \\ &\qquad = (2\pi)^{-2d} \sum_{r\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}r(\nu-\xi)} \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}z\eta} a(x,\xi-\eta;\varepsilon) b(x-z,\xi;\varepsilon)\, d\xi d\eta\,. \end{aligned}$$

Equation (B.15) gives

$$\begin{aligned} &(2\pi)^{-2d} \sum_{r\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}r(\nu-\xi)} \sum_{z\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}z\eta} a(x,\xi-\eta;\varepsilon) b(x-z,\xi;\varepsilon)\, d\xi d\eta \\ &\qquad = (2\pi)^{-d} \sum_{r\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}r(\nu-\xi)} \left(e^{-i\varepsilon D_z D_\eta} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\right)\Big|_{\substack{z=x\\ \eta=\xi}} d\xi \end{aligned}$$

and by the representation (B.8) and definition (B.7) of $\delta_\pi$ we have

$$\begin{aligned} &(2\pi)^{-d} \sum_{r\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}r(\nu-\xi)} \left(e^{-i\varepsilon D_z D_\eta} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\right)\Big|_{\substack{z=x\\ \eta=\xi}} d\xi \\ &= (2\pi)^{-d} \int_{[-\pi,\pi]^d} \delta_\pi(\nu-\xi) \left(e^{-i\varepsilon D_z D_\eta} a(x,\eta;\varepsilon) b(z,\xi;\varepsilon)\right)\Big|_{\substack{z=x\\ \eta=\xi}} d\xi \\ &= \left(e^{-i\varepsilon D_z D_\eta} a(x,\eta;\varepsilon) b(z,\nu;\varepsilon)\right)\Big|_{\substack{z=x\\ \eta=\nu}}\,. \end{aligned} \tag{B.28}$$

Inserting (B.28) in (B.27) therefore shows

$$c(x,\nu;\varepsilon) = \left(e^{-i\varepsilon D_z D_\eta} a(x,\eta;\varepsilon) b(z,\nu;\varepsilon)\right)\Big|_{\substack{z=x\\ \eta=\nu}}\,. \tag{B.29}$$

Together with the Lemmata B.2 and B.5, this proves the assertion.

□

## B.3. Norm estimates for operators on $(\varepsilon\mathbb{Z})^d$ in microlocal approximation

To prove Proposition B.9, we need in addition the following proposition, which is an adapted version of the Calderon-Vaillancourt-Theorem.

PROPOSITION B.8. *Let $a \in S^r_\delta(\mathbf{1})\left(\mathbb{R}^d \times \mathbb{T}^d\right)$ with $0 \leq \delta \leq \frac{1}{2}$. Then there exists a constant $M > 0$ such that, for the associated operator $\operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)$ given by (B.1) the estimate*

$$\| \operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)u\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \leq M\varepsilon^r \|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}$$

*holds for any $u \in s\left((\varepsilon\mathbb{Z})^d\right)$ and $\varepsilon > 0$. $\operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)$ can therefore be extended to a continuous operator: $\ell^2\left((\varepsilon\mathbb{Z})^d\right) \longrightarrow \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with $\| \operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)\|_\infty \leq M\varepsilon^r$. Moreover $M$ can be chosen depending only on a finite number of Fréchet semi-norms of the symbol $a$.*

Proof:
We have to show for all $u, v \in s\left((\varepsilon\mathbb{Z})^d\right)$ the estimate

$$|\left\langle u\,,\, \operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)v\right\rangle_{\ell^2}| \leq M\varepsilon^r \|u\|_{\ell^2}\|v\|_{\ell^2} \tag{B.30}$$

holds, where $M$ depends only on a finite number of Fréchet semi-norms $\|\partial_x^\alpha \partial_\xi^\beta a\|_\infty$. By use of the Fourier transformation defined in (2.3) and (2.4) and with the substitution $\tilde{z} = \frac{z}{\sqrt{\varepsilon}}$ for $z = x, y, \eta, \xi$, which symmetrizes the $\varepsilon$-dependance between configuration and momentum space, we have

$$\begin{aligned}
\left\langle u\,,\, \operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)v\right\rangle_{\ell^2} &= (2\pi)^{-d} \sum_{x\in(\varepsilon\mathbb{Z})^d} \bar{u}(x) \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\xi\, e^{-\frac{i}{\varepsilon}(x-y)\xi} a(x,\xi;\varepsilon)v(y) \\
&= (2\pi)^{-\frac{3d}{2}} \sum_{x\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\eta e^{-\frac{i}{\varepsilon}\eta x} \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\eta) \sum_{y\in(\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} d\xi\, e^{-\frac{i}{\varepsilon}(x-y)\xi} a(x,\xi;\varepsilon)v(y) \\
&= (2\pi)^{-\frac{3d}{2}}\varepsilon^d \sum_{\tilde{y},\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \iint_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} d\tilde{\xi}\, \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta}) e^{-i((\tilde{x}-\tilde{y})\tilde{\xi}+\tilde{x}\tilde{\eta})} \times \\
&\qquad \times a(\sqrt{\varepsilon}\tilde{x}, \sqrt{\varepsilon}\tilde{\xi};\varepsilon)v(\sqrt{\varepsilon}\tilde{y})\,.
\end{aligned}$$

Introducing a cut-off-function $\zeta(|\tilde{\xi}+\tilde{\eta}|)$ supported in a neighborhood of zero, the integral splits into two parts, i.e. $\left\langle u\,,\, \operatorname{Op}_\varepsilon^{\mathbb{T}^d}(a)v\right\rangle_{\ell^2} = I_1 + I_2$ (compare the proof of lemma B.5).
To analyze the part multiplied by $(\mathbf{1} - \zeta(|\tilde{\xi}+\tilde{\eta}|))$, which we denote by $I_1$, we use the operators

$$\begin{aligned}
L_5(\tilde{x}-\tilde{y},\tilde{\xi}) &:= \frac{\mathbf{1} - \Delta_{\tilde{\xi}}}{\langle \tilde{x}-\tilde{y}\rangle^2} \qquad \text{and} \\
L_6(\tilde{x},\tilde{\xi}+\tilde{\eta}) &:= \frac{-\varepsilon\Delta_{\tilde{x}}^{\sqrt{\varepsilon}}}{2d - 2\sum_\nu \cos(\sqrt{\varepsilon}(\tilde{\xi}_\nu+\tilde{\eta}_\nu))}\,,
\end{aligned}$$

where $\Delta_{\tilde{x}}^{\sqrt{\varepsilon}}$ denotes the discrete Laplacian defined in (B.19). Since $L_6$ and $L_5$ leave the exponential function occurring in the integral invariant, we have by summation by parts

$$\begin{aligned}
I_1 &= (2\pi)^{-\frac{3d}{2}}\varepsilon^d \sum_{\tilde{y},\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \int\int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} d\tilde{\xi}\, \left(L_6^k(\tilde{x},\tilde{\xi}+\tilde{\eta}) L_5^l(\tilde{x}-\tilde{y},\tilde{\xi}) e^{-i((\tilde{x}-\tilde{y})\tilde{\xi}+\tilde{x}\tilde{\eta})}\right) \times \\
&\qquad \times \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta})(\mathbf{1} - \zeta(|\tilde{\xi}+\tilde{\eta}|)) a(\sqrt{\varepsilon}\tilde{x}, \sqrt{\varepsilon}\tilde{\xi};\varepsilon)v(\sqrt{\varepsilon}\tilde{y}) \\
&= (2\pi)^{-\frac{3d}{2}}\varepsilon^d \sum_{\tilde{y},\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \iint_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} d\tilde{\xi}\, \left(L_5^l(\tilde{x}-\tilde{y},\tilde{\xi}) e^{-i((\tilde{x}-\tilde{y})\tilde{\xi}+\tilde{x}\tilde{\eta})}\right) \times \\
&\qquad \times \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta}) v(\sqrt{\varepsilon}\tilde{y}) \frac{\mathbf{1} - \zeta(|\tilde{\xi}+\tilde{\eta}|)}{\left(2d - 2\sum_\nu \cos(\sqrt{\varepsilon}(\tilde{\xi}_\nu+\tilde{\eta}_\nu))\right)^k} \left(-\varepsilon\Delta_{\tilde{x}}^{\sqrt{\varepsilon}}\right)^k a(\sqrt{\varepsilon}\tilde{x}, \sqrt{\varepsilon}\tilde{\xi};\varepsilon)\,,
\end{aligned}$$

which leads by integration by parts to

$$\begin{aligned} I_1 &= (2\pi)^{-\frac{3d}{2}}\varepsilon^d \sum_{\tilde y,\tilde x\in(\sqrt{\varepsilon}\mathbb{Z})^d} \iint_{[-\frac{\pi}{\sqrt\varepsilon},\frac{\pi}{\sqrt\varepsilon}]^d} d\tilde\eta d\tilde\xi\, e^{-i((\tilde x-\tilde y)\tilde\xi+\tilde x\tilde\eta)} \left(\mathscr{F}_\varepsilon{}^{-1}\bar u\right)(\sqrt\varepsilon\tilde\eta)\frac{v(\sqrt\varepsilon\tilde y)}{\langle\tilde x-\tilde y\rangle^{2l}}\times \\ &\times\sum_{|\alpha|\le 2l} Q_\alpha(D_{\tilde\xi})\frac{\mathbf{1}-\zeta(|\tilde\xi+\tilde\eta|)}{\left(2d-2\sum_\nu\cos(\sqrt\varepsilon(\tilde\xi_\nu+\tilde\eta_\nu))\right)^k} P_\alpha(D_{\tilde\xi})\left(-\varepsilon\Delta_{\tilde x}^{\sqrt\varepsilon}\right)^k a(\sqrt\varepsilon\tilde x,\sqrt\varepsilon\tilde\xi;\varepsilon)\,. \end{aligned}$$

