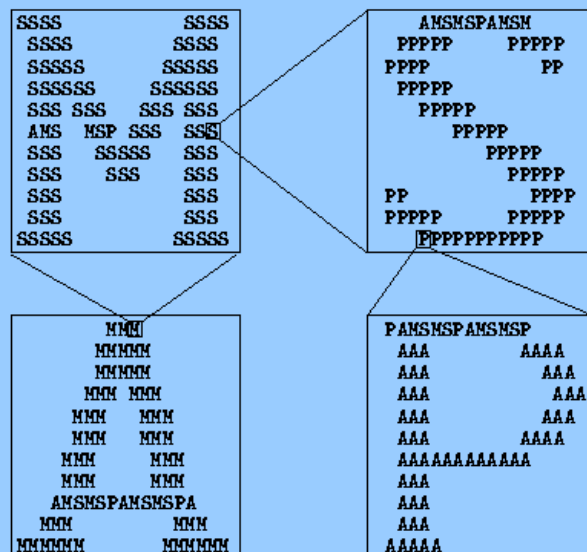


# Analysis, Modeling and Simulation of Multiscale Problems

Semiclassical resonances for two-level Schrödinger operator with a conical intersection

S. Fujiié, C. Lasser, L. Nédélec

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# Semiclassical resonances for a two-level Schrödinger operator with a conical intersection

Setsuro Fujié

Graduate School of Material Science, University of Hyogo  
2167 Shosha, Himeji, 671-2201 Japan  
fujiie@sci.u-hyogo.ac.jp \*

Caroline Lasser

Fachbereich Mathematik, Freie Universität Berlin  
Arnimallee 2-6, D-14195 Berlin, Germany  
lasser@math.fu-berlin.de †

Laurence Nédélec

L.A.G.A., Institut Galilée, Université de Paris Nord  
av. J.B. Clement, F-93430 Villetaneuse, France  
nedelec@math.univ-paris13.fr ‡

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## Abstract

We study the resonant set of a two-level Schrödinger operator with a linear conical intersection. This model operator can be decomposed into a direct sum of first order systems on the real half-line. For these ordinary differential systems we locally construct exact WKB solutions, which are connected to global solutions, amongst which are resonant states. The main results are a generalized Bohr-Sommerfeld quantization condition and an asymptotic description of the set of resonances as a distorted lattice.

## 1 Introduction

This paper is devoted to the study of the following two-dimensional, two-level Schrödinger operator

$$P = -h^2 \Delta_x + V(x) = -h^2 \Delta_x + \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}.$$

Our aim is to compute the asymptotic distribution of resonances of  $P$  with real part in an  $h$ -independent positive interval  $]a, b[$ ,  $0 < a < b$ , as the semiclassical parameter  $h \rightarrow 0$  tends to zero.

Two-level Schrödinger operators appear naturally in the study of molecular spectra: if the positions of a molecule's nuclei are denoted by  $x \in \mathbb{R}^n$ , and  $0 < h \ll 1$  is Planck's constant divided by the square-root of the nuclear mass, then a full molecular Hamiltonian reads as  $H_{\text{mol}} = -h^2 \Delta_x + H_{\text{el}}(x)$ . For every nucleonic position  $x$ , the electronic Hamiltonian  $H_{\text{el}}(x)$  is an operator on the electronic degrees of freedom. The full operator  $H_{\text{mol}}$  acts on nucleonic *and* electronic degrees of freedom, that is on wave functions in  $L^2(\mathbb{R}^N, \mathbb{C})$ , where  $N = 3 \cdot (\text{number of nuclei} + \text{electrons})$  is a notoriously large number. If one considers two eigenvalues of the electronic Hamiltonian  $H_{\text{el}}(x)$ , which are well separated from the rest of the electronic spectrum  $\sigma(H_{\text{el}}(x))$  uniformly for all  $x$ , then Born-Oppenheimer approximation allows to reduce the study of the full molecular problem to the case of two-level systems acting solely on the nucleonic degrees of freedom. The justification of this approximation can be found in [7, 19] for the time-independent and in [14, 16, 29] for the time-dependent case.

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Chapter 2 in Hagedorn's monograph [15] gives the standard classification of matrix Schrödinger operators with eigenvalue crossings of minimal multiplicity, where our model operator  $P$  appears as the normal form for a codimension two crossing: the real symmetric potential matrix  $V(x) = V(x_1, x_2)$  depends smoothly on the two real parameters  $x_1$  and  $x_2$ . It has two eigenvalues

$$\pm\sqrt{x_1^2 + x_2^2} = \pm|x|,$$

which coincide on the codimension two manifold  $\{x = 0\} \subset \mathbb{R}^2$ . The graph of the mapping  $x \mapsto \pm|x|$  shows two cones intersecting at the origin, which explains the term conical intersection, which is used in the chemical physics' literature (see for example [5, 8]). Such a degeneracy, geared by two parameters, is generic in the sense, that it cannot be removed by symmetry preserving perturbations. The matrix  $V(x)$  is in essence Rellich's celebrated example of a smooth matrix, which is not smoothly diagonalizable [27].

Let us consider the two scalar Hamiltonians

$$P^\pm = -h^2\Delta_x \pm |x|.$$

The upper level operator  $P^+$  is a Schrödinger operator with confining potential, and it has pure point spectrum only (see Appendix A). The lower level operator  $P^-$ , however, has a linearly decreasing negative potential, and one sees by a Mourre-type argument, that  $P^-$  is of purely continuous spectrum. The full operator  $P$  inherits the continuous spectrum of  $P^-$ , while spectrally echoing the discrete spectrum of  $P^+$  with resonances close to the real axis.

The study of some general systems *without* intersecting eigenpotentials has revealed resonances, which are exponentially close to the real axis with respect to  $h \rightarrow 0$ , see [23, 24, 4]. In our case, however, resonances have larger imaginary part because of the conical intersection. In fact, we will show that the imaginary part is of  $O(h \ln \frac{1}{h})$ .

