Eigenvalues and Eigenfunctions of Schrödinger Operators: Inverse Spectral Theory; and the Zeros of Eigenfunctions

by

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A dissertation submitted to The Johns Hopkins University in conformity with the requirements for the degree of Doctor of Philosophy

Baltimore, Maryland

March, 2009

Updated 2-12-09

Abstract

This dissertation contains two disjoint parts:

Part I: In the first part (which is from [H1]) we find some explicit formulas for the semi-classical wave invariants at the bottom of the well of a Schrödinger operator. As an application of these new formulas for the wave invariants, we prove similar inverse spectral results, obtained by Guillemin and Uribe in [GU], using fewer symmetry assumptions. We also show that in dimension 1, no symmetry assumption is needed to recover the Taylor coefficients of $V(x)$.

Part II: In the second part (which is from [H2]) we study the semi-classical distribution of the complex zeros of the eigenfunctions of the 1D Schrödinger operators for the class of real polynomial potentials of even degree, with fixed energy level, E. We show that as $h_n \to 0$ the zeros tend to concentrate on the union of some level curves $\Re(S(z_m, z)) = c_m$ where $S(z_m, z) = \int_{z_m}^{z} \sqrt{V(t) - E}\, dt$ is the complex action, and z_m is a turning point. We also calculate these curves for some symmetric and non-symmetric one-well and double-well potentials. The example of the non-symmetric double-well potential shows that we can obtain different pictures of complex zeros for different subsequences of h_n.

Readers: Professors Steve Zelditch (Advisor), John Toth, Bernard Shiffman, Chris Sogge, Joel Spruck, Hans Christianson and Petar Maksimovic .

Acknowledgments

First and foremost, I would like to thank my advisor Steve Zelditch for his generous support and encouragement and also for his patient guidance during my five years at Johns Hopkins. I especially appreciate that he consistently shared his ideas with me.

I also want to thank many faculty members at Johns Hopkins, especially Bernard Shiffman, Richard Wentworth, Bill Minicozzi, Chris Sogge and Joel Spruck for many helpful discussions and for instructing many interesting courses.

I also extend my gratitude to Christine for her great love and support. Also I thank my friends in Baltimore, especially Sid, Mike, Reza, Arash, Vahid, Alireza Asadpoure, Mazdak, Ramin, Rafik, Peter, Mimi, Ananda, Darius, Behzad, Marcin and Yanir for their friendship and support. Finally I thank my friends in Iran, specially Arash Alavian, Mahmood, Morteza, Nima, Milad, Hamid Ranjbar, Amir Mohammadi, Keyvan, Behrooz, Jalil, Arash Yousefi, Ali Jelvehdar, Hamed and my brothers Saeed, Vahid and Navid for being good and loyal friends.

Dedication: I dedicate this work to my Mother, Fakhri, for her never ending love and to my Father, Mohammadali for his support and care. Their unwavering love made me the person I am.

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Part I

Inverse Spectral Problems for Schrödinger Operators

Chapter 1

Introduction

1.1 Motivation and Background

In this part of the dissertation we study some inverse spectral problems of the eigenvalue problem for the semi-classical Schrödinger operator,

$$\hat{P} = -\frac{\hbar^2}{2}\triangle + V(x) \qquad \text{on} \quad L^2(\mathbb{R}^n), \tag{1.1}$$

associated to the Hamiltonian

$$P(x,\xi) = \frac{1}{2}\,\xi^2 + V(x).$$

Here the potential $V(x)$ in (1.1) satisfies

(1.2)
$$\begin{cases} V(x) \in C^\infty(\mathbb{R}^n), \\ V(x) \text{ has a unique non-degenerate global minimum at } x = 0 \text{ and } V(0) = 0, \\ \text{For some } \varepsilon > 0,\ V^{-1}[0,\varepsilon] \text{ is compact.} \end{cases}$$

Under these conditions for sufficiently small $\hbar$, say $\hbar \in (0, h_0)$, and sufficiently small δ, a classical fact tells us the spectrum of $\hat{P}$ in the energy interval $[0, \delta]$ is finite. We denote these eigenvalues by

$$\{E_j(\hbar)\}_{j=0}^m.$$

We call these eigenvalues the low-lying eigenvalues of $\hat{P}$. We notice the Weyl's law reads

$$(1.3)\qquad m = N_\hbar(\delta) = \sharp\{j; 0 \le E_j(\hbar) \le \delta\} = \frac{1}{(2\pi\hbar)^n}\Big(\int_{\frac{1}{2}\xi^2+V(x)\le\delta} dx d\xi + o(1)\Big).$$

Recently in [GU], Guillemin and Uribe raised the question whether we can recover the Taylor coefficients of V at $x = 0$ from the low-lying eigenvalues $E_j(\hbar)$. They also established that if we assume some symmetry conditions on V, namely $V(x) = f(x_1^2, ..., x_n^2)$, then the 1-parameter family of low-lying eigenvalues, $\{E_j(\hbar) \,|\, \hbar \in (0, h_0)\}$, determines the Taylor coefficients of V at $x = 0$.

In this thesis we will attempt to recover as much of V as possible from the family $E_j(\hbar)$, by establishing some new formulas for the wave invariants at the bottom of the potential (Theorem 1.2.1). Using these new expressions for the wave invariants, in Theorem 1.2.2 we improve the inverse spectral results of [GU] for a larger class of potentials.

A classical approach in studying this problem is to examine the asymptotic behavior as $\hbar \to 0$ of the truncated trace

$$(1.4)\qquad Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}),$$

where $\Theta \in C_0^\infty([0,\infty))$ is supported in $I = [0, \delta]$ and equals one in a neighborhood of 0.

The asymptotic behavior of the truncated trace around the equilibrium point $(x, \xi) = (0, 0)$ has been extensively studied in the literature. It is known that (see for example [BPU]) for t in a sufficiently small interval $(0, t_0)$, $Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}})$ has an asymptotic expansion of the following form:

$$Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}) \sim \sum_{j=0}^{\infty} a_j(t)\hbar^j, \qquad \hbar \to 0. \tag{1.5}$$

Throughout this dissertation when we refer to wave invariants at the bottom of the well, we mean the coefficients $a_j(t)$ in (1.5).

By applying an orthogonal change of variable, we can assume that V is of the form

$$V(x) = \frac{1}{2}\sum_{k=1}^{n} \omega_k^2 x_k^2 + W(x), \qquad \omega_k > 0, \tag{1.6}$$
$$W(x) = O(|x|^3), \qquad |x| \to 0.$$

In addition to conditions in (1.2), we also assume that $\{\omega_k\}$ are linearly independent over $\mathbb{Q}$. We note that we have $W(0) = 0$, $\nabla W(0) = 0$ and $\mathrm{Hess}W(0) = 0$.

1.2 Statement of Results

1.2.1 Explicit formulas for the wave invariants

Our first result finds explicit formulas for the wave invariants.

THEOREM **1.2.1.** *There exists t_0 such that for $0 < t < t_0$,*

1.

$$a_0(t) = Tr(e^{\frac{-it}{\hbar}\hat{H}_0}) = \prod_{k=1}^{n} \frac{1}{2i\sin\frac{\omega_k t}{2}}, \qquad \textit{where} \qquad \hat{H}_0 = -\frac{1}{2}\hbar^2\Delta + \frac{1}{2}\sum_{k=1}^{n}\omega_k^2 x_k^2.$$

2. For $j \geq 1$, the wave invariants $a_j(t)$ defined in (1.5) are given by

$$a_j(t) = a_0(t) \sum_{l=1}^{2j} i^{l(n-1)+\frac{n}{2}} e^{i\frac{\pi}{4} sgn H_l} \int_0^t \int_0^{s_1} ... \int_0^{s_{l-1}} P_{l+j} b_l(0) ds_l ... ds_1, \tag{1.7}$$

where for every m,

$$P_m b_l(0) = \frac{i^{-m}}{2^m\, m!} < H_l^{-1} \nabla, \nabla >^m (b_l)(0),$$

$$b_l = \prod_{i=1}^{l} W(\frac{\cos \omega_k s_i}{2}(z_{i+1}^k + z_i^k) - \frac{\sin \omega_k s_i}{\omega_k} \xi_i^k + (\frac{\sin \omega_k (t - s_i) + \sin \omega_k s_i}{\sin \omega_k t}) x^k),$$

and H_l^{-1} is the inverse matrix of the Hessian H_l =Hess $\Psi_l(0)$, where

$$\Psi_l = \Psi_l(t, x, z_1, ..., z_l, \xi_1, ..., \xi_l) = \sum_{k=1}^{n} \{(-\omega_k \tan \frac{\omega_k}{2} t) x_k^2 + (\frac{\omega_k}{2} \cot \omega_k t)(z_1^k)^2 + \sum_{i=1}^{l} (z_{i+1}^k - z_i^k) \xi_i^k\}.$$

The Hessian of Ψ_l is calculated with respect to every variable except t. Therefore the entries of the matrix H_l^{-1} are functions of t. The matrix H_l^{-1} is shown in (3.10).

3. The wave invariant $a_j(t)$ is a polynomial of degree $2j$ of the Taylor coefficients of V. The Taylor coefficients of highest order appearing in $a_j(t)$ are of order $2j+2$. In fact these highest order Taylor coefficients appear in the linear term of the polynomial and

$$a_j(t) = \frac{a_0(t)}{(2i)^{j+1}} \sum_{|\vec{\alpha}|=j+1} \frac{t}{\vec{\alpha}!} (\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega}}{2} t)^{\vec{\alpha}} D_{2\vec{\alpha}}^{2j+2} V(0) \tag{1.8}$$

$$+\{\textit{a polynomial of Taylor coefficients of order} \leq 2j+1\}$$

Notice that in (1.8), we have used the standard shorthand notations for multi-indices, i.e. $\vec{\alpha} = (\alpha_1, ...\alpha_n)$, $\vec{\omega} = (\omega_1, ...\omega_n)$, $|\vec{\alpha}| = \alpha_1 + ... + \alpha_n$, $\vec{\alpha}! = \alpha_1!...\alpha_n!$, $\vec{X}^{\vec{\alpha}} = X_1^{\alpha_1}...X_n^{\alpha_n}$, and $D_{\vec{\alpha}}^m = \frac{\partial^m}{\partial x_1^{\alpha_1}...\partial x_n^{\alpha_n}}$ with $m = |\vec{\alpha}|$.

1.2.2 Inverse spectral result

Our second result improves the result of Guillemin and Uribe in [GU]. This theorem is actually a non-trivial corollary of Theorem 1.2.1.

Theorem **1.2.2.** *Let V satisfy* (1.2), (1.6), *and be of the form*

$$V(x) = f(x_1^2, ..., x_n^2) + x_n^3 g(x_1^2, ..., x_n^2), \tag{1.9}$$

for some $f, g \in C^\infty(\mathbb{R}^n)$. Then the low-lying eigenvalues of $\hat{P} = -\frac{1}{2}\hbar^2\Delta + V$ determine $D_{\vec{\alpha}}^{|\vec{\alpha}|}V(0)$, $|\vec{\alpha}| = 2, 3$, and if $D_{3\vec{e}_n}^3 V(0) := \frac{\partial^3 V}{\partial x_n^3}(0) \neq 0$, they determine all the Taylor coefficients of V at $x = 0$.

One quick consequence of Theorem 1.2.2 is the following:

Corollary **1.2.3.** *If $n = 1$, and $V \in C^\infty(\mathbb{R})$ satisfies* (1.2), *then (with no symmetry assumptions) the low-lying eigenvalues determine $V''(0)$ and $V^{(3)}(0)$, and if $V^{(3)}(0) \neq 0$, then these eigenvalues determine all the Taylor coefficients of V at $x = 0$.*

1.2.3 Results of Guillemin and Colin de Verdière

Recently, Guillemin and Colin de Verdière in [CG1] (see also [C]) studied inverse spectral problems of 1 dimensional semi-classical Schrödinger operators. One of the main results in [CG1] is our above Corollary 1.2.3 .

1.3 Outline of proofs

Let us briefly sketch our main ideas for the proofs. First, because of a technical reason which arises in the proofs, we will need to replace the Hamiltonian P by the following Hamiltonian H

$$\begin{cases} H(x,\xi) = \frac{1}{2}\xi^2 + V_\hbar(x), \\ \\ V_\hbar(x) = \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2 + W_\hbar(x), \\ \\ W_\hbar(x) = \chi(\frac{x}{\hbar^{\frac{1}{2}-\varepsilon}})W(x), \qquad \varepsilon > 0 \text{ sufficiently small,} \end{cases}$$

where the cut off $\chi \in C_0^\infty(\mathbb{R}^n)$ is supported in the unit ball $B_1(0)$ and equals one in $B_{\frac{1}{2}}(0)$.

Then in two lemmas (Lemma 2.1.1 and Lemma 2.1.2) we show that for t in a sufficiently small interval $(0, t_0)$, in the sense of tempered distributions we have

$$Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}) = Tr(e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty).$$

This reduces the problem to studying the asymptotic of $Tr(e^{\frac{-it}{\hbar}\hat{H}})$. For this we use the construction of the kernel $k(t,x,y)$ of the propagator $U(t) = e^{\frac{-it}{\hbar}\hat{H}}$ found in [Z]. We find that

$$k(t,x,y) = C(t)e^{\frac{i}{\hbar}S(t,x,y)}\sum_{l=0}^{\infty} a_l(t,\hbar,x,y), \tag{1.10}$$

where

$$S(t,x,y) = \sum_{k=1}^n \frac{\omega_k}{\sin\omega_k t}(\frac{1}{2}(\cos\omega_k t)(x_k^2+y_k^2) - x_k y_k), \tag{1.11}$$

$a_0 = 1$, and for $l \geq 1$,

$$a_l(t,\hbar,x,y) = (\frac{-1}{2\pi})^{ln}(\frac{1}{i\hbar})^{l(n+1)}\int_0^t \dots \int_0^{s_{l-1}} \overbrace{\int \dots \int}^{2l} e^{\frac{i}{\hbar}\Phi_l} b_l(s,x,y,\vec{z},\vec{\xi})d^l z d^l \xi d^l s,$$

where

$$\Phi_l = \sum_{k=1}^n \{\frac{\omega_k}{2}\cot\omega_k t(z_1^k)^2 + \sum_{i=1}^l (z_{i+1}^k - z_i^k)\xi_i^k\},$$

and

$$b_l = \prod_{i=1}^{l} W_\hbar\left(\frac{\cos\omega_k s_i}{2}(z_{i+1}^k + z_i^k) - \frac{\sin\omega_k s_i}{\omega_k}\xi_i^k + \frac{\sin\omega_k(t-s_i)}{\sin\omega_k t}y^k + \frac{\sin\omega_k s_i}{\sin\omega_k t}x^k\right).$$

Next we apply the expression in (1.10) for $k(t,x,y)$ to the formula $Tr(e^{\frac{-it}{\hbar}\hat{H}}) = \int k(t,x,x)dx$. Then we obtain an infinite series of oscillatory integrals, each one corresponding to one a_l. Finally we apply the method of stationary phase to each oscillatory integral and we show that the resulting series is a valid asymptotic expansion. From the resulting asymptotic expansion we obtain the formulas (1.7).

1.4 Some remarks and comparison of approaches

Now let us compare our approach for the construction of $k(t,x,y)$ with the classical approach. In the classical approach (see for instance [DSj],[D], [R], [BPU] and [U]), one constructs a WKB approximation for the kernel $k_P(t,x,y)$ of the operator $\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}$, i.e.

$$k_P(t,x,y) = \int e^{\frac{i}{\hbar}(\varphi_P(t,x,\eta)-y.\eta)} b_P(t,x,y,\eta,\hbar)d\eta, \tag{1.12}$$

where $\varphi_P(t,x,\eta)$ satisfies the Hamilton-Jacobi equation (or eikonal equation in geometrical optics)

$$\partial_t\varphi_P(t,x,\eta) + P(x,\partial_x\varphi_P(t,x,\eta)) = 0, \qquad \varphi_P|_{t=0} = x.\eta,$$

and the function b_P has an asymptotic expansion of the form

$$b_P(t,x,y,\eta,\hbar) \sim \sum_{j=0}^{\infty} b_{P,j}(t,x,y,\eta)\hbar^j.$$

The functions $b_{P,j}(t,x,y,\eta)$ are calculated from the so called transport equations. See for example [R], [DSj], [EZ] or Appendix A of the paper in hand for the details of the above construction.

In this setting, when one integrates the kernel $k_P(t,x,y)$ on the diagonal and applies the stationary phase to the given oscillatory integral, one obtains very complicated expressions for the wave invariants. Of course the classical calculations above show the existence of asymptotic formulas of the form (1.5) (which can be used to get Weyl-type estimates for the counting functions of the eigenvalues, see for example [BPU]). Unfortunately these formulas for the wave invariants are not helpful when trying to establish some inverse spectral results.

Hence, one should look for more efficient methods to calculate the wave invariants $a_j(t)$. One approach is to use the semi-classical Birkhoff normal forms, which was used in the papers [Sj] and [ISjZ] and [GU]. The Birkhoff normal forms methods were also used by S. Zelditch in [Z4] to obtain positive inverse spectral results for real analytic domains with symmetries of an ellipse. Zelditch proved that for a real analytic plane domain with symmetries of an ellipse, the wave invariants at a bouncing ball orbit, which is preserved by the symmetries, determine the real analytic domain under isometries of the domain.

Recently in [Z3], Zelditch improved his earlier result to the real analytic domains with only one mirror symmetry. His approach for this new result was different. He used a direct approach (Balian-Bloch trace formula) which involves Feynman-diagrammatic calculations of the stationary phase method to obtain a more explicit formula for the wave invariants at the bouncing ball orbit.

Motivated by the work of Zelditch [Z3] mentioned above, our approach is also somehow direct and involves combinatorial calculations of the stationary phase.

Our formula in (1.10) for the kernel of the propagator, $U(t) = e^{\frac{-it}{\hbar}\hat{H}}$, is different from the WKB-expression in the sense that we only keep the quadratic part of the phase function, namely the phase function $S(t, x, y)$ in (1.11) of the propagator of Anisotropic oscillator , and we put the rest in the amplitude $\sum_{l=0}^{\infty} a_l(t, \hbar, x, y)$ in (1.10). The details of this construction are mentioned in Prop 2.2.1.

Chapter 2

Semi-classical Parametrix for the Schrödinegr Propagator

2.1 Two reductions

Because of some technical issues arising in the proof of Theorem 1.2.1, we will need to use the following tow lemmas as reductions.

In the following, we let $\chi \in C_0^\infty(\mathbb{R}^n)$ be a cut off which is supported in the unit ball $B_1(0)$ and equals one in $B_{\frac{1}{2}}(0)$.

Lemma **2.1.1.** *Let the Hamiltonians P and H be defined by*

$$\begin{cases} P(x,\xi) = \frac{1}{2}\xi^2 + V(x) \\ \\ V(x) = \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2 + W(x) \\ \\ W(x) = O(|x|^3), \quad \text{as } x \to 0 \end{cases}, \qquad \begin{cases} H(x,\xi) = \frac{1}{2}\xi^2 + V_\hbar(x), \\ \\ V_\hbar(x) = \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2 + W_\hbar(x), \\ \\ W_\hbar(x) = \chi(\frac{x}{\hbar^{\frac{1}{2}-\varepsilon}})W(x), \qquad \varepsilon > 0 \;\; \textit{sufficiently small}, \end{cases} \tag{2.1}$$

and let $\hat{P}$ and $\hat{H}$ be the corresponding Weyl (or standard) quantizations. Then for t in a sufficiently small interval $(0, t_0)$

$$Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}) = Tr(\Theta(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty).$$

In other words, the wave invariants $a_j(t)$ will not change if we replace P by H.

Proof. Proof is given in Appendix A. □

Next we use the following lemma to get rid of $\Theta(\hat{H})$.

LEMMA **2.1.2.** *Let H be defined by (2.1). Then in the sense of tempered distributions*

$$Tr(\Theta(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) = Tr(e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty).$$

This means that if we sort the spectrum of $\hat{H}$ as

$$E_1(\hbar) < E_2(\hbar) \leq ... \leq E_j(\hbar) \to +\infty,$$

then for every Schwartz function $\varphi(t) \in S(\mathbb{R})$

$$< Tr(e^{\frac{-it}{\hbar}\hat{H}}) - Tr(\Theta(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}),\, \varphi(t) >= \sum_{j=1}^{\infty}(1 - \Theta(E_j(\hbar)))\hat{\varphi}(\frac{E_j(\hbar)}{\hbar}) = O(\hbar^\infty).$$

Proof. Proof is given in Appendix B. □

Because of the above lemmas, it is enough to study the asymptotic of $Tr(e^{\frac{-it}{\hbar}\hat{H}})$.