With the notation

$$\begin{aligned} G_{lk\alpha}(\tilde x,\tilde\xi) &:= \frac{\varepsilon^{\frac d2}}{\sqrt{2\pi}^d}\int_{[-\frac{\pi}{\sqrt\varepsilon},\frac{\pi}{\sqrt\varepsilon}]^d} e^{-i\tilde x\tilde\eta}\left(\mathscr{F}_\varepsilon{}^{-1}\bar u\right)(\sqrt\varepsilon\tilde\eta)Q_\alpha(D_{\tilde\xi})\frac{\mathbf{1}-\zeta(|\tilde\xi+\tilde\eta|)}{\left(2d-2\sum_\nu\cos(\sqrt\varepsilon(\tilde\xi_\nu+\tilde\eta_\nu))\right)^k}\times \\ &\qquad\times P_\alpha(D_{\tilde\xi})\left(-\varepsilon\Delta_{\tilde x}^{\sqrt\varepsilon}\right)^k a(\sqrt\varepsilon\tilde x,\sqrt\varepsilon\tilde\xi;\varepsilon)\,d\tilde\eta \quad\text{and} \qquad (B.31) \\ F_l(\tilde x,\tilde\xi) &:= \frac{\varepsilon^{\frac d2}}{\sqrt{2\pi}^d}\sum_{\tilde y\in(\sqrt\varepsilon\mathbb{Z})^d} e^{i\tilde y\tilde\xi}\frac{v(\sqrt\varepsilon\tilde y)}{\langle\tilde x-\tilde y\rangle^{2l}} \qquad (B.32) \end{aligned}$$

we have

$$I_1 = (2\pi)^{-\frac d2}\sum_{\tilde x\in(\sqrt\varepsilon\mathbb{Z})^d}\int_{[-\frac{\pi}{\sqrt\varepsilon},\frac{\pi}{\sqrt\varepsilon}]^d} d\tilde\xi\, e^{-i\tilde x\tilde\xi}F_l(\tilde x,\tilde\xi)\sum_{|\alpha|\le 2l}G_{lk\alpha}(\tilde x,\tilde\xi)\,. \qquad (B.33)$$

By use of the Schwarz inequality, we can now estimate the $\ell^2\left((\sqrt\varepsilon\mathbb{Z}^d\right)\times\mathscr{L}^2\left((\mathbb{T}/\sqrt\varepsilon)^d\right)$-norm of $F_l$ and $G_{lk\alpha}$ separately, to get an estimate for the given integral. Since

$$\begin{aligned} F_l(\tilde x,\tilde\xi) &= \mathscr{F}_{\varepsilon}{}^{-1}_{y\to\sqrt\varepsilon\tilde\xi}\,\varepsilon^{\frac d2}\frac{v(y)}{\langle\tilde x-\frac{y}{\sqrt\varepsilon}\rangle^{2l}} \quad\text{and} \\ G_{lk\alpha}(\tilde x,\tilde\xi) &= \mathscr{F}_{\varepsilon\,\eta\to\sqrt\varepsilon\tilde x}\left(\mathscr{F}_\varepsilon{}^{-1}\bar u\right)(\eta)Q_\alpha(D_{\tilde\xi})\frac{\mathbf{1}-\zeta(|\tilde\xi+\frac{\eta}{\sqrt\varepsilon}|)}{\left(2d-2\sum_\nu\cos(\sqrt\varepsilon\tilde\xi_\nu+\eta_\nu)\right)^k}\times \\ &\qquad\times P_\alpha(D_{\tilde\xi})\left(-\varepsilon\Delta_{\tilde x}^{\sqrt\varepsilon}\right)^k a(\sqrt\varepsilon\tilde x,\sqrt\varepsilon\tilde\xi;\varepsilon)\,, \end{aligned}$$

we have by (2.8)

$$\begin{aligned} \|F_l\|^2_{\ell^2((\sqrt\varepsilon\mathbb{Z})^d)\times\mathscr{L}^2((\mathbb{T}/\sqrt\varepsilon)^d)} &= \sum_{\tilde x\in(\sqrt\varepsilon\mathbb{Z})^d}\int_{[-\frac{\pi}{\sqrt\varepsilon},\frac{\pi}{\sqrt\varepsilon}]^d}|F_l(\tilde x,\tilde\xi)|^2\,d\tilde\xi \\ &= \sum_{\tilde x\in(\sqrt\varepsilon\mathbb{Z})^d}\varepsilon^{-\frac d2}\int_{[-\pi,\pi]^d}|F_l(\tilde x,\frac{\xi}{\sqrt\varepsilon})|^2\,d\xi = \varepsilon^{-\frac d2}\sum_{\tilde x\in(\sqrt\varepsilon\mathbb{Z})^d}\sum_{y\in((\varepsilon\mathbb{Z})^d)}|\mathscr{F}_{\varepsilon\,\xi\to y}F_l(\tilde x,\frac{\xi}{\sqrt\varepsilon})|^2 \\ &\le \sum_{\tilde x\in(\sqrt\varepsilon\mathbb{Z})^d}\varepsilon^{-\frac d2}\sum_{y\in((\varepsilon\mathbb{Z})^d)}\varepsilon^d\frac{|v(y)|^2}{\langle\tilde x-\frac{y}{\sqrt\varepsilon}\rangle^{4l}} \end{aligned}$$

and thus for $l$ big enough with $\tilde t=\tilde x-\tilde y$

$$\|F_l\|^2_{\ell^2((\sqrt\varepsilon\mathbb{Z})^d)\times\mathscr{L}^2((\mathbb{T}/\sqrt\varepsilon)^d)} \le \|v\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)}\sum_{\tilde t\in(\sqrt\varepsilon\mathbb{Z})^d}\varepsilon^{\frac d2}\langle\tilde t\rangle^{-4l}\le C_l\|v\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)}\,. \qquad (B.34)$$

On the other hand by (2.7)

$$\|G_{lk\alpha}\|^2_{\ell^2((\sqrt{\varepsilon}\mathbb{Z})^d)\times\mathscr{L}^2((\mathbb{T}/\sqrt{\varepsilon})^d)} = \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\xi} \sum_{\tilde{x}\in((\sqrt{\varepsilon}\mathbb{Z})^d)} |G_{lk\alpha}(\tilde{x},\tilde{\xi})|^2$$
$$= \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\xi} \sum_{x\in((\varepsilon\mathbb{Z})^d)} |G_{lk\alpha}(\frac{x}{\sqrt{\varepsilon}},\tilde{\xi})|^2 = \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\xi} \int_{[-\pi,\pi]^d} d\eta |\mathscr{F}^{-1}_{\varepsilon x\to\eta} G_{lk\alpha}(\frac{x}{\sqrt{\varepsilon}},\tilde{\xi})|^2$$
$$\leq \int_{[-\pi,\pi]^d} d\eta \left|\left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\eta)\right|^2 \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\xi} \left| Q_\alpha(D_{\tilde{\xi}}) \frac{\mathbf{1} - \zeta(|\tilde{\xi}+\frac{\eta}{\sqrt{\varepsilon}}|)}{\left(2d - 2\sum_\nu \cos(\sqrt{\varepsilon}\tilde{\xi}_\nu + \eta_\nu)\right)^k} \right|^2 \times$$
$$\times \left| P_\alpha(D_{\tilde{\xi}}) \left(-\varepsilon\Delta^{\sqrt{\varepsilon}}_{\tilde{x}}\right)^k a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon)\right|^2 .$$

