ASYMPTOTIC EIGENFUNCTIONS FOR A CLASS OF DIFFERENCE OPERATORS

MARKUS KLEIN AND ELKE ROSENBERGER

ABSTRACT. We analyze a general class of difference operators $H_{\varepsilon} = T_{\varepsilon} + V_{\varepsilon}$ on $\ell^2((\varepsilon \mathbb{Z})^d)$, where V_{ε} is a one-well potential and ε is a small parameter. We construct formal asymptotic expansions of WKB-type for eigenfunctions associated with the low lying eigenvalues of H_{ε} . These are obtained from eigenfunctions or quasimodes for the operator H_{ε} , acting on $L^2(\mathbb{R}^d)$, via restriction to the lattice $(\varepsilon \mathbb{Z})^d$.

1. INTRODUCTION

The central topic of this paper is the construction of formal WKB-type expansions of eigenfunctions for a rather general class of families of difference operators $(H_{\varepsilon})_{\varepsilon \in (0,\varepsilon_0]}$ on the Hilbert space $\ell^2((\varepsilon \mathbb{Z})^d)$, as the small parameter $\varepsilon > 0$ tends to zero. The operator H_{ε} is given by

$$H_{\varepsilon} = (T_{\varepsilon} + V_{\varepsilon}), \quad \text{where} \quad T_{\varepsilon} = \sum_{\gamma \in (\varepsilon \mathbb{Z})^d} a_{\gamma} \tau_{\gamma},$$

$$(1.1)$$

$$(a_{\gamma}\tau_{\gamma}u)(x) = a_{\gamma}(x;\varepsilon)u(x+\gamma) \quad \text{for} \quad x,\gamma \in (\varepsilon\mathbb{Z})^d$$
(1.2)

and V_{ε} is a multiplication operator, which in leading order is given by $V_0 \in \mathscr{C}^{\infty}(\mathbb{R}^d)$.

This paper is based on the thesis Rosenberger [17]. It is the third in a series of papers (see Klein-Rosenberger [14], [15]); the aim is to develop an analytic approach to the semiclassical eigenvalue problem and tunneling for H_{ε} which is comparable in detail and precision to the well known analysis for the Schrödinger operator (see Simon [18], [19] and Helffer-Sjöstrand [11]). Our motivation comes from stochastic problems (see Klein-Rosenberger [14], Bovier-Eckhoff-Gayrard-Klein [3], [4], Baake-Baake-Bovier-Klein [2]). A large class of discrete Markov chains analyzed in [4] with probabilistic techniques falls into the framework of difference operators treated in this article.

In this paper we consider the case of a one-well potential V_{ε} and derive formal asymptotic expansions for the eigenfunctions v_j and the associated low lying eigenvalues of H_{ε} . These lead to good quasimodes for H_{ε} (in the precise sense of Theorem 1.6 below), which will be crucial for our analysis of the tunneling problem in a subsequent paper (see [17]). In general, these expansions contain half-integer powers of ε . As in [11] for the case of Schrödinger operators, we obtain sufficient conditions for the absence of these half-integer terms. We approach the construction of asymptotic expansions of type

$$v_j(x;\varepsilon) \sim e^{-\frac{\varphi(x)}{\varepsilon}} u_j(x;\varepsilon)$$

by conjugation of H_{ε} with the exponential weight $e^{-\frac{\varphi(x)}{\varepsilon}}$ and subsequent rescaling, using the variable $y = \frac{x}{\sqrt{\varepsilon}}$. Here φ is the Finsler distance of x to the potential well placed at x = 0, as constructed in Klein-Rosenberger [14]. This leads to an operator \hat{G}_{ε} treated at length in Section 3. It is analog to the approach in Klein-Schwarz [13] in the case of the Schrödinger operator. This more elementary approach avoids the use of an additional FBI-transform which was used in the original WKB-analysis of Helffer-Sjöstrand [11]. We remark that the discrete setting of the present paper introduces numerous technical difficulties. The main technical result in this respect is Proposition 3.2 on the expansion of $e^{\frac{\varphi(x)}{\varepsilon}} H_{\varepsilon} e^{-\frac{\varphi(x)}{\varepsilon}}$ (in the variable y).

We assume

HYPOTHESIS 1.1 (a) The coefficients $a_{\gamma}(x;\varepsilon)$ in (1.1) are functions

$$a: (\varepsilon \mathbb{Z})^d \times \mathbb{R}^d \times (0, \varepsilon_0] \to \mathbb{R}, \qquad (\gamma, x, \varepsilon) \mapsto a_\gamma(x; \varepsilon), \qquad (1.3)$$

for some $\varepsilon_0 > 0$, satisfying the following conditions:

(i) They have an expansion

$$a_{\gamma}(x;\varepsilon) = \sum_{k=0}^{N-1} \varepsilon^k a_{\gamma}^{(k)}(x) + R_{\gamma}^{(N)}(x;\varepsilon), \qquad N \in \mathbb{N}, \qquad (1.4)$$

where $a_{\gamma} \in \mathscr{C}^{\infty}(\mathbb{R}^d \times (0, \varepsilon_0])$ and $a_{\gamma}^{(k)} \in \mathscr{C}^{\infty}(\mathbb{R}^d)$ for $0 \le k \le N-1$.

- (ii) $\sum_{\gamma} a_{\gamma}^{(0)} = 0$ and $a_{\gamma}^{(0)} \le 0$ for $\gamma \ne 0$
- (iii) $\overline{a_{\gamma}}(x;\varepsilon) = a_{-\gamma}(x+\gamma;\varepsilon)$ for $x \in \mathbb{R}^d, \gamma \in (\varepsilon\mathbb{Z})^d$
- (iv) For any c > 0 and $\alpha \in \mathbb{N}^d$ there exists C > 0 such that for $0 \le k \le N-1$ uniformly with respect to $x \in \mathbb{R}^d$ and $\varepsilon \in (0, \varepsilon_0]$

$$\|e^{\frac{c|\cdot|}{\varepsilon}}\partial_x^{\alpha}a_{\cdot}^{(k)}(x)\|_{\ell^{2}_{\gamma}((\varepsilon\mathbb{Z})^{d})} \leq C \quad and \quad \|e^{\frac{c|\cdot|}{\varepsilon}}\partial_x^{\alpha}R_{\cdot}^{(N)}(x)\|_{\ell^{2}_{\gamma}((\varepsilon\mathbb{Z})^{d})} \leq C\varepsilon^{N} \quad (1.5)$$

- (v) $\operatorname{span}\{\gamma \in (\varepsilon \mathbb{Z})^d \mid a_{\gamma}^{(0)}(x) < 0\} = \mathbb{R}^d \text{ for } x = 0.$
- (b) (i) The potential energy V_{ε} is the restriction to $(\varepsilon \mathbb{Z})^d$ of a function $\widehat{V}_{\varepsilon} \in \mathscr{C}^{\infty}(\mathbb{R}^d, \mathbb{R})$, which has an expansion

$$\widehat{V}_{\varepsilon}(x) = \sum_{\ell=0}^{N-1} \varepsilon^l V_{\ell}(x) + R_N(x;\varepsilon), \qquad N \in \mathbb{N},$$
(1.6)

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

- (ii) V_ε is polynomially bounded and there exist constants R, C > 0 such that V_ε(x) > C for all |x| ≥ R and ε ∈ (0, ε₀].
- (iii) $V_0(x) \ge 0$ and it takes the value 0 only at the non-degenerate minimum $x_0 = 0$, which we call the potential well.

If $\mathbb{T}^d := \mathbb{R}^d/(2\pi)\mathbb{Z}^d$ denotes the *d*-dimensional torus and $b \in \mathscr{C}^\infty (\mathbb{R}^d \times \mathbb{T}^d \times (0,1])$, a pseudodifferential operator $\operatorname{Op}_{\varepsilon}^{\mathbb{T}}(b) : \mathcal{K}((\varepsilon \mathbb{Z})^d) \longrightarrow \mathcal{K}'((\varepsilon \mathbb{Z})^d)$ is defined by

$$\operatorname{Op}_{\varepsilon}^{\mathbb{T}}(b) v(x) := (2\pi)^{-d} \sum_{y \in (\varepsilon\mathbb{Z})^d} \int_{[-\pi,\pi]^d} e^{\frac{i}{\varepsilon}(y-x)\xi} b(x,\xi;\varepsilon) v(y) \, d\xi \,, \tag{1.7}$$

where

$$\mathcal{K}\left((\varepsilon\mathbb{Z})^d\right) := \{u : (\varepsilon\mathbb{Z})^d \to \mathbb{C} \mid u \text{ has compact support}\}$$
(1.8)

and $\mathcal{K}'((\varepsilon \mathbb{Z})^d) := \{f : (\varepsilon \mathbb{Z})^d \to \mathbb{C} \}$ is dual to $\mathcal{K}((\varepsilon \mathbb{Z})^d)$ by use of the scalar product $\langle u, v \rangle_{\ell^2} := \sum_x \bar{u}(x)v(x)$ (see the appendix of [15] for the basic theory of such operators).

We remark that under the assumptions given in Hypothesis 1.1, one has for T_{ε} defined in (1.1), $T_{\varepsilon} = \operatorname{Op}_{\varepsilon}^{\mathbb{T}}(t(.,.;\varepsilon))$, where $t \in \mathscr{C}^{\infty}(\mathbb{R}^d \times \mathbb{T}^d \times (0,\varepsilon_0])$ is given by

$$t(x,\xi;\varepsilon) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_{\gamma}(x;\varepsilon) \exp\left(-\frac{i}{\varepsilon}\gamma \cdot \xi\right) .$$
(1.9)

Here t is considered as a function on $\mathbb{R}^{2d} \times (0, \varepsilon_0]$, which is 2π -periodic with respect to ξ .

Furthermore, we set

$$t(x,\xi;\varepsilon) = \sum_{k=0}^{N-1} \varepsilon^k t_k(x,\xi) + \tilde{t}_N(x,\xi;\varepsilon) , \quad \text{with}$$

$$t_k(x,\xi) := \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_{\gamma}^{(k)}(x) e^{-\frac{i}{\varepsilon}\gamma\xi} , \quad 0 \le k \le N-1$$

$$\tilde{t}_N(x,\xi;\varepsilon) := \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} R_{\gamma}^{(N)}(x;\varepsilon) e^{-\frac{i}{\varepsilon}\gamma\xi} .$$

$$(1.10)$$

Thus, in leading order, the symbol of H_{ε} is $h_0 := t_0 + V_0$.

HYPOTHESIS 1.1 (c) We assume that t_0 defined in (1.10) fulfills

$$t_0(0,\xi) > 0$$
, if $|\xi| > 0$.

A simple example for an operator satisfying Hypothesis 1.1 is the discrete Laplacian. Here we have $a_{\gamma} = -1$ if $|\gamma| = \varepsilon$, $a_0 = 2d$ and $a_{\gamma} = 0$ else independent of x and ε , leading to

$$t(x,\xi;\varepsilon) = t_0(x,\xi) = 2\sum_{\nu=1}^d (1 - \cos \xi_{\nu}).$$

REMARK 1.2 It follows from (the proof of) Klein-Rosenberger [14], Lemma 1.2, that under the assumptions given in Hypothesis 1.1:

- (a) $\sup_{x,\xi} |\partial_x^{\alpha} \partial_{\xi}^{\beta} t(x,\xi;\varepsilon)| \leq C_{\alpha,\beta}$ for all $\alpha, \beta \in \mathbb{N}^d$ uniformly with respect to ε . Moreover $t_k, 0 \leq k \leq N-1$, is bounded and $\sup_{x,\xi} |\tilde{t}_N(x,\xi;\varepsilon)| = O(\varepsilon^N)$.
- (b) By Hypothesis 1.1, (a)(i), the condition (a)(v) holds for all x in a neighborhood of 0. This is sufficient to prove all statements of this paper. For the more global results of [14], it is necessary to assume (v) for all x ∈ ℝ^d.
- (c) At $\xi = 0$, for fixed $x \in \mathbb{R}^d$, the function t_0 defined in (1.10) has an expansion

$$t_0(x,\xi) = \langle \xi, B(x)\xi \rangle + \sum_{\substack{|\alpha|=2n\\n\geq 2}} B_\alpha(x)\xi^\alpha \qquad as \ |\xi| \to 0,$$
(1.11)

where $\alpha \in \mathbb{N}^d$, $B \in \mathscr{C}^{\infty}(\mathbb{R}^d, \mathcal{M}(d \times d, \mathbb{R}))$ is positive definite in a neighborhood of zero, B(x) is symmetric and B_{α} are real functions. By straightforward calculations one gets for $\mu, \nu \in \mathbb{N}$

$$B_{\nu\mu}(x) = -\frac{1}{2\varepsilon^2} \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_{\gamma}^{(0)}(x) \gamma_{\nu} \gamma_{\mu} .$$
(1.12)

- (d) By Hypothesis 1.1(a)(iii) and since the a_γ are real, the operator T_ε defined in (1.1) is symmetric. In the probabilistic context, which is our main motivation, the former is a standard reversibility condition while the latter is automatic for a Markov chain. Moreover, T_ε is bounded (uniformly in ε) by condition (a)(iv) and bounded from below by -Cε for some C > 0 by condition (a)(iv), (iii) and (ii).
- (e) A combination of the expansion (1.4) and the reversibility condition (a)(iii) establishes that the 2π -periodic function $\mathbb{R}^d \ni \xi \mapsto t_0(x,\xi)$ is even with respect to $\xi \mapsto -\xi$, i.e., $a_{\gamma}^{(0)}(x) = a_{-\gamma}^{(0)}(x)$ for all $x \in \mathbb{R}^d, \gamma \in (\varepsilon \mathbb{Z})^d$.
- (f) By condition (a),(iv) in Hypothesis 1.1, the exponential decay of the coefficients a_{γ} with respect to γ , the 2π -periodic function $\mathbb{R}^d \ni \xi \mapsto t(x,\xi;\varepsilon)$ has an analytic continuation to \mathbb{C}^d . Moreover for all B > 0

$$\sum_{\gamma} |a_{\gamma}(x;\varepsilon)| e^{\frac{B|\gamma|}{\varepsilon}} \leq C .$$

uniformly with respect to x and ε . This yields in particular

$$\sup_{x \in \mathbb{R}^d} |a_{\gamma}(x;\varepsilon)| \le C e^{-\frac{B|\gamma|}{\varepsilon}}$$
(1.13)

We further remark that condition (a),(iv) implies the estimate $|a_{\gamma}^{(k)}(x) - a_{\gamma}^{(k)}(x+h)| \leq Ch$ for $0 \leq k \leq N-1$ uniformly with respect to $\gamma \in (\varepsilon \mathbb{Z})^d$ and $h, x \in \mathbb{R}^d$.

(g) Since T_{ε} is bounded, $H_{\varepsilon} = T_{\varepsilon} + V_{\varepsilon}$ defined in (1.1) possesses a self adjoint realization on the maximal domain of V_{ε} . Abusing notation, we shall denote this realization also by H_{ε} and its domain by $\mathscr{D}(H_{\varepsilon}) \subset \ell^2((\varepsilon \mathbb{Z})^d)$. The associated symbol is denoted by $h(x, \xi; \varepsilon)$. Clearly, H_{ε} commutes with complex conjugation.

We will use the notation

$$\tilde{a}: \mathbb{Z}^d \times \mathbb{R}^d \ni (\eta, x) \mapsto \tilde{a}_\eta(x) := a_{\varepsilon\eta}^{(0)}(x) \in \mathbb{R}$$
(1.14)

and we have by Remark 1.2 (d) and (1.14)

$$-\tilde{h}_0(x,\xi) := h_0(x,i\xi) = \sum_{\eta \in \mathbb{Z}^d} \tilde{a}_\eta(x) \cosh(\eta \cdot \xi) + V_0(x) : \mathbb{R}^{2d} \to \mathbb{R} .$$
(1.15)

As shown in [14], the eigenfunctions associated to the first eigenvalues are localized in a small neighborhood of the potential well.