2.2 Construction of $k(t,x,y)$, the kernel of $U(t) = e^{\frac{-it}{\hbar}\hat{H}}$

In this section we follow the construction in [Z] to obtain an oscillatory integral representation of $k(t,x,y)$, the kernel of the propagator $e^{\frac{-it}{\hbar}\hat{H}}$. The reader should consult

[Z] for many details. In that article Zelditch uses the Dyson's Expansion of propagator to study the singularities of the kernel $k(t,x,y)$. But he does not consider the semi-classical setting $\hbar \to 0$ in his calculations (i.e. in his calculations $\hbar = 1$). So we follow the same calculations but also consider $\hbar$ carefully.

The following important proposition gives a new semi-classical approximation to the propagator $U(t)$ near the bottom of the well.

PROPOSITION **2.2.1.** *Let $k(t,x,y)$ be the Schwartz kernel of the propagator $U(t) = e^{\frac{-it}{\hbar}\hat{H}}$. Then*

(A) We have

$$k(t,x,y) = \Big(\prod_{k=1}^{n} \frac{\omega_k}{2\pi i\hbar \sin\omega_k t}\Big)^{\frac{1}{2}} e^{\frac{i}{\hbar}S(t,x,y)} \sum_{l=0}^{\infty} a_l(t,\hbar,x,y), \tag{2.2}$$

where

$$S(t,x,y) = \sum_{k=1}^{n} \frac{\omega_k}{\sin\omega_k t}\Big(\frac{1}{2}(\cos\omega_k t)(x_k^2 + y_k^2) - x_k y_k\Big).$$

Also $a_0 = 1$ and for $l \geq 1$,

(2.3)

$$a_l(t,\hbar,x,y) = \Big(\frac{-1}{2\pi}\Big)^{ln}\Big(\frac{1}{i\hbar}\Big)^{l(n+1)} \int_0^t \dots \int_0^{s_{l-1}} \overbrace{\int \dots \int}^{2l} e^{\frac{i}{\hbar}\Phi_l} b_l(s,x,y,\vec{z},\vec{\xi})\, d^l z\, d^l \xi\, d^l s,$$

where

$$\Phi_l = \sum_{k=1}^{n}\Big\{\frac{\omega_k}{2}\cot\omega_k t (z_1^k)^2 + \sum_{i=1}^{l}(z_{i+1}^k - z_i^k)\xi_i^k\Big\}, \tag{2.4}$$

and

(2.5)

$$b_l = \prod_{i=1}^{l} W_\hbar\Big(\frac{\cos\omega_k s_i}{2}(z_{i+1}^k + z_i^k) - \frac{\sin\omega_k s_i}{\omega_k}\xi_i^k + \frac{\sin\omega_k(t-s_i)}{\sin\omega_k t}y^k + \frac{\sin\omega_k s_i}{\sin\omega_k t}x^k\Big). \qquad (z_{l+1} := 0)$$

(B) For every $\vec{\alpha}$, $\vec{\beta}$, there exists $k_0 = k_0(\alpha, \beta)$ such that for every $0 < \hbar \leq h_0 \leq 1$

$$|\partial_x^{\vec{\alpha}} \partial_y^{\vec{\beta}} a_l(t, \hbar, x, y)| \leq \frac{C_{\alpha,\beta,n}(t)^l ||W_\hbar^\star||^l_{|\alpha|+|\beta|+k_0}}{l!} \hbar^{l(\frac{1}{2}-3\varepsilon)-\frac{1}{2}(|\vec{\alpha}|+|\vec{\beta}|)}, \tag{2.6}$$

where

$$W_\hbar^\star(x) = \frac{W_\hbar(\hbar^{\frac{1}{2}} x)}{\hbar^{3(\frac{1}{2}-\varepsilon)}} = \chi(\hbar^\varepsilon x) \frac{W(\hbar^{\frac{1}{2}} x)}{\hbar^{3(\frac{1}{2}-\varepsilon)}} \tag{2.7}$$

and is uniformly in $B(\mathbb{R}^n_x)$; i.e. $W_\hbar^\star$ is bounded with bounded derivatives and the bounds are independent of $\hbar$. Hence the sum $a(t, \hbar, x, y) = \sum_{l=0}^\infty a_l(t, \hbar, x, y)$ in (2.2) is uniformly convergent in $B(\mathbb{R}^n_x \times \mathbb{R}^n_y)$. In fact

$$|\partial_x^{\vec{\alpha}} \partial_y^{\vec{\beta}} a(t, \hbar, x, y)| \leq \hbar^{-\frac{1}{2}(|\vec{\alpha}|+|\vec{\beta}|)} \exp\left(\hbar^{\frac{1}{2}-\epsilon} C_{\alpha,\beta,n}(t) ||W_\hbar^\star||_{|\alpha|+|\beta|+k_0}\right).$$

Proof. Following [Z], we denote

$$\begin{cases} \hat{H}_0 = -\frac{1}{2}\hbar^2 \Delta + \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2, \qquad \text{(Anisotropic Oscillator)} \\ \\ \hat{H} = \hat{H}_0 + W_\hbar(x) = -\frac{1}{2}\hbar^2 \Delta + V_\hbar(x), \end{cases}$$

and by $U_0(t) = e^{\frac{-it}{\hbar}\hat{H}_0}$, and $U(t) = e^{\frac{-it}{\hbar}\hat{H}}$, we mean their corresponding propagators.

From

$$(i\hbar\partial_t - \hat{H}_0) U(t) = W_\hbar . U(t),$$

we obtain

$$U(t) = U_0(t) + \frac{1}{i\hbar} \int_0^t U_0(t-s) . W_\hbar . U(s) ds. \tag{2.8}$$

By iteration we get the norm convergent Dyson Expansion:

(2.9)

$$U(t) = U_0(t) + \sum_{l=1}^\infty \frac{1}{(i\hbar)^l} \int_0^t \ldots \int_0^{s_{l-1}} U_0(t) [U_0(s_1)^{-1} . W_\hbar . U_0(s_1)] \ldots [U_0(s_l)^{-1} . W_\hbar . U_0(s_l)] ds_l \ldots ds_1.$$

It is well-known that for $t \neq \frac{m\pi}{\omega_k}$, the kernel of $U_0(t)$ is given by

$$k_0(t,x,y) = (\prod_{k=1}^{n} \frac{\omega_k}{2\pi i\hbar \sin \omega_k t})^{\frac{1}{2}} e^{\frac{i}{\hbar}S(t,x,y)}, \tag{2.10}$$

where

$$S(t,x,y) = \sum_{k=1}^{n} \frac{\omega_k}{\sin \omega_k t}(\frac{1}{2}(\cos \omega_k t)(x_k^2 + y_k^2) - x_k y_k).$$

Then by taking kernels in (2.9) and after some change of variables (see [Z], pages $8-9$ and $18-19$), we get (2.2). This finishes the proof of part (A) of the proposition.

Before proving part (B), let us mention a useful estimate from [Z]. The setting in [Z] is a non-semiclassical one, i.e. $\hbar = 1$. In [Z] on pages $17-18$ the following estimate (for $\hbar = 1$) is proved using integration by parts. That there exists a positive integer $k_0 = k_0(\alpha, \beta, n)$ and a continuous function $C_{\alpha,\beta,n}(t)$ such that

$$|\partial_x^{\vec{\alpha}} \partial_y^{\vec{\beta}} a_l(t,1,x,y)| \leq \frac{1}{l!} C_{\alpha,\beta,n}(t)^l ||W_1||^l_{|\alpha|+|\beta|+k_0}, \qquad (W_1 = W_\hbar \mid_{\hbar=1}) \tag{2.11}$$

The estimates (2.11) will change if one considers $\hbar$ in the calculations. This would be part (B) of the proposition. Let us prove part (B), namely the estimate (2.6). First, in (2.3), we apply the change of variables $x \mapsto \hbar^{\frac{1}{2}}x$, $y \mapsto \hbar^{\frac{1}{2}}y$, $\vec{z} \mapsto \hbar^{\frac{1}{2}}\vec{z}$ and $\vec{\xi} \mapsto \hbar^{\frac{1}{2}}\vec{\xi}$. This gives us $\hbar^{ln}$ in front of the integral. Then we replace $W_\hbar$ by $\hbar^{3(\frac{1}{2}-\varepsilon)}W_\hbar^\star$. After collecting all the powers of $\hbar$ in front of the integral we obtain

$$a_l(t,\hbar,\hbar^{\frac{1}{2}}x,\hbar^{\frac{1}{2}}y) = (\frac{-1}{2\pi})^{ln} \hbar^{l(\frac{1}{2}-3\varepsilon)} \int_0^t \dots \int_0^{s_{l-1}} \overbrace{\int \dots \int}^{2l} e^{i\Phi_l} b_l^\star(s,x,y,\vec{z},\vec{\xi}) d^l z d^l \xi d^l s,$$

where

$$b_l^\star(s,x,y,\vec{z},\vec{\xi}) = \prod_{i=1}^{l} W_\hbar^\star(\frac{\cos \omega_k s_i}{2}(z_{i+1}^k + z_i^k) - \frac{\sin \omega_k s_i}{\omega_k}\xi_i^k + \frac{\sin \omega_k (t-s_i)}{\sin \omega_k t} y^k + \frac{\sin \omega_k s_i}{\sin \omega_k t} x^k).$$

Next we apply (2.11) to the above integral with W_1 replaced by $W_\hbar^\star$, and we get (2.6). To finish the proof we have to show that for every positive integer m we can find uniform bounds (i. e. independent of $\hbar$) for the m-th derivatives of the function $W_\hbar^\star(x)$. Since $\chi(x)$ is supported in the unit ball, from the definition (2.7) we see that $W_\hbar^\star$ is supported in $|x| < \hbar^{-\varepsilon}$. So from (2.7) it is enough to find uniform bounds in $\hbar$ for the m-th derivatives of the function $\frac{W(\hbar^{\frac{1}{2}}x)}{\hbar^{3(\frac{1}{2}-\varepsilon)}}$ in the ball $|x| < \hbar^{-\varepsilon}$. This is very clear for $m \geq 3$. For $m < 3$, we use the order of vanishing of $W(x)$ at $x = 0$. Since $W(0) = 0$, $\nabla W(0) = 0$ and $\mathrm{Hess}W(0) = 0$, the order of vanishing of W at $x = 0$ is 3. Therefore in the ball $|x| < \hbar^{-\varepsilon}$, the functions

$$\frac{W(\hbar^{\frac{1}{2}}x)}{(\hbar^{\frac{1}{2}}x)^3}, \frac{(\partial^\alpha W)(\hbar^{\frac{1}{2}}x)}{(\hbar^{\frac{1}{2}}x)^2}, \frac{(\partial^\alpha \partial^\beta W)(\hbar^{\frac{1}{2}}x)}{\hbar^{\frac{1}{2}}x},$$

are bounded functions with uniform bounds in $\hbar$, and the statement follows easily for $m < 3$. $\square$

Chapter 3

Asymptotics of the Trace

In this chapter we show that the integral $Tr\, U(t) = \int k(t,x,x)dx$ is convergent as an oscillatory integral and using (2.2) we express $Tr\, U(t)$ as an infinite sum of oscillatory integrals with an appropriate $\hbar$-estimate for the remainder term.

3.1 Trace as a tempered distribution

In this section we review some standard facts. We know that the sum

$$Tr\, U(t) = \sum e^{-\frac{it\mathbf{E}_j(\hbar)}{\hbar}}$$

is convergent in the sense of tempered distributions, i.e. $Tr\, U(t) \in S'(\mathbb{R})$. This can be shown by the Weyl's law in its high energy setting, which implies that for potentials of the form $V(x) = \frac{1}{2}\sum_{k=1}^{n} \omega_k^2 x_k^2 + W_\hbar(x)$, with $W \in B(\mathbb{R}^n)$, for fixed $\hbar$, the $j-$th eigenvalue $E_j(\hbar)$ satisfies

$$E_j(\hbar) \sim C(n,\hbar) j^{\frac{2}{n}}, \qquad j \to \infty. \tag{3.1}$$

Another way to define $Tr\, U(t)$ is to write it as the limit

$$(3.2) \qquad Tr\, U(t) = \lim_{\tau\to 0^+} Tr\, U(t-i\tau) = \lim_{\tau\to 0^+} \sum e^{-\frac{(it+\tau)\mathbf{E}_j(\hbar)}{\hbar}}.$$

This time the Weyl's law (3.1) implies that the sum $Tr\, U(t-i\tau)$ is absolutely uniformly convergent because of the rapidly decaying factor $e^{-\frac{\tau \mathbf{E}_j(\hbar)}{\hbar}}$. As a result, $U(t-i\tau)$ is a trace class operator. It is clear that the kernel of $U(t-i\tau)$ is $k(t-i\tau,x,y)$, the analytic continuation of the kernel $k(t,x,y)$ of $U(t)$. Clearly $k(t-i\tau,x,y)$ is continuous in x and y. So we can write $Tr\, U(t-i\tau) = \int k(t-i\tau,x,x)dx$. We notice that this integral is uniformly convergent. This is because up to a constant this integral equals to $\int e^{\frac{i}{\hbar}S(t-i\tau,x,x)}\, a(t-i\tau,\hbar,x,x)$, and the exponential factor in the integral is rapidly decaying for $\tau > 0$ as $|x| \to \infty$ and a is a bounded function. More precisely

$$\Re(iS(t-i\tau,x,x)) = \sum_{k=1}^{n} \Re(-i\omega_k \tan(\frac{\omega_k(t-i\tau)}{2}))x_k^2 = \sum_{k=1}^{n} \frac{\omega_k(1-e^{2\tau\omega_k})}{|1+e^{w_k(it+\tau)}|^2} x_k^2,$$

and

$$\frac{\omega_k(1-e^{2\tau\omega_k})}{|1+e^{w_k(it+\tau)}|^2} < 0.$$

The discussion above shows that the integral $\int k(t,x,x)dx$ can be defined by integrations by parts as follows: Since

$$< D_x >^2 \, e^{iS(t,x,x)} := (1-\Delta)e^{iS(t,x,x)} = (1+ \parallel 2\vec{\omega}\tan(\frac{\vec{\omega}t}{2})\vec{x} \parallel^2 + 2i \sum_{k=1}^{n} \omega_k \tan(\frac{\omega_k t}{2}))e^{iS(t,x,x)},$$

we can write

$$(3.3) \qquad \int e^{\frac{i}{\hbar}S(t,x,x)}\, a(t,\hbar,x,x)dx = \hbar^{\frac{n}{2}} \int e^{iS(t,x,x)}\, a(t,\hbar,\sqrt{\hbar}x,\sqrt{\hbar}x)dx =$$

$$\hbar^{\frac{n}{2}} \int e^{iS(t,x,x)} (< D_x >^2 \; (1+ \parallel 2\vec{\omega}\tan(\frac{\vec{\omega}t}{2})\vec{x} \parallel^2 + 2i \sum_{k=1}^{n} \omega_k \tan(\frac{\omega_k t}{2}))^{-1})^{n_0} a(t,\hbar,\sqrt{\hbar}x,\sqrt{\hbar}x)dx$$

If we assume $0 < t < \min_{1\le k\le n}\{\frac{\pi}{2w_k}\}$, then by choosing $n_0 > \frac{n}{2}$, and because $a(t,\hbar,x,y) \in B(\mathbb{R}^n_x \times \mathbb{R}^n_y)$, the integral becomes absolutely convergent.

3.2 Trace as an infinite sum of oscillatory integrals

Since by (2.6) the series $a(t,\hbar,x,y) = \sum_{l=0}^{\infty} a_l(t,\hbar,x,y)$ is absolutely uniformly convergent, we have

$$\int e^{\frac{i}{\hbar}S(t,x,x)}\, a(t,\hbar,x,x)dx = \sum_{l=0}^{\infty} \int e^{\frac{i}{\hbar}S(t,x,x)}\, a_l(t,\hbar,x,x)dx,$$

and therefore we obtain an infinite sum of oscillatory integrals. The next step is to apply the stationary phase method to each integral above and then add the asymptotic expansions to obtain an asymptotic expansion for the $Tr\, U(t)$.

3.3 Estimates for the remainder

Because we have an infinite sum of asymptotic expansions, we have to establish that the resulting asymptotic for the trace is a valid approximation. Hence we have to find some appropriate $\hbar$-estimates for the remainder term of the series. To be more precise define

$$I_l(t,\hbar) = \hbar^{-\frac{n}{2}} \int e^{\frac{i}{\hbar}S(t,x,x)}\, a_l(t,\hbar,x,x)dx. \tag{3.4}$$

Hence by this notation, $Tr\, U(t) = \prod_{k=1}^{n}(\frac{\omega_k}{2\pi i \sin \omega_k t})^{\frac{1}{2}} \sum_{l=0}^{\infty} I_l(t,\hbar)$. Now we have the following crucial proposition.

Proposition **3.3.1.** *Fix $0 < \varepsilon < \frac{1}{6}$, and $I_l(t,\hbar)$ be defined by (3.4). Then for all $m \geq 1$*

$$Tr\, U(t) = \prod_{k=1}^{n}(\frac{\omega_k}{2\pi i \sin \omega_k t})^{\frac{1}{2}} \sum_{l=0}^{m-1} I_l(t,\hbar) + O(\hbar^{m(\frac{1}{2}-3\varepsilon)}). \tag{3.5}$$

Proof. If in (3.4) we integrate by parts as we did in (3.3), and choose $n_0 = [\frac{n}{2}] + 1$, then using (2.6) we get

$$|I_l(t,\hbar)| \leq C_n'(t) \frac{C_n(t)^l ||W_\hbar^\star||_{2n_0+k_0}^l}{l!} \hbar^{l(\frac{1}{2}-3\varepsilon)},$$

where $C_n(t) = \max_{|\alpha|+|\beta|\leq 2n_0}\{C_{\alpha,\beta,n}(t)\}$. We note that $\frac{1}{2} - 3\varepsilon > 0$ because $0 < \varepsilon < \frac{1}{6}$. Now it is clear that for every positive integer m, and every $0 < \hbar \leq h_0 \leq 1$,

(3.6)
$$|\sum_{l=m}^{\infty} I_l(t,\hbar)| \leq C_n'(t) e^{\{C_n(t)||W_\hbar^\star||_{2n_0+k_0}\}} \hbar^{m(\frac{1}{2}-3\varepsilon)}.$$

Since by Proposition 2.2.1.B, $\sup_{0<\hbar\leq 1} ||W_\hbar^\star||_{2n_0+k_0} < \infty$, we get (3.5). □

The Proposition 3.3.1 is very important because it enables us to add up all the asymptotic expansions obtained by applying stationary phase method to each $I_l(t,\hbar)$.

3.4 Stationary phase calculations and the proof of parts 1 & 2 of Theorem 1.2.1

In this section we will apply the stationary phase method to each $I_l(t,\hbar)$ in (3.5). By (3.4), (2.2) and (2.3) we have

(3.7)
$$I_l(x,\hbar) = (\frac{-1}{2\pi})^{ln}(\frac{1}{i\hbar})^{l(n+1)+\frac{n}{2}} \int_0^t ... \int_0^{s_{l-1}} \overbrace{\int ... \int}^{2l+1} e^{\frac{i}{\hbar}\Psi_l} b_l(s,x,x,\vec{z},\vec{\xi}) d^l s\, d^l z\, d^l \xi\, dx,$$

where

(3.8)
$$\Psi_l = S(t,x,x) + \Phi_l = \sum_{k=1}^{n}\{(-\omega_k \tan\frac{\omega_k}{2}t)\, x_k^2 + \frac{\omega_k}{2}\cot\omega_k t(z_1^k)^2 + \sum_{i=1}^{l}(z_{i+1}^k - z_i^k)\xi_i^k\}.$$

It is easy to see that the only critical point of the phase function Ψ_l, given by (3.8), is at $(x,\vec{z},\vec{\xi}) = 0$.

Next we calculate $H_l =$Hess$\Psi_l(0)$ and H_l^{-1}. In the following we use the notation $D(\vec{v})$ for the diagonal matrix $Diag(v_1,...,v_n)$, where $\vec{v} = (v_1,...,v_n)$. From (3.8), we get

(3.9)

$$H_l = \begin{pmatrix} D(-2\vec{\omega}\tan(\frac{\vec{\omega}t}{2}))_{n\times n} & 0 & 0 \\ 0 & \begin{pmatrix} D(\vec{\omega}\cot\vec{\omega}t)_{n\times n} & 0 \\ 0 & 0 \end{pmatrix}_{ln\times ln} & \begin{pmatrix} -I & 0 & .. & & 0 \\ I & -I & 0 & .. & 0 \\ 0 & I & \ddots & & \\ \vdots & & \ddots & & \\ 0 & & & I & -I \end{pmatrix}_{ln\times ln} \\ 0 & \begin{pmatrix} -I & I & .. & & 0 \\ 0 & -I & I & .. & 0 \\ . & 0 & \ddots & \ddots & \\ . & & & & I \\ 0 & & & 0 & -I \end{pmatrix}_{ln\times ln} & 0 \end{pmatrix}_{(2l+1)n\times(2l+1)n},$$

where $I = I_{n\times n}$ is the identity matrix of size $n \times n$.