**Remark 1.1** By the scaling transformation  $x \mapsto h^{2/3}x$ , the operator  $P$  is unitarily equivalent to the  $h$ -independent operator  $P^0 = -\Delta_x + V(x)$ . We note that an  $h$ -dependent complex number  $E = E(h)$  is a resonance of  $P$  if and only if  $E(h)h^{-2/3}$  is a resonance of  $P^0$ . The semiclassical distribution of resonances of  $P$  with real part in an  $h$ -independent interval  $]a, b[$  corresponds to the high energy asymptotics of resonances of  $P^0$ .  $\diamond$

In the mathematical physics' literature, zero energy wave functions close to a conical level crossing [2, 3] have been studied, and conical intersections have also been addressed as generators of resonances [5]. Our work is complementary to the results of Avron and Gordon [2, 3], who have studied the resonant states of the linear model operator  $P$  in an energy range close to zero, using generalized hypergeometric functions.

A first mathematical proof of existence of resonances for the matrix operator  $P$  has been given by one of the authors [25]. She crucially used that  $P$  is unitarily equivalent to the direct sum of ordinary differential operators

$$\bigoplus_{\nu \in \mathbb{Z} + \frac{1}{2}} P_\nu(r, hD_r; h), \quad P_\nu(r, \rho; h) = \begin{pmatrix} r^2 - \rho & h\nu/r \\ h\nu/r & r^2 + \rho \end{pmatrix} \quad (1)$$

where  $(r, \rho) \in \mathbb{R}^+ \times \mathbb{R}$  and  $D_r = -i\partial/\partial r$ . In fact, let

$$\hat{u}(\xi) = \frac{1}{2\pi h} \int_{\mathbb{R}^2} e^{-ix \cdot \xi/h} u(x) dx$$

be the  $h$ -Fourier transform of  $u$ , and  $\xi = r(\cos \phi, \sin \phi)$  the polar coordinate. If we expand  $\hat{u}(\xi)$  as the Fourier series with respect to the angular variable  $\phi$ ,

$$\hat{u}(\xi) = r^{-1/2} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \sum_{\nu \in (\mathbb{Z} + 1/2)} e^{-ih\nu\phi} w_\nu(r),$$

then the equation  $Pu(x) = Eu(x)$  is reduced to a family of first order ordinary differential systems  $P_\nu w_\nu(r) = Ew_\nu(r)$ ,  $\nu \in \mathbb{N} - 1/2$ , see also §2.

The resonances of the operator  $P$  are defined by complex dilation. They are the eigenvalues of the complex scaled Hamiltonian

$$P_\theta = -h^2 e^{-2i\theta} \Delta_x + e^{i\theta} V(x),$$

which is a non-selfadjoint operator with discrete spectrum independent of the dilation parameter  $\theta \in ]0, \frac{\pi}{3}[$  (see for example [1, 18, 28, 31] for general theory of resonances and [25] for the model operator  $P$ ). In terms of the reduced operators  $P_\nu$ , resonances are then characterized as follows:

**Proposition 1.2**  $E \in \mathbb{C}$  is a resonance of the operator  $P = -h^2 \Delta + V$  if and only if there exist  $\nu \in \mathbb{N} - \frac{1}{2} = \{\frac{1}{2}, \frac{3}{2}, \dots\}$  and a non-trivial solution  $w$  to the equation

$$P_\nu w = Ew \tag{2}$$

satisfying

$$\lim_{r \rightarrow 0^+} w(r) = 0, \quad r^2 w(e^{-i\theta} r), \quad w'(e^{-i\theta} r) \in L^2(\mathbb{R}^+, \mathbb{C}^2), \tag{3}$$

for some  $\theta \in ]0, \pi/3[$ .

We will see later in §4, that the second and third conditions of (3) on the behavior of  $w$  on  $e^{-i\theta} \mathbb{R}^+$  can be replaced by an *incoming* condition on  $\mathbb{R}^+$ .

**Definition 1.3**  $E \in \mathbb{C}$  is called a resonance of  $P$  with angular momentum number  $\nu \in \mathbb{N} - \frac{1}{2}$ , if equation (2) has a non-trivial solution satisfying (3) for some  $\theta \in ]0, \pi/3[$ .

Let  $\nu \in \mathbb{N} - \frac{1}{2}$ . If  $0 < a < E < b$  for  $h$ -independent positive numbers  $a, b$ , and if  $h$  is sufficiently small, the energy surface

$$\{(r, \rho) \in \mathbb{R}^+ \times \mathbb{R}; \det(P_\nu(r, \rho; h) - E) = 0\},$$

consists of two connected curves, one a closed simple curve and the other unbounded, see Figure 1.

Let  $A(E, h)$  be the action associated with this closed curve,

$$A(E, h) = 2 \int_{r_0}^{r_1} \frac{\sqrt{r^2(E - r^2)^2 - h^2 \nu^2}}{r} dr,$$

where  $0 < r_0 < r_1$  are the two positive zeros of  $r^2(E - r^2)^2 - h^2 \nu^2$ , and the square root is positive. As a function of  $E$ , the action  $A(E, h)$  is extended analytically into a complex neighborhood of the interval  $(a, b)$ . We easily see that  $A(E, h) \rightarrow \frac{4}{3} E^{3/2}$  as  $h \rightarrow 0$ . More precisely, Proposition 8.2 shows

$$A(E, h) = \frac{4}{3} E^{3/2} + \pi \nu h + O(h^2 |\ln h|) \quad (h \rightarrow 0). \tag{4}$$