Since by assumption

$$\sup_{\tilde{x},\tilde{\xi}} \left|\partial^\alpha_{\tilde{x}}\partial^\beta_{\tilde{\xi}} a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon)\right| \leq \tilde{M}\varepsilon^{r+(\frac{1}{2}-\delta)(|\alpha|+|\beta|)} , \tag{B.35}$$

we can use the arguments given from equation (B.20) to (B.22) concerning the discrete Laplacian and the derivatives of $\left(2d - 2\sum_\nu \cos(\sqrt{\varepsilon}(\tilde{\xi}_\nu + \tilde{\eta}_\nu))\right)^{-1}$, to get with $\tilde{\tau} = \tilde{\xi} + \tilde{\eta}$

$$\begin{aligned} \|G_{lk\alpha}\|^2_{\ell^2((\sqrt{\varepsilon}\mathbb{Z})^d)\times\mathscr{L}^2((\mathbb{T}/\sqrt{\varepsilon})^d)} &\leq M\varepsilon^{2(r+(\frac{1}{2}-\delta)(|\alpha|+2k)+k)} \|u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)} \int_{\mathrm{supp}(\mathbf{1}-\zeta)} d\tilde{\tau} \left|\frac{C_{k\alpha}}{|\sqrt{\varepsilon}\tilde{\tau}|^{2k}}\right|^2 \\ &\leq C_{k\alpha} M\varepsilon^{2(r+(|\alpha|+2k)(\frac{1}{2}-\delta))} \|u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)} \end{aligned} \tag{B.36}$$

for $k$ big enough. Inserting (B.34) and (B.36) in (B.33) yields

$$\begin{aligned} |I_1| &\leq \sum_{|\alpha|\leq 2l} C_{lk\alpha} M\varepsilon^{r+(|\alpha|+2k)(\frac{1}{2}-\delta)} \|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \|v\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \\ &\leq C_{lk} M\varepsilon^r \|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)} \|v\|_{\ell^2((\varepsilon\mathbb{Z})^d)} . \end{aligned} \tag{B.37}$$

To get an estimate for the modulus of $I_2$, which denotes the integral over the support of $\zeta$, we use $L_5(\tilde{x}-\tilde{y},\tilde{\xi})$, so

$$I_2 = (2\pi)^{-\frac{3d}{2}} \varepsilon^d \sum_{\tilde{y},\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \iint_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} d\tilde{\xi} \left(L^l_5(\tilde{x}-\tilde{y},\tilde{\xi}) e^{-i((\tilde{x}-\tilde{y})\tilde{\xi}+\tilde{x}\tilde{\eta})}\right) \times$$
$$\times \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta}) \zeta(|\tilde{\xi}+\tilde{\eta}|) a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon) v(\sqrt{\varepsilon}\tilde{y}) =$$
$$= (2\pi)^{-\frac{3d}{2}} \varepsilon^d \sum_{\tilde{y},\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \frac{v(\sqrt{\varepsilon}\tilde{y})}{\langle\tilde{x}-\tilde{y}\rangle^{2l}} \iint_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} d\tilde{\xi}\, e^{-i((\tilde{x}-\tilde{y})\tilde{\xi}+\tilde{x}\tilde{\eta})} \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta}) \times$$
$$\times \left(\mathbf{1} - \Delta_{\tilde{\xi}}\right)^l \zeta(|\tilde{\xi}+\tilde{\eta}|) a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon) .$$

With the notation

$$\begin{aligned} G_l(\tilde{x},\tilde{\xi}) &:= \frac{\varepsilon^{\frac{d}{2}}}{\sqrt{2\pi}^d} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\eta} e^{-i\tilde{x}\tilde{\eta}} \left(\mathscr{F}_\varepsilon{}^{-1}\bar{u}\right)(\sqrt{\varepsilon}\tilde{\eta}) \left(\mathbf{1} - \Delta_{\tilde{\xi}}\right)^l \zeta(|\tilde{\xi}+\tilde{\eta}|) a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon) = \\ &= \mathscr{F}_{\varepsilon\eta\to\sqrt{\varepsilon}\tilde{x}} \left(\mathscr{F}^{-1}\bar{u}\right)(\eta) \left(\mathbf{1} - \Delta_{\tilde{\xi}}\right)^l \zeta(|\tilde{\xi} + \frac{\eta}{\sqrt{\varepsilon}}|) a(\sqrt{\varepsilon}\tilde{x},\sqrt{\varepsilon}\tilde{\xi};\varepsilon) \end{aligned}$$

and $F_l$ as given in (B.32)

$$I_2 = (2\pi)^{-\frac{d}{2}} \sum_{\tilde{x}\in(\sqrt{\varepsilon}\mathbb{Z})^d} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde{\xi} e^{-i\tilde{x}\tilde{\xi}} F_l(\tilde{x},\tilde{\xi}) G_l(\tilde{x},\tilde{\xi}) . \tag{B.38}$$

We get by (B.35), the substitution $\tilde\tau = \tilde\xi + \tilde\eta$ and the isometry of the Fourier transform in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$

$$\begin{aligned}\|G_l\|^2_{\ell^2((\sqrt{\varepsilon}\mathbb{Z})^d)\times\mathscr{L}^2((\mathbb{T}/\sqrt{\varepsilon})^d)} &\leq \int_{[-\pi,\pi]^d} d\eta \left|\left(\mathscr{F}_\varepsilon{}^{-1}\bar u\right)(\eta)\right|^2 \times \\ &\quad\times \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde\xi \left|\sum_{|\alpha|\leq 2l}\left(Q_\alpha(D_{\tilde\xi})\zeta(|\tilde\xi + \frac{\eta}{\sqrt{\varepsilon}}|)\right)\left(P_\alpha(D_{\tilde\xi})a(\sqrt{\varepsilon}\tilde x, \sqrt{\varepsilon}\tilde\xi;\varepsilon)\right)\right|^2 \\ &\leq \|u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)} \int_{[-\frac{\pi}{\sqrt{\varepsilon}},\frac{\pi}{\sqrt{\varepsilon}}]^d} d\tilde\tau \left|\sum_{|\alpha|\leq 2l} C_\alpha \varepsilon^{r+(\frac12-\delta)|\alpha|}Q_\alpha(D_{\tilde\tau})\zeta(|\tilde\tau|)\right|^2 \\ &\leq C_l\varepsilon^r\|u\|^2_{\ell^2((\varepsilon\mathbb{Z})^d)}\,. \end{aligned} \tag{B.39}$$

for $l$ big enough. Inserting (B.34) and (B.39) in (B.38) leads via the Schwarz inequality to

$$|I_2| \leq C_l\varepsilon^r\|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}\|v\|_{\ell^2((\varepsilon\mathbb{Z})^d)}$$

and therefore we finally get

$$|\left\langle u\,,\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)v\right\rangle_{\ell^2}| \leq M\varepsilon^r\|u\|_{\ell^2((\varepsilon\mathbb{Z})^d)}\|v\|_{\ell^2((\varepsilon\mathbb{Z})^d)}\,.$$

Since $s\left((\varepsilon\mathbb{Z})^d\right)$ is dense in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, the operator $\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)$ is continuous in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ with the operator norm

$$\|\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(a)\|_\infty \leq M\varepsilon^r\,.$$

□

We are now in the position to introduce the Hamilton operator analyzed in Chapter 2 and to find the norm estimate of this operator in microlocal approximation.

PROPOSITION B.9. *Let $T_\varepsilon$ be a translation operator on the lattice $(\varepsilon\mathbb{Z})^d$ as described in Hypothesis 2.7 with the symbol $t$ and let $T_{\varepsilon,q,j}$ denote the quadratic approximation of $T_\varepsilon$, associated to the symbol $t_{\pi,q,j}$ defined in (2.29). Let $\chi_{j,\varepsilon}$, $1\leq j\leq m$ and $\tilde\phi_{0,\varepsilon}$ be the cut-off-functions defined in (2.41) and (2.45) respectively. Then*

$$||\chi_{j,\varepsilon}\,\mathrm{Op}_\varepsilon^{\mathbb{T}^d}(\tilde\phi_{0,\varepsilon})(T_\varepsilon - T_{\varepsilon,q,j})\,\mathrm{Op}_\varepsilon^{T^d}(\tilde\phi_{0,\varepsilon})\chi_{j,\varepsilon}||_\infty = O(\varepsilon^{\frac65})\,.$$

Proof:
To use Proposition B.8, we have to find the symbol associated to the operator we want to estimate. Because the operator is a composition of several operators, this will be done by use of Lemma B.7. First we remark that for two symbols $a, b \in S^r_\delta(m)$, $\delta < \frac12$, where $b$ has compact support, and a function $\psi \in \mathscr{C}_0^\infty(\mathbb{R}^d\times\mathbb{T}^d)$ with $\psi(x,\xi)|_{\operatorname{supp} b} = 1$, we have

$$a\#b(x,\xi,\varepsilon) = a\psi\#b(x,\xi,\varepsilon) + O\left(\varepsilon^\infty\right)\,. \tag{B.40}$$