Since H_l is of the form $H_l = \begin{pmatrix} K & 0 & 0 \\ 0 & A & B \\ 0 & B^T & 0 \end{pmatrix}$, the inverse matrix equals $H_l^{-1} = \begin{pmatrix} K^{-1} & 0 & 0 \\ 0 & 0 & {B^T}^{-1} \\ 0 & B^{-1} & -B^{-1}A{B^T}^{-1} \end{pmatrix}$. A simple calculation shows that

(3.10)

$$H_l^{-1} = \begin{pmatrix} D(\frac{-1}{2\vec{\omega}}\cot(\frac{\vec{\omega}t}{2})) & 0 & 0 \\ 0 & 0 & \begin{pmatrix} -I & -I & ... & & -I \\ 0 & -I & -I & ... & -I \\ 0 & 0 & -I & \ddots & \vdots \\ \vdots & \ddots & \ddots & & -I \\ 0 & ... & & 0 & -I \end{pmatrix} \\ 0 & \begin{pmatrix} -I & 0 & ... & & 0 \\ -I & -I & 0 & & \vdots \\ \vdots & \vdots & \ddots & & \vdots \\ -I & \ddots & \ddots & -I & 0 \\ -I & ... & & -I & -I \end{pmatrix} & \begin{pmatrix} -\Omega & -\Omega & ... & -\Omega \\ -\Omega & -\Omega & ... & -\Omega \\ \vdots & & & \vdots \\ -\Omega & -\Omega & ... & -\Omega \end{pmatrix} \end{pmatrix},$$

where $\Omega = D(\vec{w}\cot\vec{\omega}t)$.

It is also easy to see that

$$\det H_l = (-1)^{(l+1)n}\prod_{k=1}^{n} 2\omega_k \tan\frac{\omega_k t}{2}. \tag{3.11}$$

By applying the stationary phase lemma to (3.7) and plugging into (3.5) we obtain

(3.12)

$$Tr\,U(t) = \prod_{k=1}^{n}\left(\frac{\omega_k}{\sin\omega_k t}\right)^{\frac{1}{2}}\sum_{l=0}^{m-1}\frac{\hbar^{-l}}{i^{l(n+1)+\frac{n}{2}}}\frac{(-1)^{ln}e^{i\frac{\pi}{4}\mathrm{sgn}H_l}}{\sqrt{|\det H_l|}}\int_0^t ... \int_0^{s_{l-1}}\sum_{j=0}^{\infty}\hbar^j P_j b_l(0)ds_l...ds_1 + O(\hbar^{m(\frac{1}{2}-3\varepsilon)}),$$

where

(3.13)

$$P_j b_l(x,\vec{z},\vec{\xi}) = \frac{i^{-j}}{2^j.j!} < H_l^{-1}\nabla,\nabla >^j\; b_l(x,\vec{z},\vec{\xi}) = \frac{i^{-j}}{2^j.j!}\sum_{r_1,...,r_{2j}\in\mathcal{A}_l} h_l^{r_1r_2}...h_l^{r_{2j-1}r_{2j}}\frac{\partial^{2j}b_l(x,\vec{z},\vec{\xi})}{\partial r_1...\partial r_{2j}},$$

where in the sum (3.13) the indices $r_1,...,r_{2j}$ run in the set $\mathcal{A}_l = \{x^k, z_1^k, ..z_l^k, \xi_1^k, ..\xi_l^k\}_{k=1}^n$, and $h_l^{rr'}$ with $r, r' \in \mathcal{A}_l$, corresponds to the (r,r')-th entry of the inverse Hessian H_l^{-1}.

We note that $P_j b_l(0) = 0$ if $2j < 3l$. This is true because of (2.5) and because $W(0) = 0$, $\nabla W(0) = 0$ and Hess$W(0) = 0$. This implies, first, there are not any negative powers of $\hbar$ in the expansion (as we were expecting). Second, the constant term (i.e. the 0-th wave invariant), which corresponds to the term $l = j = 0$ in the sum, equals

$$a_0(t) = TrU_0(t) = \prod_{k=1}^{n}\left(\frac{\omega_k}{\sin\omega_k t}\right)^{\frac{1}{2}}\frac{i^{-\frac{n}{2}}e^{\frac{-\pi n}{4}}}{(2\omega_k\tan\frac{\omega_k t}{2})^{\frac{1}{2}}} = \prod_{k=1}^{n}\frac{1}{2i\sin\frac{\omega_k t}{2}}.$$

And third (using (3.11)), for $j \geq 1$ the coefficient of $\hbar^j$ in (3.12) equals

$$a_j(t) = \left(\prod_{k=1}^{n}\frac{1}{2i\sin\frac{\omega_k t}{2}}\right)\sum_{l=1}^{2j} i^{l(n-1)+\frac{n}{2}}e^{i\frac{\pi}{4}\mathrm{sgn}H_l}\int_0^t\int_0^{s_1}...\int_0^{s_{l-1}} P_{l+j}b_l(0)ds_l...ds_1.$$

The sum goes only up to $2j$ because if $l > 2j$ then $2(l+j) < 3l$ and $P_{l+j}b_l(0) = 0$.

This proves the first two parts of Theorem 1.2.1.

3.5 Calculations of the wave invariants and the proof of part 3 of Theorem 1.2.1

In this section we try to calculate the wave invariants $a_j(t)$ from the formulas (1.7). First of all, let us investigate how the terms with highest order of derivatives appear in $a_j(t)$. Because b_l is the product of l copies of $W_\hbar$ functions, and because we have to put at least 3 derivatives on each $W_\hbar$ to obtain non-zero terms, the highest possible order of derivatives that can appear in $P_{j+l}b_l(0)$, is $2(j+l) - 3(l-1) = 2j - l + 3$. This implies that, because in the sum (1.7) we have $1 \leq l \leq 2j$, the highest order of derivatives in $a_j(t)$ is $2j+2$ and those derivatives are produced by the term corresponding to $l = 1$, i.e. $P_{j+1}b_1(0)$. The formula (1.7) also shows that $a_j(t)$ is a polynomial of degree $2j$. The term with the highest polynomial order is the one with $l = 2j$, i.e. $P_{3j}b_{2j}(0)$ (which has the lowest order of derivatives) and the term $P_{j+1}b_1(0)$ is the linear term of the polynomial. Now let us calculate $P_{j+1}b_1(x, \vec{z}, \vec{\xi}\,)$ and prove Theorem 1.2.1.3.

By (3.13),

$$P_{j+1}b_1 = \frac{i^{-(j+1)}}{2^{j+1}.(j+1)!} \sum_{r_1,\ldots,r_{2j+2}\in\mathcal{A}_1} h_1^{r_1r_2}\ldots h_1^{r_{2j+1}r_{2j+2}} \frac{\partial^{2j+2}b_1}{\partial r_1\ldots\partial r_{2j+2}}, \tag{3.14}$$

where here by (2.5)

$$b_1 = W_\hbar\left(\frac{\cos\omega_k s}{2} z^k - \frac{\sin\omega_k s}{\omega_k}\xi^k + \left(\frac{\sin\omega_k(t-s) + \sin\omega_k s}{\sin\omega_k t}\right)x^k\right).$$

Also by (3.10),

$$H_1^{-1} = \begin{pmatrix} D(\frac{-1}{2\vec{\omega}}\cot(\frac{\vec{\omega}t}{2})) & 0 & 0 \\ 0 & 0 & -I \\ 0 & -I & -D(\vec{w}\cot\vec{\omega}t) \end{pmatrix}.$$

Hence the only non-zero entries of H_1^{-1} are the ones of the form $h_1^{x^kx^k}, h_1^{z^k\xi^k} = h_1^{\xi^kz^k}$, and $h_1^{\xi^k\xi^k}$. Now we let

$$\begin{cases} i_{x^kx^k} = \text{the number of times } h_1^{x^kx^k} \text{ appears in } h_1^{r_1r_2}...h_1^{r_{2j+1}r_{2j+2}} \text{in (3.14)}, \\ i_{z^k\xi^k} = \text{the number of times } h_1^{z^k\xi^k} \text{ appears in } h_1^{r_1r_2}...h_1^{r_{2j+1}r_{2j+2}} \text{in (3.14)}, \\ i_{\xi^k\xi^k} = \text{the number of times } h_1^{\xi^k\xi^k} \text{ appears in } h_1^{r_1r_2}...h_1^{r_{2j+1}r_{2j+2}} \text{in (3.14)}. \end{cases}$$

By applying these notations to (3.14), (2.5) we get

$$\begin{aligned} P_{j+1}b_1 = \frac{i^{-(j+1)}}{2^{j+1}(j+1)!} \sum_{\sum_{k=1}^n i_{x^kx^k}+i_{z^k\xi^k}+i_{\xi^k\xi^k}=j+1} & \Big\{ \frac{(j+1)!\ 2^{\sum_{k=1}^n i_{z^k\xi^k}}}{\prod_{k=1}^n i_{x^kx^k}!i_{z^k\xi^k}!i_{\xi^k\xi^k}!} \\ & \times \prod_{k=1}^n \left(\frac{-\cot\frac{\omega_k t}{2}}{2\omega_k}\right)^{i_{x^kx^k}} (-1)^{i_{z^k\xi^k}} \left(-\omega_k\cot\omega_k t\right)^{i_{\xi^k\xi^k}} \\ & \times \prod_{k=1}^n \left(\frac{\sin\omega_k(t-s)+\sin\omega_k s}{\sin\omega_k t}\right)^{2i_{x^kx^k}} \left(\frac{\cos\omega_k s}{2}\right)^{i_{z^k\xi^k}} \left(\frac{-\sin\omega_k s}{\omega_k}\right)^{i_{z^k\xi^k}+2i_{\xi^k\xi^k}} \\ & \times D^{2j+2}_{2\alpha_1,...2\alpha_n} W_\hbar \Big\}, \end{aligned}$$

where $\alpha_k = i_{x^kx^k} + i_{z^k\xi^k} + i_{\xi^k\xi^k}$, for $k = 1, ..., n$.

Next we write the above big sum as

$$\begin{aligned} & \sum_{\sum_{k=1}^n i_{x^kx^k}+i_{z^k\xi^k}+i_{\xi^k\xi^k}=j+1} \frac{(j+1)!}{\prod_{k=1}^n i_{x^kx^k}!i_{z^k\xi^k}!i_{\xi^k\xi^k}!}(\star) \\ & \qquad = \sum_{\sum \alpha_k=j+1} \frac{(j+1)!}{\prod \alpha_k!} \sum_{i_{x^kx^k}+i_{z^k\xi^k}+i_{\xi^k\xi^k}=\alpha_k} \prod_{k=1}^n \frac{\alpha_k!}{i_{x^kx^k}!i_{z^k\xi^k}!i_{\xi^k\xi^k}!}(\star). \end{aligned}$$

So the coefficient of $D^{2j+2}_{2\alpha_1,...2\alpha_n} W_\hbar$ in $P_{j+1}b_1$, equals

$$\frac{i^{-(j+1)}}{2^{j+1}} \frac{(-1)^{j+1}}{(\prod\alpha_k!)(\prod\omega_k^{\alpha_k})} \prod_{k=1}^n \left(\frac{1}{2}\cot\frac{\omega_k t}{2}\left(\frac{\sin\omega_k(t-s)+\sin\omega_k s}{\sin\omega_k t}\right)^2 - \cos\omega_k s\sin\omega_k s + \cot\omega_k t\sin^2\omega_k s\right)^{\alpha_k}.$$

Now we observe that the term in the parenthesis simplifies to

$$\frac{1}{2}\cot\frac{\omega_k t}{2}\left(\frac{\sin\omega_k(t-s)+\sin\omega_k s}{\sin\omega_k t}\right)^2-\cos\omega_k s\sin\omega_k s+\cot\omega_k t\sin^2\omega_k s=\frac{1}{2}\cot\frac{\omega_k t}{2}.$$

So we get

$$P_{j+1}b_1=\frac{1}{(2i)^{j+1}}\sum_{|\vec{\alpha}|=j+1}\frac{1}{\vec{\alpha}!}\left(\frac{-1}{2\vec{\omega}}\cot\frac{\vec{\omega}t}{2}\right)^{\vec{\alpha}}D^{2j+2}_{2\vec{\alpha}}W_\hbar, \tag{3.15}$$

Finally, by plugging $(x,\vec{z},\vec{\xi}\,)=0$ into equation (3.15) and applying it to (1.7), we get (1.8). This finishes the proof of Theorem 1.2.1.3.

For future reference let us highlight the equation we just established

(3.16)
$$S_1:=\sum_{r_1,\dots,r_{2j+2}\in\mathcal{A}_1}h_1^{r_1r_2}\dots h_1^{r_{2j+1}r_{2j+2}}\frac{\partial^{2j+2}W}{\partial r_1\dots\partial r_{2j+2}}=(j+1)!\sum_{|\vec{\alpha}|=j+1}\frac{1}{\vec{\alpha}!}\left(\frac{-1}{2\vec{\omega}}\cot\frac{\vec{\omega}t}{2}\right)^{\vec{\alpha}}D^{2j+2}_{2\vec{\alpha}}W,$$

where

$$W=W\left(\frac{\cos\omega_k s}{2}z^k-\frac{\sin\omega_k s}{\omega_k}\xi^k+\left(\frac{\sin\omega_k(t-s)+\sin\omega_k s}{\sin\omega_k t}\right)x^k\right).$$

3.6 Calculations of $\int_0^t\int_0^{s_1}P_{j+2}b_2(0)$, and the proof of Theorem 1.2.2

Throughout this section we assume that V is of the form (1.9). Hence, the only non-zero Taylor coefficients are of the form $D^{2j+2}_{2\vec{\alpha}}V(0)$, or $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n}V(0)$, where $\vec{e}_n=(0,\dots,0,1)$.

We notice that based on our discussion in the previous section, the Taylor coefficients of order $2j+1$ appear in $\int_0^t\int_0^{s_1}P_{j+2}b_2(0)$, and they are of the form $D^{2j+1}_{\vec{\beta}}V(0)D^3_{\vec{\delta}}V(0)$. Therefore we look for the coefficients of the data

$$\left\{ D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0) D^3_{3\vec{e}_n} V(0); \quad |\vec{\alpha}| = j-1 \right\}. \tag{3.17}$$

in the expansion of $a_j(t)$.

PROPOSITION **3.6.1.** *In the expansion of $a_j(t)$, the coefficient of the data $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0) D^3_{3\vec{e}_n} V(0)$, $|\vec{\alpha}| = j-1$, is*

$$\frac{c_2(n)}{(2i)^{j+2}} \frac{t}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega} t}{2} \right)^{\vec{\alpha}} \left(\frac{1}{3\omega_n^2} \left(\frac{2\alpha_n + 5}{\alpha_n + 1}\right)\left(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2}\right)^2 + \frac{1}{9\omega_n^4} \right). \tag{3.18}$$

Therefore

$$a_j(t) = \frac{c_1(n)}{(2i)^{j+1}} \sum_{|\vec{\alpha}|=j+1} \frac{t}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega} t}{2}\right)^{\vec{\alpha}} D^{2j+2}_{2\vec{\alpha}} V(0) \tag{3.19}$$

$$+ \frac{c_2(n)}{(2i)^{j+2}} \sum_{|\vec{\alpha}|=j-1} \frac{t}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega} t}{2} \right)^{\vec{\alpha}} \left(\frac{1}{3\omega_n^2} \left(\frac{2\alpha_n + 5}{\alpha_n + 1}\right)\left(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2}\right)^2 + \frac{1}{9\omega_n^4} \right) D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0) D^3_{3\vec{e}_n} V(0)$$

$$+ \{\textit{a polynomial of Taylor coefficients of order} \le 2j\}.$$

Proof. As we mentioned at the beginning of Section 2.7, the data $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0) D^3_{3\vec{e}_n} V(0)$, $|\vec{\alpha}| = j-1$, appears first in $a_j(t)$ and it is a part of the term $\int_0^t \int_0^{s_1} P_{j+2} b_2(0)$. So let us calculate those terms in the expansion of $P_{j+2} b_2(0)$ which contain $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0) D^3_{3\vec{e}_n} V(0)$. By (2.5), since here $l = 2$, we have

$$b_2(s_1, s_2, x, x, z_1, z_2, \xi_1, \xi_2) = W_1 W_2, \qquad \text{where,}$$

$$W_1 = W\left(\tfrac{\cos \omega_k s_1}{2}(z_1^k + z_2^k) - \tfrac{\sin \omega_k s_1}{\omega_k} \xi_1^k + \left(\tfrac{\sin \omega_k (t - s_1) + \sin \omega_k s_1}{\sin \omega_k t}\right) x^k\right), \tag{3.20}$$

$$W_2 = W\left(\tfrac{\cos \omega_k s_2}{2} z_2^k - \tfrac{\sin \omega_k s_2}{\omega_k} \xi_2^k + \left(\tfrac{\sin \omega_k (t - s_2) + \sin \omega_k s_2}{\sin \omega_k t}\right) x^k\right).$$

Also from (3.10) we have

$$
(3.21)\quad H_2^{-1} = \begin{pmatrix} D(\frac{-1}{2\vec{\omega}}\cot(\frac{\vec{\omega}t}{2})) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -I & -I \\ 0 & 0 & 0 & 0 & -I \\ 0 & -I & 0 & -D(\vec{\omega}\cot(\vec{\omega}t)) & -D(\vec{\omega}\cot(\vec{\omega}t)) \\ 0 & -I & -I & -D(\vec{\omega}\cot(\vec{\omega}t)) & -D(\vec{\omega}\cot(\vec{\omega}t)) \end{pmatrix}_{5n\times 5n}.
$$

By (3.13) and (3.20), $P_{j+2}b_2(0) = \frac{i^{-j}}{2^j.j!}S_2$, where S_2 is the following sum

$$
(3.22)\qquad S_2 = \sum_{r_1,\dots,r_{2j+4}\in\mathcal{A}_2} h_2^{r_1r_2}\dots h_2^{r_{2j+3}r_{2j+4}}(W_1\,W_2)_{r_1\dots r_{2j+4}}(0),
$$

where $\mathcal{A}_2 = \{x^k, z_1^k, z_2^k, \xi_1^k, \xi_2^k\}_{k=1}^n$ and for every $r, r' \in \mathcal{A}_2$, $h_2^{rr'}$ is the (r,r')-entry of the matrix H_2^{-1} in (3.21). We would like to separate out those terms in S_2 which include $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n}V(0)D^3_{3\vec{e}_n}V(0)$. To do this, from the total number $2j+4$ derivatives that we want to apply to W_1W_2, we have to put 3 of them on W_1 (or W_2) and put $2j+1$ of them on W_2 (or W_1 respectively). These combinations fit into one of the following two different forms

$$
(3.23)\qquad S_2^1 = \sum_{r_1,\dots,r_{2j+4}\in\mathcal{A}_2} h_2^{r_1r_2}\dots h_2^{r_{2j+3}r_{2j+4}}(W_1)_{r_1r_2r_3}\,(W_2)_{r_4,r_5\dots r_{2j+4}}(0).
$$

There are $2(j+1)(j+2)$ terms of this form in the expansion of S_2.

$$
(3.24)\qquad S_2^2 = \sum_{r_1,\dots,r_{2j+4}\in\mathcal{A}_2} h_2^{r_1r_2}\dots h_2^{r_{2j+3}r_{2j+4}}(W_1)_{r_1r_3r_5}\,(W_2)_{r_2,r_4,r_6,r_7\dots r_{2j+4}}(0).
$$

There are $2^3 \begin{pmatrix} j+2 \\ 3 \end{pmatrix}$ terms of this form in the expansion of S_2.

Now, we calculate the sums S_2^1 and S_2^2.