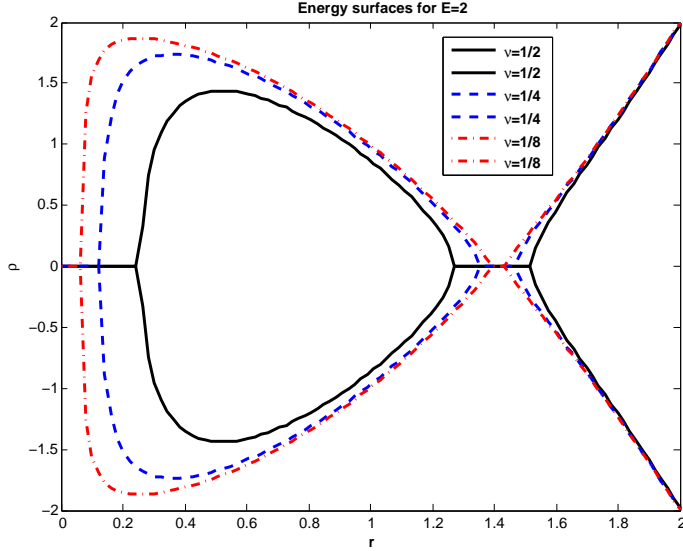


Figure 1: The energy surfaces  $\{(r, \rho) \in \mathbb{R}^+ \times \mathbb{R}; \det(P_\nu(r, \rho; h) - E) = 0\}$  for  $E = 2$  and different values of  $h\nu \in \{\frac{1}{2}, \frac{1}{4}, \frac{1}{8}\}$ .

Our main result is the following Bohr-Sommerfeld type quantization condition of resonances with fixed angular momentum.

**Theorem 1.4** *Let  $E_0 > 0$  and  $\nu \in \mathbb{N} - \frac{1}{2} = \{\frac{1}{2}, \frac{3}{2}, \dots\}$  be given. Then there exist  $\epsilon > 0$ ,  $h_0 > 0$  and a function  $\delta(E, h) : \{(E, h) \in \mathbb{C} \times \mathbb{R}_+; |E - E_0| < \epsilon, 0 < h < h_0\} \rightarrow \mathbb{C}$  with  $\delta(E, h) \rightarrow 0$  uniformly in  $E$  as  $h \rightarrow 0$ , such that  $E$  is a resonance of  $P = -h^2\Delta + V$  with angular momentum  $\nu$  if and only if  $(E, h)$  satisfies the following quantization condition:*

$$\sqrt{\frac{\pi h}{2}} \nu e^{-i\pi/4} E^{-3/4} e^{iA(E, h)/h} + 1 = \delta(E, h). \quad (5)$$

Combining this result with Proposition 1.2 and the asymptotic formula (4), one obtains the asymptotic distribution of resonances as  $h \rightarrow 0$ . Here, we take  $\lambda = E^{3/2}$  as the spectral parameter and look for resonances in the strip

$$\{\lambda \in \mathbb{C}; a < \operatorname{Re} \lambda < b, -c(h) < \operatorname{Im} \lambda < 0, \}$$

for arbitrary  $h$ -independent numbers  $0 < a < b$  and  $c(h) > 0$  which tends to 0 as  $h \rightarrow 0$ . For each

$\nu \in \mathbb{N} - \frac{1}{2}$ , we define

$$\Gamma_\nu(a, b; h) = \left\{ \lambda \in \mathbb{C}; \lambda = \lambda_{k\nu} h - i \frac{3}{8} \left( h \ln \frac{1}{h} - h \ln \frac{\pi \nu^2}{2 \lambda_{k\nu} h} \right), \right. \\ \left. k \in \mathbb{Z} \text{ s.t. } a < \lambda_{k\nu} h < b \right\},$$

where  $\lambda_{k\nu} = \frac{3\pi}{16}(8k - 4\nu + 5)$ .

**Theorem 1.5** *Let  $N \in \mathbb{N}$  and  $0 < a < b$  be given. Then there is  $h_0 > 0$  and a positive function  $r : ]0, h_0[ \rightarrow \mathbb{R}^+$  with  $r(h) = o(h)$  as  $h \rightarrow 0$  such that there exists one and only one resonance of  $P = -h^2\Delta + V$  in*

$$\left\{ E \in \mathbb{C}; |E - \lambda^{2/3}| < r(h) \right\}$$

for each  $\lambda \in \bigcup_{\nu \leq N} \Gamma_\nu(a, b; h)$ .

**Remark 1.6** Since  $a < \lambda_{k\nu} h$ , the second term of the imaginary part of  $\lambda \in \Gamma_\nu(a, b; h)$  is of  $O(h)$  and smaller than the first term  $-\frac{3}{8} h \ln \frac{1}{h}$ . Thus,  $\Gamma_\nu(a, b; h)$  is an almost horizontal sequence of complex points in the  $\lambda$ -plane, and  $\bigcup_{\nu \leq N} \Gamma_\nu(a, b; h)$  is a lattice which consists of  $N$  almost horizontal sequences. Theorem 1.5 implies that for a fixed positive interval  $]a, b[$ , we can find as many horizontal sequences of resonances as we want for sufficiently small  $h$ .  $\diamond$

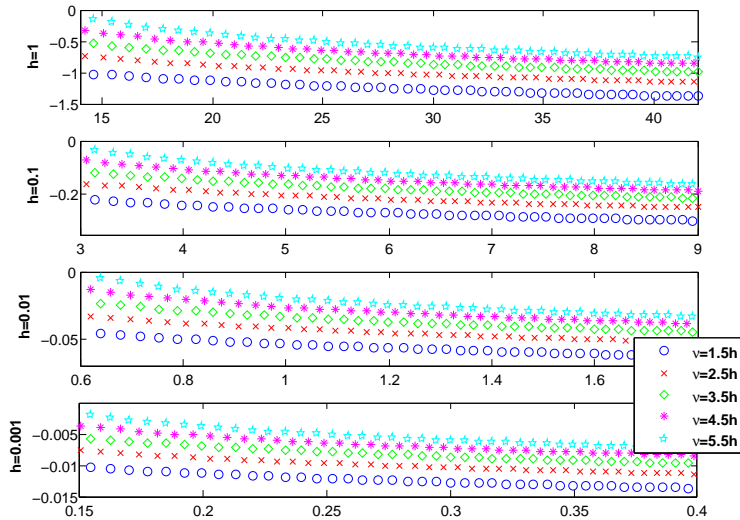


Figure 2: Resonances of the model operator  $P = -h^2\Delta + V$ . The parameter  $k$  lies in  $\{11, 12, \dots, 60\}$ , while  $\nu$  is chosen in  $\{1.5, 2.5, \dots, 5.5\}$ . The semiclassical parameter  $h$  varies from  $10^{-3}$  to 1.