(B.40) follows directly by (B.24) for the asymptotic expansion, yielding

$$(a\#b) - (a\psi\#b) \sim \sum_{\alpha\in\mathbb{N}_0^d}\frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\partial_\xi^\alpha(a - a\psi)\partial_x^\alpha b\,,$$

since on the support of $b$

$$\partial_\xi^\alpha(a - a\psi) = \partial_\xi^\alpha a(1-\psi) + \sum_{\substack{\beta,\gamma\\ 1\leq|\beta|,|\gamma|\leq|\alpha|}}\partial_\xi^\beta a\partial_\xi^\gamma\psi = 0\,.$$

Thus (B.40) holds and the operator associated to $a\psi\#b$ is equal to $A\circ B$ modulo terms of order $\varepsilon^\infty$.
Introducing the cut-off-functions

$$\widehat{\tilde\phi}_0(\xi) := \tilde\phi_{0,\varepsilon}\left(\frac{\xi}{3}\right) \quad\text{and}\quad \widehat\chi_j(x) := \chi_{j,\varepsilon}\left(\frac{x}{3}\right)\,,$$

which are equal to 1 on the support of $\tilde\phi_{0,\varepsilon}$ respectively $\chi_{j,\varepsilon}$, this allows us to analyze the symbol

$$\widehat p(x,\xi;\varepsilon) := (\chi_{j,\varepsilon}\#\tilde\phi_{0,\varepsilon}\#(t - t_{\pi,q,j})\widehat{\tilde\phi}_0\widehat\chi_j\#\tilde\phi_{0,\varepsilon}\#\chi_{j,\varepsilon})(x,\xi;\varepsilon)$$

instead of $p := (\chi_{j,\varepsilon}\#\tilde{\phi}_{0,\varepsilon}\#(t-t_{qj})\#\tilde{\phi}_{0,\varepsilon}\#\chi_{j,\varepsilon})$, which by Lemma B.7 corresponds to the considered operator.
The aim of the proof is to show $\widehat{p} \in S^{\frac{6}{5}}_{\frac{2}{5}}(1)$, since the proposition then follows directly from Proposition B.8.
To this end, we determine the symbol class of $(t-t_{\pi,q,j})\widehat{\tilde{\phi}}_0\widehat{\chi}_j$. With the notation $\widehat{\chi}_j(x) =: \widehat{\tilde{\chi}}_j(\varepsilon^{-\frac{2}{5}}x)$ and similar for $\widehat{\tilde{\phi}}_0$, let $\alpha, \beta, \alpha_i, \beta_i \in \mathbb{N}_0^d$ for $i = 1, 2$ and $|\alpha_1| + |\alpha_2| = |\alpha|$ as well as $|\beta_1| + |\beta_2| = |\beta|$, then

$$\left|\partial_x^\alpha \partial_\xi^\beta (t - t_{\pi,q,j})\widehat{\tilde{\phi}}_0\widehat{\chi}_j\right| = \left|\sum_{\alpha_1,\alpha_2,\beta_1,\beta_2} \varepsilon^{-\frac{2}{5}(|\beta_2|+|\alpha_2|)} \left(\partial_x^{\alpha_1}\partial_\xi^{\beta_1}(t - t_{\pi,q,j})\right) \left(\partial_\xi^{\beta_2}\widehat{\tilde{\phi}}_0\right) \left(\partial_x^{\alpha_2}\widehat{\tilde{\chi}}_j\right)\right| . \quad \text{(B.41)}$$

The scaling of the support of the cut-off-functions with respect to $\varepsilon$ yields $|x - x_j| = O\left(\varepsilon^{\frac{2}{5}}\right) = |\xi|$, therefore

$$\begin{aligned} &\sup_{|\xi|\in\operatorname{supp}(\widehat{\tilde{\phi}}_0)} \sup_{|x|\in\operatorname{supp}(\widehat{\chi}_j)} \left(\partial_x^{\alpha_1}\partial_\xi^{\beta_1}(t - t_{\pi,q,j})(x, \xi; \varepsilon)\right) \\ &\quad = \sup_{|\xi|\in\operatorname{supp}(\widehat{\tilde{\phi}}_0)} \sup_{|x|\in\operatorname{supp}(\widehat{\chi}_j)} \left(\partial_x^{\alpha_1}\partial_\xi^{\beta_1}(\langle\xi\,,\,(B(x) - B(x_j))\xi\rangle + O\left(|\xi|^3\right))\right) \\ &\quad \le C\varepsilon^{\frac{6}{5}-|\beta_1|\frac{2}{5}-|\alpha_1|\frac{2}{5}} . \end{aligned} \quad \text{(B.42)}$$

Inserting (B.42) in (B.41) shows

$$|\partial_x^\alpha \partial_\xi^\beta (t - t_{\pi,q,j})\widehat{\tilde{\phi}}_0\widehat{\chi}_j(x, \xi; \varepsilon)| \le C_{\alpha,\beta}\varepsilon^{\frac{6}{5}-\frac{2}{5}(|\alpha|+|\beta|)}$$

and therefore $(t - t_{\pi,q,j})\widehat{\tilde{\phi}}_0\widehat{\chi}_j \in S^{\frac{6}{5}}_{\frac{2}{5}}(1)$. The cut-off-functions $\chi_{j,\varepsilon}$ and $\tilde{\phi}_{0,\varepsilon}$ are both elements of $S^0_{\frac{2}{5}}(1)$, thus by Lemma B.6 we get $p' \in S^{\frac{6}{5}}_{\frac{2}{5}}(1)(\mathbb{R}^d \times \mathbb{T}^d)$. The estimate of the norm of the associated operator in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$ results by use of Lemma B.8.

□

The following lemma, which gives the resulting symbol class of double commutators, is an application of the Lemmata B.6 and B.7.

Lemma B.10. *Let $\chi(x) \in \mathscr{C}^\infty(\mathbb{R}^d)$ and $\phi(\xi) \in \mathscr{C}^\infty(\mathbb{T}^d)$ be multiplication operators in the configuration respectively momentum space with symbols in $S^{r_1}_{\delta_1}(m_1)(\mathbb{R}^d \times \mathbb{T}^d)$, $\delta_1 < \frac{1}{2}$. Let $H$ be an operator on $\ell^2((\varepsilon\mathbb{Z})^d)$ associated to the phase space symbol $h(x, \xi) \in S^{r_2}_{\delta_2}(m_2)(\mathbb{R}^d \times \mathbb{T}^d)$, $\delta_2 < \frac{1}{2}$. For $a \in S^{r_a}_{\delta_a}(m_a)(\mathbb{R}^d \times \mathbb{T}^d)$ and $b \in S^{r_b}_{\delta_b}(m_b)(\mathbb{R}^d \times \mathbb{T}^d)$ let*

$$[a, b]_\# := a\#b - b\#a$$

*denote the commutator in symbolic calculus.*
*Then for $\alpha, \alpha_1, \alpha_2 \in \mathbb{N}^d$ with $|\alpha| \ge 2$ and $\alpha_1 + \alpha_2 = \alpha$ with $|\alpha_k| \ge 1, k = 1, 2$ and for $\delta := \max\{\delta_1, \delta_2\}$:*

(a) *$[\chi, [\chi, h]_\#]_\# \in S^{2-2(\delta_1+\delta_2)}_\delta(m_1^2 m_2)$ and it has the expansion*

$$[\chi(x), [\chi(x), h(x, \xi)]_\#]_\# \sim \sum_\alpha \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!} \left(\partial_\xi^\alpha h\right)(x, \xi) \sum_{\alpha_1,\alpha_2} \left(\partial_x^{\alpha_1}\chi\right)(x) \left(\partial_x^{\alpha_2}\chi\right)(x) .$$

(b) *$[\phi(\xi), [\phi(\xi), h(x, \xi)]_\#]_\# \in S^{2-2(\delta_1+\delta_2)}_\delta(m_1^2 m_2)$ and it has the expansion*

$$[\phi(\xi), [\phi(\xi), h(x, \xi)]_\#]_\# \sim \sum_\alpha \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!} \left(\partial_x^\alpha h\right)(x, \xi) \sum_{\alpha_1,\alpha_2} \left(\partial_\xi^{\alpha_1}\phi\right)(\xi) \left(\partial_\xi^{\alpha_2}\phi\right)(\xi) .$$