3.6.1 Calculation of S_2^1

We rewrite S_2^1 as

$$S_2^1 = \sum_{r_1,\dots,r_4} h_2^{r_1r_2} h_2^{r_3r_4} \Big(\sum_{r_5,\dots,r_{2j+4}} h_2^{r_5r_6} \dots h_2^{r_{2j+3}r_{2j+4}} (W_2)_{r_5\dots r_{2j+4}} \Big)_{r_4} (W_1)_{r_1r_2r_3}(0).$$

Then from the definition of W_2 in (3.20) and also from (3.21) it is clear that we can apply (3.16) to the sum in the big parenthesis above. Hence we get

(3.25)
$$S_2^1 = (j+1)! \sum_{|\vec{\alpha}|=j} \frac{1}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega} t}{2} \right)^{\vec{\alpha}} \Big(\sum_{r_1,\dots,r_4} h_2^{r_1r_2} h_2^{r_3r_4} \big(D_{2\vec{\alpha}}^{2j} W_2 \big)_{r_4} (W_1)_{r_1r_2r_3} \Big)(0).$$

This reduces the calculation of S_2^1 to calculating the small sum

$$A_2^1 = \sum_{r_1,\dots,r_4} h_2^{r_1r_2} h_2^{r_3r_4} (\tilde{W}_2)_{r_4} (W_1)_{r_1r_2r_3}(0), \qquad (\tilde{W}_2 = D_{2\vec{\alpha}}^{2j} W_2).$$

Computation of the sum A_2^1 is straight forward and we omit writing the details of this computation. Using Maple, we obtain

$$\int_0^t \int_0^{s_1} A_2^1 \, ds_2 \, dt = -\frac{t}{2\omega_n^2} \left(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2} \right) \big(D_{\vec{e}_n}^1 \tilde{W}_2 \, D_{3\vec{e}_n}^3 W_1 \big)(0).$$

If we plug this into (3.25), after a change of variable $\alpha_n \to \alpha_n + 1$ in indices, we get

(3.26)
$$\int_0^t \int_0^{s_1} S_2^1\, ds_2\, dt = \frac{(j+1)!}{\alpha_n + 1} \sum_{|\vec{\alpha}|=j-1} \frac{1}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega}t}{2} \right)^{\vec{\alpha}} (-\frac{t}{2\omega_n^2})(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2})^2 D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0)\, D^3_{3\vec{e}_n} V(0).$$

3.6.2 Calculation of S_2^2

We rewrite S_2^2 as

$$S_2^2 = \sum_{r_1,\ldots,r_6} h_2^{r_1 r_2} h_2^{r_3 r_4} h_2^{r_5 r_6} \Big(\sum_{r_7,\ldots,r_{2j+4}} h_2^{r_7 r_8} \ldots h_2^{r_{2j+3} r_{2j+4}} (W_2)_{r_7 \ldots r_{2j+4}} \Big)_{r_2, r_4, r_6} (W_1)_{r_1 r_3 r_5}(0).$$

Again from (3.21) it is clear that we can apply (3.16) to the sum in the big parenthesis above. So

(3.27)
$$S_2^2 = (j+1)! \sum_{|\vec{\alpha}|=j-1} \frac{1}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega}t}{2} \right)^{\vec{\alpha}} \Big(\sum_{r_1,\ldots,r_6} h_2^{r_1 r_2} h_2^{r_3 r_4} \big(D^{2j-2}_{2\vec{\alpha}} W_2 \big)_{r_2, r_4, r_6} (W_1)_{r_1 r_3 r_5} \Big)(0).$$

So we need to compute

$$A_2^2 = \sum_{r_1,\ldots,r_6} h_2^{r_1 r_2} h_2^{r_3 r_4} h_2^{r_5 r_6} (\tilde{W}_2)_{r_2, r_4, r_6} (W_1)_{r_1 r_3 r_5}(0), \qquad (\tilde{W}_2 = D^{2j-2}_{2\vec{\alpha}} W_2).$$

Using Maple

$$\int_0^t \int_0^{s_1} A_2^2\, ds_2\, dt = \big(-\frac{t}{2\omega_n^2} (\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2})^2 - \frac{t}{12\omega_n^4} \big) \big(D^3_{3\vec{e}_n} \tilde{W}_2\, D^3_{3\vec{e}_n} W_1 \big)(0).$$

If we plug this into (3.27) we get

(3.28)
$$\int_0^t \int_0^{s_1} S_2^2\, ds_2\, dt = (j+1)! \sum_{|\vec{\alpha}|=j-1} \frac{1}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega}t}{2} \right)^{\vec{\alpha}} (-\frac{t}{2\omega_n^2} (\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2})^2 - \frac{t}{12\omega_n^4}) D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0)\, D^3_{3\vec{e}_n} V(0).$$

We note that the part of the expansion of $\int_0^t \int_0^{s_1} P_{j+2} b_2(0)$ which contains the data $D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0)\, D^3_{3\vec{e}_n} V(0)$, equals

$$\frac{i^{-j}}{2^j.j!}\Big(2(j+2)(j+1)\int_0^t\int_0^{s_1} S_2^1 + 2^3\binom{j+2}{3}\int_0^t\int_0^{s_1} S_2^2\Big).$$

Finally, by applying equations (3.26) and (3.28) to this we obtain (3.19).

$\square$

Now using Proposition 3.6.1, we give a proof for Theorem 1.2.2.

PROOF OF THEOREM 1.2.2. First of all, we prove that for all $\vec{\alpha}$, the functions

$$\big(\cot\frac{\vec{\omega}}{2}t\big)^{\vec{\alpha}},$$

are linearly independent over $\mathbb{C}$. To show this we define

$$\begin{cases} \vec{\cot} : (0,\pi)^n \longrightarrow \mathbb{R}^n, \\ \vec{\cot}(x_1,...,x_n) = (\cot(x_1),...,\cot(x_n)). \end{cases}$$

Because ω_k are linearly independent over $\mathbb{Q}$, the set $\{(\frac{\omega_1}{2}t,...,\frac{\omega_n}{2}t)+\pi\mathbb{Z}^n;\ t\in\mathbb{R}\}\cap(0,\pi)^n$ is dense in $(0,\pi)^n$. Since $\vec{\cot}$ is a homeomorphism and is π-periodic, we conclude that the set $\{(\cot(\frac{\omega_1}{2}t),...,\cot(\frac{\omega_n}{2}t);\ t\in\mathbb{R}\}$ is dense in $\mathbb{R}^n$. Now assume

$$\sum_{\vec{\alpha}} c_{\vec{\alpha}}\big(\cot\frac{\vec{\omega}}{2}t\big)^{\vec{\alpha}} = 0.$$

Since $\{(\cot(\frac{\omega_1}{2}t),...,\cot(\frac{\omega_n}{2}t);\ t\in\mathbb{R}\}$ is dense in $\mathbb{R}^n$, we get

$$\sum_{\vec{\alpha}} c_{\vec{\alpha}}\vec{X}^{\vec{\alpha}} = 0,$$

for every $\vec{X}=(X_1,...,X_n)\in\mathbb{R}^n$. But the monomials $\vec{X}^{\vec{\alpha}}$ are linearly independent over $\mathbb{C}$. So $c_{\vec{\alpha}}=0$.

Next we argue inductively to recover the Taylor coefficients of V from the wave invariants. Since

$$a_0(t) = \prod_{k=1}^{n} \frac{1}{2i \sin \frac{\omega_k t}{2}},$$

we can recover $\prod_{k=1}^{n} \sin \frac{\omega_k t}{2}$, and therefore we can recover $\{\omega_k\}$ up to a permutation. This can be seen by Taylor expanding $\prod_{k=1}^{n} \sin \frac{\omega_k t}{2}$. We fix this permutation and we move on to recover the third order Taylor coefficient $D^3_{3\vec{e}_n} V(0)$. This term appears first in $a_1(t)$. By Proposition 3.6.1, we have

$$\begin{aligned} a_1(t) &= c_1(n) \frac{t}{(2i)^2} \sum_{|\vec{\alpha}|=2} \frac{1}{\vec{\alpha}!} \left(\frac{-1}{2\vec{\omega}} \cot \frac{\vec{\omega}}{2} t\right)^{\vec{\alpha}} D^4_{2\vec{\alpha}} V(0) \\ &\quad + c_2(n) \frac{t}{(2i)^3} \left(\frac{5}{3\omega_n^2} \left(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2}\right)^2 + \frac{1}{9\omega_n^4} \right) \left(D^3_{3\vec{e}_n} V(0) \right)^2 \\ &\quad + \{\text{a rational function of } \omega_k\}. \end{aligned}$$

Now since the functions $\{(\cot \frac{\vec{\omega}}{2} t)^{\vec{\alpha}}\}_{|\vec{\alpha}|=2}$ and $\left(\frac{5}{3\omega_n^2} (\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2})^2 + \frac{1}{9\omega_n^4} \right)$ are linearly independent over $\mathbb{C}$, we can therefore recover the data $\{D^4_{2\vec{\alpha}} V(0)\}_{|\vec{\alpha}|=2}$ and $\{D^3_{3\vec{e}_n} V(0)^2\}$ from $a_1(t)$. So we have determined the third order term $D^3_{3\vec{e}_n} V(0)$ up to a minus sign from the first invariant $a_1(t)$. This choice of minus sign corresponds to a reflection. We fix this reflection and we move on to determine the higher order Taylor coefficients inductively.

Next we assume $D^3_{3\vec{e}_n} V(0) \neq 0$ and that we know all the Taylor coefficients $D^m_{\vec{\beta}} V(0)$ with $m \leq 2j$. We wish to determine the data $\{D^{2j+1}_{2\vec{\alpha}+3\vec{e}_n} V(0)\}_{|\vec{\alpha}|=j-1}$ and $\{D^{2j+2}_{2\vec{\alpha}} V(0)\}_{|\vec{\alpha}|=j+1}$, from the wave invariant $a_j(t)$. At this point we use Proposition 3.6.1, and to finish the proof of Theorem 1.2.2 we have to show that the set of functions

$$\left\{ (\cot \frac{\vec{\omega}}{2} t)^{\vec{\alpha}}; \quad |\vec{\alpha}| = j+1 \right\} \cup \left\{ (\cot \frac{\vec{\omega} t}{2})^{\vec{\alpha}} \left(\frac{1}{3\omega_n^2} \left(\frac{2\alpha_n + 5}{\alpha_n + 1}\right) \left(\frac{-1}{2\omega_n} \cot \frac{\omega_n t}{2}\right)^2 + \frac{1}{9\omega_n^4} \right); \quad |\vec{\alpha}| = j-1 \right\},$$

are linearly independent over $\mathbb{C}$. But this is clear from our discussion at the beginning of the proof.

Chapter 4

Appendix A

In this appendix we prove Lemma 2.1.1.

PROOF. First of all we would like to change the function Θ slightly by rescaling it. We choose $0 < \tau < 2\varepsilon$ so that $\hbar^{1-\tau} = o(\hbar^{1-2\varepsilon})$. Then we define

$$\Theta_\hbar(x) := \Theta(\frac{x}{\hbar^{1-\tau}}). \tag{4.1}$$

Thus $\Theta_\hbar \in C_0^\infty([0,\infty))$ is supported in the interval $I_\hbar = [0, \hbar^{1-\tau}\delta]$. In Appendix B, using min-max principle we show that

$$Tr(\Theta(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) = Tr(\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty) = Tr(e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty).$$

Hence to prove the lemma it is enough to show

$$Tr(\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}) = Tr(\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty).$$

To prove this identity we use the WKB construction of the kernel of the operators $\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}$ and $\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}$ and make a compression between them.

4.1 WKB construction for $\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}$

In [DSj], chapter 10, a WKB construction is made for $\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}$ for symbols P in the symbol class $S_0^0(1)$ which are independent of $\hbar$ or of the form $P(x,\xi,\hbar) \sim P_0(x,\xi) + \hbar P_1(x,\xi) + \ldots$, where $P_j \in S_0^0$ are independent of $\hbar$ (but not for symbols $H = H(x,\xi,\hbar) \in S_{\delta_0}^0$).

It is shown that we can approximate $\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}}$ for small time t, say $t \in (-t_0, t_0)$, by a fourier integral operator of the form

$$U_P(t)u(x) = (2\pi\hbar)^{-n} \int\int e^{i(\varphi_P(t,x,\eta)-y.\eta)/\hbar} b_P(t,x,y,\eta,\hbar)u(y)dyd\eta,$$

where $b_P \in C^\infty((-t_0,t_0);\ S(1))$ have uniformly compact support in (x,y,η), and φ_P is real, smooth and is defined near the support of b_P. The functions φ_P and b_P are found in such a way that for all $t \in (-t_0, t_0)$

$$||\Theta(\hat{P})e^{\frac{-it}{\hbar}\hat{P}} - U_P(t)||_{tr} = O(\hbar^\infty).$$

Let us briefly review this construction, made in [DSj]. First of all, in Chapter 8, Theorem 8.7, it is proved that for every symbol $P \in S_0^0(1)$, we have $\Theta(\hat{P}) = Op^w(a_P(x,\xi,\hbar))$ for some $a_P(x,\xi,\hbar) \in S_0^0(1)$, where here $\hat{P}$ and $Op^w(a_P(x,\xi,\hbar))$ are respectively the Weyl quantization of P and $a_P(x,\xi,\hbar)$. It is also shown that $a_P \sim a_{P,0}(x,\xi) + ha_{P,1}(x,\xi) + \ldots$ for some $a_{P,j}(x,\xi) \in S_0^0(1)$. The idea of proof is as follows. In Theorem 8.1 of [DSj] it is shown that if $\Theta \in C_0^\infty(\mathbb{R})$, and if $\tilde{\Theta} \in C_0^1(\mathbb{C})$ is an almost analytic extension of Θ (i.e. $\bar{\partial}\tilde{\Theta}(z) = O(|\Im z|^\infty)$), then

$$\Theta(\hat{P}) = \frac{-1}{\pi}\int_{\mathbb{C}} \frac{\bar{\partial}\tilde{\Theta}(z)}{z-\hat{P}} L(dz). \tag{4.2}$$

Then it is verified that for some symbol $r(x,\xi,z;\hbar)$, we have $(z-\hat{P})^{-1} = Op^w(r(x,\xi,z;\hbar))$. By symbolic calculus, one can find a formal asymptotic expansion of the form

$$r(x,\xi,z;\hbar) \sim \frac{1}{z-P} + \hbar\frac{q_1(x,\xi,z)}{(z-P)^3} + \hbar^2\frac{q_2(x,\xi,z)}{(z-P)^5} + ...,$$

by formally solving $Op^w(r(x,\xi,z;\hbar))\sharp_\hbar(z-\hat{P}) = (z-\hat{P})\sharp_\hbar Op^w(r(x,\xi,z;\hbar)) = 1$. We can see that $q_j(x,\xi,z)$ are polynomials in z with smooth coefficients. Finally it is shown that $\Theta(\hat{P}) = Op^w(a_P(x,\xi,\hbar))$, where $a_P \in S_0^0$ is given by

$$a_P(x,\xi,\hbar) = \frac{-1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Theta}(z) r(x,\xi,z;\hbar) L(dz).$$

By the above asymptotic expansion for $r(x,\xi,z;\hbar)$ one obtains an asymptotic $a_P \sim a_{P,0} + \hbar a_{P,1} + ...$, where

$$a_{P,j} = \frac{-1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Theta}(z)\frac{q_j(x,\xi,z)}{(z-P)^{2j+1}}L(dz) = \frac{1}{(2j)!}\partial_t^{2j}(q_j(x,\xi,t)\Theta(t))|_{t=P(x,\eta)}. \tag{4.3}$$

Then, again in Chapter 10 of [DSj], it is shown that $\varphi_P(t,x,\eta)$ and $b_P(t,x,y,\eta,\hbar)$ satisfy

$$\partial_t\varphi_P(t,x,\eta) + P(x,\partial_x\varphi_P(t,x,\eta)) = 0, \qquad \varphi_P|_{t=0} = x.\eta, \tag{4.4}$$

$$b_P \sim b_{P,0} + \hbar b_{P,1} + \dots, \qquad b_{P,j} = b_{P,j}(t,x,y,\eta) \in C^\infty((-t_0,t_0);\ S_0^0(1)),$$

where

(4.5)
$$\begin{cases} \partial_t b_{P,j} + \langle \partial_x\varphi_P, \partial_x b_{P,j}\rangle + \frac{1}{2}\Delta_x\varphi_P.\, b_{P,j} = -\frac{1}{2}\Delta_x b_{P,j-1}, & j \geq 0, \qquad (b_{P,-1}=0), \\ \\ b_{P,j}|_{t=0} = \psi(x,\eta)a_{P,j}(\frac{x+y}{2},\eta)\psi(y,\eta). \end{cases}$$

In (4.5), $a_{P,j}$ is given by (4.3) and $\psi(x,\eta)$ is any C_0^∞ function which equals 1 in a neighborhood of $\overline{P^{-1}(I)}$ where $I = [0,\delta]$ is, as before, the range of our low-lying eigenvalues and where Θ is supported.

There exists a similar construction for $\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}$, except here $H \in S^0_{\delta_0}$.

4.2 WKB construction for $\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}$

Since in (2.1), $H = H(x,\xi,\hbar) \in S^0_{\delta_0}$, with $\delta_0 = \frac{1}{2} - \varepsilon$, we can not simply use the construction in [DSj] mentioned above. Here in two lemmas we show that the same construction works for the operator $\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}$. We will closely follow the proofs in [DSj].

LEMMA **4.2.1.**

1) *Let $\Theta_\hbar$ be given by (4.1) and $H \in S^0_{\delta_0}$ by (2.1). Then for some $a_H \in S^0_{\delta_0}$ we have $\Theta(\hat{H}) = Op^w(a_H(x,\xi,\hbar))$. Moreover $a_H(x,\xi,\hbar) \sim a_{H,0}(x,\xi,\hbar) + \hbar a_{H,1}(x,\xi,\hbar) + \dots$, where $a_{H,j}(x,\xi,\hbar) \in S^0_{\delta_0}$ is given by*

$$a_{H,j} = \frac{-1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{\Theta}(z)\frac{q_{H,j}(x,\xi,z,\hbar)}{(z-H)^{2j+1}}L(dz) = \frac{1}{(2j)!}\partial_t^{2j}(q_{H,j}(x,\xi,t,\hbar)\Theta_\hbar(t))|_{t=H(x,\xi,\hbar)}. \tag{4.6}$$

2) *Choose c such that $0 < c < \min\{1, \omega_k^2\}_{k=1}^n \leq \max\{1, \omega_k^2\}_{k=1}^n < \frac{1}{c}$. Let $\psi_\hbar(x,\eta)$ be a function in $C_0^\infty(\mathbb{R}^{2n}) \cap S^0_{\delta_0}(\mathbb{R}^{2n})$ which is supported in the ball $\{x^2+\eta^2 < 4c^{-1}\hbar^{1-\tau}\delta\}$ and equals 1 in a neighborhood of $\overline{H^{-1}(I)}$, where $I_\hbar = [0, \hbar^{1-\tau}\delta]$ ($I_\hbar$ is where $\Theta_\hbar$ is supported). Then*

$$\Theta_\hbar(\hat{H})u(x) = (2\pi\hbar)^{-n}\int\int e^{i(x-y).\eta/\hbar}\psi_\hbar(x,\eta)a_H(\frac{x+y}{2},\eta,\hbar)\psi_\hbar(y,\eta)u(y)dyd\eta + K(\hbar)u(x), \tag{4.7}$$

where $||K(\hbar)||_{tr} = O(\hbar^\infty)$.

PROOF OF LEMMA 4.2.1: Since $H \in S^0_{\delta_0}$ and $\delta_0 = \frac{1}{2} - \varepsilon < \frac{1}{2}$, the symbolic calculus mentioned in the last section can be followed similarly to prove Lemma 4.2.1.1. It is also easy to check that in (4.6), $a_{H,j} \in S^0_{\delta_0}$. The second part of the Lemma is stated in [DSj] , equation 10.1, for the case $P \in S^0_0$. The same argument works for $H \in S^0_{\delta_0}$, precisely because the factor $\hbar^N$ on the right hand side of the inequality in Proposition 9.5 of [DSj] changes to $\hbar^{N-\delta_0\alpha}$. Thus the discussion on pages $115-116$ still follows.

LEMMA **4.2.2.** *There exists $t_0>0$ such that for every $t \in (-t_0,t_0)$, there exist functions $\varphi_H(t,x,\eta,\hbar)$ and $b_H(t,x,y,\eta,\hbar)$ such that the operator $U_H(t)$ defined by*

$$U_H(t)u(x) = (2\pi\hbar)^{-n}\int\int e^{i(\varphi_H(t,x,\eta,\hbar)-y.\eta)/\hbar} b_H(t,x,y,\eta,\hbar)u(y)dyd\eta, \tag{4.8}$$

satisfies

$$||\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}} - U_H(t)||_{tr} = O(\hbar^\infty).$$

Moreover, we can choose φ_H and b_H such that

1) φ_H satisfies the eikonal equation

$$\partial_t\varphi_H(t,x,\eta,\hbar) + H(x,\partial_x\varphi_H(t,x,\eta,\hbar)) = 0, \qquad \varphi_H|_{t=0} = x.\eta. \tag{4.9}$$

This equation can be solved in $(-t_0,t_0)\times\{x^2+\eta^2 < C\hbar^{1-\tau}\delta\}$ where C is an arbitrary constant. In fact φ_H is independent of $\hbar$ in this domain. (Only the domain of φ_H depends on $\hbar$. See (4.12).)