We shall construct asymptotic expansions of WKB-type for the eigenfunctions and associated low lying eigenvalues of H_{ε} . It is crucial for our approach that our actual constructions of quasimodes are done for the operator on $L^2(\mathbb{R}^d)$

$$\widehat{H}_{\varepsilon} = \widehat{T}_{\varepsilon} + \widehat{V}_{\varepsilon} , \qquad \widehat{T}_{\varepsilon} = \sum_{\gamma \in (\varepsilon \mathbb{Z})^d} a_{\gamma}(x;\varepsilon) \tau_{\gamma} , \qquad (1.16)$$

where $a_{\gamma}(x;\varepsilon)$ and $\widehat{V}_{\varepsilon}$ satisfy Hypothesis 1.1. Alternatively, $\widehat{H}_{\varepsilon} = \operatorname{Op}_{\varepsilon}(t+\widehat{V}_{\varepsilon})$, where $\operatorname{Op}_{\varepsilon}$ denotes the usual ε -dependent quantization for symbols in $S^r_{\delta}(m)(\mathbb{R}^{2d})$ (see [15]) and the symbol t is defined in (1.9). For $\widehat{H}_{\varepsilon}$, it is easy to change coordinates by translations and rotations. One then observes that restriction of an eigenfunction (or a quasi-mode) of $\widehat{H}_{\varepsilon}$ to the lattice $(\varepsilon \mathbb{Z})^d$ gives an eigenfunction (or a quasi-mode) of H_{ε} with the same (approximate) eigenvalue. More precisely, for $x_0 \in \mathbb{R}^d$, let us denote by $\mathscr{G}_{x_0} = (\varepsilon \mathbb{Z})^d + x_0$ the corresponding affine lattice. Then H_{ε} acts in a natural way on $\ell^2(\mathscr{G}_{x_0})$, since restriction to \mathscr{G}_{x_0} and translation by $\gamma \in (\varepsilon \mathbb{Z})^d$ commutes. If $r_{\mathscr{G}_{x_0}}$ denotes restriction to \mathscr{G}_{x_0} , we have

$$H_{\varepsilon} r_{\mathscr{G}_{x_0}} = r_{\mathscr{G}_{x_0}} \widehat{H}_{\varepsilon} , \qquad x_0 \in \mathbb{R}^d .$$
(1.17)

We remark that in this context the choice of $x_0 = 0$ in Hypothesis 1.1,(b)(iii) is arbitrary. In this paper we shall systematically analyze spectrum and eigenfunctions of H_{ε} by constructing quasimodes for \hat{H}_{ε} . We shall, however, not discuss the spectrum and the eigenfunctions of \hat{H}_{ε} as an operator on $L^2(\mathbb{R}^d)$. This would involve a discussion of the infinite degeneracy of each eigenvalue of \hat{H}_{ε} , which is not relevant in the context of this paper.

We denote the operator associated to the symbol h_0 by

$$\widehat{H}_{0}u(x) := \sum_{\gamma \in (\varepsilon \mathbb{Z})^{d}} a_{\gamma}^{(0)}(x)u(x+\gamma) + V_{0}(x)u(x) .$$
(1.18)

Furthermore for B defined in (1.12) we set $B_0 := B(0)$. The harmonic approximation of H_{ε} (associated with a small neighborhood of $(x, \xi) = (0, 0)$, see [15]) is given by

$$\widehat{H}_{q}^{0}(x,\varepsilon D) = -\varepsilon^{2} \langle D, B_{0}D \rangle + \langle x, Ax \rangle + \varepsilon(t_{1}(0,0) + V_{1}(0)) , \qquad (1.19)$$

where $A = D^2 V_0(0)$. It follows from the assumptions given in Hypotheses 1.1 that the matrix, $\tilde{A} := B_0^{\frac{1}{2}} A B_0^{\frac{1}{2}}$ is symmetric and there exists an orthogonal matrix $R \in \text{SO}(d, \mathbb{R})$ such that $R \tilde{A} R^t = \Lambda$, where $\Lambda = \text{diag}(\lambda_1^2, \ldots, \lambda_d^2)$ and $\lambda_{\nu} > 0$ for $1 \leq \nu \leq d$. Therefore, by means of the unitary transformation

$$Uf(x) = \sqrt{|B_0^{-\frac{1}{2}}|f(RB_0^{-\frac{1}{2}}x)}, \qquad (1.20)$$

 \widehat{H}^0_q is unitarily equivalent to the associated harmonic oscillator

$$\widehat{H}_{q}^{'0}(x,\varepsilon D) := -\varepsilon^{2}\Delta + \sum_{\nu=1}^{d} \lambda_{\nu} x_{\nu}^{2} + \varepsilon(t_{1}(0,0) + V_{1}(0)) = U^{-1} \widehat{H}_{q}^{0} U, \qquad x \in \mathbb{R}^{d}.$$
(1.21)

and we set

$$\widehat{H}_{\varepsilon}' := U^{-1} \widehat{H}_{\varepsilon} U = \widehat{T}_{\varepsilon}' + \widehat{V}_{\varepsilon}' , \qquad (1.22)$$

where, with the notation $C := RB_0^{-\frac{1}{2}}$,

$$\widehat{V}_{\varepsilon}'(x) = \widehat{V}_{\varepsilon}\left(C^{-1}x\right) \tag{1.23}$$

$$\widehat{T}_{\varepsilon}'f(x) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_{\gamma}(C^{-1}x;\varepsilon)f(x+C\gamma) = \sum_{\mu \in \Gamma_C} \left(a'_{\mu}\tau_{\mu}\right)f(x) , \qquad (1.24)$$

where in the last equation we set $\Gamma_C := C(\varepsilon \mathbb{Z})^d$ and for $\mu \in \Gamma_C$

$$(a'_{\mu}\tau_{\mu})f(x) = a'_{\mu}(x;\varepsilon)f(x+\mu) \quad \text{with} \quad a'_{\mu}(x;\varepsilon) := a_{C^{-1}\mu}(C^{-1}x;\varepsilon) . \tag{1.25}$$

Since C has maximal rank, it follows at once by direct calculation, that Hypothesis 1.1(a) holds for a', if $(\varepsilon \mathbb{Z})^d$ is replaced by Γ_C and γ by μ . By $h'_0 = t'_0 + V'_0$ we denote the symbol associated to the operator $U^{-1}\hat{H}_0 U$ with respect to the ε -quantization given in (1.7). Then

$$t'_0(x,\xi) = \langle \xi, B'(x)\xi \rangle_{\ell^2} + O(|\xi|^3), \qquad B'(x) = \mathbf{1} + o(\mathbf{1})$$
(1.26)

and

$$V_0'(x) = \sum_{\nu=1}^d \lambda_\nu^2 x_\nu^2 + O(|x|^3) =: V_{0,q}'(x) + O(|x|^3), \quad \lambda_\nu > 0.$$
 (1.27)

Moreover the symbol associated to $\widehat{T}'_{\varepsilon}$ is given by

$$t'_{\varepsilon}(x,\xi) = \sum_{\gamma \in (\varepsilon\mathbb{Z})^d} a_{\gamma}(C^{-1}x;\varepsilon) \exp\left(-\frac{i}{\varepsilon}C\gamma \cdot \xi\right) = \sum_{\mu \in \Gamma_C} a'_{\mu}(x;\varepsilon) \exp\left(-\frac{i}{\varepsilon}\mu \cdot \xi\right) \,. \tag{1.28}$$

The eigenfunctions of $\widehat{H}_q^{\prime 0}$ are given by

$$g_{\alpha}(x) = \varepsilon^{-\frac{d}{4}} h_{\alpha}\left(\frac{x}{\sqrt{\varepsilon}}\right) e^{-\frac{\varphi_0(x)}{\varepsilon}} .$$
(1.29)

where $h_{\alpha}(x) = h_{\alpha_1}(x_1) \dots h_{\alpha_d}(x_d)$. Each $h_{\alpha_{\nu}}$ is a one-dimensional Hermite polynomial, which is assumed to be normalized in the sense that $\|g_{\alpha}\|_{L^2} = 1$. The phase function φ_0 is given by

$$\varphi_0(x) := \sum_{\nu=1}^d \frac{\lambda_\nu}{2} x_\nu^2, \qquad x \in \mathbb{R}^d, \qquad (1.30)$$

solving the harmonic eikonal equation $|\nabla \varphi_0(x)|^2 = V'_{0,q}(x)$. The eigenfunctions of \hat{H}^0_q are thus given by $\tilde{g}_{\alpha} := Ug_{\alpha}$.

The following lemma concerns the existence of a local solution of a generalized eikonal equation.

LEMMA 1.3 Under the assumptions given in Hypothesis 1.1, there exists a unique \mathscr{C}^{∞} -function φ defined in a neighborhood Ω of 0, with $\varphi(0) = 0$, solving

$$\hat{h}_0'(x, \nabla\varphi(x)) := -h_0'(x, i\nabla\varphi(x)) = 0, \qquad x \in \Omega.$$
(1.31)

Furthermore

$$|\varphi(x) - \varphi_0(x)| = O(|x|^3) \quad as \quad |x| \to 0,$$
 (1.32)

and the homogeneous Taylor polynomials φ_k of degree k + 2, $k \ge 1$, of φ are constructively determined by solving transport equations depending on the Taylor expansion of h'_0 at $(x,\xi) = (0,0)$.

REMARK 1.4 It follows from the proof of Theorem 1.5 in Klein-Rosenberger [14], that φ coincides in Ω with the Finsler distance $d^0(x)$. This proof uses Lemma 1.3, which is taken from the dissertation [17]. For the sake of the reader, we shall recall the proof of Lemma 1.3 here.

HYPOTHESIS 1.5 For Ω, φ as in Lemma 1.3, we choose a neighborhood $\Omega_1 \subset \Omega$ of 0 such that for any $\delta > 0$ and for some C > 0 the estimate $|\nabla \varphi(x)| \geq C$ holds for $x \in \Omega_1 \setminus \{|x| \leq \delta\}$. We consider some set Ω_2 such that $\overline{\Omega_2} \subset \Omega_1$ and define a smooth cut-off function χ supported in Ω_1 such that $\chi(x) = 1$ for any $x \in \Omega_2$. Then we set for any b > 0

$$\tilde{\varphi}(x) := \chi(x)\varphi(x) + (1 - \chi(x))b|x|, \qquad x \in \mathbb{R}^d.$$
(1.33)

The central result of this paper is the construction of the following system of quasimodes of WKB-type, both for the operators $\widehat{H}'_{\varepsilon}$ on $L^2(\mathbb{R}^d)$ and H_{ε} on $\ell^2((\varepsilon \mathbb{Z})^d)$.

THEOREM 1.6 Let, for $\varepsilon > 0$, \hat{H}_{ε} and H_{ε} respectively be an Hamilton operator satisfying Hypotheses 1.1. Let $\tilde{\varphi}, \Omega_1$ and Ω_2 satisfy Hypothesis 1.5. Furthermore we assume that εE denotes an eigenvalue of $\hat{H}_{q}^{(0)}$ defined in (1.21) with multiplicity m.

(a) Then there are functions $u_j \in \mathscr{C}_0^{\infty} \left(\mathbb{R}^d \times [0, \varepsilon_0) \right)$, $u_{j\ell} \in \mathscr{C}_0^{\infty}(\mathbb{R}^d)$, $j = 1, \ldots, m$, $\ell \in \frac{\mathbb{Z}}{2}$, $\ell \geq -N$ for some N, such that for all $M \in \frac{\mathbb{Z}}{2}$ there are $C_M < \infty$ satisfying

$$u_j(x;\varepsilon) - \sum_{\substack{\ell \in \frac{\mathbb{Z}}{2}\\ \ell \ge -N}}^M \varepsilon^\ell u_{j\ell}(x) \right| \le C_M \varepsilon^M, \quad (x \in \mathbb{R}^d), \qquad (1.34)$$

and real functions $E_i(\varepsilon)$ with asymptotic expansion

$$E_j(\varepsilon) \sim E + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk} , \qquad (1.35)$$

solving the equation

$$\left(\widehat{H}_{\varepsilon}' - \varepsilon E_{j}(\varepsilon)\right) \left(u_{j}(x,\varepsilon)e^{-\frac{\widetilde{\varphi}(x)}{\varepsilon}}\right) = O\left(\varepsilon^{\infty}\right)e^{-\frac{\widetilde{\varphi}(x)}{\varepsilon}}, \quad (x \in \Omega_{3}, \ \varepsilon \to 0),$$
(1.36)

for some neighborhood $\Omega_3 \subset \Omega_2$ of zero, where the rhs of (1.36) is $O(|x|^{\infty})$ as $|x| \to 0$. (b) The approximate eigenfunctions

$$v_j := U\left(u_j e^{-\frac{\tilde{\varphi}}{\varepsilon}}\right)$$

of $\widehat{H}_{\varepsilon}$ are almost orthonormal in the sense that

$$\langle v_j, v_k \rangle_{L^2} = \delta_{jk} + O(\varepsilon^{\infty}) .$$
 (1.37)

- (c) We set $I_E := \{ \alpha \in \mathbb{N}^d \mid \hat{H}_q^{\prime 0} g_\alpha = \varepsilon E g_\alpha \}$, where g_α is given by (1.29). If $|\alpha|$ is even (or odd resp.) for all $\alpha \in I_E$, then all half integer terms (or integer terms resp.) in the expansion (1.34) vanish. Moreover if $|\alpha|$ is even or odd for all $\alpha \in I_E$, the half integer terms in (1.35) vanish.
- (d) For any $x_0 \in \mathbb{R}^d$, the restriction $v_j^{\varepsilon} := r_{\mathscr{G}_{x_0}} v_j$ of the approximate eigenfunctions to the lattice $\mathscr{G}_{x_0} = (\varepsilon \mathbb{Z})^d + x_0$ are approximate eigenfunctions for the operator H_{ε} with respect to the approximate eigenvalues given in (1.35), i.e.,

$$(H_{\varepsilon} - \varepsilon E_j(\varepsilon))v_j^{\varepsilon}(x) = O(\varepsilon^{\infty}) U e^{-\frac{\varphi}{\varepsilon}}(x), \quad (x \in \Omega_3 \cap \mathscr{G}_{x_0}, \ \varepsilon \to 0),$$
(1.38)

where the rhs of (1.38) is $O(|x|^{\infty})$ as $|x| \to 0$.

(e) For the restricted approximate eigenfunctions we have

$$\langle v_j^{\varepsilon}, v_k^{\varepsilon} \rangle_{\ell^2} = \varepsilon^{-d} \left(\delta_{jk} + O(\sqrt{\varepsilon}) \right) .$$
 (1.39)

We shall use Theorem 1.6 in a forthcoming paper to obtain sharp estimates on tunneling (see also [17]). The plan of the paper is as follows. Section 2 consists of the proof of Lemma 1.3. In Section 3 we prove asymptotic results for the operator \hat{G}_{ε} , which is a unitary transform of \hat{H}_{ε} . Here we change variables and introduce an exponential weight. Then we use this expansion of \hat{G}_{ε} to define an operator G on spaces of formal symbols. In Section 4, we construct asymptotic expansions of eigenfunctions of G. Section 5 gives the proof of Theorem 1.6. We emphasize that the results of Sections 3 and 4 concern expansions for operators on spaces of formal symbols. These results are crucial for the proof of Theorem 1.6.

2. Proof of Lemma 1.3

If we formally compute the left hand side of (1.36) and expand the coefficients of $e^{-\frac{\varphi}{\varepsilon}}$ in powers of ε , the equation of order zero determines the function φ . 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 $u \in L^2(\mathbb{R}^d)$ given by

$$e^{\frac{\varphi}{\varepsilon}}\widehat{T}'_{\varepsilon}e^{-\frac{\varphi}{\varepsilon}}u(x)=\sum_{\gamma\in\Gamma_C}a'_{\gamma}(x;\varepsilon)e^{\frac{1}{\varepsilon}(\varphi(x)-\varphi(x+\gamma))}u(x+\gamma)\;.$$

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

$$\sum_{\gamma \in \Gamma_C} a'_{\gamma}(x;\varepsilon) e^{\frac{1}{\varepsilon}(-\gamma \cdot \nabla \varphi(x) - \sum_{\nu\mu} \gamma_{\nu} \gamma_{\mu} \int_0^1 \partial_{\mu} \partial_{\nu}(\varphi(x+t\gamma))(1-t) dt} \left(u(x) + \int_0^1 \nabla u(x+t\gamma) \cdot \gamma dt \right) . \quad (2.1)$$

The term of order zero in ε is for $\gamma = \varepsilon \eta$ and \tilde{a}_{η} defined in (1.14)

$$\sum_{\eta \in C\mathbb{Z}^d} \tilde{a}'_{\eta}(x) e^{-\eta \cdot \nabla \varphi(x)} u(x) = t'_0(x, -i\nabla \varphi(x)) u(x) .$$
(2.2)

Thus the resulting order zero part of (1.36) is the generalized eikonal equation (1.31).