The plots in Figure 2 illustrate the distorted lattice of resonances given by Theorem 1.5. The larger the angular momentum  $\nu \in \mathbb{N} - \frac{1}{2}$ , the closer the resonance to the real axis and the longer the life time of the corresponding resonant states. Studies of the dynamical properties [9, 21, 22] of the model operator  $P$  complement this observation:

The one-level operators  $P^\pm = -h^2\Delta \pm |x|$  induce Hamiltonian systems conserving angular momentum  $x \wedge \xi = x_1\xi_2 - x_2\xi_1$ , which also encodes how close classical trajectories arrive near the crossing manifold  $\{x = 0\}$ . On the one hand, a high angular momentum number  $\nu$  of a resonance mirrors a periodic orbit of the upper level with high angular momentum. Such orbits in turn imply existence of localized quasimodes and long-living resonant states. On the other hand, small angular momentum numbers  $\nu$  correspond to orbits close to the crossing manifold. Nearby the crossing, non-adiabatic transitions to the unbounded motion of the minus-system are possible. In this regime shorter life-times and resonances far away from the real axis have to be expected. The prefactor before the exponential of the action integral in the Bohr-Sommerfeld condition (5) stems from these non-adiabatic transitions.

The proof of our main results, Theorem 1.4 and Theorem 1.5, proceeds as follows: In §2, we reduce the study of the full operator  $P$  to that of the ordinary differential operators  $P_\nu$ ,  $\nu \in \mathbb{N} - \frac{1}{2}$ , and prove Proposition 1.2. Then, we construct *exact WKB solutions* of  $P_\nu w = Ew$ , which are not only asymptotic solutions with respect to  $h$  but also exact solutions. Several theories of exact WKB analysis for ordinary differential equations have recently been developed and applied. In §3, we extend the method of Gérard and Grigis for scalar Schrödinger equations [13] to a family of  $2 \times 2$  first order differential systems. These exact solutions are locally defined in turning point free complex domains. A turning point  $r$  satisfies  $\det(P_\nu(r, 0) - E) = 0$ . That is, turning points lie in the intersection of the energy surface with  $\{\rho = 0\}$ . We have three positive turning points  $r_0 < r_1 < r_2$ , where  $r_0$  tends to 0 while  $r_1$  and  $r_2$  tend to  $\sqrt{E}$  as  $h \rightarrow 0$ . The strategy to obtain globally defined solutions by connecting the exact WKB solutions at the turning points is outlined in §4. More precisely, the aim is to construct an exact solution, which vanishes at the origin, and to represent it after several connection procedures as a linear combination of Jost solutions, which are defined at infinity. The quantization condition of resonances will then be given as the condition that the connection coefficient of the outgoing Jost solution vanishes (Proposition 4.1). §5 defines Jost solutions and represents them as exact WKB solutions. The origin is a regular singular point of the equation  $P_\nu w = Ew$  of indices  $\pm\nu$ . In §6, we construct an exact WKB solution in a small complex neighborhood of  $r = 0$ , which corresponds to the index  $+\nu$ , that is satisfies the boundary condition at the origin. Studying the two parameter asymptotics of this solution as  $(r, h) \rightarrow (0, 0)$ , we face the same difficulties, which are met in the context of the so-called *Langer modification* at a regular singular point (cf. [12, 20]). The bad error estimates in Theorem 1.4 and Theorem 1.5 come only from here. The connection procedure at  $r = \sqrt{E}$ , where the second and third turning point coalesce, is the core of our construction.  $r = \sqrt{E}$ , or microlocally  $(r, \rho) = (\sqrt{E}, 0)$ , is a double turning point or an unstable fixed point and is similar to a non-degenerate barrier top of scalar Schrödinger operators. Note that the conical intersection at  $x = 0$  of the original operator  $P$  corresponds to this point. Hence, roughly speaking, the transition at the conical intersection of the partial differential operator is reduced to that at an unstable fixed point of a family of ordinary differential operators. The connection formula at  $r = \sqrt{E}$  is calculated in §7, using a microlocal reduction to a normal form [17, 6, 26], which passes by the famous Landau-Zener problem for non-adiabatic transitions. The term  $\sqrt{h}$  in the quantization condition (5), which gives the principal part of the imaginary part of the resonances, comes from the connection here. In §8, we compute the quantization condition (Theorem 1.4) from the connection formulae obtained in the preceding sections. This condition is given in the form of Bohr-Sommerfeld using the action  $A(E, h)$ . Analysing the asymptotic behavior of the action  $A(E, h)$ , we finally get the semiclassical distribution of resonances (Theorem 1.5).



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## 2 Reduction to the first order system

Let

$$P = -h^2 \Delta_x + V(x), \quad V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}. \quad (6)$$

If one equips its complex scaled counterpart

$$P_\theta = -e^{-2i\theta} h^2 \Delta_x + e^{i\theta} V(x), \quad \theta \in ]0, \frac{\pi}{3}[$$

with the domain

$$\mathcal{D} = \{u \in H^2(\mathbb{R}^2, \mathbb{C}^2); |x|u \in L^2(\mathbb{R}^2, \mathbb{C}^2)\},$$

then  $P_\theta$  is a closed operator with purely discrete spectrum,  $\sigma(P_\theta) = \sigma_{\text{disc}}(P_\theta)$ , see Theorem 2.1 in [25]. The spectrum is independent of the scaling parameter  $\theta \in ]0, \frac{\pi}{3}[$  in the sense that

$$\sigma_{\text{disc}}(P_\theta) = \sigma_{\text{disc}}(P_{\theta'}) \quad (0 < \theta < \theta' < \frac{\pi}{3}).$$

The eigenvalues of the dilated operator  $P_\theta$  are the resonances of the operator  $P = -h^2 \Delta_x + V(x)$ . We note, that the choice of the dilation angle  $\theta \in ]0, \frac{\pi}{3}[$  is crucial: under  $x \mapsto -x$ , the dilated operator  $P_{\pi/3}$  is unitarily equivalent to the original operator  $P$ , which has absolutely continuous spectrum.