2) For all $t \in (-t_0,t_0)$, we have $b_H(t,x,y,\eta,\hbar) \in S^0_{\delta_0}$ with supp $b_H \subset \{x^2+\eta^2, y^2+\eta^2 < C_1\hbar^{1-\tau}\delta\}$ for some constant C_1. Also b_H has an asymptotic expansion of the form

(4.10)
$$b_H \sim b_{H,0} + \hbar b_{H,1} + \ldots, \qquad b_{H,j} = b_{H,j}(t,x,y,\eta,\hbar) \in C^\infty((-t_0,t_0);\ S^0_{\delta_0}(1)),$$

and the functions $b_{H,j}$ satisfy the transport equations

(4.11)
$$\begin{cases} \partial_t b_{H,j} + \left\langle \partial_x \varphi_H, \partial_x b_{H,j} \right\rangle + \frac{1}{2}\Delta_x \varphi_H .\, b_{H,j} = -\frac{1}{2}\Delta_x b_{H,j-1}, \qquad j \geq 0, \qquad (b_{H,-1} = 0), \\ \\ b_{H,j}|_{t=0} = \psi_\hbar(x,\eta) a_{H,j}(\frac{x+y}{2}, \eta, \hbar) \psi_\hbar(y,\eta), \end{cases}$$

where in (4.11) we let $\psi_\hbar(x,\eta)$ be a function in $C_0^\infty(\mathbb{R}^{2n}) \cap S^0_{\delta_0}(\mathbb{R}^{2n})$ which is supported in the ball $\{x^2+\eta^2 < 4c\hbar^{1-\tau}\delta\}$ and equals 1 in a neighborhood of $\overline{H^{-1}(I_\hbar)}$, where $I_\hbar = [0, \hbar^{1-\tau}\delta]$. Here c is defined in Lemma 4.2.1.2. Also in (4.11), the functions $a_{H,j}$ are defined by (4.6).

3) *For all $t \in (-t_0, t_0)$*

(4.12)
$$\varphi_H(t,x,\eta,\hbar) = \varphi_P(t,x,\eta) \qquad on \qquad \{x^2+\eta^2, y^2+\eta^2 < C_1\hbar^{1-\tau}\delta\} \supset supp\,(b_H(x,y,\eta,\hbar)).$$

4) *For all $t \in (-t_0, t_0)$*

(4.13) $$b_{H,j}(t,x,y,\eta,\hbar) = b_{P,j}(t,x,y,\eta) \qquad on \qquad \left\{x^2+\eta^2,\ y^2+\eta^2 < c\hbar^{1-\tau}\delta\right\}.$$

Proof of Lemma 4.2.2: First of all we assume $U_H(t)$ is given by (4.8) and we try to solve the equation

$$\begin{cases} ||(\frac{\hbar}{i}\partial_t + \hat{H})U_H(t)||_{tr} = O(\hbar^\infty), \\ \\ U_H(0) = \Theta_\hbar(\hat{H}). \end{cases}$$

for φ_H and b_H, for small time t.

Using (4.7), this leads us to

$$\begin{cases} e^{-i\varphi_H/\hbar}(\frac{\hbar}{i}\partial_t + \hat{H})(e^{i\varphi_H/\hbar}b_H) \in C^\infty((-t_0,t_0);\ S_{\delta_0}^{-\infty}(1)), \\ \\ b|_{t=0} = \psi_\hbar(x,\eta)a_H(\frac{x+y}{2},\eta,\hbar)\psi_\hbar(y,\eta). \end{cases}$$

We choose the phase function $\varphi_H = \varphi_H(t,x,\eta,\hbar)$ to satisfy the eikonal equation (4.9). This equation can be solved in a neighborhood of the support of b_H, for small time $t \in (-t_0,t_0)$ with t_0 independent of $\hbar$. Let us explain how to solve this equation. We let $(x(t,z,\eta;\hbar),\xi(t,z,\eta;\hbar))$ be the solution to the Hamilton equation

$$\begin{cases} \partial_t x = \partial_\xi H(x,\xi,\hbar) = \xi, & x(0,z,\eta;\hbar) = z \\ \\ \partial_t \xi = -\partial_x H(x,\xi,\hbar) = -\partial_x V_\hbar(x), & \xi(0,z,\eta;\hbar) = \eta \end{cases} . \tag{4.14}$$

We can show that (see section 4 of [Ch]) there exists t_0 independent of $\hbar$ such that for all $|t| \leq t_0$ we have

$$\begin{cases} |\partial_z x(t,z,\eta;\hbar) - I| \leq \frac{1}{2}, & |\partial_\eta x(t,z,\eta;\hbar)| \leq \frac{1}{2} \\ \\ |\partial_z \xi(t,z,\eta;\hbar)| \leq \frac{1}{2}, & |\partial_\eta \xi(t,z,\eta;\hbar) - I| \leq \frac{1}{2} \end{cases} . \tag{4.15}$$

We can choose t_0 independent of $\hbar$, precisely because in equation 4.4 of [Ch] we have a uniform bound in $\hbar$ for $\mathrm{Hess}(V_\hbar(x))$. Now, we define

$$\lambda : (z,\eta) \longmapsto (x(t,z,\eta;\hbar),\eta).$$

It is easy to see that $\lambda(0,0) = (0,0)$. This is because if $(z,\eta) = (0,0)$ then $H(x,\xi) = H(z,\eta) = 0$. By (2.1) and (1.2), and $W(x) = O(|x|^3)$, we can see that $H(x,\xi) = 0$

implies $(x(t,0,0;\hbar),\xi(t,0,0;\hbar)) = (0,0)$. On the other hand from (4.15) we have $\frac{1}{2} < |\partial_z x(t,z,\eta;\hbar)| < \frac{3}{2}$. Therefore λ is invertible in a neighborhood of origin. We define the inverse function by

$$\lambda^{-1}(x,\eta) = (z(t,x,\eta;\hbar),\eta),$$

which is defined in a neighborhood of $(x,\eta) = (0,0)$. Then we have

(4.16)

$$\varphi_H(t,x,\eta,\hbar) = z(t,x,\eta;\hbar).\eta + \int_0^t \frac{1}{2}|\xi(s,z(t,x,\eta;\hbar),\eta;\hbar)|^2 - V_\hbar(x(s,z(t,x,\eta;\hbar),\eta;\hbar))ds,$$

A similar formula holds for φ_P except in (4.14) H should be replaced by P and in (4.16) $V_\hbar$ by V. It is known that the eikonal equation for φ_P can be solved near $\mathrm{supp} b_P$, for small time $t \in (-t_0,t_0)$ (Of course t_0 is independent of $\hbar$). Now, we want to show that

$$(4.17) \qquad \varphi_H(t,x,\eta,\hbar) = \varphi_P(t,x,\eta) \qquad \text{in} \qquad (-t_0,t_0) \times \{x^2+\eta^2 < C\hbar^{1-\tau}\delta\}.$$

Let (x,η) be in $\{x^2+\eta^2 < C\hbar^{1-\tau}\delta\}$. First, we show that $|z(t,x,\eta;\hbar)| < 8C^{\frac{1}{2}}\hbar^{\frac{1-\tau}{2}}\delta^{\frac{1}{2}}$. Because $z(t,0,0;\hbar) = 0$, by Fundamental Theorem of Calculus we have

$$|z(t,x,\eta;\hbar)| \leq \big(|x|+|\eta|\big)\sup\{(|\partial_x|+|\partial_\eta|)(z(t,x,\eta;\hbar))\}.$$

From $x(t,z(t,x,\eta;\hbar),\eta;\hbar) = x$, we get

$$\partial_\eta z = -(\partial_z x)^{-1}\partial_\eta x.$$

Thus by (4.15), $|\partial_x z|+|\partial_\eta z| \leq 4$. Hence $|z(t,x,\eta;\hbar)| < 4(|x|+|\eta|) < 8C^{\frac{1}{2}}\hbar^{\frac{1-\tau}{2}}\delta^{\frac{1}{2}}$. This implies that for all $|t| \leq t_0$, $(x(s,z(t,x,\eta;\hbar),\eta;\hbar),\xi(s,z(t,x,\eta;\hbar),\eta;\hbar))$ will stay in a ball of radius $O(\hbar^{1-\tau})$ centered at the origin (this can be seen from the conservation of energy i.e. $H(x,\xi) = H(z,\eta)$). On the other hand, by definition (2.1), P and H agree in the ball $\{x^2+\eta^2 < \frac{1}{4}\hbar^{1-2\varepsilon}\}$ and $\tau < 2\varepsilon$. So for all $t,s \in (-t_0,t_0)$ and $(x,\eta) \in \{x^2+\eta^2 < C\hbar^{1-\tau}\delta\}$ we have

$$z_P(t,x,\eta) = z(t,x,\eta;\hbar),$$

(4.18)
$$x_P(s, z_P(t,x,\eta),\eta) = x(s, z(t,x,\eta;\hbar),\eta;\hbar),$$

$$\xi_P(s, z_P(t,x,\eta),\eta) = \xi(s, z(t,x,\eta;\hbar),\eta;\hbar),$$

where $z_P(t,x,\eta)$, $x_P(s, z_P(t,x,\eta),\eta)$ and $\xi_P(s, z_P(t,x,\eta),\eta)$ are corresponded to the Hamilton flow of P. Hence by (4.16) and a similar formula for φ_P, we have (4.17). This also shows that we can solve (4.9) in $(-t_0,t_0) \times \{x^2+\eta^2 < C\hbar^{1-\tau}\delta\}$.

To find b_H we assume it is of the form (4.10) and we search for functions $b_{H,j}$ such that $e^{-i\varphi_H/\hbar}(\frac{\hbar}{i}\partial_t + \hat{H})(e^{i\varphi_H/\hbar}b_H) \sim 0$. After some straightforward calculations and using the eikonal equation for φ_H we obtain the so called transport equations (4.11). Now let us solve the transport equations inductively (see [Ch]).

In [Ch] it is shown that the solutions to the transport equation (4.11) are given by

(4.19)
$$b_{H,0}(t,x,y,\eta,\hbar) = J^{-\frac{1}{2}}(t,x,\eta,\hbar) b_{H,0}(0, z(t,x,\eta;\hbar),\eta;\hbar), y,\eta,\hbar)$$

$$\begin{aligned} b_{H,j}(t,x,y,\eta,\hbar) = J^{-\frac{1}{2}}(t,x,\eta,\hbar)\Big(& b_{H,j}(0, z(t,x,\eta;\hbar),\eta;\hbar), y,\eta,\hbar) \\ & -\tfrac{1}{2}\int_0^t J^{\frac{1}{2}}(s,x,\eta,\hbar)\Delta b_{H,j-1}(s, x(s, z(t,x,\eta;\hbar),\eta;\hbar), y,\eta,\hbar)ds\Big). \end{aligned}$$

where

$$J(t,x,\eta,\hbar) = \det(\partial_x z(t,x,\eta;\hbar))^{-1}.$$

Now, we notice by the assumption on $\psi_\hbar$, we have $\mathrm{supp}(b_{H,j}(0,x,y,\eta;\hbar)) \subset \{x^2+\eta^2, x^2+\eta^2 < 4c^{-1}\hbar^{1-\tau}\delta\}$. So by our previous discussion on $z(t,x,\eta,\hbar)$, we can argue inductively that for all $t \in (-t_0,t_0)$, $\mathrm{supp}(b_{H,j}) \subset \{x^2+\eta^2, y^2+\eta^2 < C_1\hbar^{1-\tau}\delta\}$

for some constant C_1. Since $b_{H,j}|_{t=0} \in S^0_{\delta_0}$, we can also see inductively from (4.19) that $b_{H,j} \in S^0_{\delta_0}$. Finally, Borel's theorem produces a compactly supported amplitude $b_H \in S^0_{\delta_0}$ from the compactly supported functions $b_{H,j} \in S^0_{\delta_0}$. This finishes the proof of items $1, 2$ and 3 of Lemma 4.2.2.

Now we give a proof for item 4 of Lemma 4.2.2.

By choosing $C > C_1$, equation (4.12) is clearly true from (4.17). Next we prove that equation (4.13) holds. Using (4.3) and (4.6), and because P and H agree in the ball $\{x^2+\eta^2 < \frac{1}{4}\hbar^{1-2\varepsilon}\}$, we observe that the functions $a_{P,j}(x,\eta)$ and $a_{H,j}(x,\xi,\hbar)$ agree in this ball. Therefore, because $\text{supp}\psi_\hbar(x,\eta) \subset \{x^2+\eta^2 < 4c^{-1}\hbar^{1-\tau}\delta\}$ and $\psi_\hbar = 1$ in $\{x^2+\eta^2 < c\hbar^{1-\tau}\delta\}$, by (4.5) and (4.11)

$$b_{H,j}(0,x,y,\eta,\hbar) = b_{P,j}(0,x,y,\eta) \qquad \text{on} \quad \{(x,y,\eta);\, x^2+\eta^2,\ y^2+\eta^2 < c\hbar^{1-\tau}\delta\}.$$

This proves (4.13) only at $t = 0$. But by applying (4.18) to (4.19) and a similar formula for b_P, we get (4.13). This finishes the proof of Lemma 4.2.2.

To finish the proof of Lemma 2.1.1, we have to show that for t sufficiently small $TrU_H(t) = TrU_P(t) + O(\hbar^\infty)$, or equivalently

$$\int\int e^{i(\varphi_H(t,x,\eta,\hbar)-x.\eta)/\hbar} b_H(t,x,x,\eta,\hbar)dxd\eta = \int\int e^{i(\varphi_P(t,x,\eta)-x.\eta)/\hbar} b_P(t,x,x,\eta,\hbar)dxd\eta + O(\hbar^\infty).$$

By (4.12), the phase function φ_H of the double integral on the left hand side equals φ_P on the support of the amplitude b_H, so φ_H is independent of $\hbar$ in this domain. Now, if $t \in (0,t_0)$ where t_0 is smaller than the smallest non-zero period of the flows of P and H respectively in the energy balls

$$\{(x,\eta)|\ H(x,\eta)\leq \delta\hbar^{1-\tau}C_1\}\ \subset\ \{(x,\eta)|\ P(x,\eta)\leq\delta\},$$

then for every such t, $(x,\eta)=(0,0)$ is the only critical point of the phase functions $\varphi_H(t,x,\eta,\hbar)-x.\eta$ and $\varphi_P(t,x,\eta)-x.\eta$ in these energy balls.

Obviously both integrals in the equation above are convergent because their amplitudes are compactly supported. But the question is whether or not we can apply the stationary phase lemma to these integrals around their unique non-degenerate critical points. By Lemma 4.2.2 the phase functions φ_H and φ_P are independent of $\hbar$ on the support of their corresponding amplitudes. Hence $\varphi_H,\varphi_P\in S^0_0$ on $\operatorname{supp} b_H$ and $\operatorname{supp} b_P$ respectively. On the other hand $b_H(t,x,x,\eta,\hbar)\in S^0_{\delta_0}$, $\delta_0<\frac{1}{2}$; and $b_P(t,x,x,\eta,\hbar)\in S^0_0$. These facts can be used to get the required estimates for the remainder term in the stationary phase lemma (for an estimate for the remainder term of the stationary phase lemma, see for example Proposition 5.2 of [DSj]).

Finally, by (4.12) and (4.13) it is obvious that the integrals above must have the same stationary phase expansions.

Chapter 5

Appendix B

In this appendix we prove Lemma 2.1.2. In fact we prove that if $\Theta_\hbar$ is given by (4.1) then in the sense of tempered distributions

$$Tr(\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) = Tr(e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty). \tag{5.1}$$

Proof of Lemma 2.1.2 follows similarly.

We will use the min-max principle.

Min-max principle. Let H be a self-adjoint operator that is bounded from below, i.e. $H \geq cI$, with purely discrete spectrum $\{E_j\}_{j=0}^\infty$. Then

$$E_j = \sup_{\varphi_1,\dots,\varphi_{j-1}} \inf_{\substack{\psi \in D(H);\, \|\psi\|=1 \\ \psi \in \mathrm{span}(\varphi_1,\dots,\varphi_{j-1})^\perp}} (\psi, H\psi). \tag{5.2}$$

As before we put $\hat{H} = -\frac{1}{2}\hbar^2\Delta + V_\hbar(x) = -\frac{1}{2}\hbar^2\Delta + \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2 + W_\hbar(x)$, and $\hat{H}_0 = -\frac{1}{2}\hbar^2\Delta + \frac{1}{2}\sum_{k=1}^n \omega_k^2 x_k^2$. Then if we let $C = \|W_\hbar(x)\|_{L^\infty\left(\mathbb{R}^n\times(0,\hbar_0)\right)}$, we have

$$(\psi, \hat{H}_0\psi) - C \leq (\psi, \hat{H}\psi) \leq (\psi, \hat{H}_0\psi) + C,$$

and therefore by applying the min-max principle to the operators $\hat{H}$ and $\hat{H}_0$ we get

$$E_j^0(\hbar) - C \leq E_j(\hbar) \leq E_j^0(\hbar) + C. \tag{5.3}$$

Notice we have explicit formulas for the eigenvalues $E_j^0(\hbar)$ of $\hat{H}_0$. They are given by the lattice points in the first quadrant of $\mathbb{R}^n$. More precisely

$$\sigma(\hat{H}_0) = \Big\{ E_{\vec{\gamma}}^0(\hbar) = \hbar\sum_{k=1}^n \omega_k(\gamma_k + \frac{1}{2});\ \ \gamma_k \in \mathbb{Z}^{\geq 0} \Big\}.$$

Since in the sense of tempered distributions

$Tr(\Theta_\hbar(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) = Tr(\chi_{[0,\delta\hbar^{1-\tau}]}(\hat{H})e^{\frac{-it}{\hbar}\hat{H}}) + O(\hbar^\infty);$ (see for example [Ca], Proposition 6),

to prove (5.1), it is clearly enough to show that for every φ in $S(\mathbb{R})$

$$\sum_{\{j;\, E_j(\hbar) > \delta\hbar^{1-\tau}\}} \hat{\varphi}(\frac{E_j(\hbar)}{\hbar}) = O(\hbar^\infty).$$

Since $\hat{\varphi}$ is in $S(\mathbb{R})$, for every $p \geq 0$ there exists a constant C_p such that

$$|\hat{\varphi}(x)| \leq C_p|x|^{-p}.$$

Hence by (5.3)

$$\varphi(\frac{E_j(\hbar)}{\hbar}) \leq C_p\Big|\frac{E_j(\hbar)}{\hbar}\Big|^{-p} \leq C_p\Big|\frac{E_j^0(\hbar) - C}{\hbar}\Big|^{-p}.$$

Again using (5.3) and because $C = \|W_\hbar(x)\|_{L^\infty\left(\mathbb{R}^n\times(0,\hbar_0)\right)} < A\hbar^{\frac{3}{2}-3\varepsilon} < \frac{\delta}{4}\hbar^{1-\tau}$ we get

$$\varphi(\frac{E_j(\hbar)}{\hbar}) \leq C_p(\frac{\delta\hbar^{1-\tau}-C}{\delta\hbar^{1-\tau}-2C})^p\Big|\frac{E^0_j(\hbar)}{\hbar}\Big|^{-p} < 2C_p\Big|\frac{E^0_j(\hbar)}{\hbar}\Big|^{-p}, \qquad \text{for } E_j(\hbar) > \delta\hbar^{1-\tau}.$$

Now let m be an arbitrary positive integer. So in order to prove the lemma it is enough to find a uniform bound for

$$A(\hbar) := \hbar^{-m} \sum_{\{\vec{\gamma};\ \sum\omega_k(\gamma_k+\frac{1}{2})>\frac{\delta\hbar^{1-\tau}-C}{\hbar}\}} |\sum_{k=1}^{n}\omega_k(\gamma_k+\frac{1}{2})|^{-p}.$$

By applying the geometric-arithmetic mean value inequality we get

$$A(\hbar) \leq n^{-p}\hbar^{-m} \sum_{\{\vec{\gamma};\ \sum\omega_k(\gamma_k+\frac{1}{2})>\frac{\delta\hbar^{1-\tau}-C}{\hbar}\}} |\prod_{k=1}^{n}\omega_k(\gamma_k+\frac{1}{2})|^{-p}$$

$$\leq n^{-p}\sum_{k=1}^{n}\Big\{\Big(\hbar^{-m}\sum_{\{\gamma_k\in\mathbb{Z}^{\geq 0};\ \omega_k(\gamma_k+\frac{1}{2})>\frac{\delta\hbar^{1-\tau}-C}{n\hbar}\}}|\omega_k(\gamma_k+\frac{1}{2})|^{-p}\Big)\prod_{k'\neq k}\Big(\sum_{\gamma_{k'}}|\omega_{k'}(\gamma_{k'}+\frac{1}{2})|^{-p}\Big)\Big\}.$$

We claim for p large enough there is a uniform bound for the sum on the right hand side of the above inequality. It is clear that if $p \geq 2$ then the series $\sum_{\gamma_{k'}}|\omega_{k'}(\gamma_{k'}+\frac{1}{2})|^{-p}$ is convergent. Also if for some γ_k we have $\omega_k(\gamma_k+\frac{1}{2}) > \frac{\delta\hbar^{1-\tau}-C}{n\hbar}$, then because $C = O(\hbar^{\frac{3}{2}-3\varepsilon})$, for $\hbar$ small enough we have $\big(\omega_k(\gamma_k+\frac{1}{2})\big)^{1/\tau} > (\frac{\delta}{2n})^{1/\tau}\frac{1}{\hbar}$. Thus

$$\sum_{\{\gamma_k\in\mathbb{Z}^{\geq 0};\ \omega_k(\gamma_k+\frac{1}{2})>\frac{\delta\hbar^{1-\tau}-C}{n\hbar}\}} \hbar^{-m}|\omega_k(\gamma_k+\frac{1}{2})|^{-p} \leq (\frac{2n}{\delta})^{m/\tau}\sum_{\gamma_k}|\omega_k(\gamma_k+\frac{1}{2})|^{\frac{m}{\tau}-p}.$$

So if we choose $p > \max\{\frac{m}{\tau}, 2\}$, then the sum on the right hand side is convergent and therefore we have a uniform bound for the sum on the left hand side and hence for $A(\hbar)$. This finishes the proof of (5.1).