Following Helffer ([9]), the idea of the proof is to determine φ as generating function of a lagrangian manifold $\Lambda_{+} = \{(x, \nabla \varphi(x)) \mid (x, \xi) \in \mathscr{N}\}$ lying in the "energy shell" $(\tilde{h}'_{0})^{-1}(0)$, where

 \mathscr{N} is a neighborhood of (0,0). By Hypothesis 1.1, \tilde{h}'_0 expands in a neighborhood of (0,0) in $T^*\mathbb{R}^d$ as

$$\tilde{h}_0'(x,\xi) = \langle \xi, B'(x)\xi \rangle - \sum_{\nu=1}^d \lambda_\nu^2 x_\nu^2 + O\left(|\xi|^3 + |x|^3\right) , \qquad (2.3)$$

where $B'(0) = \mathbf{1}$. Thus by the symmetry of the matrix B', the Hamiltonian vector field of h'_0 in a neighborhood of (0,0) expands as

$$X_{\tilde{h}'_{0}} = 2\sum_{\nu=1}^{d} \left(\sum_{\mu=1}^{d} B'_{\nu\mu}(x)\xi_{\mu} \frac{\partial}{\partial x_{\nu}} + \left(\lambda_{\nu}^{2}x_{\nu} + \sum_{\mu,\eta=1}^{d} \frac{\partial B'_{\mu\eta}}{\partial x_{\nu}}(x)\xi_{\mu}\xi_{\eta} \right) \frac{\partial}{\partial \xi_{\nu}} \right) + O\left(|\xi|^{2} + |x|^{2} \right) =$$
$$= 2\sum_{\nu=1}^{d} \left(\sum_{\mu=1}^{d} B'_{\nu\mu}(x)\xi_{\mu} \frac{\partial}{\partial x_{\nu}} + \lambda_{\nu}^{2}x_{\nu} \frac{\partial}{\partial \xi_{\nu}} \right) + O\left(|\xi|^{2} + |x|^{2} \right) .$$
(2.4)

The linearization of $X_{\tilde{h}'_{\alpha}}$ at the critical point (0,0) yields the fundamental matrix

$$L := DX_{\tilde{h}'_0}(0,0) = 2 \begin{pmatrix} & 1 & 0 \\ 0 & & \ddots \\ & 0 & 1 \\ \lambda_1^2 & 0 & & \\ & \ddots & & 0 \\ 0 & & \lambda_d^2 & & \end{pmatrix}.$$
 (2.5)

L has the eigenvalues $\pm 2\lambda_{\nu}$, $\nu = 1, \ldots d$. An eigenvector (x, ξ) with respect to $\pm \lambda_{\nu}$ fulfills $\xi_{\nu} = \pm \lambda_{\nu} x_{\nu}$. By Λ^{0}_{\pm} we denote the positive (resp. negative) eigenspace of *L*. Λ^{0}_{\pm} can be characterized as the subsets of phase space, which consist of all points (x, ξ) such that $e^{-tL}(x, \xi) \to 0$ for $t \to \pm \infty$. Moreover, Λ^{0}_{\pm} are Lagrangian subspaces of $T_{(0,0)}(T^*\mathbb{R}^d)$ of the form $\xi = \pm \nabla \varphi_0(x)$ with φ_0 defined in (1.30).

Denote by F_t the flow of the hamiltonian vector field $X_{\tilde{h}'_0}$. By the Local Stable Manifold Theorem ([1]), there is an open neighborhood \mathcal{N} of (0,0) in $T^*\mathbb{R}^d$, such that

$$\Lambda_{\pm} := \{ (x,\xi) \in \mathscr{N} \mid F_t(x,\xi) \to (0,0) \quad \text{for} \quad t \to \mp \infty \}$$

$$(2.6)$$

are d-dimensional submanifolds tangent to Λ^0_{\pm} at (0,0) (the stable (Λ_-) and unstable (Λ_+) manifold of $X_{\tilde{h}'_0}$ at the critical point (0,0)). Λ_+ and Λ_- 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 $T_{(x,\xi)}(T^*\mathbb{R}^d)$, 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 $(u,v) \in T_{(x,\xi)}(\Lambda_{\pm})$

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

In the limit $t \to -\infty$, the elements of $T_{(x,\xi)}(\Lambda_+)$ lie in the Lagrangian plane Λ^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 Ω of 0 in \mathbb{R}^d . Therefore we can parameterize Λ_+ 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 Λ_+ 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

$$\nabla \varphi(x) = \Psi(x)$$
 and $\varphi(0) = 0$.

Since $T_{(0,0)}(\Lambda_{\pm}) = \Lambda_{\pm}^{0}$, the leading order term of this function φ is equal to φ_{0} , thus φ can be written as (1.32). Furthermore φ solves the eikonal equation (1.31), because $\Lambda_{+} \subset \left(\tilde{h}_{0}'\right)^{-1}(0)$.

With the ansatz (1.32), we have a constructive procedure to iteratively find the terms φ_k . The coefficients of the eikonal equation (1.31) of the lowest order in x vanish and the coefficients belonging to higher orders in x iteratively fix the φ_k . To this end, we expand B'(x) and $B'_{\alpha}(x)$ at x = 0 as

$$B'(x) = \mathbf{1} + DB'|_0 x + O(|x|^2)$$
(2.7)

$$B'_{\alpha}(x) = B'_{\alpha}(0) + DB'_{\alpha}|_{0}x + O\left(|x|^{2}\right) .$$
(2.8)

Furthermore we write

$$V_0'(x) = V_{0,q}'(x) + \sum_{k\geq 3}^N W_k(x) + O\left(|x|^{N+1}\right)$$

where W_k denotes a homogeneous polynomial of degree k. The third order equation

$$-\langle \nabla \varphi_0, DB'|_0 x \rangle \nabla \varphi_0 \rangle - 2 \sum_{\nu=0}^d \lambda_\nu x_\nu \frac{\partial \varphi_1}{\partial x_\nu}(x) + W_3(x) = 0, \qquad x \in \Omega$$

fixes φ_1 for a given W_3 , the fourth order

$$-2\langle \nabla\varphi_0, (DB'|_0 x)\nabla\varphi_1 \rangle + \sum_{|\alpha|=4} B'_{\alpha} (\nabla\varphi_0)^{\alpha} - 2\sum_{\nu=0}^d \lambda_{\nu} x_{\nu} \frac{\partial\varphi_2}{\partial x_{\nu}}(x) - \sum_{\nu=0}^d \left(\frac{\partial\varphi_1}{\partial x_{\nu}}\right)^2 + W_4(x) = 0$$

is an equation for φ_2 and the higher orders in φ are inductively given by the higher order parts of the eikonal equation, which all take the form

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

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

3. EXPANSION OF THE TRANSFORMED OPERATOR

DEFINITION 3.1 Let ψ denote any real valued function on \mathbb{R}^d . We introduce an ε -dependent unitary map

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

by

$$(U_{\varepsilon}(\psi)f)(y) = \varepsilon^{\frac{d}{4}} e^{\frac{\psi(\sqrt{\varepsilon}y)}{\varepsilon}} f(\sqrt{\varepsilon}y)$$
(3.1)

and set for $\widehat{H}'_{\varepsilon}$ as defined in (1.22)

$$\widehat{G}_{\varepsilon,\psi} := \frac{1}{\varepsilon} U_{\varepsilon}(\psi) \widehat{H}'_{\varepsilon} U_{\varepsilon}^{-1}(\psi) .$$
(3.2)

Then $\widehat{G}_{\varepsilon,\psi}$ defines a self adjoint operator on \mathscr{H}_{ψ} , whose domain contains the set of all polynomials $\mathbb{C}[y]$, if $\psi \geq C|x|$ for some C > 0 and for all large x. Choosing in particular $\psi = \tilde{\varphi} \in \mathscr{C}^{\infty}(\mathbb{R}^d)$ satisfying Hypothesis 1.5, we remark that for any $M \in \mathbb{N}$, uniform with respect to $\varepsilon \in (0, \varepsilon_0)$,

$$\|\langle . \rangle^M\|_{\mathscr{H}_{\tilde{\varphi}}} \le C_M , \quad \text{where} \quad \langle y \rangle := \sqrt{1+|y|^2} .$$

$$(3.3)$$

In fact by the definition of $\tilde{\varphi}$, for some $A, C_1, C_2 > 0$,

$$\tilde{\varphi}(\sqrt{\varepsilon}y) \ge \begin{cases} C_1 \varepsilon |y|^2, & \text{for } |y| \le \frac{A}{\sqrt{\varepsilon}} \\ C_2 \sqrt{\varepsilon} |y|, & \text{otherwise} \end{cases}$$
(3.4)

and therefore

$$\|\langle \,.\,\rangle^M\|_{\mathscr{H}_{\tilde{\varphi}}} \leq \int_{\mathbb{R}^d} e^{-2C_1|y|^2} \langle y \rangle^M \, dy + \int_{|y| > \frac{A}{\sqrt{\varepsilon_0}}} e^{-\frac{C_2|y|}{\sqrt{\varepsilon_0}}} \langle y \rangle^M \, dy \leq C_M$$

PROPOSITION 3.2 For $\Omega_2, \tilde{\varphi}$ as in Hypothesis 1.5, let $\zeta \in \mathscr{C}_0^{\infty}(\mathbb{R}^d)$ be a cut-off-function, such that supp $\zeta \subset \Omega_2$ and set $\zeta_{\varepsilon}(y) := \zeta(\sqrt{\varepsilon}y)$. Then the operator $\hat{G}_{\varepsilon} := \hat{G}_{\varepsilon,\tilde{\varphi}}$ defined in (3.2) has an expansion

$$\widehat{G}_{\varepsilon} = \sum_{\frac{\mathbb{N}}{2} \ni k \le N - \frac{1}{2}} \varepsilon^k G_k + R_N, \qquad N \in \frac{\mathbb{N}}{2}.$$
(3.5)

Here

$$G_k = \left(b_k + \sum_{|\alpha|=1}^{2k+2} b_{k,\alpha} \partial^{\alpha}\right) , \qquad (3.6)$$

where b_k is a polynomial of degree 2k, which is even (odd) with respect to $y \mapsto -y$ if 2k is even (odd), and $b_{k,\alpha}$ is a polynomial of degree $2k + 2 - |\alpha|$, which is even (odd) if $2k - |\alpha|$ is even (odd). Moreover there exist constants C_N and $\varepsilon_0 > 0$ such that for any $\varepsilon \in (0, \varepsilon_0]$ and for any $u, v \in \mathbb{C}[y] \subset \mathscr{H}_{\tilde{\varphi}}$

$$\left| \langle u, \zeta_{\varepsilon} R_N v \rangle_{\mathscr{H}_{\tilde{\varphi}}} \right| \le C_N \varepsilon^N \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| \le 4N+4}} \| y^{\alpha} u \|_{\mathscr{H}_{\tilde{\varphi}}} \sum_{\beta \in \mathbb{N}^d \\ |\beta| \le N} \| |\cdot|^{2N+2} \partial^{\beta} v \|_{\mathscr{H}_{\tilde{\varphi}}} .$$
(3.7)

REMARK 3.3 (a) As a map on $\mathbb{C}[y]$, G_k , $k \in \frac{\mathbb{N}}{2}$, 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_{ℓ} in the representation of G_k .

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

$$G_0 = \Delta_y \varphi_0(y) + \sum_{\nu=1}^d (2(\partial_{y_\nu} \varphi_0(y))\partial_{y_\nu}) - \Delta_y + V_1(0) + t_1(0,0)$$
(3.8)

This is shown below the proof of Proposition 3.2.

Proof of Proposition 3.2. Step 1: We start by analyzing the terms arising from the potential energy \hat{V}_{ε}' . We have

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

and, using Hypothesis 1.1,(b), for any $N \in \frac{\mathbb{N}}{2}$ by Taylor expansion of $V'_{\ell}(\sqrt{\varepsilon}y)$ for $\ell \in \mathbb{N}, \ell < N$, at $\sqrt{\varepsilon}y = 0$, we get for $N_{\ell} = 2(N - \ell + 1) \in \mathbb{N}$

$$V_0'(\sqrt{\varepsilon}y) = \varepsilon \sum_{j=1}^d \lambda_j^2 y_j^2 + \sum_{k=3}^{N_0-1} \varepsilon^{\frac{k}{2}} D_x^k V_0'|_{x=0}[y]^k + R_{N,0}(y,\varepsilon)$$
(3.9)

$$\varepsilon^{\ell} V_{\ell}'(\sqrt{\varepsilon}y) = \sum_{k=0}^{N_{\ell}-1} \varepsilon^{\ell+\frac{k}{2}} D_x^k V_{\ell}'|_{x=0}[y]^k + R_{N,\ell}(y,\varepsilon) , \qquad 1 \le \ell < N , \qquad (3.10)$$

where $D_x^k f|_x [y]^k := D_x^k f|_x (y, \dots, y)$ and for $0 \le \ell < N$

$$R_{N,\ell}(y,\varepsilon) = \varepsilon^{N+1} \frac{1}{(2N-2\ell)!} \int_0^1 (1-t)^{2(N-\ell)} D_x^{2(N-\ell+1)} V_\ell'|_{x=t\sqrt{\varepsilon}y} [y]^{2(N-\ell+1)} dt .$$
(3.11)

Thus for $u, v \in \mathbb{C}[y]$ and for $0 \le \ell < N$

$$\left| \left\langle u \,,\, \zeta_{\varepsilon} \frac{1}{\varepsilon} R_{N,\ell}(.,\varepsilon) v \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \right| \leq C_{N,\ell} \varepsilon^{N} \| u \|_{\mathscr{H}_{\tilde{\varphi}}} \sum_{\substack{\alpha \in \mathbb{N}^{d} \\ |\alpha| = 2(N-\ell+1)}} \| y^{\alpha} v \|_{\mathscr{H}_{\tilde{\varphi}}} \,. \tag{3.12}$$

We will need the following notations for $N \in \frac{\mathbb{N}}{2}$:

$$[N] := \max\{n \in \mathbb{N} \mid n < N+1\} \text{ and } [[N]] := \max\{n \in \mathbb{N} \mid n \le N\}.$$
(3.13)

Combining the terms in (3.9) and (3.10) for $0 \le \ell < N$, leads together with the expansion (1.6) in Hypothesis 1.1,(b),(i) and the estimates on $R_{[N]}$ given there, to

$$\frac{1}{\varepsilon} U_{\varepsilon}(\tilde{\varphi}) \widehat{V}_{\varepsilon}' U_{\varepsilon}^{-1}(\tilde{\varphi})(y) = \sum_{j=2}^{2N+1} \varepsilon^{\frac{j}{2}-1} D_x^j V_0'|_{x=0}[y]^j + R_{N,0}(y,\varepsilon)$$

$$+ \sum_{\ell=1}^{[N-1]} \left(\sum_{j=0}^{2(N-\ell)+1} \varepsilon^{\frac{j}{2}-1+\ell} D_x^j V_\ell'|_{x=0}[y]^j + R_{N,\ell}(y,\varepsilon) \right) + R_{[N]}(y,\varepsilon)$$

$$= \sum_{\substack{k \in \frac{N}{2} \\ k \le N - \frac{1}{2}}} \varepsilon^k p_k(y) + R_N'(y,\varepsilon) ,$$
(3.14)

where

$$p_{k}(y) = \sum_{\ell=0}^{[[k+1]]} D_{x}^{2(k+1-\ell)} V_{\ell}'|_{x=0}[y]^{2(k+1-\ell)} \quad \text{and}$$
(3.15)
$$R_{N}'(y,\varepsilon) = \sum_{\ell=0}^{[N-1]} R_{N,\ell}(y,\varepsilon) + \zeta_{\varepsilon}(y) R_{[N]}(y,\varepsilon) .$$

Thus p_k is a polynomial of degree 2k + 2, which is even (odd) if 2k + 2 is even (odd) (or if k is integer (half-integer)).