(c) *the symbol associated to the operator $[A, B]$ is given by $[a, b]_\#$.*

*If we split the asymptotic series given in (a) and (b) in the finite sum of terms with $2 \le |\alpha| \le N-1$ and a remainder $R_N$, the remainder is an element of the symbol class $S^{N(1-\delta_1-\delta_2)}_\delta(m_1^2 m_2)$ and it depends linearly on a finite number of Fréchet semi-norms of the single symbols. Furthermore it depends only on the derivatives of $h$, which are at least of order $N$ and of the product of derivatives of the cut-off functions of order $N_1$ and $N_2$, such that $N_1 + N_2 \ge N$.*

Proof:
(a):
The double commutator is given by

$$[\chi(x), [\chi(x), h(x,\xi)]_\#]_\# = \chi\#\chi\#h(x,\xi) + h\#\chi\#\chi(x,\xi) - 2\chi\#h\#\chi(x,\chi)\,. \tag{B.43}$$

By Lemma B.6, these terms are given by

$$\begin{aligned}
\chi\#\chi\#h(x,\xi) &= \chi\cdot\chi\cdot h(x,\xi)\\
h\#\chi\#\chi(x,\xi) &= \sum_{\substack{\alpha\in\mathbb{N}^d\\|\alpha|\leq N-1}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\left(\partial_\xi^\alpha h\right)\left(\partial_x^\alpha\chi^2\right)(x,\xi) + R_N(x,\xi;\varepsilon\\
\chi\#h\#\chi(x,\chi) &= \sum_{\substack{\alpha\in\mathbb{N}^d\\|alpha|\leq N-1}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\chi\left(\partial_\xi^\alpha h\right)\left(\partial_x^\alpha\chi\right)(x,\xi) + \tilde{R}_N(x,\xi;\varepsilon)\,.
\end{aligned}$$

where $R_N, \tilde{R}_N \in S_\delta^{N(1-\delta_1-\delta_2)}(m_1^2 m_2)$. The terms with $|\alpha| = 0$ and $|\alpha| = 1$ cancel in (B.43) Furthermore all terms with $2\chi_j\partial_x^\alpha\chi_j$ cancel. Thus it remains by use of the Leibnitz formula with $\alpha_1+\alpha_2=\alpha$ and $|\alpha_k|\geq 1, k=1,2$ the expansion

$$[\chi(x), [\chi(x), h(x,\xi)]_\#]_\# = \sum_{\substack{\alpha\in\mathbb{N}^d\\2\leq|\alpha|\leq N-1}} (i\varepsilon)^{|\alpha|}\left(\partial_\xi^\alpha h\right)\sum_{\substack{\alpha_1,\alpha_2\in\mathbb{N}^d\\\alpha_1+\alpha_2=\alpha}}\frac{1}{|\alpha_1|!|\alpha_2|!}\left(\partial_x^{\alpha_1}\chi\right)\left(\partial_x^{\alpha_2}\chi\right)(x,\xi) + R_N(x,\xi;\varepsilon)$$

with $R_N \in S_\delta^{N(1-\delta_1-\delta_2)}(m_1^2 m_2)$. The statement on the symbol class follows at once from this expansion, since each summand is at least of order $\varepsilon^{2(1-\delta_1-\delta_2)}$ and by use of the Leibnitz rule.
(b):
As above the double commutator consists of the terms

$$[\phi(\xi), [\phi(\xi), h(x,\xi)]_\#]_\# = \phi\#\phi\#h(x,\xi) + h\#\phi\#\phi(x,\xi) - 2\phi\#h\#\phi(x,\chi) \tag{B.44}$$

and the summands have the expansions

$$\begin{aligned}
\phi\#\phi\#h(x,\xi) &= \sum_{\substack{\alpha\in\mathbb{N}^d\\|\alpha|\leq N-1}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\left(\partial_x^\alpha h\right)\left(\partial_\xi^\alpha\phi^2\right)(x,\xi) + R_N(x,\xi;\varepsilon)\\
h\#\chi\#\chi(x,\xi) &= h\cdot\phi\cdot\phi(x,\xi)\\
\chi\#h\#\chi(x,\chi) &= \sum_{\substack{\alpha\in\mathbb{N}^d\\|\alpha|\leq N-1}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\phi\left(\partial_x^\alpha h\right)\left(\partial_\xi^\alpha\phi\right)(x,\xi) + \tilde{R}_N(x,\xi;\varepsilon)\,,
\end{aligned}$$

where $R_N, \tilde{R}_N \in S_\delta^{N(1-\delta_1-\delta_2)}(m_1^2 m_2)$. Therefore in (B.44) remains as discussed in (a) with $\alpha_1 + \alpha_2 = \alpha$ and $|\alpha_k|\geq 1, k=1,2$

$$[\phi(\xi), [\phi(\xi), h(x,\xi)]_\#]_\# \sim \sum_{\substack{\alpha\in\mathbb{N}^d\\2\leq|\alpha|\leq N-1}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\left(\partial_x^\alpha h\right)\sum_{\substack{\alpha_1,\alpha_2\in\mathbb{N}^d\\\alpha_1+\alpha_2=\alpha}}\left(\partial_\xi^{\alpha_1}\phi\right)\left(\partial_\xi^{\alpha_2}\phi\right)(x,\xi) + R_N(x,\xi;\varepsilon)$$

with $R_N \in S_\delta^{N(1-\delta_1-\delta_2)}(m_1^2 m_2)$. The statement on the symbol class follows from this expansion as discussed in (a).
(c): This is a direct consequence of Lemma B.7.
The additional properties of $R_N$ follow immediately from the properties of remainder in Corollary B.6.

□

## B.4. Definition of Pseudo-differential Operators on $\mathscr{L}^2(\mathbb{R}^d)$

We follow the definitions of $h$-scaled symbol classes and associated pseudo-differential operators given in Dimassi-Sjöstrand ([**16**]) and Robert ([**50**]). These definitions are analogue to the lattice case and for several results on the composition of symbols and the Calderon-Vaillancourt Theorem, we refer to the books just mentioned.

Definition B.11. (a) *A function $m : \mathbb{R}^n \to [0, \infty)$ is called an order function, if there exist constants $C_0 > 0$ and $N_0 > 0$, such that*

$$m(x) \le C_0 \langle x - y\rangle^{N_0} m(y)\,, \qquad x, y \in \mathbb{R}^d,$$

*with the notation $\langle x\rangle := \sqrt{1 + |x|^2}$.*

(b) *For an order function $m$ on $\mathbb{R}^n$, the symbol space $S(m)\left(\mathbb{R}^n\right)$ consists of all $a \in \mathscr{C}^\infty(\mathbb{R}^n)$, for which for all $\alpha \in \mathbb{N}^d$ there is a constant $C_\alpha$ such that*

$$|\partial_x^\alpha a(x)| \le C_\alpha m(x)\,, \qquad x \in \mathbb{R}^d\,.$$

*We often write $S(m)$, if the underlying space is clear.*

(c) *If the symbol $a(x;\varepsilon)$ depends on a small parameter $\varepsilon \in (0,1]$, $a$ is said to be in $S(m)$, if $a(\cdot\,;\varepsilon)$ is uniformly bounded in $S(m)$ for $\varepsilon$ varying in $(0,1]$. Let $S^k(m) := \varepsilon^k S(m)$ describe for $k \in \mathbb{R}$ the space of symbols of the form $\varepsilon^k a(x;\varepsilon)$ for $a \in S(m)$. For $\delta \in [0,1]$, the space $S^k_\delta(m)\left(\mathbb{R}^d\right)$ consists of functions $a(x;\varepsilon)$ on $\mathbb{R}^d \times (0,1]$, belonging to $S(m)\left(\mathbb{R}^d\right)$ for every fixed $\varepsilon$ and satisfying*

$$|\partial_x^\alpha a(x;\varepsilon)| \le C_\alpha m(x,\xi)\varepsilon^{k-\delta|\alpha|}\,, \quad x \in \mathbb{R}^d\,.$$

(d) *Let $a_j \in S^{k_j}_\delta(m), k_j \nearrow \infty$, then $a \sim \sum_{j=0}^\infty a_j$ means that $a - \sum_{j=0}^N a_j \in S^{k_{N+1}}_\delta(m)$ for every $N \in \mathbb{N}$.*

(e) *A pseudo-differential operator $\mathrm{Op}_\varepsilon : \mathscr{C}_0^\infty\left(\mathbb{R}^d\right) \to \left(\mathscr{C}_0^\infty\right)'\left(\mathbb{R}^d\right)$ associated to a symbol $a \in S^k_\delta(m)\left(\mathbb{R}^{2d}\right)$ is defined by*

$$\mathrm{Op}_\varepsilon\, u(x) = \frac{1}{(\varepsilon 2\pi)^n} \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}(y-x)\xi} a(x,\xi;\varepsilon) u(y)\, dy d\xi\,, \qquad u \in \mathscr{C}_0^\infty\left(\mathbb{R}^d\right)\,.$$

Using the symbolic calculus introduced in Dimassi-Sjöstrand [**16**], in particular Proposition 7.7, Theorem 7.9 and Theorem 7.11, it is possible to show by similar considerations as in the lattice case, that for $\widehat{T}, \widehat{T_{qj}}$ defined in (2.30) and (2.33) respectively and the cut-off functions $\chi_{j,\varepsilon}, \phi_k$ defined in (2.41) and (2.44) the norm estimate

$$||\chi_{j,\varepsilon}(x)\tilde{\phi}_{0,\varepsilon}(\varepsilon D)(T_\varepsilon - T_{\varepsilon qj})\tilde{\phi}_{0,\varepsilon}(\varepsilon D)\chi_{j,\varepsilon}(x)||_\infty = O(\varepsilon^{\frac{6}{5}}) \tag{B.45}$$

holds.