Part II

Complex Zeros of $1D$ Schrödinger Operators

Chapter 6

Introduction

6.1 Motivation and Background

This part of the dissertation is concerned with the eigenvalue problem for a one-dimensional semi-classical Schrödinger operator

$$(6.1) \qquad (-h^2\frac{d^2}{dx^2} + V(x))\psi(x,h) = E(h)\psi(x,h), \qquad \psi(x,h) \in L^2(\mathbb{R}) \quad h \to 0^+$$

Using the spectral theory of the Shrödinger operators [BS], we know that if $\lim_{x\to\pm\infty} V(x) = +\infty$ then the spectrum is discrete and can be arranged in an increasing sequence $E_0(h) < E_1(h) < E_2(h) < \cdots \uparrow \infty$. Notice that each eigenvalue has multiplicity one. We let $\{\psi_n(x,h)\}$ be a sequence of eigenfunctions associated to $E_n(h)$. If we assume the potential $V(x)$ is a real polynomial of even degree with positive leading coefficient, then we can arrange the eigenvalues as above and the eigenfunctions $\psi_n(x,h)$ possess analytic continuations $\psi_n(z,h)$ to $\mathbb{C}$. Our interest is in the distribution of complex zeros of $\psi_n(z,h)$ as $h \to 0^+$ when an energy level E is fixed. The substitutions $\lambda = \frac{1}{h}$, and $q(x) = V(x) - E$ changes the eigenvalue problem (6.1) to the problem:

$$(6.2) \qquad y''(x,\lambda) = \lambda^2 q(x)y(x,\lambda), \qquad y(x,\lambda) \in L^2(\mathbb{R}), \qquad \lambda \to \infty.$$

Since $\lim_{x \to \pm\infty} q(x) = +\infty$, again the spectrum is discrete and can be arranged as

$$\lambda_0 < \lambda_1 < \lambda_2 < \cdots < \lambda_n \cdots \uparrow \infty. \tag{6.3}$$

We define the discrete measure Z_{λ_n} by

$$Z_{\lambda_n} = \frac{1}{\lambda_n} \sum_{\{z \mid y(z,\lambda_n)=0\}} \delta_z. \tag{6.4}$$

In this thesis we study the limits of weak* convergent subsequences of the sequence $\{Z_{\lambda_n}\}$ as $n \to \infty$. We say

$$Z_{\lambda_{n_k}} \longrightarrow Z, \quad \text{(in weak* sense)}$$

if for every test function $\varphi \in C_c^\infty(\mathbb{R}^2)$ we have

$$Z_{\lambda_{n_k}}(\varphi) \longrightarrow Z(\varphi).$$

We will call these weak limits, *the zero limit measures.* But before stating our results let us mention some background and motivation for the problem.

Form the classical Sturm-Liouville theory we know everything about the real zeros of solutions of (6.2). We know that on a classical interval (i.e. an interval where $q(x) < 0$), every real-valued solution $y(x, \lambda)$ of (6.2) (not necessarily L^2-solution) is oscillatory and becomes highly oscillatory as $\lambda \to \infty$. In fact the spacing between the real zeros on a classical interval, measured by the Ağmon metric, is $\frac{\pi}{\lambda}$. On the other hand there is at most one real zero on each connected forbidden interval where $q(x) > 0$. This shows that every limit Z in (6.5) has the union of classical intervals in its support.

It turns out that other than the harmonic oscillator $q(z) = z^2 - a^2$ where the eigenfunctions do not have any non-real zeros, the complex zeros are more complicated. It is easy to see that when $q(z) = z^4 + az^2 + b$, the eigenfunctions have infinitely many zeros on the imaginary axis. For $q(z) = z^4 \pm a^4$, Titchmarsh in [T] made a conjecture that all the non-real zeros are on the imaginary axis. This conjecture was proved by Hille in [H1]. In general one can only hope to study the asymptotics of large zeros of $y(z, \lambda)$ rather than finding the exact locations of zeros. The asymptotics of zeros of solutions to (6.2) for a fixed λ and large z, have been extensively studied mainly by E. Hille, R. Nevanlinna, H. Wittich and S. Bank (see [N], [W], [B]). But it seems the semi-classical limit of complex zeros has not been studied in the literature, at least not from the perspective that was mentioned in Theorem 6.2.1, which is closely related to the quantum limits of eigenfunctions. This problem was raised around fifteen years ago when physicists were trying to find a connection between eigenfunctions of quantum systems and the dynamics of the classical system. It was noticed that for the ergodic case the complex zeros tend to distribute uniformly in the phase space but for the integrable systems the zeros tend to concentrate on one-dimensional lines. An article which made this point and contains very interesting graphics is [LV]. The problem of complex zeros of complexified eigenfunctions and relations to quantum limits is suggested by S. Zelditch mainly in [Z5]. There, the author proves that if a sequence $\{\varphi_{\lambda_n}\}$ of eigenfunctions of the Laplace-Beltrami operator on a real analytic manifold M is quantum ergodic then the sequence $\{Z_{\lambda_n}\}$ of zero distributions associated to the complexified eigenfunctions $\{\varphi^{\mathbb{C}}_{\lambda_n}\}$ on $M^{\mathbb{C}}$, the complexification of M, is weakly convergent to an explicitly calculable measure. A natural problem is to generalize the results in [Z5] for Schrödinger eigenfunctions on real analytic manifolds. This is indeed a difficult problem. Perhaps the first step to study such a problem is to consider the one dimensional case which we do in this paper. The main reason to study the complex zeros rather than the real zeros is that the problem is much easier in this case (in higher dimensions). For example in studying the zeros of polynomials as a model for eigenfunctions, the Fundamental Theorem of Algebra and Hilbert's Nullstellensatz are two good examples of how the complex zeros are easier and somehow richer. See [Z6] for some background of the problem and some motivation in higher dimensions.

6.2 Statement of results

Throughout this part of the thesis we assume that $q(z)$ has simple zeros. We may be able to extend the results in the case of multiple turning points using the methods in [F1, O2] on the asymptotic expansions around multiple turning points. Notice that $q(x)$ has to change its sign on the real axis, because if it is positive everywhere then (6.2) does not have any solution in $L^2(\mathbb{R})$. Hence $q(z)$ has at least two simple real zeros. We say $q(x)$ is a one-well potential if it has exactly two (simple) real zeros and a double-well potential if it has exactly four (simple) real zeros. One of our results is

THEOREM **6.2.1.** *Let $q(z)$ be a real polynomial of even degree with positive leading coefficient. Then every weak limit Z (zero limit measure) of the sequence $\{Z_{\lambda_n}\}$ is of the form*

$$Z = \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma|, \tag{6.5}$$

$$|d\gamma| = |\gamma'(t)|\,dt,$$

where γ is a union of finitely many smooth connected curves γ_m in the plane. For each γ_m there exists a constant c_m, a canonical domain D_m and a turning point z_m on the boundary of D_m such that γ_m is given by

$$\Re(S(z_m, z)) = c_m, \qquad z \in D_m, \tag{6.6}$$

where $S(z_m, z) = \int_{z_m}^{z} \sqrt{q(t)}\,dt$ and the integral is taken along any path in D_m joining z_m to z.

This theorem shows that if Z in (6.5) is the limit of a subsequence $\{Z_{\lambda_{n_k}}\}$, then the complex zeros of $\{y(z, \lambda_{n_k})\}$ tend to concentrate on γ as $k \to \infty$ and in the limit they cover γ. The factor $|\sqrt{q(z)}| = |\sqrt{V(z) - E}|$ indicates that the limit distribution of the zeros on γ is measured by the Ağmon metric. We call the curves γ_m the *zeros lines* of the limit Z. The next question after seeing Theorem 6.2.1 is "what are all the possible zero limit measures and corresponding zero lines for a given polynomial $q(z)$?" We answer this question for some one-well and double-well potentials.

One of our results is that for a symmetric quartic oscillator the full sequence $\{Z_{\lambda_n}\}$ is convergent, i.e. there is a unique zero limit measure. Here, by $q(z)$ being symmetric we mean that after a translation on the real axis, q(z) is an even function. But for a non-symmetric quartic oscillator there are at least two zero limit measures. The Stokes lines play an important role in the description of the zero lines. In fact the infinite zero lines are asymptotic to Stokes lines. This fact was observed in [B].

Our proofs are elementary. We use the complex WKB method, connection formulas and asymptotics of the eigenvalues by Fedöryuk in [F1].

At the end of this manuscript (§8.4) we will briefly mention some interesting examples of one-well and double-well potentials where $\deg(q(z)) = 4, 6$.

Theorem **6.2.2.** *Let $q(z) = (z^2 - a^2)(z^2 - b^2)$, where $0 < a < b$. Then as $n \to \infty$*

$$Z_{\lambda_n} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma|, \qquad \gamma = (a, b) \cup (-b, -a) \cup (-\infty i, +\infty i).$$

Notice in Theorem 6.2.2 we can express γ by three equations

$$\gamma = \{\Re S(a, z) = 0\} \cup \{\Re S(-a, z) = 0\} \cup \{\Re S(a, z) = -\frac{1}{2}\xi\},$$

where $\xi = \int_{-a}^{a} \sqrt{q(t)}\,dt$, and each equation is written in some canonical domain.

Theorem **6.2.3.** *Let $q(z) = (z^2 - a^2)(z^2 + b^2)$, where $a, b > 0$. Then as $n \to \infty$*

$$Z_{\lambda_n} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma|, \qquad \gamma = (-a, a) \cup (bi, +\infty i) \cup (-\infty i, -bi).$$

We also note that in Theorem 6.2.3 we can express γ by three equations

$$\gamma = \{\Re S(a,z) = 0\} \cup \{\Re S(bi,z) = 0\} \cup \{\Re S(-bi,z) = 0\},$$

where each equation is written in some canonical domain.

Theorems 6.2.2 and 6.2.3 state that for a symmetric quartic polynomial there is a unique zero limit measure. This is not always the case when $q(z)$ is not symmetric. Let $q(z) = (z-a_0)(z-a_1)(z-a_2)(z-a_3)$ where $a_0 < a_1 < a_2 < a_3$. Using the quantization formulas (for example in [S, F1]), we have two sequences of eigenvalues

$$\lambda_n^{(1)} = \frac{2n+1}{2\alpha_1}\pi + O(\frac{1}{n}), \qquad \alpha_1 = \int_{a_0}^{a_1} |\sqrt{q(t)}|dt, \tag{6.7}$$

$$\lambda_n^{(2)} = \frac{2n+1}{2\alpha_2}\pi + O(\frac{1}{n}), \qquad \alpha_2 = \int_{a_2}^{a_3} |\sqrt{q(t)}|dt. \tag{6.8}$$

Now with this notation we have the following theorem:

THEOREM **6.2.4.** *Let $q(z) = (z-a_0)(z-a_1)(z-a_2)(z-a_3)$, where $a_0 < a_1 < a_2 < a_3$ are real numbers. Then*

1. *if $\frac{\alpha_1}{\alpha_2}$ is irrational then for each $\ell \in \{1,2\}$ there is a full density subsequence $\{\lambda_{n_k}^{(\ell)}\}$ of $\{\lambda_n^{(\ell)}\}$ such that*

$$Z_{\lambda_{n_k}^{(\ell)}} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma_\ell|\,,$$

where

$$\begin{aligned}\gamma_1 &= (a_0,a_1) \cup (a_2,a_3) \cup \{\Re(S(a_2,z) = 0\},\\ \gamma_2 &= (a_0,a_1) \cup (a_2,a_3) \cup \{\Re(S(a_1,z) = 0\}.\end{aligned} \tag{6.9}$$

2. *if $\frac{\alpha_1}{\alpha_2}$ is rational and of the form $\frac{2r_1}{2r_2+1}$ or $\frac{2r_1+1}{2r_2}$ then for each $\ell \in \{1,2\}$*

$$Z_{\lambda_n^{(\ell)}} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma_\ell|.$$

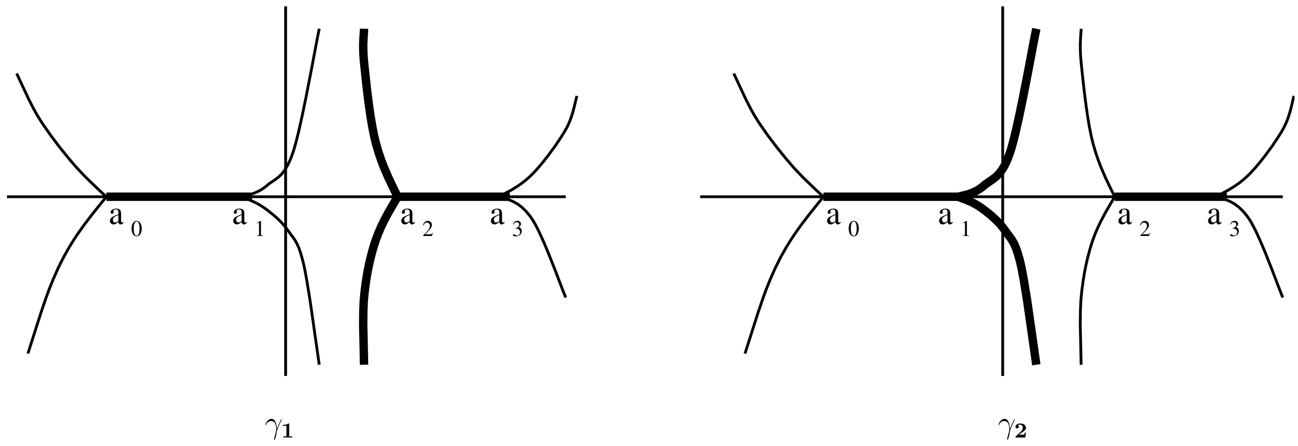


Figure 6.1: The zero lines of the non-symmetric quartic oscillator. The thick lines are the zeros lines γ_1 and γ_2 given by (6.9).

3. *if* $\frac{\alpha_1}{\alpha_2}$ *is rational and of the form* $\frac{2r_1+1}{2r_2+1}$ *where* $\gcd(2r_1+1, 2r_2+1) = 1$*, then for each* $\ell \in \{1, 2\}$ *there exists a subsequence* $\{\lambda^{(\ell)}_{n_k}\}$ *of* $\{\lambda^{(\ell)}_n\}$ *of density* $\frac{2r_\ell}{2r_\ell+1}$ *such that*

$$Z_{\lambda^{(\ell)}_{n_k}} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma_\ell|.$$

In fact $\{\lambda^{(\ell)}_{n_k}\} = \{\lambda^{(\ell)}_n | 2n+1 \neq 0 \ (mod\, 2r_\ell + 1)\}$.

Figure (6.1) shows the zero lines γ_1 and γ_2 defined in (6.9). As we see in this case the zero lines are made of Stokes lines. We should mention that in Theorem 6.2.4, when $\frac{\alpha_1}{\alpha_2}$ is irrational or of the form $\frac{2r_1+1}{2r_2+1} \neq 1$, we do not know what happens to the rest of the subsequences. There might be some exceptional subsequences (of positive density in the case $\frac{\alpha_1}{\alpha_2} = \frac{2r_1+1}{2r_2+1}$) for which the zero lines are different from γ_ℓ. As we saw in Theorem 6.2.2, this is the case for the symmetric double-well potential when $\frac{\alpha_1}{\alpha_2} = 1$. We probably need a more detailed analysis of the eigenvalues in order to answer this question.

6.3 Results of Eremenko, Gabrielov and Shapiro

Here we mention some recent results of A. Eremenko, A. Gabrielov, B. Shapiro in [EGS1] and [EGS2], and compare them to ours as their interests and their approach are very similar to ours.

1. Theorems 6.2.2 and 6.2.3 do not say anything about the exact location of the zeros but they only state that as $n \to \infty$ the zeros approach to γ with the distribution law in [6.5]. It is easy to see that for both of these symmetric cases, for each n, all the zeros of $y(z, \lambda_n)$ except finitely many of them lie on γ. In [EGS1], the authors prove that for the solutions of the equation

$$-y'' + P(x)y = \lambda y, \qquad y \in L^2(\mathbb{R}), \tag{6.10}$$

where $P(x)$ is an even real monic polynomial of degree 4, all the zeros of $y(z)$ belong to the union of the real and imaginary axis. This result indeed implies that for all n, all the zeros of $y(z, \lambda_n)$ in Theorem 6.2.2 and Theorem 6.2.3 are on the corresponding γ.

2. In [EGS2], the authors show that the complex zeros of the scaled eigenfunctions $Y_n(z) = y(\lambda_n^{1/d} z)$ of (6.10), where d =degree($P(x)$), have a unique limit distribution in the complex plane as $\lambda_n \to \infty$. The scaled eigenfunctions satisfy an equation of the form

$$Y_n''(z) = k_n^2(z^d - 1 + o(1))Y_n(z), \qquad k_n \to \infty.$$

The main reason that they could establish a uniqueness result for the limit distribution of complex zeros of $Y_n(z)$ is due the special structure of the Stokes graph of the polynomial $z^d - 1$ which is proved in Theorem 1 in [EGS2].

Chapter 7

Background on Complex WKB Method

In this chapter we review some basic definitions and facts about complex WKB method. We follow [F1]. See [O1, S, EF] for more references on this subject.

We consider the equation

$$y''(z, \lambda) = \lambda^2 q(z) y(z, \lambda), \qquad \lambda \to \infty, \tag{7.1}$$

on the complex plane $\mathbb{C}$, where $q(z)$ is a polynomial with simple zeros.

7.1 Stokes lines and Stokes graphs

A zero z_0, of $q(z)$ is called a turning point. We let $S(z_0, z) = \int_{z_0}^{z} \sqrt{q(t)}dt$. This function, is in general, a multi-valued function. The maximal connected component of the level curve $\Re(S(z_0, z)) = 0$ with initial point z_0 and having no other turning points are called the Stokes lines starting from z_0. Stokes lines are independent of the choice of the branches for $S(z_0, z)$. The union of the Stokes lines of all the turning points is called the Stokes graph of (7.1).

Figure (7.1) shows the Stokes graphs of many polynomials.

Since the turning points are simple, from each turning point three Stokes lines emanate with equal angles. In general if z_0 is a turning point of order n, then $n+2$ Stokes lines with equal angles emanate from z_0.

7.2 Canonical Domains, Asymptotic Expansions of Eigenfunctions

Since $q(z)$ is a polynomial, the Stokes graph divides the complex plane into two type of domains:

1. Half-plane type: A simply connected domain D which is bounded by Stokes lines is a half-plane type domain if under the map $S = S(z_0, z)$, it is biholomorphic to a half-plane of the form $\Re S > a$ or $\Re S < a$. Here z_0 is a turning point on the boundary of D.

2. Band-type: D as above, is of band-type if under S, it is biholomorphic to a band of the form $a < \Re S < b$.

A domain D in the complex plane is called canonical if $S(z_0, z)$ is a one-to-one map of D onto the whole complex plane with finitely many vertical cuts such that none cross the real axis. A canonical domain is the union of two half-plane type domains and some band type domains. For example, the union of two half-plane type domains sharing a Stokes line is a canonical domain.