By Theorem 5.1 in [25], the resonances of  $P$  can be characterized as follows: Let us fix  $\theta \in ]0, \frac{\pi}{3}[$ . Then  $E \in \mathbb{C}$  is a resonance of  $P$  if and only if there exists  $\nu \in \mathbb{Z} + \frac{1}{2}$  such that  $E \in \mathbb{C}$  is an eigenvalue of the operator

$$P_{\theta, \nu} = \begin{pmatrix} e^{-2i\theta} r^2 - e^{i\theta} h D_r & e^{i\theta} h \nu / r \\ e^{i\theta} h \nu / r & e^{-2i\theta} r^2 + e^{i\theta} h D_r \end{pmatrix}$$

with domain

$$\mathcal{D}_\nu = \{w \in H^1(\mathbb{R}^+); r^{-1}w, r^2w \in L^2(\mathbb{R}^+)\}$$

if  $\nu \neq \frac{1}{2}$ , and

$$\mathcal{D}_{\pm \frac{1}{2}} = \{w \in L^2(\mathbb{R}^+); (-D_r w_1 \pm \frac{1}{2r} w_2), (D_r w_2 \pm \frac{1}{2r} w_1), r^2 w \in L^2(\mathbb{R}^+)\}.$$

*Proof of Proposition 1.2:* Let  $E$  be a resonance of  $P = -h^2 \Delta + V$ . Then, there exist  $\nu \in \mathbb{Z} + \frac{1}{2}$  and  $w_\theta \in \mathcal{D}_\nu$  such that  $P_{\theta, \nu} w_\theta = E w_\theta$ . The origin  $r = 0$  is a regular singular point for the operator  $P_{\theta, \nu}$  with indicial roots  $\pm \nu$ . Hence, by the theory of Fuchs,  $w_\theta$  is a linear combination

$$w_\theta(r) = C_0 w^0(r) + C_\infty w^\infty(r)$$

of the two solutions  $w^0(r)$  and  $w^\infty(r)$  to the equation  $P_{\theta, \nu} w = E w$  such that

$$w^0(r) \sim r^{|\nu|} \begin{pmatrix} 1 \\ -\text{sgn}(\nu) i \end{pmatrix}, \quad w^\infty(r) \sim r^{-|\nu|} \begin{pmatrix} 1 \\ \text{sgn}(\nu) i \end{pmatrix} \quad (r \rightarrow 0),$$

see also §4. Then, the condition  $w_\theta \in \mathcal{D}_\nu$  implies  $C_\infty = 0$ , and  $w_\theta$  behaves like  $r^{|\nu|}$  near the origin. In §5, the construction of exact WKB solutions with base points at infinity shows

$$w_\theta(r) = C_+ w_+^\infty(r) + C_- w_-^\infty(r),$$

where  $w_+^\infty(r)$  is exponentially growing and  $w_-^\infty(r)$  is exponentially decaying as  $r \rightarrow \infty$ . Hence,  $C_+ = 0$ , and  $w_\theta(r)$  decays exponentially as  $r \rightarrow \infty$ . Setting  $w(r) := w_\theta(e^{i\theta}r)$ , one obtains a solution to  $P_\nu w = Ew$  with the claimed properties.

Let  $E \in \mathbb{C}$  and  $w$  be a solution of  $P_\nu w = Ew$  for some  $\nu \in \mathbb{Z} + \frac{1}{2}$  such that  $\lim_{r \rightarrow 0^+} w(r) = 0$  and  $r^2 w(e^{-i\theta}r), w'(e^{-i\theta}r) \in L^2(\mathbb{R}^+, \mathbb{C}^2)$ . The preceding arguments yield, that  $w_\theta(r) := w(e^{-i\theta}r)$  is a solution to the equation  $P_{\theta,\nu} w_\theta = Ew_\theta$  with  $w_\theta \in \mathcal{D}_\nu$ . Hence,  $E$  is a resonance of  $P = -h^2 \Delta + V$ .  $\square$

**Remark 2.1** Let  $E \in \mathbb{C}$  and  $\nu \in \mathbb{Z} + \frac{1}{2}$ . Then the following equivalence holds:  $u = (u_1, u_2)$  is a solution of  $P_\nu u = Eu$ , if and only if  $\tilde{u} = (-u_1, u_2)$  is a solution of  $P_{-\nu} \tilde{u} = E\tilde{u}$ . The same holds for the dilated operators  $P_{\nu,\theta}$  and  $P_{-\nu,\theta}$ ,  $\theta \in ]0, \frac{\pi}{3}[$ . Hence, we will restrict our studies to the case  $\nu \in \mathbb{N} - \frac{1}{2}$ .  $\diamond$

### 3 Exact WKB method for $2 \times 2$ systems

We now aim at a representation formula for the solutions of  $P_\nu w = Ew$ , from which it is possible to deduce an asymptotic expansion in  $h$ . The method we will extend in the following is known as exact WKB method. We derive it in a somewhat more general context, and then apply it to our specific equation.