## B.5. Analogue of the Persson Theorem in the discrete setting

In this section we will prove a theorem on the infimum of the essential spectrum of $H_\varepsilon$ acting in $\ell^2\left((\varepsilon\mathbb{Z})^d\right)$, which is similar to Persson's Theorem for Schrödinger operators. The proof follows the proof of Persson's Theorem in the Schrödinger setting given in Helffer [**30**] and Agmon [**3**] respectively.

Theorem B.12. *Let $H_\varepsilon = T_\varepsilon + V_\varepsilon$ satisfy Hypothesis 2.7, denote by $\sigma_{ess}(H_\varepsilon)$ the essential spectrum of $H_\varepsilon$ and define*

$$\Sigma(H_\varepsilon) := \sup_{\substack{K \subset (\varepsilon\mathbb{Z})^d \\ finite}} \inf \left\{ \frac{\langle H_\varepsilon \phi\,,\, \phi\rangle_{\ell^2}}{\|\phi\|^2_{\ell^2}} \,|\, \phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus K\right) \right\}\,, \tag{B.46}$$

*where $c_0(D)$ denote the space of real-valued functions on $(\varepsilon\mathbb{Z})^d$ with compact, i.e. finite, support in $((\varepsilon\mathbb{Z})^d \setminus D)$. Then*

$$\inf \sigma_{ess}\left(H_\varepsilon\right) = \Sigma\left(H_\varepsilon\right)\,.$$

The proof of Theorem B.12 is divided in two Lemmata and the main part.

Lemma B.13. *For $x \in (\varepsilon\mathbb{Z})^d$ and $R > 0$ let $B_x(R) := \{y \in (\varepsilon\mathbb{Z})^d \,|\, |x - y| < R\}$ denote the ball around $x$ with radius $R$ and*

$$\Lambda_R(x, H_\varepsilon) := \inf \left\{ \frac{\langle H_\varepsilon \phi\,,\, \phi\rangle_{\ell^2}}{\|\phi\|^2_{\ell^2}}\,;\, \phi \in c_0\left(B_x(R)\right) \right\}\,. \tag{B.47}$$

*Then for all $\delta > 0$ there exists a radius $R_\delta > 0$, such that for all $R > R_\delta$ and $\phi \in c_0\left((\varepsilon\mathbb{Z})^d\right)$*

$$\langle H_\varepsilon \phi\,,\, \phi\rangle_{\ell^2} \ge \sum_{x \in (\varepsilon\mathbb{Z})^d} \left(\Lambda_R(x, H_\varepsilon) - \delta\right) |\phi(x)|^2\,.$$

Proof of Lemma B.13:

Let $\rho \in \mathscr{C}_0^\infty\left(\mathbb{R}^d\right)$ be real valued with $\rho(x) = 0$ for $|x| \geq \frac{1}{2}$ and $\int_{\mathbb{R}^d} |\rho(x)|^2\, dx = 1$ and define

$$\rho_{y,R} := \rho\left(\frac{y-x}{R}\right) .$$

Then $\rho_{y,R}\phi \in c_0\left(B_y\left(\frac{R}{2}\right)\right)$ and therefore by the definition of $\Lambda_R$

$$\langle H_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} \geq \Lambda_{\frac{R}{2}}(y, H_\varepsilon)\|\rho_{y,R}\phi\|^2_{\ell^2} .$$

Since $B_y\left(\frac{R}{2}\right) \subset B_x(R)$ for $|x-y| < \frac{R}{2}$ and thus $\Lambda_{\frac{R}{2}}(y) \geq \Lambda_R(x)$, we get the estimate

$$\langle H_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} \geq \sum_{x\in(\varepsilon\mathbb{Z})^d} \Lambda_R(x, H_\varepsilon)(\rho_{y,R}\phi)^2(x) . \tag{B.48}$$

To analyze the scalar product we use that $T_\varepsilon$ is self adjoint and $\phi, \rho$ are real valued, yielding

$$\begin{aligned}\langle T_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} &= \frac{1}{2}\left(\langle T_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} + \langle \rho_{y,R}\phi\, ,\, T_\varepsilon\rho_{y,R}\phi\rangle_{\ell^2}\right) = \\ &= \frac{1}{2}\Big(\left\langle T_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} + \langle [T_\varepsilon, \rho_{y,R}]\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} + \left\langle \rho^2_{y,R}\phi\, ,\, T_\varepsilon\phi\right\rangle_{\ell^2} + \langle \rho_{y,R}\phi\, ,\, [T_\varepsilon, \rho_{y,R}]\phi\rangle_{\ell^2}\Big) = \\ &= \left\langle T_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} + \frac{1}{2}\left(\langle [T_\varepsilon, \rho_{y,R}]\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} + \langle \rho_{y,R}\phi\, ,\, [T_\varepsilon, \rho_{y,R}]\phi\rangle_{\ell^2}\right) .\end{aligned}$$

Since $[T_\varepsilon, \rho_{y,R}]^* = -[T_\varepsilon, \rho_{y,R}]$ it follows that

$$\langle T_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} = \left\langle T_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} + \frac{1}{2}\langle (\rho_{y,R}[T_\varepsilon, \rho_{y,R}] - [T_\varepsilon, \rho_{y,R}]\rho_{y,R})\phi\, ,\, \phi\rangle_{\ell^2}$$

and since $V_\varepsilon$ commutes with $\rho_{y,R}$, we therefore get

$$\left\langle H_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} = \langle H_\varepsilon \rho_{y,R}\phi\, ,\, \rho_{y,R}\phi\rangle_{\ell^2} - \frac{1}{2}\langle [\rho_{y,R}, [T_\varepsilon, \rho_{y,R}]]\phi\, ,\, \phi\rangle_{\ell^2} . \tag{B.49}$$

To analyze the double commutator, we use the symbolic calculus introduced in Appendix B. By Lemma B.10, the symbol associated to the operator $[\rho_{y,R}, [T_\varepsilon, \rho_{y,R}]]$ is given by

$$\begin{aligned}&\rho_{y,R}(x), [t(x,\xi), \rho_{y,R}(x)]_\#]_\# = \\ &= \sum_{\substack{\alpha\in\mathbb{N}^d\\ 2\leq|\alpha|<N}} \frac{(i\varepsilon)^{|\alpha|}}{|\alpha|!}\left(\partial_\xi^\alpha t\right)(x,\xi) \sum_{\substack{\alpha_1,\alpha_2\\ |\alpha_1|+|\alpha_2|=|\alpha|}} \left(\partial_x^{\alpha_1}\rho_{y,R}\right)(x)\left(\partial_x^{\alpha_2}\rho_{y,R}\right)(x) + R_N(t, \rho_{y,R}) ,\end{aligned} \tag{B.50}$$

where $R_N$ depends of a finite number of derivatives of $\rho_{y,R}$, which are at least of order $N$. By the scaling of $\rho_{y,R}$, it follows that $|\nabla_x \rho_{y,R}(x)| \leq \frac{C}{R}$ for $C$ suitable. Since all terms in the finite sum in (B.50) and the remainder $R_N$ depend on a product of two (at least first order) derivatives of $\rho_{y,R}$, any Fréchet semi-norm of the symbol of the double commutator is of order $\frac{1}{R^2}$. By Proposition B.8, the same statement follows for the operator-norm of the associated operator, thus there is a constant $C > 0$ such that

$$\|[\rho_{y,R}, [T_\varepsilon, \rho_{y,R}]]\|_\infty \leq \frac{C}{R^2} \tag{B.51}$$