It follows from the assumptions given in Hypothesis 1.1,(b) together with (3.12) that for $u, v \in \mathbb{C}[y]$

$$\left| \left\langle u \,,\, \zeta_{\varepsilon \frac{1}{\varepsilon}} R'_N(.,\varepsilon) v \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \right| \leq C_N \varepsilon^N \| u \|_{\mathscr{H}_{\tilde{\varphi}}} \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| = 2N+2}} \| y^{\alpha} v \|_{\mathscr{H}_{\tilde{\varphi}}} .$$
(3.16)

Step 2:

Now we investigate the coefficients in the expansion of the kinetic energy $\widehat{T}_{\varepsilon}$ after conjugation with $U_{\varepsilon}(\widetilde{\varphi})$ on the support of ζ_{ε} and give estimates for the remainder. By the expansion of $a'_{\gamma}(x,\varepsilon)$ with respect to ε following from the assumptions in Hypothesis 1.1,(a), we can write for $N \in \frac{\mathbb{N}}{2}$

$$\widehat{T}_{\varepsilon}' = \sum_{k=0}^{[N-1]} \varepsilon^k \widehat{T}_k + \widetilde{R}_{[N]}(\varepsilon) , \quad \text{where}$$
(3.17)

$$\widehat{T}_k := \sum_{\gamma \in \Gamma_C} a_{\gamma}^{\prime(k)} \tau_{\gamma} \quad \text{and} \quad \widetilde{R}_{[N]}(\varepsilon) = \sum_{\gamma \in \Gamma_C} R_{\gamma}^{([N])}(\,.\,;\varepsilon) \tau_{\gamma} \,. \tag{3.18}$$

Using (1.25), we get by Taylor-expansion for $N_k \in \mathbb{N}^*$

$$\widehat{T}_k g(x) = \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| < N_k}} \varepsilon^{|\alpha|} B_{\alpha}^{(k)}(x) \partial_x^{\alpha} g|_x + \widetilde{R}'_{N_k}(\varepsilon) g(x), \qquad g \in L^2(\mathbb{R}^d, dx) \cap \mathscr{C}^{\infty}(\mathbb{R}^d)$$
(3.19)

where we set

$$B_{\alpha}^{(k)}(x) = \sum_{\eta \in C\mathbb{Z}^d} a_{\varepsilon\eta}^{\prime(k)}(x) \frac{\eta^{\alpha}}{\alpha!} = \frac{1}{\alpha!} \partial_{\xi}^{\alpha} t_k(x, i\nabla\tilde{\varphi}(x)) \quad \text{and}$$
(3.20)

$$\tilde{R}'_{N_k}(\varepsilon)g(x) = \sum_{\alpha \in \mathbb{N}^d \mid \alpha \mid = N_k} \sum_{\eta \in C\mathbb{Z}^d} \varepsilon^{|\alpha|} a_{\varepsilon\eta}^{\prime(k)}(x) \frac{N_k}{\alpha!} \eta^{\alpha} \int_0^1 (1-t)^{N_k-1} \partial_x^{\alpha} g|_{x+t\varepsilon\eta} dt$$
(3.21)

From Remark 1.2,(b) it follows that $B_{\alpha}^{(0)} = B_{\alpha}' = 0$ if $|\alpha|$ is odd or $|\alpha| = 0$. Inserting (3.19) into (3.17) gives for $\alpha \in \mathbb{N}^d$

$$\begin{aligned} \widehat{T}_{\varepsilon}'g(x) &= \sum_{\substack{|\alpha|=2n,n\in\mathbb{N}\\2\leq |\alpha|< N_0}} \varepsilon^{|\alpha|} B_{\alpha}'(x) \partial_x^{\alpha} g|_x + \widetilde{R}'_{N_0}(\varepsilon)g(x) \\ &+ \sum_{k=1}^{[N-1]} \varepsilon^k \left[\sum_{|\alpha|< N_k} \varepsilon^{|\alpha|} B_{\alpha}^{(k)}(x) \partial_x^{\alpha} g|_x + \widetilde{R}'_{N_k}(\varepsilon)g(x) \right] + \widetilde{R}_{[N]}(\varepsilon)g(x). \end{aligned}$$
(3.22)

To analyze the unitary transform of the explicit terms on the right hand side of (3.22) we use the following generalized Faa di Bruno formula (see e.g. Hardy [8]) for $g \in \mathscr{C}^{\infty}(\mathbb{R}^d, \mathbb{R}), f \in \mathscr{C}^{\infty}(\mathbb{R})$ and $\beta \in \mathbb{N}^d$

$$\partial^{\beta} f \circ g = \sum_{n=\min\{1,|\beta|\}}^{|\beta|} \sum_{\substack{p \in (\mathbb{N}^d)^n \\ \sum_{j=1}^n p_j = \beta, |p_j| \ge 1}} C_p f^n |_g \prod_{j=1}^n \partial^{p_j} g .$$
(3.23)

(3.23) together with the Leibnitz formula yields for $f \in \mathscr{H}_{\tilde{\varphi}}$ and $\alpha, \beta, \beta' \in \mathbb{N}^d$

$$U_{\varepsilon}(\tilde{\varphi}) \left[\varepsilon^{k} B_{\alpha}^{(k)}(\varepsilon \partial_{x})^{\alpha} \right] U_{\varepsilon}(\tilde{\varphi})^{-1} f(y)$$

$$= \varepsilon^{k+|\alpha|} B_{\alpha}^{(k)}(\sqrt{\varepsilon}y) \sum_{\beta+\beta'=\alpha} \sum_{n=\min\{1,|\beta|\}}^{|\beta|} \sum_{\substack{p \in \mathbb{N}^{d} \\ \sum_{j=1}^{n} p_{j}=\beta, |p_{j}| \ge 1}} C_{p} \prod_{j=1}^{n} \left(\partial_{x}^{p_{j}} \frac{\tilde{\varphi}}{\varepsilon} \right) |_{\sqrt{\varepsilon}y} \varepsilon^{-\frac{|\beta'|}{2}} \partial_{y}^{\beta'} f(y) . \quad (3.24)$$

To analyze the right hand side of (3.24) in detail, we fix β and n. Since on the support of ζ_{ε} the phase function $\tilde{\varphi}$ is given by the asymptotic sum (1.32), we have on $\sup \zeta_{\varepsilon}$

$$\left|\nabla_x \tilde{\varphi}\right|_{\sqrt{\varepsilon}y} = O(\sqrt{\varepsilon}) \quad \text{and} \quad \partial_x^{\alpha} \tilde{\varphi}|_{\sqrt{\varepsilon}y} = O(1), \ |\alpha| > 1, \qquad (\varepsilon \to 0) \ . \tag{3.25}$$

Thus, for each partition p of β of length n (i.e. each $p = (p_1, \ldots, p_n) \in (\mathbb{N}^d)^n$ with $\sum_{j=1}^n p_j = \beta$), we set $m_p := m(\beta, n, p) := \#\{p_j \in \mathbb{N}^d \mid |p_j| = 1\}$. Then (3.25) together with (1.32) yield on the support of ζ_{ε} for any $N_{\alpha,k} \in \mathbb{N}$ and for $p \in (\mathbb{N}^d)^n$ with $\sum_{j=1}^n p_j = \beta$ and $|p_j| \ge 1$

$$\sum_{p,|p_j|\ge 1} \prod_{j=1}^n \left(\partial_x^{p_j} \frac{\tilde{\varphi}}{\varepsilon}\right) \Big|_{\sqrt{\varepsilon}y} = \varepsilon^{-n} \sum_{p,|p_j|\ge 1} \left[\sum_{\ell=0}^{N_{\alpha,k}-1} \rho_{m_p+\ell}(y) \varepsilon^{\frac{m_p+\ell}{2}} + R_{N_{\alpha,k}}''(y;\varepsilon,m_p) \right] , \quad (3.26)$$

where ρ_k denotes a homogeneous polynomial of degree k and for $u, v \in \mathbb{C}[y]$

$$\left| \left\langle u \,, \, \zeta_{\varepsilon} R_{N_{\alpha,k}}^{\prime\prime}(.;\varepsilon,m_p) v \right\rangle_{\mathscr{H}_{\bar{\varphi}}} \right| \leq C_{N_{\alpha,k}} \varepsilon^{\frac{N_{\alpha,k}+m_p}{2}} \|u\|_{\mathscr{H}_{\bar{\varphi}}} \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha|=N_{\alpha,k}+m_p}} \|y^{\alpha} v\|_{\mathscr{H}_{\bar{\varphi}}} \,. \tag{3.27}$$

Note that the polynomials ρ_k depend on β, n, p and ℓ , but are independent of the choice of the truncation N, N_k and $N_{\alpha,k}$. For fixed $\beta \in \mathbb{N}^d$ and $n \in \mathbb{N}$, it follows from the definition of m_p that for any partition $p \in (\mathbb{N}^d)^n$ of β with length n and $|p_j| \ge 1$

$$\begin{cases} m_p = n & \text{if } n = |\beta| \\ (2n - |\beta|)_+ \le m_p \le n - 1 & \text{if } n < |\beta| \end{cases}$$
(3.28)

Thus setting

$$M_{n} := \begin{cases} n-1 & \text{for } n < |\beta| \\ n & \text{for } n = |\beta| \end{cases} , \qquad (3.29)$$

the sum over all p on the right hand side of (3.26) can be substituted by the sum over all $m(=m_p)$ running from $(2n - |\beta|)_+$ to M_n . To expand the right hand side of (3.24) with respect to $\sqrt{\varepsilon}$, we take Taylor expansion of $B_{\alpha}^{(k)}(\sqrt{\varepsilon}y)$, defined in (3.20), at zero up to order $N_{\alpha,k}$, analog to the expansion of the potential energy given in (3.10), (we notice that $B_{\alpha}^{(0)} = 0$ if $|\alpha| = 0$ or $|\alpha|$ is odd). This yields for any $k \in \mathbb{N}$ together with (3.26) and (3.24) on the support of ζ_{ε} for $\alpha, \beta, \beta' \in \mathbb{N}^d$

$$U_{\varepsilon}(\tilde{\varphi}) \left[\varepsilon^{k} B_{\alpha}^{(k)}(\varepsilon \partial_{x})^{\alpha} \right] U_{\varepsilon}(\tilde{\varphi})^{-1}$$

$$= \sum_{\beta+\beta'=\alpha} \sum_{n=\min\{1,|\beta|\}}^{|\beta|} \sum_{m=(2n-|\beta|)_{+}}^{M_{n}} \sum_{\ell=0}^{N_{\alpha,k}-1} \varepsilon^{k+|\alpha|-n+\frac{m+\ell-|\beta'|}{2}} q_{m+\ell}^{(k)}(y) \partial_{y}^{\beta'} + \tilde{\tilde{R}}'_{N_{\alpha,k}}(y;\varepsilon) , \quad (3.30)$$

where $q_s^{(k)}$ denotes a homogeneous polynomial of degree s (which does not depend on the truncation $N, N_k, N_{\alpha,k}$, but depends on $\alpha, \beta, n, m, \ell$). Moreover $q_r^{(0)} = 0$ for all $m \leq r < N_{\alpha,k}$, if $|\alpha| = 0$ or

 $|\alpha|$ is odd and

$$\tilde{\tilde{R}}_{N_{\alpha,k}}'(y;\varepsilon) = \sum_{\beta+\beta'=\alpha} \sum_{n=\min\{1,|\beta|\}}^{|\beta|} \varepsilon^{k+|\alpha|-n-\frac{\beta'}{2}} \sum_{m=(2n-|\beta|)_{+}}^{M_{n}} \left[\sum_{\ell=0}^{N_{\alpha,k}-1} \varepsilon^{\frac{\ell}{2}} \left(D^{\ell} B_{\alpha}^{(k)} \Big|_{\sqrt{\varepsilon}y} [y]^{\ell} R_{N_{\alpha,k}}''(y;\varepsilon,m) \right) + \sum_{\ell=0}^{N_{\alpha,k}-1} \left(\varepsilon^{\frac{m+\ell}{2}} \rho_{m+\ell} \tilde{R}_{N_{\alpha,k}}''(y,\varepsilon) \right) + \tilde{R}_{N_{\alpha,k}}''(y,\varepsilon) R_{N_{\alpha,k}}''(y;\varepsilon,m) \right] \partial_{y}^{\beta'}.$$
 (3.31)

where $\tilde{R}_{N_{\alpha,k}}^{\prime\prime}$ denotes the remaining term in the Taylor expansion of $B_{\alpha}^{(k)}$ analog to (3.11) and $R_{N_{\alpha,k}}^{\prime\prime}$ is the remaining term on the right hand side of (3.26). Analog to (3.12) we get for $u, v \in \mathbb{C}[y]$

$$\left| \left\langle u \,, \, \zeta_{\varepsilon} \tilde{R}_{N_{\alpha,k}}^{\prime\prime}(.,\varepsilon) v \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \right| \leq C_{N_{\alpha,k}} \varepsilon^{\frac{N_{\alpha,k}}{2}} \|u\|_{\mathscr{H}_{\tilde{\varphi}}} \sum_{\alpha \in \mathbb{N}^d \atop |\alpha| = N_{\alpha,k}} \|y^{\alpha}v\|_{\mathscr{H}_{\tilde{\varphi}}} \,. \tag{3.32}$$

Since for fixed $\alpha, \beta, \beta' \in \mathbb{N}^d$ we have $-n + \frac{m}{2} \ge -\frac{|\beta|}{2}$ for all possible values of n and m, it follows that $k - 1 + |\alpha| - n + \frac{m - |\beta'| + \ell}{2} \ge k - 1 + \frac{|\alpha|}{2}$, thus by (3.30) and since $|\alpha| > 2$ for k = 0 the leading order of $\zeta_{\varepsilon} \frac{1}{\varepsilon} U_{\varepsilon}(\tilde{\varphi}) \widehat{T}_{\varepsilon}' U_{\varepsilon}(\tilde{\varphi})^{-1}$ is ε^0 . Moreover these considerations yield by (3.32), (3.31) and (3.27)

$$\left| \left\langle u \,, \, \zeta_{\varepsilon} \tilde{R}'_{N_{\alpha,k}}(.,\varepsilon) v \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \right| \leq C_{N_{\alpha,k}} \varepsilon^{k + \frac{|\alpha|}{2} - 1 + \frac{N_{\alpha,k}}{2}} \sum_{|\alpha| = N_{\alpha,k}}^{2N_{\alpha,k}} \|y^{\alpha} u\|_{\mathscr{H}_{\tilde{\varphi}}} \sum_{|\beta'| = 0}^{|\alpha|} \|\partial^{\beta'} v\|_{\mathscr{H}_{\tilde{\varphi}}} \,. \tag{3.33}$$

Combining (3.30) and (3.22) leads to

$$\frac{1}{\varepsilon} U_{\varepsilon}(\tilde{\varphi}) \widehat{T}'_{\varepsilon} U_{\varepsilon}(\tilde{\varphi})^{-1} =: (S_1 + S_2 + S_3 + S_4) (., \varepsilon), \quad \text{where for } v \in \mathscr{H}_{\tilde{\varphi}}$$
(3.34)

$$S_{1}(y,\varepsilon) = \sum_{k=0}^{\lfloor N-1 \rfloor} \sum_{\substack{\alpha \in \mathbb{N}^{d} \\ |\alpha| < N_{k}}} \sum_{\beta+\beta'=\alpha} \sum_{\substack{n=\min\{1,|\beta|\}}}^{|\beta|} \varepsilon^{k+|\alpha|-1-n}$$
$$\times \sum_{m=(2n-|\beta|)_{+}}^{M_{n}} \sum_{\ell=0}^{N_{\alpha,k}} \varepsilon^{\frac{m+\ell-|\beta'|}{2}} q_{m+\ell}^{(k)}(y) \partial_{y}^{\beta'}$$
(3.35)

$$S_2(y,\varepsilon) = \sum_{k=0}^{[N-1]} \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| < N_k}} \tilde{\tilde{R}}'_{N_{\alpha,k}}(\varepsilon)$$
(3.36)

$$S_{3}(y,\varepsilon)v(y) = e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} \sum_{k=0}^{[N-1]} \varepsilon^{k-1} \tilde{R}'_{N_{k}}(\varepsilon) e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} v\left(\frac{x}{\sqrt{\varepsilon}}\right) \Big|_{x=\sqrt{\varepsilon}y}$$
(3.37)

$$S_4(y,\varepsilon)v(y) = e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} \tilde{R}_{[N]}(\varepsilon)e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} v\left(\frac{x}{\sqrt{\varepsilon}}\right)\Big|_{x=\sqrt{\varepsilon}y} .$$
(3.38)