Let $\varepsilon > 0$ be arbitrary. We denote D^ε for the pre-image of $S(D)$ with ε-neighborhoods of the cuts and ε-neighborhoods of the turning points removed. A canonical path in D is a path such that $\Re(S)$ is monotone along the path. For example, the anti-Stokes lines (lines where, $\Im(S) = 0$), are canonical paths. For every

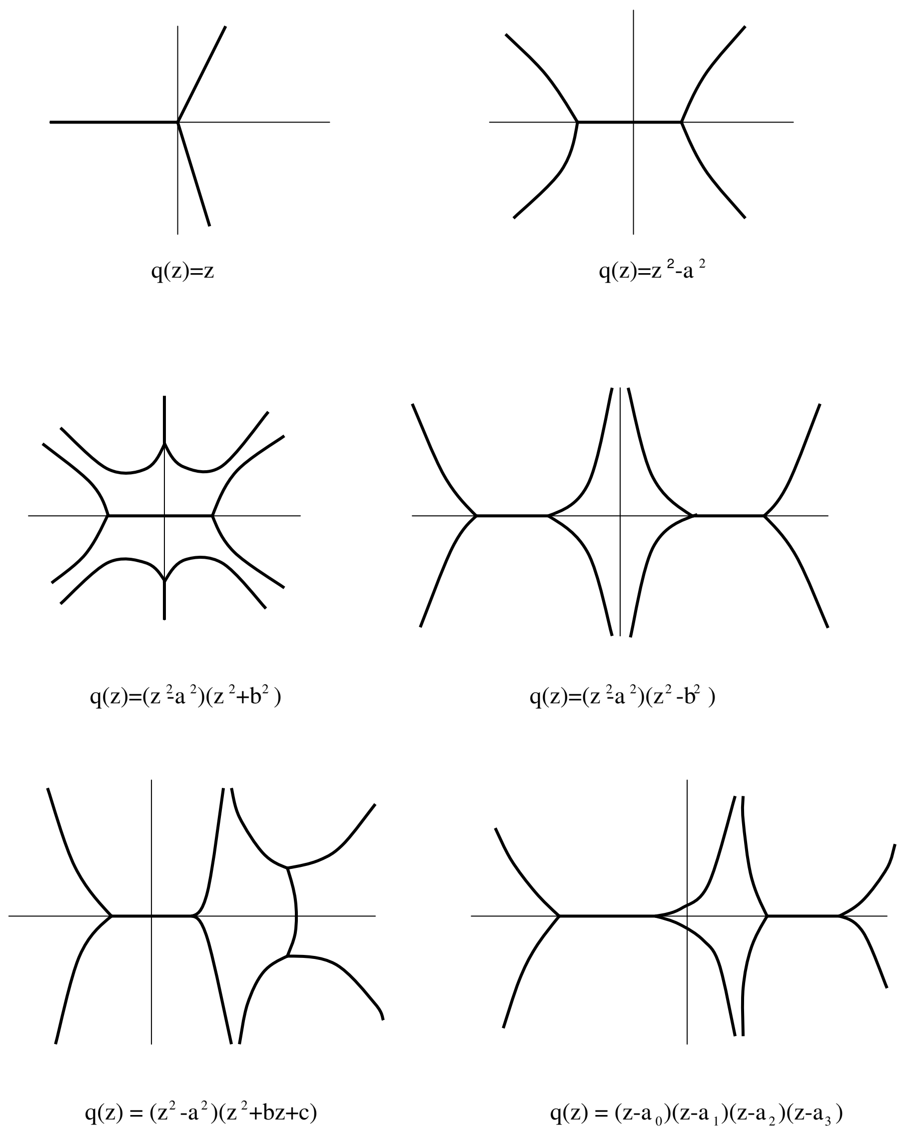


Figure 7.1: Stokes lines for some polynomials

point z in D^ε, there are always canonical paths $\gamma^-(z)$ and $\gamma^+(z)$ from z to ∞, such that $\Re S \downarrow -\infty$ and $\Re S \uparrow \infty$, respectively.

Now we have the following fact:

With D, γ^+, γ^- as above, to within a multiple of a constant, equation (7.1) has a unique solution $y_1(z, \lambda)$, such that

$$\lim_{z\to\infty, z\in\gamma^-} y_1(z,\lambda) = 0, \qquad \Re S(z_0, z) \downarrow -\infty, \tag{7.2}$$

and a unique solution $y_2(z, \lambda)$ (up to a constant multiple), such that

$$\lim_{z\to\infty, z\in\gamma+} y_2(z,\lambda) = 0, \qquad \Re S(z_0, z) \uparrow \infty. \tag{7.3}$$

The solutions y_1 and y_2 in (7.2) and (7.3) have uniform asymptotic expansions in D^ε in powers of $\frac{1}{\lambda}$. Here we only state the principle terms:

$$y_1(z,\lambda) = q^{\frac{-1}{4}}(z)e^{\lambda S(z_0,z)}(1 + \varepsilon_1(z,\lambda)) \qquad \lambda \to \infty, \tag{7.4}$$

$$y_2(z,\lambda) = q^{\frac{-1}{4}}(z)e^{-\lambda S(z_0,z)}(1 + \varepsilon_2(z,\lambda)) \qquad \lambda \to \infty, \tag{7.5}$$

where

$$\varepsilon_1(z,\lambda) = O(\frac{1}{\lambda}), \qquad \text{uniformly in } D^\varepsilon, \quad \lambda \to \infty, \tag{7.6}$$

$$\varepsilon_2(z,\lambda) = O(\frac{1}{\lambda}), \qquad \text{uniformly in } D^\varepsilon, \quad \lambda \to \infty. \tag{7.7}$$

Notice that the equalities (7.6) and (7.7) would not necessarily be uniformly in D^ε if $q(z)$ was not a polynomial.

7.3 Elementary Basis

Let D be a canonical domain, l a Stokes line in D, and $z_0 \in l$ a turning point. We use the triple (D, l, z_0) to denote this data. We select the branch of $S(z_o, z)$ in D

such that $\Im S(z_0, z) > 0$ for $z \in l$. The elementary basis $\{u(z), v(z)\}$ associated to (D, l, z_0) is uniquely defined by

$$
(7.8) \qquad \begin{cases} u(z,\lambda) = c y_1(z,\lambda), \quad \text{and} \quad v(z,\lambda) = c y_2(z,\lambda), \\ \\ |c| = 1, \text{ and } \arg(c) = \lim_{z \to z_0, z \in l} \arg(q^{1/4}(z)), \end{cases}
$$

where $y_1(z, \lambda)$, $y_2(z, \lambda)$ are given by (7.4) and (7.5).

7.4 Transition Matrices

Assume $(D, l, z_0)_j$ and $(D, l, z_0)_k$ are two triples and $\beta_j = \{u_j, v_j\}$ and $\beta_k = \{u_k, v_k\}$ their corresponding elementary basis. The matrix $\Omega_{jk}(\lambda)$ which changes the basis β_j to β_k is called the transition matrix from β_j to β_k.

Fedöryuk, in [EF], introduced three types of transition matrices that he called elementary transition matrices, and he proved that any transition matrix is a product of a finitely many of these elementary matrices. The three types are

1) $(D, l, z_1) \mapsto (D, l, z_2)$. This is the transition from one turning point to another along a finite Stokes line remaining in the same canonical domain D. The transition matrix is given by

$$
(7.9) \qquad \Omega(\lambda) = e^{i\varphi} \begin{pmatrix} 0 & e^{-i\lambda\alpha} \\ e^{i\lambda\alpha} & 0 \end{pmatrix}, \qquad \alpha = |S(z_1, z_2)|, \quad e^{i\varphi} = \frac{c_2}{c_1}.
$$

2) $(D, l_1, z_1) \mapsto (D, l_2, z_2)$. Here the rays $S(l_1)$ and $S(l_2)$ are directed to one side. This is the transition from one turning point to another along an anti-Stokes line, remaining in the same domain D. The transition matrix is

$$
(7.10) \qquad \Omega(\lambda) = e^{i\varphi} \begin{pmatrix} e^{-\lambda a} & O \\ 0 & e^{\lambda a} \end{pmatrix}, \qquad a = |S(z_1, z_2)|, \quad e^{i\varphi} = \frac{c_2}{c_1}.
$$

3) $(D_1, l_1, z_0) \mapsto (D_2, l_2, z_0)$ This is a simple rotation around a turning point z_0 so that D_1 and D_2 have a common sub-domain. More precisely, let $\{l_j; j = 1, 2, 3\}$ be the Stokes lines starting at z_0 and ordered counter-clockwise so that l_{j+1} is located on the left side of l_j. We choose the canonical domain D_j so that the part of D_j on the left of l_j equals the part of D_{j+1} on the right of l_{j+1}. Then

$$\text{(7.11)} \qquad \begin{cases} \Omega_{j,j+1}(\lambda) = e^{-\frac{\pi}{6}} \begin{pmatrix} 0 & \alpha_{j,j+1}^{-1}(\lambda) \\ 1 & i\alpha_{j+1,j+2}(\lambda) \end{pmatrix}, \\ \\ \alpha_{j,j+1}(\lambda) = 1 + O(\frac{1}{\lambda}), \quad 1 \leq j \leq 3, \\ \\ \alpha_{1,2}(\lambda)\alpha_{2,3}(\lambda)\alpha_{3,1}(\lambda) = 1, \quad \text{and} \quad \alpha_{j,j+1}(\lambda)\alpha_{j+1,j}(\lambda) = 1. \end{cases}$$

7.4.1 Polynomials with real coefficients

We finish this section with a review of some properties of the Stokes lines and transition matrices in (7.11) when the polynomial $q(z)$ has real coefficients.

1) The turning points and Stokes lines are symmetric about the real axis. If $x_1 < x_2$ are two real turning points and $q(x) < 0$ on the line segment $l = [x_1, x_2]$, then l is a Stokes line (See Figure 7.1). Similarly, if $q(x) > 0$ on l, then l is an anti-Stokes line. Let x_0 be a simple turning point on the real axis, and let l_0, l_1, l_2 be the Stokes lines starting at x_0. Then one of the Stokes lines, say l_0, is an interval of the real axis, and $l_2 = \bar{l_1}$. The Stokes lines l_1 and l_2 do not intersect the real axis other than at the point x_0. If a Stokes line l intersects the real axis at a non-turning point, then l is a finite Stokes line and it is symmetric about the real axis.

   If $\lim_{x\to\infty} q(x) = \infty$, and x^+ is the the largest zero of $q(x)$, and l_0, l_1, l_2 are the corresponding Stokes lines, then there is a half type domain D^+ such that

$$[x^+, +\infty] \subset D^+, \qquad D^+ = \overline{D^+}, \quad l_1 \cup l_2 \subset \partial D^+.$$

Clearly $[x_0, +\infty]$ is an anti-Stokes line and $S(x_0, \infty) = \infty$. By (7.2), there exists a unique solution $y^+(z, \lambda)$ such that

$$\lim_{x \to \infty} y^+(x, \lambda) = 0.$$

Similarly by (7.3) if $\lim_{x \to -\infty} q(x) = \infty$ and x^- is the smallest root of $q(x)$, and D^- a half type domain containing $[-\infty, x_0]$, there exists a unique solution $y^-(z, \lambda)$ such that

$$\lim_{x \to -\infty} y^-(x, \lambda) = 0.$$

Therefore if $y(x, \lambda)$ is an L^2-solution to (6.2) , then for some constants c^+, c^-

$$y(x, \lambda) = c^+ y^+(x, \lambda) = c^- y^-(x, \lambda).$$

Now let $\Omega_{+,-}(\lambda)$ be the transition matrix connecting D^+ to D^- and let

$$\begin{pmatrix} a(\lambda) \\ b(\lambda) \end{pmatrix} = \Omega_{+,-}(\lambda) \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The fact that $y^+(x, \lambda)$ is a constant multiple of $y^-(x, \lambda)$ is equivalent to

$$b(\lambda) = 0, \tag{7.12}$$

which is the equation that determines the eigenvalues λ_n. To calculate $\Omega_{+,-}(\lambda)$ and hence $b(\lambda)$ we have to write this matrix as a product of finitely many elementary transition matrices connecting D^+ to D^-.

2) When the polynomial $q(z)$ has real coefficients, the transitions matrices in (7.11) have some symmetries. Let x_0 be a simple turning point and $q(x) > 0$ on the

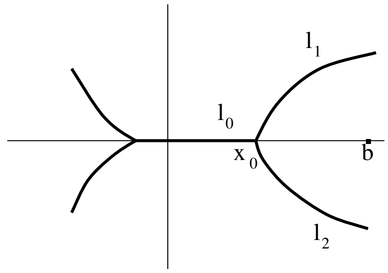


Figure 7.2:

interval $[x_0, b]$. We index the Stokes lines l_0, l_1, l_2 as in Figure (7.13). We define the canonical domains D_0, D_1, D_2 by their internal Stokes lines and their boundary Stokes lines as the following

$$D_0 = \overline{D_0}, \qquad l_0 \subset D_0, l_1 \cup l_2 \subset \partial D,$$

$$[x_0, b] \subset D_1, \qquad l_0 \cup l_2 \subset \partial D_1,$$

$$D_2 = \overline{D}_1.$$

Now with the same notation as in (7.11), we have

$$\alpha_{0,1} = \overline{\alpha_{0,2}}, \qquad |\alpha_{1,2}| = 1. \tag{7.13}$$

Chapter 8

Proofs of Results

8.1 The complex zeros in a canonical domain D

The following lemma determines how the complex zeros are distributed in a canonical domain:

LEMMA **8.1.1.** *Let $T = (D, l, z_0)$ be a triple as in §7.3 and let $\{u(z,\lambda), v(z,\lambda)\}$ be the elementary basis associated to T in (7.8). We write $y(z,\lambda_n)$ in this basis as*

$$y(z,\lambda_n) = a(\lambda_n)u(z,\lambda_n) + b(\lambda_n)v(z,\lambda_n). \tag{8.1}$$

If $\{\lambda_{n_k}\}$ is a subsequence of $\{\lambda_n\}$ such that the limit

$$t = \lim_{k\to\infty} \frac{1}{2\lambda_{n_k}} \log |\frac{b(\lambda_{n_k})}{a(\lambda_{n_k})}|, \tag{8.2}$$

exists, then in D^ε we have

$$Z_{\lambda_{n_k}} \longrightarrow \frac{1}{\pi}|\sqrt{q(z)}|\,|d\gamma|, \qquad \gamma = \{z \in D|\, \Re S(z_0, z) = t\}.$$

The last expression means that for every $\varphi \in C_c^\infty(D^\varepsilon)$ we have

$$Z_{\lambda_{n_k}}(\varphi) \to \frac{1}{\pi}\int_\gamma \varphi(z)|\sqrt{q(z)}||d\gamma|.$$

Proof of Lemma. For simplicity we omit the subscript n_k in λ_{n_k}, but we remember that the limit in (8.2) is taken along λ_{n_k}. Using (8.1), (7.8), (7.4), and (7.5), the equation $y(z,\lambda)=0$ in D^ε, is equivalent to

(8.3)
$$S(z_0,z)-\frac{1}{2\lambda}\log(\frac{1+\varepsilon_1(z,\lambda)}{1+\varepsilon_2(z,\lambda)})=\frac{1}{2\lambda}\log\mid\frac{b(\lambda)}{a(\lambda)}\mid+i(\frac{2k+1}{2\lambda}\pi+\frac{1}{2\lambda}\arg(\frac{b(\lambda)}{a(\lambda)})),\qquad k\in\mathbb{Z}.$$

where we have chosen $\log z=\log r+i\theta$, $-\pi<\theta<\pi$. We use $\tilde{S}(z)$ for the function on the left hand side of (8.3) and a_k for the sequence of complex numbers on the right hand side. As we see $\tilde{S}(z)$ is the sum of the biholomorphic function $S(z_0,z)$ and the function

(8.4)
$$\mu(z,\lambda):=-\frac{1}{2\lambda}\log(\frac{1+\varepsilon_1(z,\lambda)}{1+\varepsilon_2(z,\lambda)})=O(\frac{1}{\lambda^2}),\qquad \text{uniformly in } D^\varepsilon,\ \text{by (7.6), (7.7)}.$$

Now suppose $\varphi\in C_c^\infty(D^\varepsilon)$ and $K=\mathrm{supp}(\varphi)$. We also define $K'=S(K)$ where $S(z)=S(z_0,z)$. Without loss of generality we can assume that $\{x=t\}\cap\mathrm{int}(K')$ is a connected subset of the vertical line $x=t$, because we can follow the same argument for each connected component. Now let $s=\mathrm{length}(\{x=t\}\cap\mathrm{int}(K'))$. It is clear that because of (8.2)

$$N:=\#\{\,a_k\in\mathrm{int}(K')\}\sim s\lambda. \tag{8.5}$$

We call this finite set $\{a_k\}_{m+1\le k\le m+N}$. Now let $K\subset V\subset D^\varepsilon$ be an open set with compact closure in D^ε. We choose λ large enough such that

$$|\mu(z,\lambda)|<|S(z_0,z)-a|\qquad\forall\,a\in K',\quad\forall\,z\in\partial V.$$

Since S is a biholomorphic map, by Rouché's theorem the equation

$$\tilde{S}(z)=a_k,\qquad m+1\le k\le m+N,$$

has a unique solution z_k in V for each k. Now by (8.2), (8.3), and (8.4), we have

$$z_k=S^{-1}\Big(\frac{1}{2\lambda}\log\mid\frac{b(\lambda)}{a(\lambda)}\mid-\mu(z_k,\lambda)+i\big(\frac{2k+1}{2\lambda}\pi+O(\frac{1}{\lambda})\big)\Big)$$

$$= S^{-1}\Big(t + o(1) + i\big\{\frac{2k+1}{2\lambda}\pi - \Im\big(\mu(z_k,\lambda)\big) + O(\frac{1}{\lambda}))\big\}\Big).$$

It follows that

$$Z_\lambda(\varphi) = \frac{1}{\lambda}\sum_{k=m+1}^{m+N}\varphi(z_k) = \frac{1}{\lambda}\sum_{k=m+1}^{m+N}(\varphi\circ S^{-1})\Big(t+o(1)+i\big\{\frac{2k+1}{2\lambda}\pi-\Im\big(\mu(z_k,\lambda)\big)+O(\frac{1}{\lambda}))\big\}\Big).$$

Using the mean value theorem on the $x-$axis and (8.5), we obtain

(8.6)

$$\lim_{\lambda\to\infty} Z_\lambda(\varphi) = \lim_{\lambda\to\infty}\frac{1}{\lambda}\sum_{k=m+1}^{m+N}\big\{\Big[(\varphi\circ S^{-1})\Big(t+i\big\{\frac{2k+1}{2\lambda}\pi-\Im\big(\mu(z_k,\lambda)\big)+O(\frac{1}{\lambda}))\big\}\Big]+o(1)\big\}.$$

Because of (8.4), we know that $\Im(\mu(z_k,\lambda)) = O(\frac{1}{\lambda^2})$ uniformly in k. Also the term $O(\frac{1}{\lambda})$ is independent of k. Therefore the set

$$\wp = \{(t, \frac{2k+1}{2\lambda}\pi - \Im(\mu(z_k,\lambda)) + O(\frac{1}{\lambda}))|\ m+1 \leq k \leq m+N\}$$

is a partition of the vertical interval $\{x = t\} \cap \operatorname{int}(K')$ with $\operatorname{mesh}(\wp) \to 0$ as $\lambda \to \infty$. This together with (8.6) implies that

$$\lim_{\lambda\to\infty} Z_\lambda(\varphi) = \frac{1}{\pi}\int_{\{x=t\}} \varphi\circ S^{-1}dy.$$

Now, if in the last integral we apply the change of variable $z \mapsto S(z)$, then by the Cauchy-Riemann equations for S, we obtain

$$\frac{1}{\pi}\int_{\{x=t\}}\varphi\circ S^{-1}dy = \frac{1}{\pi}\int_{\{\Re S(z)=t\}}\varphi(z)|\sqrt{q(z)}|\,|d\gamma|.$$

This proves the Lemma.

8.2 Zeros in the complex plane and the proof of Theorem 6.2.1

First of all, we cover the plane by finitely many canonical domains D_m. Let $\varepsilon > 0$ be sufficiently small as before. Assume $\{Z_{\lambda_{n_k}}\}$ is a weak* convergent subsequence converging to a measure Z. Clearly $\{Z_{\lambda_{n_k}}\}$ converges to Z in each D^{ε}_m. We claim that the limit (8.2) exists for every triple $T_m = (D_m, z_m, l_m)$. This is clear from Lemma 8.1.1. This is because if in (8.2) we get two distinct limits t_1 and t_2 for two subsequences of $\{Z_{\lambda_{n_k}}\}$, then we get two corresponding distinct limits Z_1 and Z_2 which contradicts our assumption about $\{Z_{\lambda_{n_k}}\}$. We should also notice that if in (8.2), $t = \pm\infty$ then in the proof of Lemma 8.1.1 for λ large enough we have $\{x = \frac{1}{2\lambda}\log|\ \frac{b(\lambda)}{a(\lambda)}\ |\} \cap \mathrm{int}(K') = \emptyset$, and therefore $Z|_{D^{\varepsilon}_m} = 0$. This means that we do not obtain any zero lines in this canonical domain. In other words the zeros run away from this canonical domain as $\lambda \to \infty$. But as we mentioned in the introduction, all the Stokes lines on the real axis are contained in the set of zero lines of every limit Z, meaning that in Theorem 6.2.1, γ is never empty.

Now notice that because $\bigcup_m D^{\varepsilon}_m$ covers the plane except the ε-neighborhoods around the turning points, we have proved that

$$Z(\varphi) = \tfrac{1}{\pi}\int_{\gamma} \varphi(z)|\sqrt{q(z)}|\,|d\gamma|, \qquad \varphi \in C^{\infty}_c(\mathbb{C}\backslash \textstyle\bigcup_m B(z_m, \varepsilon)).$$

8.2.1 Complex zeros near the turning points

To finish the proof we have to show that if $\varphi_{\varepsilon} \in C^{\infty}_c(\bigcup_m B(z_m, \varepsilon))$ is a bounded function of ε, then

$$\lim_{\varepsilon\to 0}\limsup_{\lambda_{n_k}\to\infty} Z_{\lambda_{n_k}}(\varphi_{\varepsilon}) = 0.$$

This is clearly equivalent to showing that if z_0 is a turning point, then

$$\lim_{\varepsilon\to 0}\limsup_{\lambda\to\infty} \frac{\#\{z \in B(z_0, \varepsilon)|\ y(z, \lambda) = 0\}}{\lambda} = 0. \tag{8.7}$$

To prove this we use the following fact in [F1] pages $104 - 105$ or [EF] pages $39 - 41$, which enables us to improve the domain D^{ε} in (7.6) and (7.7) from a fixed ε to $\varepsilon(\lambda)$

dependent of λ such that $\varepsilon(\lambda) \to 0$ as $\lambda \to \infty$.