By the Cauchy-Schwarz inequality, we get by inserting (B.48) and (B.51) in (B.49)

$$\left\langle H_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} \geq \sum_{x\in(\varepsilon\mathbb{Z})^d} \Lambda_R(x, H_\varepsilon)|\rho_{y,R}\phi(x)|^2 - \frac{C}{R^2}\sum_{x\in B_y(R)} |\phi(x)|^2 . \tag{B.52}$$

We remark that by setting $z = \frac{y-x}{R}$

$$\int_{\mathbb{R}^d} \rho^2_{y,R}(x)\, dy = R^d \int_{\mathbb{R}^d} \rho^2(z)\, dz = R^d \tag{B.53}$$

and

$$\int_{\mathbb{R}^d} \mathbf{1}_{\{|x-y|<R\}}\; dy = R^d \int_{\mathbb{R}^d} \mathbf{1}_{\{|z|<1\}}\; dz = CR^d . \tag{B.54}$$

Thus integration of the left hand side of (B.52) with respect to $y$ yields by (B.53)

$$\int_{\mathbb{R}^d} \left\langle H_\varepsilon \phi\, ,\, \rho^2_{y,R}\phi\right\rangle_{\ell^2} dy = \left\langle H_\varepsilon\phi\, ,\, \textstyle\int_{\mathbb{R}^d} \rho^2_{y,R}\, dy\phi\right\rangle_{\ell^2} = R^d\langle H_\varepsilon\phi\, ,\, \phi\rangle_{\ell^2} . \tag{B.55}$$

If we integrate the right hand side of (B.52) with respect to $y$ and use (B.54), we get

$$\int_{\mathbb{R}^d}\left(\sum_{x\in(\varepsilon\mathbb{Z})^d}\Lambda_R(x,H_\varepsilon)\rho_{y,R}^2(x)\phi^2(x)-\frac{C}{R^2}\sum_{x\in(\varepsilon\mathbb{Z})^d}\mathbf{1}_{\{|x-y|<R\}}\,|\phi(x)|^2\right)\,dy=$$

$$=R^d\left(\sum_{x\in(\varepsilon\mathbb{Z})^d}\Lambda_R(x,H_\varepsilon)\phi^2(x)-\frac{C'}{R^2}\sum_{x\in(\varepsilon\mathbb{Z})^d}|\phi(x)|^2\right)\ . \qquad \text{(B.56)}$$

The Integration of both sides of (B.52) with respect to $y$ and division by $R^d$ gives by (B.55) and (B.56)

$$\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}\geq\sum_{x\in(\varepsilon\mathbb{Z})^d}\left(\Lambda_R(x,H_\varepsilon)-\frac{C}{R^2}\right)|\phi(x)|^2\ . \qquad \text{(B.57)}$$

By choosing for $\delta>0$ the radius $R_\delta=\sqrt{\frac{C}{\delta}}$, the statement of Lemma B.13 follows for all $R>R_\delta$ by (B.57).

□

The family $\Lambda_R(x,H_\varepsilon)$ describes the lowest eigenvalue of the Dirichlet problem with respect to the ball $B_x(R)$. The next lemma relates this family with $\Sigma(H_\varepsilon)$.

LEMMA B.14. *Let* $\Lambda_R(x,H_\varepsilon)$ *and* $\Sigma(H_\varepsilon)$ *defined in* (B.47) *and* (B.46) *respectively, then*

$$\Sigma(H_\varepsilon)=\lim_{R\to+\infty}\liminf_{|x|\to\infty}\Lambda_R(x,H_\varepsilon)\ . \qquad \text{(B.58)}$$

Proof of Lemma B.14:

We split the proof in two parts showing the two fundamental inequalities.

*Step 1:* Estimate from above

$$\Sigma(H_\varepsilon)\leq\lim_{R\to+\infty}\liminf_{|x|\to\infty}\Lambda_R(x,H_\varepsilon) \qquad \text{(B.59)}$$

Let $K\subset(\varepsilon\mathbb{Z})^d$ compact and $R>0$ fixed. Then $B_x(R)\subset(\varepsilon\mathbb{Z})^d\setminus K$ for $|x|$ large enough and thus

$$\inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|_{\ell^2}^2}\,;\,\phi\in c_0\left((\varepsilon\mathbb{Z})^d\setminus K\right)\right\}\leq\inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|_{\ell^2}^2}\,;\,\phi\in c_0\left(B_x(R)\right)\right\}(=\Lambda_R(x,H_\varepsilon))\ .$$

This inequality is satisfied for all $|x|$ large enough and the left hand side is independent of $x$, thus

$$\inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|_{\ell^2}^2}\,;\,\phi\in c_0\left((\varepsilon\mathbb{Z})^d\setminus K\right)\right\}\leq\liminf_{|x|\to\infty}\Lambda_R(x,H_\varepsilon)\ .$$

The left hand side of this inequality is independent of $R$ and the right hand side understood as a function in $R$ is monotonically decreasing and bounded from below, thus the limit $R\to\infty$ is well defined and

$$\inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|_{\ell^2}^2}\,;\,\phi\in c_0\left((\varepsilon\mathbb{Z})^d\setminus K\right)\right\}\leq\lim_{R\to+\infty}\liminf_{|x|\to\infty}\Lambda_R(x,H_\varepsilon)\ .$$

Now the right hand side is independent of the choice of $K$, thus we can take the supremum over all compact sets $K\subset(\varepsilon\mathbb{Z})^d$ and by the definition of $\Sigma(H_\varepsilon)$, this shows (B.59).

*Step 2:* Estimate from below

$$\Sigma(H_\varepsilon)\geq\lim_{R\to+\infty}\liminf_{|x|\to\infty}\Lambda_R(y,H_\varepsilon)\ . \qquad \text{(B.60)}$$

By the definition of lim inf, it follows that for all $\delta>0$ and all $R>0$ there exists an $R_0$ such that for all $|x|>R_0$

$$\Lambda_R(x,H_\varepsilon)\geq\liminf_{|x|\to\infty}\Lambda_R(x,H_\varepsilon)-\delta\ .$$

It follows immediately that for all $\phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus \overline{B_0(R_0)}\right)$

$$\sum_{x\in(\varepsilon\mathbb{Z})^d} \Lambda_R(x,H_\varepsilon)|\phi(x)|^2 \geq \left(\liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon) - \delta\right) \|\phi\|^2_{\ell^2} \ . \tag{B.61}$$

By Lemma B.13 we know that for all $\delta > 0$ and $\phi \in c_0\left((\varepsilon\mathbb{Z})^d\right)$ there exists $R_\delta$ such that for all $R > R_\delta$

$$\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2} \geq \sum_{x\in(\varepsilon\mathbb{Z})^d} \left(\Lambda_R(x,H_\varepsilon) - \delta\right)|\phi(x)|^2 \ . \tag{B.62}$$

Inserting (B.62) in (B.61) it follows that for all $\delta > 0$ there exists $R_\delta$ such that for all $R > R_\delta$ there exists $R_0$ such that for all $\phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus \overline{B_0(R_0)}\right)$

$$\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|^2_{\ell^2}} \geq \liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon) - 2\delta\,. \tag{B.63}$$

By the definition of $\Sigma(H_\varepsilon)$ it follows directly that

$$\Sigma(H_\varepsilon) \geq \inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|^2_{\ell^2}} \mid \phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus \overline{B_0(R_0)}\right)\right\} . \tag{B.64}$$

The equation (B.62) holds for all $\phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus \overline{B_0(R_0)}\right)$, thus we can take on the left hand side the infimum over all these functions, which together with (B.64) yields

$$\Sigma(H_\varepsilon) \geq \liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon) - 2\delta\ . \tag{B.65}$$

The left hand side is independent of $R$ and since the relation holds for all $R > R_\delta$, it is possible to take the limit $R \to \infty$, which yields for all $\delta > 0$

$$\Sigma(H_\varepsilon) \geq \lim_{R\to+\infty} \liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon) - 2\delta\ .$$

Thus in the limit $\delta$ the estimate (B.60) follows.

□

Proof of Theorem B.12:

We discuss the cases $\Sigma(H_\varepsilon) = \infty$ and $\Sigma(H_\varepsilon) < \infty$ separately.

*Case 1:* $\Sigma(H_\varepsilon) < \infty$:
As in the preceding proof, we conclude the equality by showing that both inequalities hold.