Recall that \tilde{R}'_{N_k} and $\tilde{R}_{[N]}$ denote operators acting on functions of x. Choosing $N_{\alpha,k} = 2(N+1-k) - |\alpha|$ gives by (3.33) and (3.36) for $u, v \in \mathbb{C}[y]$

$$\left| \langle u, \zeta_{\varepsilon} S_{2}(.,\varepsilon) v \rangle_{\mathscr{H}_{\bar{\varphi}}} \right| \leq C_{N} \varepsilon^{N} \sum_{|\alpha|=0}^{4N+4} \| y^{\alpha} u \|_{\mathscr{H}_{\bar{\varphi}}} \sum_{|\beta|=0}^{2N+2} \| \partial^{\beta} v \|_{\mathscr{H}_{\bar{\varphi}}} .$$

$$(3.39)$$

To estimate the $\mathscr{H}_{\tilde{\varphi}}$ -norm of $S_3 v$, we have to analyze the remainder $R_{N_k} g$ given in (3.21) in the case $g(x) = e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} v(\frac{x}{\sqrt{\varepsilon}})$. We first remark that by (3.4), for $y \in \operatorname{supp} \zeta_{\varepsilon}$ and for some $C, C_0 > 0$, the estimate

$$\left|\nabla\tilde{\varphi}(\sqrt{\varepsilon}y + t\varepsilon\eta)\right| \le C \begin{cases} \left|\sqrt{\varepsilon}y + \varepsilon\eta\right|, & \left|\eta\right| \le \frac{C_0}{\sqrt{\varepsilon}}\\ 1, & \left|\eta\right| > \frac{C_0}{\sqrt{\varepsilon}} \end{cases}$$
(3.40)

holds uniformly with respect to $t \in [0, 1]$. Thus for some C > 0 independent of $t \in [0, 1]$, $y \in \sup \zeta_{\varepsilon}$, by first order Taylor expansion, we have for any $\eta \in C\mathbb{Z}^d$

$$\left| e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}y+t\varepsilon\eta)}{\varepsilon}} \right| \le e^{C|\eta|} .$$
(3.41)

Moreover by the Leibnitz formula,

$$\partial_x^{\alpha} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} = e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \left(\nabla_x - \frac{1}{\varepsilon} \nabla \tilde{\varphi}(x) \right)^{\alpha}$$
(3.42)

holds. This gives together with (3.40) for $C, C_0 > 0$ and $|\alpha| = N_k$ the estimate

$$\left| \int_{0}^{1} (1-t)^{N_{k}-1} \partial_{x}^{\alpha} e^{-\frac{\tilde{\varphi}}{\varepsilon}} v\left(\frac{1}{\sqrt{\varepsilon}}\right) \right|_{x+t\varepsilon\eta} dt \right| \\ \leq C \sum_{|\tilde{\alpha}| \leq |\alpha|} \int_{0}^{1} \left\{ \frac{\varepsilon^{-\frac{N_{k}}{2}}}{\varepsilon^{-N_{k}}} \left| \tau_{t\sqrt{\varepsilon}\eta} \left(|\cdot|^{N_{k}} e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}\cdot\cdot)}{\varepsilon}} \partial^{\tilde{\alpha}} v \right)(y) \right| dt, \quad \text{if } |\eta| \leq \frac{C_{0}}{\sqrt{\varepsilon}} \\ \varepsilon^{-N_{k}} \left| \tau_{t\sqrt{\varepsilon}\eta} \left(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}\cdot)}{\varepsilon}} \partial^{\tilde{\alpha}} v \right)(y) \right| dt, \quad \text{if } |\eta| > \frac{C_{0}}{\sqrt{\varepsilon}} .$$

$$(3.43)$$

By (3.21), (3.37) and (3.43) it follows that for $v \in \mathbb{C}[y]$

$$\|\zeta_{\varepsilon}S_{3}(..\varepsilon)v\|_{\mathscr{H}_{\tilde{\varphi}}} \leq C \sum_{k=0}^{\lfloor N-1 \rfloor} \varepsilon^{k-1+N_{k}} \sum_{\substack{\alpha \in \mathbb{N}^{d} \\ |\alpha|=N_{k}}} \|\zeta_{\varepsilon} \{A_{1,\alpha}(..,\varepsilon) + A_{2,\alpha}(..,\varepsilon)\}\|_{\mathscr{H}_{\tilde{\varphi}}},$$
(3.44)

where

$$A_{1,\alpha}(y,\varepsilon) := \sum_{|\eta| \le \frac{C_0}{\sqrt{\varepsilon}}} \varepsilon^{-\frac{N_k}{2}} \left| a_{\varepsilon\eta}^{\prime(k)}(\sqrt{\varepsilon}y) \right| |\eta|^{N_k} \sum_{|\tilde{\alpha}| \le |\alpha|} e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} \int_0^1 \left| \tau_{t\sqrt{\varepsilon}\eta} \left(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}\cdot)}{\varepsilon}} \right| \cdot |^{N_k} \partial^{\tilde{\alpha}}v \right) \right| dt$$

$$(3.45)$$

$$A_{2,\alpha}(y,\varepsilon) := \sum_{|\eta| > \frac{C_0}{\sqrt{\varepsilon}}} \varepsilon^{-N_k} \left| a_{\varepsilon\eta}^{\prime(k)}(\sqrt{\varepsilon}y) \right| |\eta|^{N_k} \sum_{|\tilde{\alpha}| \le |\alpha|} e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} \int_0^1 \left| \tau_{t\sqrt{\varepsilon}\eta} \left(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}\cdot)}{\varepsilon}} \partial^{\tilde{\alpha}} v \right) \right| \, dt \; .$$

$$(3.46)$$

By Cauchy-Schwarz-Inequality, we have for any c > 0

$$\begin{split} \|\zeta_{\varepsilon}A_{2,\alpha}(.,\varepsilon)v\|_{\mathscr{H}_{\bar{\varphi}}} &\leq C\varepsilon^{-N_{k}} \left\| \left(\sum_{|\eta| > \frac{C_{0}}{\sqrt{\varepsilon}}} \left| a_{\varepsilon\eta}^{\prime(k)}(\sqrt{\varepsilon} \, . \,) \right|^{2} e^{2c|\eta|} \right)^{\frac{1}{2}} \right. \\ & \times \left(\sum_{|\eta| > \frac{C_{0}}{\sqrt{\varepsilon}}} e^{-2c|\eta|} |\eta|^{2N_{k}} \left[\sum_{|\tilde{\alpha}| \leq |\alpha|} e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon} \, . \,)}{\varepsilon}} \int_{0}^{1} \left| \tau_{t\sqrt{\varepsilon}\eta} \left(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon} \, . \,)}{\varepsilon}} \partial^{\tilde{\alpha}}v \right) \right| \, dt \right]^{2} \right)^{\frac{1}{2}} \right\|_{\mathscr{H}_{\bar{\varphi}}} \\ & \leq C\varepsilon^{-N_{k}} \sup_{x \in \mathbb{R}^{d}} \left\| a_{\varepsilon}^{\prime(k)}(x)e^{c|\cdot|} \right\|_{\ell^{2}_{\gamma}} \sum_{|\eta| > \frac{C_{0}}{\sqrt{\varepsilon}}} e^{-c|\eta|} |\eta|^{N_{k}} e^{C|\eta|} \times \\ & \sum_{|\tilde{\alpha}| \leq |\alpha|} \int_{0}^{1} \left\| e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon} \, . \,)}{\varepsilon}} \tau_{t\sqrt{\varepsilon}\eta} \left(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon} \, . \,)}{\varepsilon}} \partial^{\tilde{\alpha}}v \right) \right\|_{\mathscr{H}_{\bar{\varphi}}} \, dt \end{split}$$

We remark that

$$\|e^{\frac{\tilde{\varphi}(\sqrt{\varepsilon}\,\cdot\,)}{\varepsilon}}\tau_{t\sqrt{\varepsilon}\eta}(e^{-\frac{\tilde{\varphi}(\sqrt{\varepsilon}\,\cdot\,)}{\varepsilon}}\partial^{\tilde{\alpha}}v)\|_{\mathscr{H}_{\tilde{\varphi}}} = \|\partial^{\tilde{\alpha}}v\|_{\mathscr{H}_{\tilde{\varphi}}}.$$
(3.47)

Thus using Hypothesis 1.1(a)(iv), we get for each $\alpha \in \mathbb{N}^d$, $|\alpha| = N_k$ and for any c' > 0 the estimate

$$\|\zeta_{\varepsilon}A_{2,\alpha}(.,\varepsilon)v\|_{\mathscr{H}_{\varphi}} \le C'e^{-\frac{\alpha'}{\sqrt{\varepsilon}}} \sum_{|\tilde{\alpha}| \le |\alpha|} \|\partial^{\tilde{\alpha}}v\|_{\mathscr{H}_{\varphi}} .$$

$$(3.48)$$

By analog arguments using (3.43) and (3.47), we get

$$\|\zeta_{\varepsilon}A_{1,\alpha}(.,\varepsilon)v\|_{\mathscr{H}_{\tilde{\varphi}}} \leq C\varepsilon^{-\frac{N_{k}}{2}}C''\sum_{|\tilde{\alpha}|\leq |\alpha|} \left\||.|^{N_{k}}\partial^{\tilde{\alpha}}v\right\|_{\mathscr{H}_{\tilde{\varphi}}}.$$
(3.49)

Setting $N_k = 2(N - k + 1)$ and inserting (3.48) and (3.49) into (3.44) gives

$$\|\zeta_{\varepsilon}S_{3}(,\varepsilon)v\|_{\mathscr{H}_{\tilde{\varphi}}} \leq C\varepsilon^{N} \sum_{|\alpha| \leq 2+2N} \left\| |\cdot|^{N_{k}} \partial^{\alpha}v \right\|_{\mathscr{H}_{\tilde{\varphi}}} .$$

$$(3.50)$$

To estimate S_4 , we use (3.18) and the Cauchy-Schwarz-inequality to get

$$\begin{aligned} \|\zeta_{\varepsilon}S_{4}(,.\varepsilon)v\|_{\mathscr{H}_{\bar{\varphi}}} &= \left\|\zeta_{\varepsilon}e^{\frac{\bar{\varphi}}{\varepsilon}}\sum_{\gamma\in(\varepsilon\mathbb{Z})^{d}}R_{\gamma}^{([N])}(\sqrt{\varepsilon}\,.\,,\varepsilon)e^{\frac{c|\gamma|}{\varepsilon}}e^{-\frac{c|\gamma|}{\varepsilon}}\tau_{\gamma}e^{-\frac{\bar{\varphi}}{\varepsilon}}v\right\|_{\mathscr{H}_{\bar{\varphi}}} \\ &\leq \sup_{x\in\mathbb{R}^{d}}\left\|R_{(.)}^{([N])}(x,\varepsilon)e^{\frac{c|.|}{\varepsilon}}\right\|_{\ell_{\gamma}^{2}}\left\|\left(\sum_{\gamma}\zeta_{\varepsilon}^{2}e^{-\frac{2c|\gamma|}{\varepsilon}}e^{\frac{2\bar{\varphi}}{\varepsilon}}\left[\tau_{\gamma}e^{-\frac{\bar{\varphi}}{\varepsilon}}v\right]^{2}\right)^{\frac{1}{2}}\right\|_{\mathscr{H}_{\bar{\varphi}}}. \end{aligned}$$
(3.51)

(3.47) and Hypothesis 1.1(a)(iv) yields

$$\begin{aligned} \|\zeta_{\varepsilon}S_{4}(,.\varepsilon)v\|_{\mathscr{H}_{\tilde{\varphi}}} &\leq \varepsilon^{N}C\sum_{\gamma} e^{-\frac{c|\gamma|}{\varepsilon}} \left\|\zeta_{\varepsilon}e^{\frac{\tilde{\varphi}}{\varepsilon}} \left[\tau_{\gamma}e^{-\frac{\tilde{\varphi}}{\varepsilon}}v\right]\right\|_{\mathscr{H}_{\tilde{\varphi}}} \\ &\leq C\varepsilon^{N}\|v\|_{\mathscr{H}_{\tilde{\varphi}}}. \end{aligned}$$
(3.52)

Step 3:

In the last step we are going to combine the terms resulting from the kinetic and potential energy. The sum over all $0 \le k \le [N-1]$ of lhs(3.24) with $|\beta'| = 0$ and $n = |\beta| (= m_p)$ is given by

$$\sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha|=2n, 1 \le n \le \frac{N_0}{2}}} \varepsilon^{\frac{|\alpha|}{2}-1} B_{\alpha}^{(0)}(x) \left(\nabla \tilde{\varphi}|_x\right)^{\alpha} + \sum_{k=1}^{[N-1]} \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| < N_k}} \varepsilon^{\frac{|\alpha|}{2}-1+k} B_{\alpha}^{(k)}(x) \left(\nabla \tilde{\varphi}|_x\right)^{\alpha} , \qquad (3.53)$$

which, by the definition (3.20) of $B_{\alpha}^{(k)}$, converges to $\varepsilon^{-1}t(x, i\nabla\tilde{\varphi}|_x)$ as $N \to \infty$. Since by Hypothesis 1.5, $\tilde{\varphi}$ solves the eikonal equation (1.31) in a neighborhood of x = 0, it follows that the first sum in (3.53) (which for $N_0 \to \infty$ converges to $\varepsilon^{-1}t_0(x, i\nabla\tilde{\varphi}(x))$) cancels with the potential term $\varepsilon^{-1}V_0(x)$ in each order of ε . Eliminating the case $\alpha = \beta, n = |\alpha|, k = 0$ from the the sum in S_1 in (3.34) and eliminating the case $\ell = 0$ in (3.15) yields

$$\widehat{G}_{\varepsilon} = \frac{1}{\varepsilon} U_{\varepsilon}(\widetilde{\varphi}) \left(\widehat{V}_{\varepsilon}' - V_{0}' \right) U_{\varepsilon}(\widetilde{\varphi})^{-1} + \frac{1}{\varepsilon} U_{\varepsilon}(\widetilde{\varphi}) \left(\widehat{T}_{\varepsilon}' - t_{0}(., i\nabla\widetilde{\varphi}(.)) \right) U_{\varepsilon}(\widetilde{\varphi})^{-1}$$

$$=: A_{N} + B_{N} + R_{N}(\varepsilon).$$

$$(3.54)$$

The potential part of order N is

$$A_N = \sum_{\substack{k \in \frac{N}{2} \\ k < N}} \varepsilon^k p'_k , \qquad (3.55)$$

where

$$p_k(y) = \sum_{\ell=1}^{\lfloor \lfloor k+1 \rfloor \rfloor} D_x^{2(k+1-\ell)} V_\ell'|_{x=0} [y]^{2(k+1-\ell)} , \qquad (3.56)$$

which is a polynomial of degree 2k - 2, which is even (odd) if 2k is even (odd) (or if k is integer (half-integer)). Setting $N_{\alpha,k} = 2(N + 1 - k) - |\alpha|$ and $N_k = 2(N + 1 - k)$ in (3.34), the kinetic part of order N in (3.54) is

$$B_{N} = \sum_{\substack{|\alpha|=2n\\1\le n\le \frac{2N+2}{2}}} \sum_{\beta+\beta'=\alpha} \sum_{n=\min\{1,|\beta|\}}^{\min\{|\beta|,|\alpha|-1\}} \sum_{m=(2n-|\beta|)_{+}}^{M_{n}} \sum_{\ell=0}^{2N+2-|\alpha|} \varepsilon^{|\alpha|-1-n+\frac{m+\ell-|\beta'|}{2}} q_{m+\ell}^{(0)} \partial^{\beta'}$$
(3.57)

$$+\sum_{k=1}^{[N-1]}\sum_{\substack{\alpha\in\mathbb{N}^{d}\\|\alpha|<2(N+1-k)}}\sum_{\beta+\beta'=\alpha}\sum_{n=\min\{1,|\beta|\}}^{|\beta|}\varepsilon^{k-1+|\alpha|-n}\sum_{m=(2n-|\beta|)_{+}}^{M_{n}}\sum_{\ell=0}^{2(N+1-k)-|\alpha|}\varepsilon^{\frac{m+\ell-|\beta'|}{2}}q_{m+\ell}^{(k)}\partial^{\beta'},\quad(3.58)$$

where we recall from (3.30) that $q_s^{(k)}$ is a homogeneous polynomial of degree s, which is independent from the truncation N. First we analyze B_N . In order to get the stated result in (3.6), we collect all terms with the fixed order $r \in \frac{\mathbb{N}}{2}$ in ε . Setting

$$r = |\alpha| - 1 - n + \frac{m + \ell - |\beta'|}{2} + k , \qquad (3.59)$$

we may rewrite (3.57) as

$$B_N = \sum_{\substack{r \in \frac{\mathbb{N}}{2} \\ r < N}} \sum_{\substack{\beta' \in \mathbb{N}^d \\ |\beta'| \le n_r}} \rho_{r,\beta'} \partial^{\beta'} .$$
(3.60)

We shall determine $n_r \in \mathbb{N}$ and the properties of $\rho_{r,\beta'}$. From (3.59) we get

$$m + \ell = 2r + 2(1 + n - |\alpha| - k) + |\beta'|.$$
(3.61)

By (3.57) and (3.61), the polynomial $\rho_{r,\beta'}$ is even (odd) with respect to $y \mapsto -y$, if $2r - |\beta'|$ resp. is even (odd), since $q_{m+\ell}^{(k)}$ is homogeneous of order $m + \ell$ and $1 + n - |\alpha| - k \in \mathbb{Z}$. Using (3.61) and $\deg q_{m+\ell}^{(k)} = m + \ell$ again, we see that

$$\deg \rho_{r,\beta'} = \max_{(n,\alpha,k)} \left(2r - 2(1+n-|\alpha|-k) + |\beta'| \right) , \qquad (3.62)$$

where (n, α, k) runs through all values occurring in (3.57). Inspection of (3.57) gives the maximal value

$$n_{\max} = \begin{cases} \min\{|\alpha| - |\beta'|, |\alpha| - 1\} & \text{if } k = 0\\ |\alpha| - |\beta'| & \text{if } k > 0 \end{cases}$$

Thus, using (3.62),

$$\deg \rho_{r,\beta'} = \begin{cases} 2r+2-|\beta'|, & |\beta'| > 0\\ 2r, & |\beta'| = 0 \end{cases}$$
(3.63)

It follows from (3.62), that the maximal value n_r of $|\beta'|$ occurring in the sum on the right hand side of (3.60) is given by $n_r = 2r + 2$.