We study  $2 \times 2$  systems of first order differential equations in a complex domain  $D$ , which are of the form

$$\begin{pmatrix} p_1(x) - \frac{h}{i} \frac{d}{dx} & \omega(x) \\ \omega(x) & p_2(x) + \frac{h}{i} \frac{d}{dx} \end{pmatrix} u(x) = 0, \quad (7)$$

or equivalently

$$\frac{h}{i} \frac{d}{dx} u(x) = \begin{pmatrix} p_1(x) & \omega(x) \\ -\omega(x) & -p_2(x) \end{pmatrix} u(x). \quad (8)$$

The functions  $p_1, p_2$ , and  $\omega$  are holomorphic in  $D$ . The following considerations will lead to the construction of exact WKB solutions for this type of systems.

#### 3.1 Formal construction

A usual change of variables (using oscillatory part) and some other basic transformations reduce the operator to a more computable one. Let us put

$$g_+(x) = \frac{1}{2}(p_1(x) + p_2(x)) + \omega(x), \quad g_-(x) = -\frac{1}{2}(p_1(x) + p_2(x)) + \omega(x).$$

After conjugation by

$$M(x) = \exp\left(\frac{i}{2h} \int_0^x (p_1(t) - p_2(t)) dt\right) \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} =: m(x) \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

the system (7) is transformed into the trace-free system

$$\frac{h}{i} \frac{d}{dx} v(x) = \begin{pmatrix} 0 & g_+(x) \\ -g_-(x) & 0 \end{pmatrix} v(x)$$

with  $u(x) = M(x)v(x)$ . Introducing a new complex coordinate

$$z(x) = z(x; x_0) = \int_{x_0}^x \sqrt{g_+(t)g_-(t)} dt, \quad x_0 \in D, \quad (9)$$

we look for solutions of the form  $e^{\pm \frac{x}{h}} \tilde{w}_{\pm}(z)$ .

**Definition 3.1** Let  $p_1, p_2$ , and  $\omega$  be holomorphic in  $D$ . The zeros of the function  $g_+(x)g_-(x) = -\frac{1}{4}(p_1 + p_2)^2 + \omega^2$  are called the *turning points* of the system (7).

We note that due to the possible presence of such turning points the square root in the definition of  $z(x)$  might be defined only *locally*.

By formal calculations, the amplitude vector  $\tilde{w}_{\pm}(z)$  has to satisfy

$$\frac{h}{i} \frac{d}{dz} \tilde{w}_{\pm}(z) = \begin{pmatrix} \pm i & H(z)^{-2} \\ -H(z)^2 & \pm i \end{pmatrix} \tilde{w}_{\pm}(z),$$

where the function  $H$  is given by

$$H(z(x)) = \left( \frac{g_-(x)}{g_+(x)} \right)^{1/4}.$$

The preceding system's matrix is degenerate. For a decomposition with respect to image and kernel, we choose eigenprojectors  $P_{\pm}(z)$ , such that the matrix  $P_{\pm}(z) dP_{\pm}^{-1}(z)/dz$  is purely off-diagonal. We conjugate by

$$P_{\pm}(z) = 2^{-1} \begin{pmatrix} H(z) & \pm i H(z)^{-1} \\ H(z) & \mp i H(z)^{-1} \end{pmatrix}, \quad P_{\pm}^{-1}(z) = \begin{pmatrix} H(z)^{-1} & H(z)^{-1} \\ \mp i H(z) & \pm i H(z) \end{pmatrix}$$

and obtain a system for  $w_{\pm}(z) = P_{\pm}(z)\tilde{w}_{\pm}(z)$ ,

$$\frac{d}{dz} w_{\pm}(z) = \begin{pmatrix} 0 & \frac{H'(z)}{H(z)} \\ \frac{H'(z)}{H(z)} & \mp \frac{2}{h} \end{pmatrix} w_{\pm}(z),$$

where  $H'(z)$  is shorthand for  $dH(z)/dz$ . The series ansatz

$$w_{\pm}(z) = \sum_{n \geq 0} \begin{pmatrix} w_{2n, \pm}(z) \\ w_{2n+1, \pm}(z) \end{pmatrix} \quad (10)$$

with  $w_{0, \pm} \equiv 1$  and for  $n \geq 1$ , the recurrence equations

$$\left( \frac{d}{dz} \pm \frac{2}{h} \right) w_{2n+1, \pm}(z) = \frac{H'(z)}{H(z)} w_{2n, \pm}(z), \quad (11)$$

$$\frac{d}{dz} w_{2n+2, \pm}(z) = \frac{H'(z)}{H(z)} w_{2n+1, \pm}(z) \quad (12)$$

give us a formal solution up to some additive constants, which are fixed by setting

$$w_{n, \pm}(\tilde{z}) = 0, \quad n \geq 1,$$

for a base point  $\tilde{z} = z(\tilde{x})$  where  $\tilde{x} \in D$  is not a turning point. We note that the preceding equations for  $w_{n,\pm}$  are the same as the ones obtained by an exact WKB construction for scalar Schrödinger equations. See for example the work of C. Gérard and A. Grigis [13] or T. Ramond [26].

Let  $\Omega$  be a simply connected subset of  $D$  which does not contain any turning point. Then the function  $z = z(x)$  is conformal from  $\Omega$  onto  $z(\Omega)$ . Assume that  $\tilde{z} \in z(\Omega)$ . If  $\Gamma_{\pm}(\tilde{z}, z)$  denotes a path of finite length in  $z(\Omega)$  connecting  $\tilde{z}$  and  $z \in z(\Omega)$ , we can formally rewrite the above differential equations for  $n \geq 0$  as

$$\begin{aligned} w_{2n+1,\pm}(z) &= \int_{\Gamma_{\pm}(\tilde{z}, z)} \exp\left(\pm \frac{2}{h}(\zeta - z)\right) \frac{H'(\zeta)}{H(\zeta)} w_{2n,\pm}(\zeta) d\zeta, \\ w_{2n+2,\pm}(z) &= \int_{\Gamma_{\pm}(\tilde{z}, z)} \frac{H'(\zeta)}{H(\zeta)} w_{2n+1,\pm}(\zeta) d\zeta \end{aligned}$$