*Step 1:* Estimate from below

$$\inf\sigma_{ess}(H_\varepsilon) \geq \Sigma(H_\varepsilon) \tag{B.66}$$

As a function of $R$, the term $\liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon)$ is monotonically decreasing, thus it follows by Lemma B.14, that for fixed $R > 0$

$$\Sigma(H_\varepsilon) \leq \liminf_{|x|\to\infty} \Lambda_R(x,H_\varepsilon)$$

and thus for all $\delta > 0$ there exists $a_\delta$ such that for all $x \in (\varepsilon\mathbb{Z})^d$ with $|x| > a_\delta$

$$\Sigma(H_\varepsilon) - \frac{\delta}{2} \leq \Lambda_R(x,H_\varepsilon)\ . \tag{B.67}$$

On the other hand denoting by $\sigma(H_\varepsilon)$ the spectrum of $H_\varepsilon$, it is clear by the definition of $\Lambda_R(x,H_\varepsilon)$ and the Min-Max-principle that

$$\Lambda_R(x,H_\varepsilon) \geq \inf\sigma(H_\varepsilon)\ . \tag{B.68}$$

Since $H_\varepsilon$ is bounded from below, it follows by (B.67) and (B.68) that there exists a constant $C > 0$ such that for all $x \in (\varepsilon\mathbb{Z})^d$

$$\Lambda_R(x,H_\varepsilon) \geq \Sigma(H_\varepsilon) - C\ . \tag{B.69}$$

We choose a function $W \in c_0\left((\varepsilon\mathbb{Z})^d\right)$ such that $W(x) \geq C$ for $|x| < a_\delta$ and $W(x) \geq 0$ everywhere. Then for $H_\varepsilon + W$ it follows by Lemma B.13, (B.67) and (B.69), that for $\phi \in c_0\left((\varepsilon\mathbb{Z})^d\right)$

$$\begin{aligned}\langle (H_\varepsilon + W)\phi\,,\,\phi\rangle_{\ell^2} &\geq \sum_{x\in(\varepsilon\mathbb{Z})^d} (W(x) - \Lambda_R(x, H_\varepsilon) - \frac{\delta}{2})|\phi(x)|^2\\ &\geq \sum_{|x|\leq a_\delta} (\Sigma(H_\varepsilon) - \frac{\delta}{2})|\phi(x)|^2 + \sum_{|x|>a_\delta} (W(x) + \Sigma(H_\varepsilon) - \delta)|\phi(x)|^2\\ &\geq (\Sigma(H_\varepsilon) - \delta) \sum_{x\in(\varepsilon\mathbb{Z})^d} |\phi(x)|^2\,.\end{aligned}$$

Thus it follows

$$\inf \sigma_{ess}(H_\varepsilon + W) \geq \inf \sigma(H_\varepsilon + W) \geq \Sigma(H_\varepsilon) - \delta\,, \tag{B.70}$$

where the first estimate follows directly by the definition of the spectra. The perturbation $W$ is compactly supported, thus each $u \in \ell^2((\varepsilon\mathbb{Z})^d)$ is mapped by $W$ to a lattice function with compact support, i.e. which is non-zero only at finitely many lattice points. Thus $W$ is a finite rank operator and in particular compact. This allows to use the Theorem of Weyl (see for example [**30**], [**49**]), telling us that a perturbation of a closed operator by means of a relatively compact operator does not change the essential spectrum. Since each compact operator is relatively compact to any closed operator, it follows that

$$\sigma_{ess}(H_\varepsilon + W) = \sigma_{ess}(H_\varepsilon)$$

and since (B.70) holds for all $\delta > 0$ the estimate (B.66) is shown.

*Step 2:* Estimate from above

$$\inf \sigma_{ess}(H_\varepsilon) \leq \Sigma(H_\varepsilon) \tag{B.71}$$

Fix $\mu < \inf \sigma_{ess}(H_\varepsilon)$ and denote by $\Pi_\mu := \Pi_{(-\infty,\mu]}$ the spectral projection to the eigenspace of energies smaller or equal to $\mu$. Since $\mu$ lies below the essential spectrum and $H_\varepsilon$ is semi-bounded from below, it follows that $\Pi_\mu$ has finite rank. Thus there exists an orthonormal system of eigenfunctions $\psi_1, \ldots, \psi_n \in \ell^2\left((\varepsilon\mathbb{Z})^d\right)$ such that

$$\Pi_\mu = \sum_{j=1}^n \langle\,.\,,\,\psi_j\rangle_{\ell^2}\psi_j$$

and for all $\delta > 0$ there exists an $R_\delta$ such that

$$\sum_{|x|>R_\delta} |\psi_j(x)|^2 \leq \delta\,.$$

Therefore (by the Cauchy-Schwarz inequality) for all $\phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus B_0(R_\delta)\right)$

$$\|\Pi_\mu\phi(x)\|^2_{\ell^2} = \sum_{j=1}^n |\langle\phi\,,\,\psi_j\rangle_{\ell^2}|^2 \leq \|\phi\|^2_{\ell^2} \sum_{j=1}^n \sum_{|x|>R_\delta} |\psi_j(x)|^2 \leq \delta\|\phi\|^2_{\ell^2}\,. \tag{B.72}$$

By the definition of $\Pi_\mu$ and since there exists a constant $C > 0$ such that $H_\varepsilon \geq -C$, we have

$$\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2} \geq \mu\langle(\mathbf{1} - \Pi_\mu)\phi\,,\,(\mathbf{1} - \Pi_\mu)\phi\rangle_{\ell^2} - C\langle\Pi_\mu\phi\,,\,\Pi_\mu\phi\rangle_{\ell^2}\,. \tag{B.73}$$

Therefore

$$\begin{aligned}\Sigma(H_\varepsilon) &\geq \inf\left\{\frac{\langle H_\varepsilon\phi\,,\,\phi\rangle_{\ell^2}}{\|\phi\|^2_{\ell^2}} \,|\, \phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus B_0(R_\delta)\right)\right\}\\ &\geq \inf\left\{\mu\frac{\|(\mathbf{1} - \Pi_\mu)\phi\|^2}{\|\phi\|^2_{\ell^2}} - C\frac{\|\Pi_\mu\phi\|^2}{\|\phi\|^2} \,|\, \phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus B_0(R_\delta)\right)\right\} =\\ &= \inf\left\{\mu - (C+\mu)\frac{\|\Pi_\mu\phi\|^2}{\|\phi\|^2_{\ell^2}} \,|\, \phi \in c_0\left((\varepsilon\mathbb{Z})^d \setminus B_0(R_\delta)\right)\right\}\end{aligned}$$

and by (B.72)

$$\Sigma(H_\varepsilon) \geq \mu - (C+\mu)\delta\,.$$

The left hand side is independent of $\delta$, thus for $\delta \to 0$ we get

$$\Sigma(H_\varepsilon) \geq \mu$$

for any $\mu < \inf \sigma_{ess}(H_\varepsilon)$ and thus in the limit $\mu \to \inf \sigma_{ess}(H_\varepsilon)$ the estimate (B.71) follows and thus Theorem B.12 is proven.

*Case 2:* $\Sigma(H_\varepsilon) = \infty$:
By Lemma B.14 it follows at once that $\lim_{|x|\to\infty} \Lambda_R(x, H_\varepsilon) = \infty$, because $\Lambda_R(x, H_\varepsilon)$ is monotonically decreasing with respect to $R$. Thus for all $M > 0$ there exists a $a_M$ such that for all $x \in (\varepsilon\mathbb{Z})^d$ with $|x| > a_M$ the estimate $\Lambda_R(x, H_\varepsilon) \geq M$ holds. On the other hand by (B.68) and the semi-boundedness of $H_\varepsilon$ it follows that there exists a constant $C > 0$ such that

$$\Lambda_R(x, H_\varepsilon) \geq -C\,, \qquad \text{for all} \quad x \in (\varepsilon\mathbb{Z})^d\,.$$

We can choose a function $W \in c_0\left((\varepsilon\mathbb{Z})^d\right)$ such that $W(x) \geq C + M$ for $|x| < a_M$ and $W(x) \geq 0$ everywhere. Then

$$\langle (H_\varepsilon + W)\phi\,,\, \phi\rangle_{\ell^2} \geq \left\langle (W + \Lambda_R(.,H_\varepsilon) - \tfrac{\delta}{2})\phi\,,\, \phi\right\rangle_{\ell^2} \geq \left(M - \frac{\delta}{2}\right) \|\phi\|^2_{\ell^2}$$

and thus for all $M > 0$ there exists a function $W \in c_0\left((\varepsilon\mathbb{Z})^d\right)$ such that

$$\sigma_{ess}(H_\varepsilon + W) \geq \sigma(H_\varepsilon + W) \geq M\,.$$

As in the case $\Sigma(H_\varepsilon) < \infty$ we have $\sigma(H_\varepsilon + W) = \sigma(H_\varepsilon)$ and therefore $\sigma_{ess}(H_\varepsilon) \geq M$ for all $M > 0$ and thus $\sigma_{ess}(H_\varepsilon) = \infty$.

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