Let D be a canonical domain with turning points z_m on its boundary. Assume $N(\lambda)$ is a positive function such that $N(\infty) = \infty$. Now if we denote

$$D(\lambda) = D \setminus \bigcup_m B(z_m, |q'(z_m)|^{-1/3} N(\lambda)\lambda^{-2/3}),$$

Then in place of equations (7.6) and (7.7) we have

$$\varepsilon_1(z,\lambda),\ \varepsilon_2(z,\lambda) = O(N(\lambda)^{-3/2}), \qquad \text{uniformly in } D(\lambda), \quad \lambda \to \infty.$$

In fact this implies that Lemma 8.1.1 is true for every φ supported in D. This is because we can follow the proof of the lemma line by line except that in (8.4) we get $\mu(z,\lambda) = O(N(\lambda)^{-3/2}\lambda^{-1})$ uniformly in $D(\lambda)$ and therefore, using $N(\infty) = \infty$, we can still conclude $\mathrm{mesh}(\wp) \to 0$ as $\lambda \to \infty$.

We choose $N(\lambda) = \lambda^{1/12}$. By the discussion in the last paragraph in (8.7) we can replace ε by $\varepsilon(\lambda) = cN(\lambda)\lambda^{-2/3} = c\lambda^{-7/12}$, where $c = |q'(z_0)|^{-1/3}$. Let us find a bound for the number of zeros of $y(z,\lambda)$ in $B(z_0, \varepsilon(\lambda))$. Let $M = \sup_{B(z_0,\delta)}(|q(z)|)$ where $\delta > 0$ is fixed and is chosen such that the ball $B(z_0, \delta)$ does not contain any other turning points. We also choose λ large enough so that $\varepsilon(\lambda) < \delta$. If ζ is a zero of $y(z,\lambda)$ in the ball $B(z_0, \varepsilon(\lambda))$ then by Corollary 11.1.1 page 579 of [H1] we know that there are no zeros of $y(z,\lambda)$ in the ball of radius $\frac{\pi}{\sqrt{M}}\lambda^{-1}$ around ζ except ζ. Therefore

$$\#\{z \in B(z_0, \varepsilon(\lambda)) |\ y(z,\lambda) = 0\} \leq \frac{\mathrm{area}(B(z_0, \varepsilon(\lambda) + \frac{\pi}{2\sqrt{M}}\lambda^{-1}))}{\mathrm{area}(B(\zeta, \frac{\pi}{2\sqrt{M}}\lambda^{-1}))} = O(\lambda^{5/6}),$$

and so

$$\lim_{\lambda\to\infty} \frac{\#\{z \in B(z_0, \varepsilon(\lambda)) |\ y(z,\lambda) = 0\}}{\lambda} = 0.$$

This finishes the proof of Theorem 6.2.1.

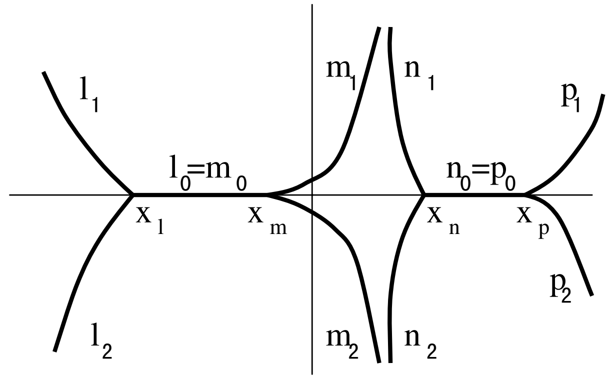


Figure 8.1:

8.3 Zeros for symmetric and non-symmetric double well potentials

In this section we give proofs for Theorems 6.2.2 and 6.2.4. We will not prove Theorem 6.2.3, because the proof is similar to (in fact easier than) the proof of the two well potential. To simplify our notations let us rename the turning points as $x_l = a_0, x_m = a_1, x_n = a_2, x_p = a_3$. Then we can index the Stokes lines as in Fig (8.1).

We define the canonical domains D_l, D_{m_0}, D, D_{n_0}, and D_p by

$$
\begin{aligned}
& l_1 \subset D_l, \qquad m_1, m_0, l_2 \subset \partial D_l, \\
& m_0 \subset D_{m_0}, \qquad l_1, l_2, m_1, m_2 \subset \partial D_{m_0}, \\
& m_1, n_1 \subset D, \qquad l_1, l_0, m_2, n_2, p_0, p_1 \subset \partial D, \\
& n_0 \subset D_{n_0}, \qquad p_1, p_2, n_1, n_2 \subset \partial D_{n_0}, \\
& p_1 \subset D_p, \qquad n_1, n_0, p_2 \subset \partial D_p \ .
\end{aligned} \tag{8.8}
$$

Notice that the complex conjugates of the these canonical domains are also canonical domains and in fact if we include these complex conjugates then we obtain a covering of the plane by canonical domains. But because $q(x)$ is real, the zeros are symmetric with respect to the x-axis, and it is therefore enough to find the zeros in $D_l \cup D_{m_0} \cup D \cup D_{n_0} \cup D_p$. By lemma 8.1.1 we only need to discuss the limit (8.2) in each of these canonical domains. First of all let us compute the equation of the eigenvalues (7.12).

Here, the transition matrix $\Omega_{+,-}$, is the product of the seven elementary matrices associated to the following sequence of triples:

$$(D_p, l_1, x_p) \mapsto (D_{n_0}, n_0, x_p) \mapsto (D_{n_0}, n_0, x_n) \mapsto (D, n_1, x_n)$$
$$\mapsto (D, m_1, x_m) \mapsto (D_{m_0}, m_0, x_m) \mapsto (D_{m_0}, m_0, x_l) \mapsto (D_l, l_1, x_l).$$

In fact if we define

$$\alpha_1 = \int_{x_l}^{x_m} |\sqrt{q(t)}|dt, \quad \alpha_2 = \int_{x_n}^{x_p} |\sqrt{q(t)}|dt, \quad \xi = \int_{x_m}^{x_n} \sqrt{q(t)}dt,$$

then by (7.9),(7.10) and (7.11), we have

$$\begin{pmatrix} a(\lambda) \\ b(\lambda) \end{pmatrix} = \Omega_{+,-} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & \alpha_{l_0 l_1}^{-1} \\ 1 & i\alpha_{l_1 1_2} \end{pmatrix} \begin{pmatrix} 0 & e^{-i\lambda\alpha_1} \\ e^{i\lambda\alpha_1} & 0 \end{pmatrix} \begin{pmatrix} 0 & \alpha_{m_1 m_0}^{-1} \\ 1 & i\alpha_{m_0 m_2} \end{pmatrix} \begin{pmatrix} e^{-\lambda\xi} & 0 \\ 0 & e^{\lambda\xi} \end{pmatrix}$$
$$\times \begin{pmatrix} 0 & \alpha_{n_0 n_1}^{-1} \\ 1 & i\alpha_{n_1 n_2} \end{pmatrix} \begin{pmatrix} 0 & e^{-i\lambda\alpha_2} \\ e^{i\lambda\alpha_2} & 0 \end{pmatrix} \begin{pmatrix} 0 & \alpha_{p_1 p_0}^{-1} \\ 1 & i\alpha_{p_0 p_2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A simple calculation shows that

$$b(\lambda) = \alpha_{p_1 p_0}^{-1}\alpha_{n_0 n_1}^{-1} e^{i\lambda(\alpha_2-\alpha_1)}e^{-\lambda\xi} - (\alpha_{m_0 m_2}e^{-i\lambda\alpha_1} + \alpha_{l_1 l_2}\alpha_{m_1 m_0}^{-1}e^{i\lambda\alpha_1})(\alpha_{p_0 p_2}e^{-i\lambda\alpha_2} + \alpha_{n_1 n_2}\alpha_{p_1 p_0}^{-1}e^{i\lambda\alpha_2})e^{\lambda\xi}.$$

Hence $b(\lambda) = 0$ implies that

$$\Gamma_1(\lambda)\Gamma_2(\lambda) = \alpha_{p_1 p_0}^{-1}\alpha_{n_0 n_1}^{-1} e^{i\lambda(\alpha_2-\alpha_1)}e^{-2\lambda\xi}, \tag{8.9}$$

where

$$\Gamma_1(\lambda) = \alpha_{m_0m_2}e^{-i\lambda\alpha_1} + \alpha_{l_1l_2}\alpha^{-1}_{m_1m_0}e^{i\lambda\alpha_1} = 2\cos(\alpha_1\lambda) + O(\tfrac{1}{\lambda}),$$

(8.10)

$$\Gamma_2(\lambda) = \alpha_{p_0p_2}e^{-i\lambda\alpha_2} + \alpha_{n_1n_2}\alpha^{-1}_{p_1p_0}e^{i\lambda\alpha_2} = 2\cos(\alpha_2\lambda) + O(\tfrac{1}{\lambda}).$$

Now let us discuss the limit in (8.2) for each of the canonical domains defined in (8.8). Even though the coefficients $a(\lambda)$, $b(\lambda)$ are different for different canonical domains, we do not consider it in our notation.

By (7.4), (7.5) , (7.6), and (7.7), it is clear that for λ large enough there are no zeros in D_l^ε and D_p^ε. For (D_{n_0}, n_0, x_p) we have

$$\begin{pmatrix} a(\lambda) \\ b(\lambda) \end{pmatrix} = \begin{pmatrix} 0 & \alpha^{-1}_{p_1p_0} \\ 1 & i\alpha_{p_0p_2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha^{-1}_{p_1p_0} \\ i\alpha_{p_0p_2} \end{pmatrix}.$$

Using (7.11),(7.13), for the full sequence λ_n we have

$$\frac{1}{2\lambda_n}\log|\frac{b(\lambda_n)}{a(\lambda_n)}| = \frac{1}{2\lambda_n}\log|\alpha_{p_1p_2}| = 0.$$

Hence $t = 0$ and, by Lemma 8.1.1, the Stokes line $n_0 = (a_2, a_3)$ is a zero line in D_{n_0}. The same proof shows that the Stokes line $[a_0, a_1]$ is a zero line for the full sequence Z_{λ_n} in D_{m_0}. Now it only remains to discuss the limit in (8.2) in the canonical domain D. For the triple (D, n_1, x_n) we have

$$\begin{pmatrix} a(\lambda) \\ b(\lambda) \end{pmatrix} = \begin{pmatrix} 0 & \alpha^{-1}_{n_0n_1} \\ 1 & i\alpha_{n_1n_2} \end{pmatrix} \begin{pmatrix} 0 & e^{-i\lambda\alpha_2} \\ e^{i\lambda\alpha_2} & 0 \end{pmatrix} \begin{pmatrix} 0 & \alpha^{-1}_{p_1p_0} \\ 1 & i\alpha_{p_0p_2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} e^{i\lambda\alpha_2}\alpha^{-1}_{p_1p_0}\alpha^{-1}_{n_0n_1} \\ i\Gamma_2(\lambda) \end{pmatrix}.$$

Therefore, by the second equation in (7.11), we obtain

$$t = \lim_{n\to\infty}\frac{1}{2\lambda_n}\log|\frac{i\Gamma_2(\lambda_n)}{e^{i\lambda_n\alpha_2}\alpha^{-1}_{p_1p_0}\alpha^{-1}_{n_0n_1}}| = \lim_{n\to\infty}\frac{1}{2\lambda_n}\log|\Gamma_2(\lambda_n)|. \tag{8.11}$$

The limit (8.11) does not necessarily exist for the full sequence $\{\lambda_n\}$. We study this limit in different cases as follows:

1. $\frac{\boldsymbol{\alpha_1}}{\boldsymbol{\alpha_2}} = \mathbf{1}$:

This is exactly the symmetric case in Theorem 6.2.2. It is easy to see that if $\alpha_1 = \alpha_2$, then there exists a translation on the real line which changes $q(z)$ to an even function. When $q(z)$ is even, because of the symmetry in the problem, we have $\Gamma_1(\lambda) = \Gamma_2(\lambda)$. On the other hand equation (8.9) implies that

$$|\Gamma_1(\lambda)||\Gamma_2(\lambda)| = e^{-2\lambda\xi}(1 + O(\frac{1}{\lambda})). \tag{8.12}$$

This means that in the symmetric case, the full sequence λ_n satisfies

$$|\Gamma_1(\lambda_n)| = |\Gamma_2(\lambda_n)| = e^{-\lambda_n\xi}(1 + O(\frac{1}{\lambda_n})).$$

Therefore, by (8.11) we have $t = -\frac{1}{2}\xi$ and using the lemma the line $\Re S(a, z) = -\frac{1}{2}\xi$, is the zero line in D. We note that this in fact determines the whole imaginary axis, because $\Re S(a, 0) = -\frac{1}{2}\xi$. Also notice that in the symmetric case, by our notations we have $a = a_2 = x_n$. This proves Theorem 6.2.2.2.

2. $\frac{\boldsymbol{\alpha_1}}{\boldsymbol{\alpha_2}} \neq \mathbf{1}$:

In this case as we mentioned in the introduction, there are more than one zero limit measures. Here the limit (8.11) behaves differently for the two subsequences in (6.7) and (6.8) (notice that the equations (6.7) and (6.8) in fact follow from (8.9)). It is clear from (8.10) that if for a subsequence $\{\lambda_{n_k}\}$ we have a lower bound δ for $|\cos(\alpha_2\lambda_{n_k})|$, then we have t=$\lim_{k\to\infty} \frac{1}{2\lambda_{n_k}} \log|\Gamma_2(\lambda_{n_k})| = 0$. Also if we have a lower bound δ for $|\cos(\alpha_1\lambda_{n_k})|$ then $\lim_{k\to\infty} \frac{1}{2\lambda_{n_k}} \log|\Gamma_1(\lambda_{n_k})| = 0$, and by (8.12) we have $t = \lim_{k\to\infty} \frac{1}{2\lambda_{n_k}} \log|\Gamma_2(\lambda_{n_k})| = -\xi$. To find such subsequences we denote for each $\ell = 1, 2$

$$A_\delta^{(\ell)} = \{\lambda_n;\ |\cos(\alpha_\ell \lambda_n)| > \delta\}.$$

By (6.7) and (6.8), it is clear that up to some finite sets $A_\delta^{(1)} \subset \{\lambda_n^{(2)}\}$ and $A_\delta^{(2)} \subset \{\lambda_n^{(1)}\}$. We would like to find the density of the subsets $A_\delta^{(1)}$ and $A_\delta^{(2)}$ in $\{\lambda_n^{(2)}\}$ and $\{\lambda_n^{(1)}\}$ respectively. Here by the density of a subsequence $\{\lambda_{n_k}\}$ of $\{\lambda_n\}$ we mean

$$d = \lim_{n\to\infty} \frac{\#\{k;\ \lambda_{n_k} \le \lambda_n\}}{n}.$$

If we set $\tau = \arcsin(\delta)$ then we have

$$A_\delta^{(1)} = \{n \in \mathbb{N};\ |(n+\frac{1}{2})\frac{\alpha_1}{\alpha_2} + (m+\frac{1}{2})| > \tau + O(\frac{1}{n}), \quad \forall\, m \in \mathbb{Z}\},$$

$$A_\delta^{(2)} = \{n \in \mathbb{N};\ |(n+\frac{1}{2})\frac{\alpha_2}{\alpha_1} + (m+\frac{1}{2})| > \tau + O(\frac{1}{n}), \quad \forall\, m \in \mathbb{Z}\}.$$

We only discuss the density of the subset $A_\delta^{(1)}$. We rewrite this subset as

$$A_\delta^{(1)} = \{n \in \mathbb{N};\ |(2n+1)\alpha_1 + (2m+1)\alpha_2| > 2\alpha_2\tau + O(\frac{1}{n}), \quad \forall\, m \in \mathbb{Z}\}.$$

From this we see that if $\frac{\alpha_1}{\alpha_2}$ is a rational of the from $\frac{2r_1}{2r_2+1}$ (or $\frac{2r_1+1}{2r_2}$), then because for every m and n we have

$$|(2n+1)(2r_1) + (2m+1)(2r_2+1))| \ge 1,$$

therefore $d(A_\delta^{(1)}) = 1$ for $\tau = \frac{1}{8r_2+4}$. This proves Theorem 6.2.4.2. When $\frac{\alpha_1}{\alpha_2}$ is a rational of the form $\frac{2r_1+1}{2r_2+1}$, we define

$$B_\delta^{(1)} = \{n \in A_\delta^{(1)};\ 2n+1 \ne 0 \pmod{2r_2+1}\}.$$

Since for every $n \in B_\delta^{(1)}$ and $m \in \mathbb{Z}$ we have

$$|(2n+1)(2r_1+1) + (2m+1)(2r_2+1))| \geq 1,$$

for $\tau = \frac{1}{8r_2+4}$, we get $d(A_\delta^{(1)}) \geq d(B_\delta^{(1)}) = \frac{2r_2}{2r_2+1}$. This completes the proof of Theorem 6.2.4.3.

To prove Theorem 6.2.4.1, when $\frac{\alpha_1}{\alpha_2}$ is irrational, we use the fact that the set $\mathbb{Z}\alpha_1 \oplus \mathbb{Z}\alpha_2$ is dense in $\mathbb{R}$. In fact it is easy to see that the subset $A = \{n\alpha_1 + m\alpha_2 | \; n \in \mathbb{N}, \; m \in \mathbb{Z}\}$ is also dense. Now if we rewrite $A_\delta^{(1)}$ as

$$A_\delta^{(1)} = \{n \in \mathbb{N}; \; |(n\alpha_1 + m\alpha_2) + \frac{1}{2}(\alpha_1 + \alpha_2)| > \alpha_2\tau + O(\frac{1}{n}), \quad \forall \, m \in \mathbb{Z}\},$$

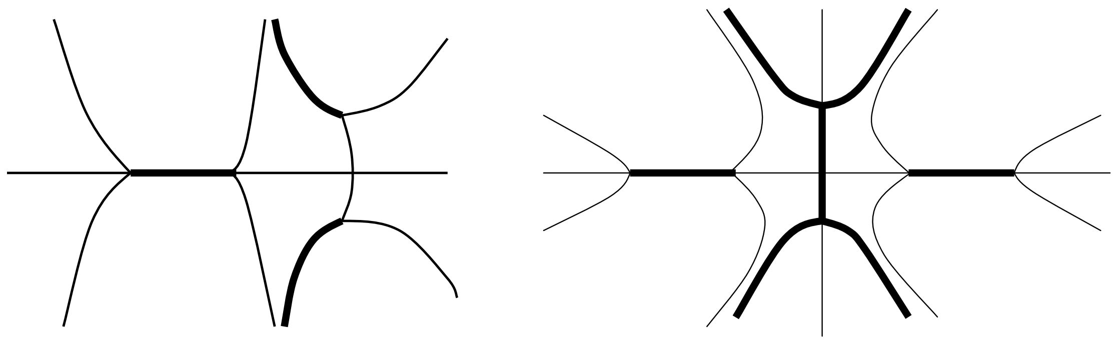
then from the denseness of the set A, it is not hard to see that in this case $d(A_\delta^{(1)}) = 1 - \frac{2\alpha_2}{\alpha_1}\tau$. Hence we conclude that when $l = 1$ there is a subsequence $\{\lambda_{n_k}^{(\ell)}\}$ of $\{\lambda_n^{(\ell)}\}$ of density 1. The same argument works for $l = 2$. This finishes the proof.

8.4 More examples of the zero lines for some polynomial potentials

In Figure (8.2) we have illustrated the zero lines for the polynomials

$$q(z) = (z^2 - a^2)(z^2 + bz + c) \qquad \text{and} \qquad q(z) = (z^2 - a^2)(z^2 - b^2)(z^2 + c^2).$$

The thickest lines in these figures are the zero lines. In fact for these examples there is a unique zero limit measure as in the other symmetric cases we mentioned in Theorems 6.2.2 and 6.2.3. We will not give the proofs, as they follow similarly, but we



$q(z) = (z^2 - a^2)(z^2 + bz + c)$ $\qquad$ $q(z) = (z^2 - a^2)(z^2 - b^2)(z^2 + c^2)$

Figure 8.2:

would like to raise the following question:

QUESTION: Is there any polynomial potential with n wells, $n \geq 3$ for which there is a unique zero limit measure for the zeros of eigenfunctions?

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Vitae

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