or after iterated integration as

$$\begin{aligned} w_{2n+1,\pm}(z) &= \int_{\Gamma_{\pm}(\tilde{z}, z)} \int_{\Gamma_{\pm}(\tilde{z}, \zeta_{2n+1})} \cdots \int_{\Gamma_{\pm}(\tilde{z}, \zeta_2)} d\zeta_1 \cdots d\zeta_{2n+1} \\ &\quad \exp\left(\pm \frac{2}{h}(\zeta_2 - \zeta_3 + \cdots + \zeta_{2n+1} - z)\right) \frac{H'(\zeta_1)}{H(\zeta_1)} \cdots \frac{H'(\zeta_{2n+1})}{H(\zeta_{2n+1})}, \\ w_{2n+2,\pm}(z) &= \int_{\Gamma_{\pm}(\tilde{z}, z)} \int_{\Gamma_{\pm}(\tilde{z}, \zeta_{2n+2})} \cdots \int_{\Gamma_{\pm}(\tilde{z}, \zeta_2)} d\zeta_1 \cdots d\zeta_{2n+2} \\ &\quad \exp\left(\pm \frac{2}{h}(\zeta_2 - \zeta_3 + \cdots - \zeta_{2n+2})\right) \frac{H'(\zeta_1)}{H(\zeta_1)} \cdots \frac{H'(\zeta_{2n+2})}{H(\zeta_{2n+2})}. \end{aligned}$$

### 3.2 Convergence, $h$ -dependence, and Wronskians

We now give the preceding formal construction some mathematical meaning in turning point-free compact sets  $\Omega \subset D$ .

**Lemma 3.2** *For any fixed  $h > 0$ , the formal series (10) converges uniformly in any compact subset of  $\Omega$ , and*

$$w_{\pm}^{\text{even}}(x, h) = \sum_{n \geq 0} w_{2n,\pm}(z(x)), \quad w_{\pm}^{\text{odd}}(x, h) = \sum_{n \geq 0} w_{2n+1,\pm}(z(x)) \quad (13)$$

are holomorphic functions in  $D$ .

*Proof:* In  $\Omega$ , all the functions defined above are well-defined analytic functions. For compact subsets  $K \subset \Omega$  and  $\tilde{z}, z \in z(K)$  there exist positive constants  $C_{\pm}^h(K) > 0$  depending on the semiclassical parameter  $h$  and the compact set  $K$  such that

$$\sup_{\zeta \in \Gamma_{\pm}(\tilde{z}, z)} \left| \exp\left(\pm \frac{2}{h}\zeta\right) \frac{H'(\zeta)}{H(\zeta)} \right| \leq C_{\pm}^h(K). \quad (14)$$

If we denote the maximal length of the paths  $\Gamma_{\pm}(\tilde{z}, \cdot) \subset K$  in the preceding iterated integrations by  $0 < L < \infty$ , then

$$\sup_{z \in z(K)} |w_{n,\pm}(z)| \leq \frac{C_{\pm}^h(K)^n L^n}{n!}, \quad n \geq 0,$$

where the bound  $\frac{L^n}{n!}$  comes from the volume of a simplex with length  $L$ .  $\square$

Thus, we have uniform convergence of the series (10) for  $w_{\pm}(z)$  and exact solutions

$$u_{\pm}(x) = e^{\pm \frac{z(x)}{h}} m(x) T_{\pm}(z(x)) \begin{pmatrix} w_{\pm}^{\text{even}}(x) \\ w_{\pm}^{\text{odd}}(x) \end{pmatrix}$$

of the original problem (7) on turning point free sets  $\Omega$ , where

$$\begin{aligned} T_{\pm}(z) &= \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} H(z)^{-1} & H(z)^{-1} \\ \mp iH(z) & \pm iH(z) \end{pmatrix} \\ &= \begin{pmatrix} H(z)^{-1} \mp iH(z) & H(z)^{-1} \pm iH(z) \\ -H(z)^{-1} \mp iH(z) & -H(z)^{-1} \pm iH(z) \end{pmatrix}, \quad z \in z(\Omega). \end{aligned} \tag{15}$$

We write these solutions  $u_{\pm}(x)$  as

$$u_{\pm}(x; x_0, \tilde{x})$$

indicating the particular choice of the phase base point  $x_0$  in (9), which defines the phase function  $z(x) = z(x; x_0)$ , and the choice of the amplitude base point  $\tilde{z} = z(\tilde{x})$ , which is the initial point of the path  $\Gamma_{\pm}(\tilde{z}, \cdot)$ .

For a fixed  $\tilde{x} \in \Omega$ , let  $\Omega_{\pm}$  be the set of  $x \in \Omega$  such that there exists a path  $\Gamma_{\pm}(z(\tilde{x}), z(x))$  along which  $x \mapsto \pm \text{Re } z(x)$  increases strictly. Then,

**Proposition 3.3** *The identities in (13) for  $w_{\pm}^{\text{even}}(x, h)$  and  $w_{\pm}^{\text{odd}}(x, h)$  give asymptotic expansions in  $\Omega_{\pm}$ . More precisely, we have for any  $\alpha \in \mathbb{N}$  and  $N \in \mathbb{N}$*

$$\begin{aligned} \partial^{\alpha} \left( w_{\pm}^{\text{even}}(x, h) - \sum_{n=0}^N w_{2n, \pm}(z(x)) \right) &= O(h^{N+1}), \\ \partial^{\alpha} \left( w_{\pm}^{\text{odd}}(x, h) - \sum_{n=0}^N w_{2n+1, \pm}(z(x)) \right) &= O(h^{N+2}). \end{aligned}$$

uniformly in compact subsets of  $\Omega_{\pm}$ . In particular,

$$w_{\pm}^{\text{even}}(x, h) = 1 + O(h), \quad w_{\pm}^{\text{odd}}(x, h) = O(h).$$

The proof is just the same as that of Proposition 1.2 of [13]. The key point is the following: Since the iterated integrations defining  $w_{n, \pm}(z)$  contain terms of the form  $\exp(\pm \zeta/h)$ , one has to make sure that  $\zeta \mapsto \pm \text{Re}(\zeta)$  is a strictly increasing function along the path  $\Gamma_{\pm}(\tilde{z}, z)$ . In other words, the paths  $\Gamma_{\pm}(z(\tilde{x}), z(x))$  have to intersect the *Stokes lines*, that is the level curves of  $x \mapsto \text{Re}(z(x))$ , transversally in a suitable direction.