Thus, setting $b_r := \rho_{r,0} + p_r$ and $b_{r,\beta'} := \rho_{r,\beta'}$, we have by (3.54), (3.55) and (3.60) for any $r \in \frac{\mathbb{N}}{2}, r < N$

$$G_r = b_{2r} + \sum_{\substack{\beta \in \mathbb{N}^d \\ 1 \le |\beta| \le 2r+2}} b_{2r+2-|\beta|} \partial^{\beta} ,$$

where, by the considerations below (3.56) and (3.61), b_r denotes a polynomial of degree 2r which is even (odd) with respect to $y \mapsto -y$, if 2r is even (odd) and $b_{r,\beta}$ denotes a polynomial of degree $2r + 2 - |\beta|$, which is even (odd) if $2r - |\beta|$ is even (odd).

The estimate (3.7) on the remainder $R_N(\varepsilon)$ in (3.54) follows at once from (3.52), (3.50), (3.39) and (3.47).

Proof of Remark 3.3,(b):

The kinetic part of the term of order ε^0 results from the terms in (3.24), for which the pair $(k, |\alpha|)$ takes the values (0, 2), (1, 1) and (2, 0). These have to be combined with the potential part of this term given by $j = 2, \ell = 0$ and $j = 0, \ell = 1$ respectively in (3.14). Again, by use of the eikonal equation (1.31), the terms $V'_{0,q}(x)$ and $|\nabla \tilde{\varphi}_0(x)|^2$ cancel. Since $B'(x) = \mathbf{1} + o(\mathbf{1}), (3.8)$ follows by direct calculation.

We introduce the following formal symbol spaces. Let for $n \in \mathbb{N}^*$

$$\mathcal{K}_{\frac{1}{n}} := \left\{ \mu = \sum_{j \in \frac{\mathbb{Z}}{n}} \mu_j \varepsilon^j \ \middle| \ \mu_j \in \mathbb{C} \quad \text{and} \quad c_\mu := \inf\{j \mid \mu_j \neq 0\} > -\infty \right\}$$
(3.64)

$$\mathcal{V} := \left\{ p = \sum_{j \in \frac{\mathbb{Z}}{2}} p_j \varepsilon^j \middle| p_j \in \mathbb{C}[y] \quad \text{and} \quad c_p := \inf\{j \mid p_j \neq 0\} > -\infty \right\}.$$
(3.65)

Defining addition component-by-component and multiplication by the Cauchy product, $\mathcal{K}_{\frac{1}{n}}$ 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 \hat{G}_{ε} a well defined linear operator G on \mathcal{V} by setting, for $\mathcal{V} \ni p = \sum_{\substack{j \geq k \\ j \in \frac{Z}{2}}} \varepsilon^j p_j$,

$$Gp(y) = \sum_{j \ge k} \varepsilon^j \sum_{r \in \frac{N}{2}} \varepsilon^r G_r p_j(y) = \sum_{j+r=\ell \ge k} \varepsilon^\ell G_r p_j(y) \in \mathcal{V} .$$
(3.66)

We denote the set of linear operators on \mathcal{V} by $\mathcal{L}(\mathcal{V})$.

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

$$\langle p, q \rangle_{\mathcal{V}} = \int_{\mathbb{R}^d} \overline{p(\varepsilon, y)} q(\varepsilon, y) e^{-2\frac{\tilde{\varphi}(\sqrt{\varepsilon}y)}{\varepsilon}} dy.$$
 (3.67)

To this end, using (1.32), we define real polynomials $\omega_k \in \mathbb{R}[y]$ by $\omega_0 := 1$ and

$$e^{-2\frac{\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} =: e^{-\sum_{\nu=1}^{d} \lambda_{\nu} y_{\nu}^{2}} \left(\sum_{\substack{k \in \frac{\mathbb{N}}{2} \\ k < N}} \varepsilon^{k} \omega_{k}(y) + \tilde{R}_{N}(\varepsilon, y) \right).$$
(3.68)

Then

$$\omega_j(y) = \sum_{\ell=1}^{2j} \sum_{\substack{k_1 + \dots + k_\ell = j \\ k_i \in \frac{\mathbb{N}^*}{2}}} \frac{(-2)^\ell}{\ell!} \varphi_{2k_1}(y) \dots \varphi_{2k_\ell}(y) , \qquad (3.69)$$

where the summands are homogeneous polynomials of degree $2j + 2\ell$ with parity $(-1)^{2j}$ and

$$|\tilde{R}_N(\varepsilon, y)| = O\left(\varepsilon^N \langle y \rangle^{6N}\right) .$$
(3.70)

DEFINITION 3.4 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 sesquilinear form $\langle . , . \rangle_{\mathcal{V}} : \mathcal{V} \times \mathcal{V} \to \mathcal{K}_{\frac{1}{2}}$ by

$$\langle p, q \rangle_{\mathcal{V}} := \sum_{m \in \mathbb{Z} \atop 2} \varepsilon^m \sum_{j+k+\ell=m} \int_{\mathbb{R}^d} \overline{p_j(y)} q_k(y) \omega_\ell(y) e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2} \, dy \,. \tag{3.71}$$

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

LEMMA 3.5 The sesquilinear form defined in (3.71) is non-degenerate, i.e.,

$$\langle p, q \rangle_{\mathcal{V}} = 0 \quad \text{for all} \quad p \in \mathcal{V} \quad \text{implies} \quad q = 0.$$
 (3.72)

Proof. If $q \neq 0$ we have $q = \sum_{j \geq k} q_j \varepsilon^j$, $k, j \in \frac{\mathbb{Z}}{2}$ with $q_k \neq 0$ for some k. For $p := \varepsilon^k q_k$, the lowest order of the sesquilinear form is given by

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

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

PROPOSITION 3.6 Let G be the operator (3.66) on \mathcal{V} induced by $\widehat{G}_{\varepsilon}$ defined in (3.2) and let $\langle ., . \rangle_{\mathcal{V}}$ be the non-degenerate sesquilinear form introduced in Definition 3.4. Then for all $p, q \in \mathcal{V}$

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

Proof. We will consider $Y = \mathbb{C}[y]$ as a subset of the form domain of $\widehat{G}_{\varepsilon}$ for $\varepsilon > 0$. This can canonically be identified with a subset \mathcal{Y} of \mathcal{V} . By the linearity of $\langle . , . \rangle_{\mathcal{V}}$, it is sufficient to prove the proposition for $p, q \in \mathcal{Y}$.

We need the following lemma:

LEMMA 3.7 Let $p, q \in Y$, then the function

$$(0,\sqrt{\varepsilon_0}) \ni \sqrt{\varepsilon} \mapsto \left\langle p, \widehat{G}q \right\rangle (\sqrt{\varepsilon}) := \left\langle p, \widehat{G}_{\varepsilon}q \right\rangle_{\mathscr{H}_{\widetilde{\varphi}}}$$
(3.73)

has an asymptotic expansion at $\sqrt{\varepsilon} = 0$. In particular, for any $N \in \frac{\mathbb{N}}{2}$, we have

$$\langle p, \widehat{G}q \rangle(\sqrt{\varepsilon}) = \sum_{\substack{\ell,k \in \frac{N}{2}\\ \ell > 0, k+\ell < N}} \varepsilon^{k+\ell} \int_{\mathbb{R}^d} \bar{p}(y) G_k q(y) e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2} \omega_\ell(y) \, dy + O\left(\varepsilon^N\right)$$
(3.74)

where G_k is given in Proposition 3.2 and the polynomials ω_{ℓ} are defined in (3.68).

Proof of Lemma 3.7. Step 1:

We will show that, for ζ_{ε} as in Proposition 3.2, there exists some C > 0 such that

$$\langle p, \widehat{G}q \rangle(\sqrt{\varepsilon}) = \int_{\mathbb{R}^d} e^{-\frac{\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} \zeta_{\varepsilon}(y)\overline{p}(y)\widehat{G}_{\varepsilon}q(y)\,dy + O\left(e^{-\frac{O}{\varepsilon}}\right) \,. \tag{3.75}$$

In fact, we can write

$$\left\langle p, \widehat{G}q \right\rangle (\sqrt{\varepsilon}) = J_1(\sqrt{\varepsilon}) + J_2(\sqrt{\varepsilon}), \quad \text{where}$$
 (3.76)

$$J_1(\sqrt{\varepsilon}) := \left\langle \zeta_{\varepsilon} p \,, \, \widehat{G}_{\varepsilon} q \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \quad \text{and} \quad J_2(\sqrt{\varepsilon}) := \left\langle (1 - \zeta_{\varepsilon}) p \,, \, \widehat{G}_{\varepsilon} q \right\rangle_{\mathscr{H}_{\tilde{\varphi}}} \,. \tag{3.77}$$

Since by Hypothesis 1.5 and the definition of ζ in Proposition 3.2 we have $\tilde{\varphi}(x) = \varphi(x)$ for $x \in \operatorname{supp} \zeta$, it remains to show that $|J_2(\sqrt{\varepsilon})| = O(e^{-\frac{C}{\varepsilon}})$.

By the definition of $\widehat{G}_{\varepsilon}$ and with $x = \sqrt{\varepsilon}y$ we can write

$$J_2(\sqrt{\varepsilon}) = \varepsilon^{-\frac{d}{2}-1} \int_{\mathbb{R}^d} \bar{p}(\frac{x}{\sqrt{\varepsilon}}) e^{-\frac{\bar{\varphi}(x)}{\varepsilon}} \widehat{H}'_{\varepsilon} \left(q(\frac{x}{\sqrt{\varepsilon}}) e^{-\frac{\bar{\varphi}(x)}{\varepsilon}} \right) (1-\zeta(x)) \, dx \;. \tag{3.78}$$

By Hypothesis 1.1 and (1.22) we have $\widehat{H}'_{\varepsilon} = \widehat{T}'_{\varepsilon} + \widehat{V}'_{\varepsilon}$, where $\widehat{T}'_{\varepsilon}$ is bounded (see Remark 1.2,(c)) and $\widehat{V}'_{\varepsilon}$ is a polynomially bounded multiplication operator on $L^2(\mathbb{R}^d)$, thus

$$(1-\zeta(x))\widehat{H}'_{\varepsilon}\left(q(\frac{x}{\sqrt{\varepsilon}})e^{-\frac{\widetilde{\varphi}(x)}{\varepsilon}}\right) =: u_{\varepsilon}(x) \in L^{2}(\mathbb{R}^{d}), \qquad (3.79)$$

where $||u_{\varepsilon}||_{L^2} = O(\varepsilon^{-m})$ for some m > 0 depending on the dimension d. We therefore have by (3.4) for some C > 0, using the Cauchy-Schwarz-inequality in (3.78),

$$|J_2(\sqrt{\varepsilon})| \le \varepsilon^{-\frac{d}{2}-1} ||u_{\varepsilon}||_{L^2} \left(\int_{|x|>\eta} e^{-\frac{\tilde{C}|x|}{\varepsilon}} |p(\frac{x}{\sqrt{\varepsilon}})|^2 \, dx \right)^{\frac{1}{2}} = O\left(e^{-\frac{C}{\varepsilon}}\right) \,. \tag{3.80}$$

Step 2:

We will show that for all $N \in \mathbb{N}$

$$\int_{\mathbb{R}^d} e^{-\frac{2\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} \zeta_{\varepsilon}(y)\bar{p}(y)\widehat{G}_{\varepsilon}q(y)\,dy = \sum_{\substack{\ell,k\in\frac{\mathbb{N}}{2}\\\ell>0,\ell+k< N}} \varepsilon^{\ell+k} \int_{\mathbb{R}^d} e^{-\sum_{\nu=1}^d \lambda_\nu y_\nu^2} \zeta_{\varepsilon}(y)\omega_\ell(y)\bar{p}(y)G_kq(y)\,dy + O(\varepsilon^N)\,,$$
(3.81)

which together with (3.75) shows (3.74).

By Proposition 3.2

$$lhs(3.81) = \sum_{\substack{k \in \frac{\mathbb{N}}{2} \\ 0 \le k < N}} \varepsilon^k \int_{\mathbb{R}^d} e^{-\frac{2\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} \zeta_{\varepsilon}(y)\bar{p}(y)G_kq(y)\,dy + O(\varepsilon^N) \,.$$
(3.82)

By the definition of ω_{ℓ} in (3.68) together with (3.70), it follows by the expansion of the exponential function that

$$\zeta_{\varepsilon}(y)e^{-\frac{2\varphi(\sqrt{\varepsilon}y)}{\varepsilon}} = \zeta_{\varepsilon}(y)e^{-\sum_{\nu=1}^{d}\lambda_{\nu}y_{\nu}^{2}} \left(1 + \sum_{\substack{k \in \frac{\mathbb{N}^{*}}{2} \\ k < N}} \varepsilon^{k}\omega_{k}(y) + \widehat{R}_{N}(\varepsilon, y)\right), \quad (3.83)$$

where for some $\hat{C}_N > 0$

$$|\widehat{R}_N(\varepsilon, y)| \le \varepsilon^N \widehat{C}_N \langle y \rangle^{6N} .$$
(3.84)

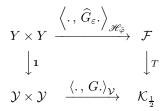
Inserting (3.83) into (3.82), using (3.84) and Remark 3.3, gives (3.81).

We come back to the proof of Proposition 3.6.

In order to use the symmetry of $\widehat{G}_{\varepsilon}$ on $\mathscr{H}_{\widetilde{\varphi}}$, we use the function $\langle p, \widehat{G}q \rangle$ on $(0, \sqrt{\varepsilon_0})$ defined in (3.73). By Lemma 3.7 it has an asymptotic expansion at $\sqrt{\varepsilon} = 0$, which induces a mapping

$$\left\langle \, . \, , \widehat{G} \, . \, \right\rangle : Y \times Y \to \mathcal{K}_{\frac{1}{2}} \, .$$

By (3.66), (3.71) and (3.74) we see that this function coincides with the quadratic form $\langle \cdot, G \cdot \rangle_{\mathcal{V}}$ restricted to $\mathcal{Y} \times \mathcal{Y}$. Using the definition (3.73), we see that the diagram



is commutative. Here \mathcal{F} denotes the set of functions on $(0, \sqrt{\varepsilon_0})$, which possess an asymptotic expansion in integer powers of $\sqrt{\varepsilon}$ and T denotes asymptotic expansion.

Since for $\langle \widehat{G}_{\varepsilon} . , . \rangle_{\mathscr{H}_{\widetilde{\varphi}}}$ and $\langle G . , . \rangle_{\mathcal{V}}$ we have an analog commutative diagram, the proposition is traced back to the symmetry of $\widehat{G}_{\varepsilon}$ on $\mathscr{H}_{\widetilde{\varphi}}$.

4. Construction of formal asymptotic expansions

In this section we construct formal asymptotic expansions for the eigenfunctions and eigenvalues of \hat{H}_{ε} .

First we recall that the operator εG_0 on \mathscr{H}_{φ} , given in (3.8), is unitary equivalent to the harmonic oscillator $\widehat{H}_q^{\prime 0}$ defined in (1.21), where the unitary transformation $U_{\varepsilon}(\varphi_0)$ is defined in (3.1). Therefore the spectrum of G_0 is given by

$$\sigma(G_0) = \left\{ e_{\alpha} = \sum_{\nu=1}^d \left(\lambda_{\nu} (2\alpha_{\nu} + 1) \right) + V_1(0) + t_1(0, 0) \mid \alpha \in \mathbb{N}^d \right\} .$$
(4.1)

The eigenfunctions of $\widehat{H}_q^{\prime 0}$ are the functions g_{α} defined in (1.29) with φ_0 introduced in (1.30), thus the $\mathscr{H}_{\tilde{\varphi}}$ -normalized eigenfunctions of εG_0 are given by

$$(U_{\varepsilon}(\varphi_0)g_{\alpha})(y) = h_{\alpha}(y), \qquad G_0h_{\alpha} = e_{\alpha}h_{\alpha}$$
(4.2)

where h_{α} denotes a product of Hermite polynomials $h_{\alpha_{\nu}} \in \mathbb{R}[y_{\nu}]$. Since $h_k(-x) = (-1)^k h_k(x)$ for any $k \in \mathbb{N}$, it follows that h_{α} 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 4.1 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

$$R(z) := \sum_{k=0}^{\infty} \left[-R_0(z) \sum_{j \in \frac{\mathbb{N}^*}{2}} \varepsilon^j G_j \right]^k R_0(z) = -\sum_{j \in \frac{\mathbb{N}}{2}} \varepsilon^j r_j(z) \qquad with$$
(4.3)

$$r_j := \sum_{k=1}^{2j} (-1)^k \sum_{\substack{j=J_1+\dots+j_k\\j_1,\dots,j_k \in \frac{N^*}{2}}} \left(\prod_{m=1}^k -R_0 G_{j_m}\right) R_0 .$$
(4.4)

(b)

$$\langle p, R(z)q \rangle_{\mathcal{V}} = \langle R(\bar{z})p, q \rangle_{\mathcal{V}}.$$
 (4.5)

(c) For r_j defined in (4.4)

$$\langle p, r_j(z)q \rangle_{\mathcal{V}} = \langle r_j(\bar{z})p, q \rangle_{\mathcal{V}}, \qquad j \in \frac{\mathbb{N}}{2}.$$
 (4.6)

Proof. (a): Clearly, $R_0(z)$, G_j and r_j are linear operators in \mathcal{V} (i.e. elements of $\mathcal{L}(\mathcal{V})$ (see Remark 3.3), thus $R(z) \in \mathcal{L}(\mathcal{V})$. A short calculation (in the sense of formal power series) shows that indeed $R(z) = (G-z)^{-1}$.

(b): By (a) and Proposition 3.6, we can write

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

(c): This follows directly from the expansion (4.3).

In the following we will use the resolvent operator R(z) (as a map on \mathcal{V}) to define a spectral projection for G associated to an eigenvalue of G_0 .

By (4.3), 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 3.2, that G_j raises the degree of each polynomial by 2j. Thus there exist real numbers $c_{\alpha\beta}^j$ such that for all $\alpha, \beta \in \mathbb{N}^d$, $j \in \frac{\mathbb{N}}{2}$ we have

$$G_j h_{\alpha} = \sum_{|\beta| \le |\alpha| + 2j} c^j_{\alpha\beta} h_{\beta} .$$

$$(4.7)$$

Combining (4.7), (4.4) and (4.2), 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

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

$$(4.8)$$

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.

Since $r_j(z)$ is well defined on \mathcal{V} for each $j \in \frac{\mathbb{N}}{2}$ and depends in a meromorphic way on z, we can define for $p = \sum_{k \ge M} \varepsilon^k p_k \in \mathcal{V}$

$$\Pi_E p := \sum_{\substack{k+\ell=j\\\ell\in\frac{N}{2},k\ge M}} \varepsilon^j \frac{1}{2\pi i} \oint_{\Gamma(E)} r_\ell(z) p_k \, dz \,.$$

$$\tag{4.9}$$

We denote this operator by

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

This is analog to the familiar Riesz projection for operators on a Hilbert space.

PROPOSITION 4.2 Let $E \in \sigma(G_0)$ with multiplicity m. Then the operator Π_E defined in (4.9) is a symmetric projection in \mathcal{V} of dimension m, which commutes with G.

Proof. Symmetry:

The symmetry of Π_E is a consequence of (4.6):

$$\left\langle p, \oint_{\Gamma(E)} r_j(z) \, dzq \right\rangle_{\mathcal{V}} = -\left\langle \oint_{\Gamma(E)} r_j(z) \, dzp, \, q \right\rangle_{\mathcal{V}},$$

where the negative sign results from the conjugation of z.

1

 $\Pi_E^2 = \Pi_E:$

Using (4.3), (4.9) and the resolvent equation, this follows from standard arguments (see [13] or [11] for the computation in the setting of formal power series).

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

We introduce the set

$$I_E := \left\{ \alpha \in \mathbb{N}^d \mid G_0 h_\alpha = E h_\alpha \right\} =: \left\{ \alpha^1, \dots, \alpha^m \right\}$$

$$(4.10)$$

numbering the *m* Hermite polynomials with eigenvalue (energy) *E* for G_0 . As a consequence of the representation (4.3) of R(z) (recall $r_0(z) = R_0(z)$) and of the definition (4.9) of Π_E , we can write for $\alpha \in I_E$

$$\Pi_E h_\alpha = h_\alpha + \sum_{j \in \frac{\mathbb{N}^*}{2}} \varepsilon^j p_j \tag{4.11}$$

for some polynomials $p_j \in \mathbb{C}[y]$ of degree less than or equal to $|\alpha| + 2j$ (this follows from (4.8)). Since the Hermite polynomials form a basis, (4.11) implies that the functions $\Pi_E h_{\alpha^k}$, $k = 1, \ldots m$, are linearly independent over $\mathcal{K}_{\frac{1}{2}}$. Thus their span has dimension m. It remains to show that this span coincides with the range of Π_E , i.e., we have to show that for all $\beta \in \mathbb{N}_0^d$ there exist $\mu_{\alpha} \in \mathcal{K}_{\frac{1}{2}}$, $\alpha \in I_E$, such that

$$\Pi_E h_\beta = \sum_{\alpha \in I_E} \mu_\alpha h_\alpha \,. \tag{4.12}$$

Let $\beta \notin I_E$, then

$$\Pi_E h_\beta = \sum_{j \in \frac{\mathbb{N}^*}{2}} \varepsilon^j p_j \tag{4.13}$$

for some $p_j \in \mathbb{C}[y]$. Since the Hermite polynomials form a basis in $\mathbb{C}[y]$, the polynomial $p_{\frac{1}{2}}$ expands to

$$p_{\frac{1}{2}} = \sum_{\alpha \in I_E} c_{\alpha} h_{\alpha} + \sum_{\beta' \notin I_E} c_{\beta'} h_{\beta'} \,. \tag{4.14}$$

Applying Π_E on both sides of (4.13) and using $\Pi_E^2 = \Pi_E$, (4.14) and again (4.13) for the second equality, we get

$$\Pi_E h_{\beta} = \varepsilon^{\frac{1}{2}} \sum_{\alpha \in I_E} c_{\alpha} \Pi_E h_{\alpha} + \varepsilon^{\frac{1}{2}} \sum_{\beta' \notin I_E} c_{\beta'} \Pi_E h_{\beta'} + \sum_{\substack{j \ge 1\\j \in \frac{\mathbb{N}^*}{2}}} \varepsilon^j \Pi_E p_j = \varepsilon^{\frac{1}{2}} \sum_{\alpha \in I_E} c_{\alpha} \Pi_E h_{\alpha} + \sum_{\substack{j \ge 1\\j \in \frac{\mathbb{N}^*}{2}}} \varepsilon^j \tilde{p}_j$$

for $\tilde{p}_j \in \mathbb{C}[y]$. Thus by expanding the terms of the next order we gain the order $\varepsilon^{\frac{1}{2}}$ in the remaining term and inductively obtain $\mu_{\alpha} \in \mathcal{K}_{\frac{1}{2}}$ satisfying equation (4.12). The case $\beta \in I_E$ can easily be reduced to this case.

 $\Pi_E G = G \Pi_E$: This follows from the fact that G commutes with R(z) together with the definition (4.9).

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 set $f_j := \prod_E h_{\alpha^j}$, $\alpha^j \in I_E$. Then equation (4.11) and Definition 3.4 for the sesquilinear form in \mathcal{V} imply for some $\gamma_k \in \mathbb{R}$

$$\langle f_i, f_j \rangle_{\mathcal{V}} = \delta_{ij} + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k \gamma_k \in \mathcal{K}_{\frac{1}{2}}, \qquad 1 \le i, j \le m,$$
(4.15)

since the Hermite polynomials are orthogonal and the $g_{\alpha j}$ are normalized in the L^2 -norm. The matrix $F = (F_{ij}) := (\langle f_i, f_j \rangle_{\mathcal{V}})$ is symmetric, because the f_k are real functions. Furthermore the elements of the symmetric matrix $B := F^{-\frac{1}{2}}$ (given by a binomial series) are in $\mathcal{K}_{\frac{1}{2}}$. Then

$$e := (e_1, \dots, e_m) := (f_1, \dots, f_m)B =: fB$$
(4.16)

defines an orthonormal basis $\{e_1, \ldots, e_m\}$ of $\operatorname{Ran} \Pi_E$ (the orthonormalization of $\{f_1, \ldots, f_m\}$). In this basis, the matrix $M = (M_{ij})$ of $G|_{\operatorname{Ran} \Pi_E}$ is given by

$$M = e^t G e = B f^t G f B = B F^G B, \qquad (4.17)$$

where $F_{kl}^G := \langle f_k, Gf_l \rangle_{\mathcal{V}} \in \mathcal{K}_{\frac{1}{2}}$. Thus M is a finite symmetric matrix with entries in $\mathcal{K}_{\frac{1}{2}}$. Using Proposition 3.2 and 4.2 together with (4.7) and (4.15) and the fact, that $h_{\alpha^j}, \alpha^j \in I_E$, are the eigenfunctions of G_0 for the eigenvalue E, we can conclude

$$F_{ij}^G = E\delta_{ij} + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k \mu_k, \quad \text{where} \quad \mu_k \in \mathbb{R}.$$
(4.18)

It is shown in [13], 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 [13] (see also [6]), 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 4.3 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 $E_1, \ldots E_m$ 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 4.3 and the special form of the elements of M defined in (4.17) that this matrix possesses m (not necessarily distinct) eigenvalues in $\mathcal{K}_{\frac{1}{2}}$ of the form

$$E_j(\varepsilon) = E + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk} = \sum_{k \in \frac{\mathbb{N}}{2}} \varepsilon^k E_{jk}, \quad j = 1, \dots m$$
(4.19)

where $E_{j0} = E$ and the corresponding eigenfunctions are

$$\psi_j(\varepsilon) = \sum_{k \in \frac{\mathbb{N}}{2}} \varepsilon^k \psi_{jk}, \quad \text{where} \quad \psi_{jk} \in \mathbb{C}[y] \quad \text{with} \quad \deg \psi_{jk} = \max_{\alpha \in I_E} (|\alpha| + 2k).$$
(4.20)

The statement on the degree of ψ_{jk} follows from (4.11) and the fact that every eigenfunction can be written as linear combination

$$\psi = \sum_{\alpha \in I_E} \lambda_\alpha \Pi_E h_\alpha \tag{4.21}$$

with coefficients λ_{α} without negative powers in $\sqrt{\varepsilon}$.

Using the parity results in Proposition 3.2 and Remark 3.3, we can prove the next proposition about the absence of half integer terms in the expansion (4.19).

PROPOSITION 4.4 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 (4.10). Let M denote the matrix specified in equation (4.17) and $E_j(\varepsilon)$ its eigenvalues given in (4.19). Then $M_{ij} \in \mathcal{K}_1$ and $E_j(\varepsilon) \in \mathcal{K}_1$ for $1 \leq i, j \leq m$.

Proof. By Theorem 4.3 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} . We will change notation during this proof to $f_{\alpha} = \prod_E h_{\alpha}$ and $F_{\alpha\beta}^G$ 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 (4.9) the coefficients in the power series of f_{α} are given by

$$f_{\alpha j} = \frac{1}{2\pi i} \oint_{\Gamma} r_j(z) h_\alpha \, dz \,. \tag{4.22}$$

The $r_j(z)$ are determined by G_{j_ℓ} and $R_0(z)$ via formula (4.4), and since G_{j_ℓ} changes the parity of a polynomial in $\mathbb{C}[y]$ by the factor $(-1)^{2j_\ell}$, $j_\ell \in \frac{\mathbb{N}^*}{2}$ (see Remark 3.3), we can conclude that $r_j(z)$ changes the parity by $(-1)^{2j}$. Using that the parity of h_α is given by $(-1)^{|\alpha|}$, we obtain $(-1)^{|\alpha|+2j}$ as parity of $f_{\alpha j}$. By Definition 3.4 we have

$$\langle f_{\alpha}, f_{\beta} \rangle_{\mathcal{V}} = \sum_{n \in \frac{\mathbb{Z}}{2}} \varepsilon^n \sum_{\substack{j,k,\ell \in \frac{\mathbb{Z}}{2} \\ j+k+\ell=n}} \int_{\mathbb{R}^d} f_{\alpha j}(y) f_{\beta k}(y) \omega_{\ell}(y) e^{-\sum_{\nu=1}^d \lambda_{\nu} y_{\nu}^2} \, dy$$

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 (3.69) the parity of ω_{ℓ} is $(-1)^{2\ell}$, the scalar product therefore vanishes if $(|\alpha|+2j+|\beta|+2k+2\ell)$ is odd. Since by assumption α and β have the same parity, $|\alpha| + |\beta|$ is even. Thus the integral vanishes if $2(j + k + \ell) = 2n$ is 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

$$\langle f_{\alpha}, Gf_{\beta} \rangle_{\mathcal{V}} = \sum_{n \in \frac{\mathbb{Z}}{2}} \varepsilon^n \sum_{\substack{j,k,\ell,r \in \frac{\mathbb{Z}}{2}\\ j+k+\ell+r=n}} \int_{\mathbb{R}^d} f_{\alpha j}(y) G_r f_{\beta k}(y) \omega_{\ell}(y) e^{-\sum_{\nu=1}^d \lambda_{\nu} y_{\nu}^2} \, dy \, .$$

The operator G_r changes the parity by $(-1)^{2r}$ as already mentioned, so as before the integral vanishes if $j + k + \ell + r = n$ is half integer.

We will now return to our original variable $x = \sqrt{\varepsilon}y$. Substituting it in equation (4.20) and rearranging with respect to powers in $\sqrt{\varepsilon}$ yields for $d_{jk} := \deg \psi_{jk}$ and $N := \frac{d_{jk}}{2} - k = \max_{\alpha \in I_E} \frac{|\alpha|}{2}$ to

$$\psi_j(y;\varepsilon) = \sum_{k \in \frac{\mathbb{N}}{2}} \varepsilon^k \psi_{jk} \left(\frac{x}{\sqrt{\varepsilon}}\right) = \sum_{k \in \frac{\mathbb{N}}{2}} \sum_{\substack{\beta \in \mathbb{N}^d \\ 0 \le |\beta| \le d_{jk}}} \varepsilon^{k - \frac{|\beta|}{2}} \rho_{j,k,\beta} x^\beta$$
$$=: \sum_{\substack{\ell \in \frac{\mathbb{N}}{2} \\ \ell \ge -N}} \varepsilon^\ell \widehat{u}_{j\ell}(x) \,,$$

where (with $\ell = k - \frac{|\beta|}{2}$)

$$\widehat{u}_{j\ell}(x) = \sum_{\substack{\beta \in \mathbb{N}^d \\ -2\ell \le |\beta|}} \rho_{j,\ell+\frac{|\beta|}{2},\beta} x^{\beta}$$
(4.23)

and we set

$$\widehat{u}_j(x;\varepsilon) := \sum_{\substack{\ell \in \frac{\mathbb{Z}}{2} \\ \ell \ge -N}} \varepsilon^{\ell} \widehat{u}_{j\ell}(x) \,. \tag{4.24}$$

We denote by \mathcal{A} the set of formal symbols \hat{u}_j given by a power series as in (4.24) with arbitrary N. Then \mathcal{A} is a vector space over $\mathcal{K}_{\frac{1}{2}}$, on which

$$\left. e^{\frac{\tilde{\varphi}(x)}{\varepsilon}} \widehat{H}'_{\varepsilon} e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \right|_{\mathcal{A}} =: H'_{\varepsilon,\mathcal{A}}$$

$$(4.25)$$

acts as an operator with eigenfunctions \hat{u}_j , where \hat{H}_{ε} fulfills Hypothesis 1.1 and $\tilde{\varphi}$ is constructed in Hypothesis 1.5. The following theorem will summarize these results and give a condition on the absence of half integer terms in the expansion.

THEOREM 4.5 Let \hat{H}_{ε} satisfy Hypothesis 1.1, \hat{H}'_{ε} be defined in (1.22), and $\tilde{\varphi}$ be the real function described in Hypothesis 3.1. Let E be an eigenvalue with multiplicity m of the harmonic approximation G_0 of \hat{G}_{ε} given in (3.8).

(a) Then the operator $H'_{\varepsilon,\mathcal{A}}$ defined in (4.25) has an orthonormal system of m eigenfunctions \widehat{u}_j of the form (4.24) in \mathcal{A} , where the lowest order monomial in $\widehat{u}_{j\ell} \in \mathbb{C}[[x]]$ is of degree $\max\{-2\ell, 0\}$.

The associated eigenvalues are

$$\varepsilon E_j(\varepsilon) = \varepsilon \left(E + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk} \right).$$
(4.26)

(b) If $|\alpha|$ is even (resp. odd) for all $\alpha \in I_E$, then all half integer (resp. integer) terms in the expansion (4.24) vanish.

Proof. (a): This point is already shown in the discussion succeeding equation (4.24).

(b): By equation (4.21) and Proposition 4.4 together with Theorem 4.3 we can write any eigenfunction ψ as a linear combination of $\Pi_E h_{\alpha}$ with coefficients in \mathcal{K}_1 , thus we get explicitly

$$\psi\left(\frac{x}{\sqrt{\varepsilon}}\right) = \sum_{\alpha \in I_E} \sum_{\substack{j \in \mathbb{N}_0\\k \in \mathbb{N}_0/2}} \varepsilon^{j+k} \lambda_{\alpha j} f_{\alpha k}\left(\frac{x}{\sqrt{\varepsilon}}\right) \,.$$

As discussed below (4.22), 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 degree $|\alpha|+2k-2\ell$ for $0 \leq 2\ell \leq |\alpha|+2k, \ell \in \mathbb{N}$. If we combine the powers in ε arising in the sum, we get $\varepsilon^{j+\ell-\frac{|\alpha|}{2}}$, 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 \hat{u}_j is just a reordering, this is also true for \hat{u}_j . The assertion for (4.26) follows from Proposition 4.4.

5. Proof of Theorem 1.6

We shall now construct the quasimodes of Theorem 1.6. For \hat{u}_j given by (4.24), we can use the Theorem of Borel with respect to x, to find \mathscr{C}^{∞} -functions $\tilde{\hat{u}}_{jl}$ possessing \hat{u}_{jl} as Taylor series at zero. We define a formal asymptotic series in a neighborhood Ω'_3 of 0 by

$$\tilde{\hat{u}}_j(x;\varepsilon) := \sum_{\substack{l \in \frac{\mathbb{Z}}{2} \\ l \ge -N}} \varepsilon^l \tilde{\hat{u}}_{jl}(x) \, .$$

Then

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}}(\hat{H}'_{\varepsilon} - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}}\tilde{\hat{u}}_j(x,\varepsilon) = b_j(x;\varepsilon) , \qquad (5.1)$$

where $b_j(x;\varepsilon) = \sum_{\substack{l \in \frac{\mathbb{Z}}{2} \\ \ell \geq -N}} \varepsilon^\ell b_{j\ell}(x)$ has the property, that each $b_{j\ell} \in \mathscr{C}^{\infty}(\Omega'_3)$ vanishes to infinite order at x = 0. It remains to show that it is possible to modify the functions $\tilde{u}_{j\ell}$ by uniquely determined functions $c_{j\ell}$ vanishing at zero to infinite order such that for the resulting functions $\tilde{u}_{j\ell} := \tilde{u}_{j\ell} - c_{j\ell}$, the formal series

$$\tilde{u}_j(x;\varepsilon) := \sum_{\substack{\ell \ge -N\\\ell \in \mathbb{Z}/2}} \varepsilon^\ell \tilde{u}_{j\ell}(x)$$
(5.2)

solves for $x \in \Omega'_3$ the equation

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}}(\hat{H}'_{\varepsilon} - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}}\tilde{u}_j(x,\varepsilon) = 0.$$
(5.3)

To this end, we have to show that the equation

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}}(\hat{H}'_{\varepsilon} - \varepsilon E_j(\varepsilon))e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}}c_j(x,\varepsilon) = b_j(x;\varepsilon) .$$
(5.4)

has a unique formal power solution $c_j(x;\varepsilon) \sim \sum_{\ell \geq -N} \varepsilon^\ell c_{j\ell}(x)$ with coefficients $c_{j\ell} \in \mathscr{C}^{\infty}(\Omega'_3)$ vanishing to infinite order at x = 0. By the definition of $\widehat{T}'_{\varepsilon}$ and $\widehat{V}'_{\varepsilon}$ in (1.24) and (1.23) and the assumptions in Hypothesis 1.1, we have (setting $E = E_{j0}$)

$$e^{\frac{\tilde{\varphi}(x)}{\varepsilon}} \left[\widehat{T}_{\varepsilon}' + \widehat{V}_{\varepsilon}' - \varepsilon \left(E + \sum_{k \in \mathbb{N}^*/2} \varepsilon^k E_{jk} \right) \right] e^{-\frac{\tilde{\varphi}(x)}{\varepsilon}} \sum_{\substack{\ell \ge -N \\ \ell \in \mathbb{Z}/2}} \varepsilon^\ell c_j(x)$$

$$= \sum_{\substack{\ell \ge -N \\ \ell \in \mathbb{Z}/2}} \varepsilon^\ell \left\{ \sum_{\gamma \in (\varepsilon \mathbb{Z})^d} \left[\sum_{k \in \mathbb{N}} \varepsilon^k a_{\gamma}'^{(k)}(x;\varepsilon) e^{\frac{1}{\varepsilon} (\tilde{\varphi}(x) - \tilde{\varphi}(x+\gamma))} c_j(x+\gamma;\varepsilon) \right] + \sum_{k \in \mathbb{N}/2} \varepsilon^k \left(V_k'(x) - \varepsilon E_{jk} \right) c_j(x;\varepsilon) \right\}.$$

To get the different orders in ε of the kinetic term, we expand a'_{γ} , $\tilde{\varphi}$ and $c_{j\ell}$ at x and set $\eta := \frac{\gamma}{\varepsilon} \in \mathbb{Z}^d$. Taylor expansion gives

$$\frac{1}{\varepsilon}\left(\tilde{\varphi}(x) - \tilde{\varphi}(x + \varepsilon\eta)\right) = -\nabla\tilde{\varphi}(x) \cdot \eta - \frac{\varepsilon}{2}D^2\tilde{\varphi}|_x[\eta]^2 - \frac{\varepsilon^2}{2}\int_0^1 (1 - t)^2 D^3\tilde{\varphi}|_{x + t\varepsilon\eta}[\eta]^3 dt$$
(5.5)

and

$$c_{j\ell}(x+\varepsilon\eta) = c_{j\ell}(x) + \varepsilon\eta \cdot \nabla c_{j\ell}(x) + \varepsilon^2 \int_0^1 (1-t)D^2 c_{j\ell}|_{x+t\varepsilon\eta}[\eta]^2 dt .$$
(5.6)

Combining (5.5) with the expansion of the exponential function at zero gives

$$e^{\frac{1}{\varepsilon}(\tilde{\varphi}(x)-\tilde{\varphi}(x+\gamma))} = e^{-\nabla\tilde{\varphi}(x)\cdot\eta} \left(1 - \frac{\varepsilon}{2}D^{2}\tilde{\varphi}|_{x}[\eta]^{2} + \frac{\varepsilon^{2}}{4}\left(D^{2}\tilde{\varphi}|_{x}[\eta]^{2}\right)^{2} + O\left(\varepsilon^{4}\right)\right) \times \\ \times \left(1 - \frac{\varepsilon^{2}}{2}\int_{0}^{1}(1-t)^{2}D^{3}\tilde{\varphi}|_{x+t\varepsilon\eta}[\eta]^{3}dt + O\left(\varepsilon^{4}\right)\right)\left(1 + O\left(\varepsilon^{3}\right)\right) .$$
(5.7)

The lowest order equation in (5.4) is that of order -N. By the eikonal equation (1.31), the left hand side of it vanishes and the same argument applies for the $-N + \frac{1}{2}$ order equation of (5.4). The

first non-vanishing term arises from the action of the first order part of the conjugated operator on $c_{j,-N}(x)$, which is given by

$$\left\{\sum_{\gamma \in (\varepsilon\mathbb{Z})^d} e^{-\frac{1}{\varepsilon}\nabla\tilde{\varphi}(x)\cdot\gamma} \left[a_{\gamma}^{\prime(0)}(x) \left(\frac{1}{\varepsilon}\gamma \cdot \nabla - \frac{1}{2\varepsilon}\langle\gamma, D^2\tilde{\varphi}|_x\gamma\rangle \right) + a_{\gamma}^{\prime(1)}(x) \right] + V_1(x) - E \right\} c_{j,-N}(x) = b_{j,-N+1}. \quad (5.8)$$

This equation takes the form

$$\left(\mathcal{P}(x,\partial_x) + f(x)\right)u(x) = v(x) \tag{5.9}$$

for the differential operator

$$\mathcal{P}(x,\partial_x) := \sum_{\eta \in \mathbb{Z}^d} \tilde{a}'_{\eta}(x) e^{-\nabla \tilde{\varphi}(x) \cdot \eta} \eta \cdot \nabla , \qquad (5.10)$$

which is well defined by the exponential decay of \tilde{a}'_{η} (see Hypothesis 1.1(a)(iv) and (1.14)) and by (3.25). The next and all higher order equations in (5.4) result from the action of the first order part of the conjugated operator given in (5.8) on the respective highest order part of c_j , which for the k-th order is the term $c_{j,k-1}$. 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 c_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 (5.9). Thus all transport equation take the form (5.9) with $f, v \in \mathscr{C}^{\infty}(\Omega'_3)$ and v vanishing to infinite order at x = 0 by the construction of the formal series (4.24). The differential operator \mathcal{P} defined in (5.10) is of the form $\langle Z, \nabla \rangle$ for the vector field $Z(x) = (z_1(x), \ldots, z_d(x))$ given by

$$z_{\nu}(x) = \sum_{\eta \in \mathbb{Z}^d} \tilde{a}'_{\eta}(x) e^{-\nabla \tilde{\varphi}(x) \cdot \eta} \eta_{\nu} \quad .$$
(5.11)

Since $a_{\gamma}^{'(0)}(x) = a_{-\gamma}^{'(0)}(x)$ (Remark 1.2(d)) we have

$$\sum_{\eta \in \mathbb{Z}^d} \tilde{a}'_{\eta}(x)\eta_{\nu} = 0 \quad \text{for all} \quad \nu = 1, \dots, d , \qquad (5.12)$$

thus by (5.11) x = 0 is a singular point of the vector field Z. In order to linearize at zero, we compute

$$\partial_{x_{\mu}}|_{0}z_{\nu} = \sum_{\eta \in \mathbb{Z}^{d}} \left[(\partial_{x_{\mu}}|_{0}\tilde{a}_{\eta}')e^{-\nabla\tilde{\varphi}(0)\cdot\eta}\eta_{\nu} - \tilde{a}_{\eta}'(0)e^{-\nabla\tilde{\varphi}(0)\cdot\eta}\partial_{x_{\mu}}|_{0}(\langle\nabla\tilde{\varphi}\,,\,\eta\rangle)\eta_{\nu} \right]$$
$$= \partial_{x_{\mu}}|_{0}\sum_{\eta \in \mathbb{Z}^{d}}\tilde{a}_{\eta}'\eta_{\nu} - \sum_{\eta \in \mathbb{Z}^{d}}\tilde{a}_{\eta}'(0)\lambda_{\mu}\eta_{\mu}\eta\nu\,, \qquad (5.13)$$

where for the second equation we used that for $x \in \Omega$ the phase function $\tilde{\varphi}$ is given by (1.32) and thus $\nabla \tilde{\varphi}(0) = 0$ and $\partial_{x_{\mu}}|_0 \langle \nabla \tilde{\varphi}, \eta \rangle = \lambda_{\mu} \eta_{\mu}$. By (5.12) the first term on the right hand side of (5.13) vanishes and therefore

$$\partial_{x_{\mu}}|_{0}z_{\nu} = -\sum_{\eta \in \mathbb{Z}^{d}} \tilde{a}_{\eta}'(0)\lambda_{\mu}\eta_{\mu}\eta_{\nu}$$

By (1.12) and (1.26) we get

$$-\sum_{\eta\in\mathbb{Z}^d}\tilde{a}'_{\eta}(0)\eta_{\mu}\eta_{\nu}\lambda_{\mu} = \begin{cases} 2\lambda_{\mu} > 0 & \text{for } \nu = \mu\\ 0 & \text{for } \nu \neq \mu \end{cases}$$

Therefore the linearization of Z at 0 is $Z_0 := (z_{10}, \ldots, z_{d0})$ with $z_{\nu 0}(x) = 2\lambda_{\nu}x_{\nu}$ and the corresponding differential operator is given by

$$\mathcal{P}_0(x,\partial_x) = \sum_{\nu=1}^d 2\lambda_\nu x_\nu \partial_{x_\nu}$$

with $\lambda_{\nu} > 0$ for $\nu = 1, \ldots, d$. By Dimassi-Sjöstrand [5] (Proposition 3.5), the differential equation (5.9) has a unique \mathscr{C}^{∞} -solution in a sufficiently small star-shaped neighborhood Ω'_{3} , vanishing to infinite order at x = 0. This gives the required solution of (5.4), and thus defines \tilde{u}_{j} in (5.2) solving (5.3) in Ω'_{3} .

Again by a Borel procedure, but now with respect to ε , we can find a function $u'_j \in \mathscr{C}^{\infty}(\Omega'_3 \times [0, \varepsilon_0))$ representing the asymptotic sum $\tilde{u}_i(x; \varepsilon)$ given in (5.2), which we denote by

$$u_j'(x;\varepsilon) \sim \sum_{\substack{l \in \frac{\pi}{2} \\ l \ge -N}} \varepsilon^l \tilde{u}_{jl}(x) .$$
(5.14)

In order to get a function, which is defined on $\mathbb{R}^d \times [0, \varepsilon_0)$, we multiply with a cut-off function $k \in \mathscr{C}_0^{\infty}(\mathbb{R}^d)$, with supp $k \subset \Omega'_3$ and such that for some Ω_3 with $\overline{\Omega_3} \subset \Omega'_K 3$ we have k(x) = 1 for $x \in \Omega_3$. We denote the resulting function $u_j \in \mathscr{C}_0^{\infty}(\mathbb{R}^d \times [0, \varepsilon_0))$ by

$$u_j(x;\varepsilon) := k(x)u'_j(x;\varepsilon) \sim k(x) \sum_{\substack{\ell \in \frac{\mathbb{Z}}{2} \\ \ell \ge -N}} \varepsilon^\ell \tilde{u}_{j\ell}(x) =: \sum_{\substack{\ell \in \frac{\mathbb{Z}}{2} \\ \ell \ge -N}} \varepsilon^\ell u_{j\ell}(x) ,$$

where $u_{j\ell} := k \tilde{u}_{j\ell}$. Analogously we define a real function $E_j(\varepsilon)$ as an asymptotic sum

$$E_j(\varepsilon) \sim E + \sum_{k \in \frac{\mathbb{N}^*}{2}} \varepsilon^k E_{jk}$$

We have therefore proven (a), the main part of the Theorem 1.6.

The approximate orthonormality (1.37) follows from the orhonormality of the expansion \hat{u}_j given in (4.24) proven in Theorem 4.5, combined with a standard estimate of Laplace type $(\int e^{-\frac{x^2}{\varepsilon}} O(x^{\infty}) dx = O(x^{\infty}))$. The estimate (1.39) for the restricted approximate eigenfunctions follows from (1.37) together with Lemma 3.4 in [15].

The statement on the absence of half-integer terms in (1.35) follows from Proposition 4.4, the statement on the absence of half integer or integer terms respectively in (1.34) is a direct consequence of Theorem 4.5.

To make the step from $\widehat{H}'_{\varepsilon}$ acting on $\mathscr{C}_{0}^{\infty}(\mathbb{R}^{d})$ to the operator H_{ε} acting on lattice functions $\mathcal{K}((\varepsilon\mathbb{Z})^{d})$, we use that $\mathscr{G}_{x_{0}}$ is invariant under the action of $\widehat{H}_{\varepsilon}$ as discussed above (1.17). Thus the restriction to the lattice commutes with $\widehat{H}_{\varepsilon}$ and applying the restriction operator $r_{\mathscr{G}_{x_{0}}}$ to (1.36) yields (1.38).

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MARKUS KLEIN AND ELKE ROSENBERGER

UNIVERSITÄT POTSDAM, INSTITUT FÜR MATHEMATIK, AM NEUEN PALAIS 10, 14469 POTSDAM E-mail address: mklein@math.uni-potsdam.de, erosen@uni-potsdam.de