One defines the Wronskian of two  $\mathbb{C}^2$ -valued functions  $u, v$  as  $\mathcal{W}(u, v) = u_1 v_2 - u_2 v_1$ . If  $z = \alpha u + \beta v$  with  $\alpha, \beta \in \mathbb{C}$ , then

$$\alpha = \frac{\mathcal{W}(z, v)}{\mathcal{W}(u, v)}, \quad \beta = -\frac{\mathcal{W}(z, u)}{\mathcal{W}(u, v)}.$$

Elementary computations give the following exact Wronskian formulas for WKB solutions with different phase and amplitude base points, using  $w_{\pm}^{\text{even}}$  and  $w_{\pm}^{\text{odd}}$ .

**Lemma 3.4** *Let  $x, x_0, y_0, \tilde{x}, \tilde{y} \in \Omega$ . Then,*

$$\begin{aligned} \mathcal{W}(u_{\pm}(x; x_0, \tilde{x}), u_{\pm}(x; y_0, \tilde{y})) &= \pm 2 i m(x)^2 \exp\left(\pm \frac{1}{h} (z(x; x_0) + z(x; y_0))\right) \\ &\times \left(w_{\pm}^{\text{even}}(x; x_0, \tilde{x}) w_{\pm}^{\text{odd}}(x; y_0, \tilde{y}) - w_{\pm}^{\text{odd}}(x; x_0, \tilde{x}) w_{\pm}^{\text{even}}(x; y_0, \tilde{y})\right), \end{aligned} \quad (16)$$

$$\begin{aligned} \mathcal{W}(u_{\pm}(x; x_0, \tilde{x}), u_{\mp}(x; y_0, \tilde{y})) &= \pm 2 i m(x)^2 \exp\left(\pm \frac{1}{h} (z(x; x_0) - z(x; y_0))\right) \\ &\times \left(w_{\pm}^{\text{even}}(x; x_0, \tilde{x}) w_{\mp}^{\text{even}}(x; y_0, \tilde{y}) - w_{\pm}^{\text{odd}}(x; x_0, \tilde{x}) w_{\mp}^{\text{odd}}(x; y_0, \tilde{y})\right). \end{aligned} \quad (17)$$

*In particular, if  $p_1 = p_2$ , then  $m = 1$ , all the Wronskians are independent of  $x$ , and we have for solutions with the same phase base point*

$$\mathcal{W}(u_{\pm}(\cdot; x_0, \tilde{x}), u_{\pm}(\cdot; x_0, \tilde{y})) = \mp 2 i \exp\left(\pm \frac{2}{h} z(\tilde{y}; x_0)\right) w_{\pm}^{\text{odd}}(\tilde{y}; x_0, \tilde{x}), \quad (18)$$

$$\mathcal{W}(u_{\pm}(\cdot; x_0, \tilde{x}), u_{\mp}(\cdot; x_0, \tilde{y})) = \pm 2 i w_{\pm}^{\text{even}}(\tilde{y}; x_0, \tilde{x}). \quad (19)$$

## 4 Formulation of the resonance condition

We now go back to our system

$$(P_{\nu} - E) u(r) = \begin{pmatrix} r^2 - E - \frac{h}{i} \frac{d}{dr} & \frac{h\nu}{r} \\ \frac{h\nu}{r} & r^2 - E + \frac{h}{i} \frac{d}{dr} \end{pmatrix} u(r) = 0, \quad r \in \mathbb{R}^+, \quad (20)$$

for  $E \in \mathbb{C}$  and  $\nu \in (\mathbb{N} - \frac{1}{2})$ , and study in particular their behavior as  $r \rightarrow 0$  and  $r \rightarrow \infty$ . In what follows, we use  $x$  instead of  $r$  and rewrite the equation (20) in the form

$$hD_x u = Au, \quad A = \begin{pmatrix} x^2 - E & \frac{h\nu}{x} \\ -\frac{h\nu}{x} & E - x^2 \end{pmatrix}. \quad (21)$$

The origin is a regular singular point of the equation with indicial roots  $\pm\nu$ . Indeed, (21) can be rewritten as

$$x \frac{d}{dx} u = (A_0 + O(x)) u \quad (x \rightarrow 0), \quad A_0 = \begin{pmatrix} 0 & i\nu \\ -i\nu & 0 \end{pmatrix},$$

and  $\pm\nu$  are the eigenvalues of  $A_0$ , and  ${}^t(1, \mp i)$  are the corresponding eigenvectors. Let  $u_0(x)$  be a solution corresponding to the index  $+\nu$ ,

$$u_0(x) \sim x^{\nu} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

as  $x \rightarrow 0$ . We will see in §5, that there exist Jost solutions  $f^{\pm}(x)$ , which are characterised by their asymptotic behavior at infinity,

$$f^+(x) \sim e^{+i(x^3 - 3Ex)/3h} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad f^-(x) \sim e^{-i(x^3 - 3Ex)/3h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (22)$$

as  $x \rightarrow +\infty$ . If  $\theta \in ]0, \pi/3[$ , then the dilated solution  $f^+(xe^{-i\theta})$  is exponentially growing and  $f^-(xe^{-i\theta})$  exponentially decaying as  $x \rightarrow +\infty$ . Since  $f^+$  and  $f^-$  are linearly independent,  $u_0$  can be expressed as a linear combination of these solutions,

$$u_0(x) = c^+(E, h)f^+(x) + c^-(E, h)f^-(x). \quad (23)$$

By Proposition 1.2, we obtain the following characterization of resonances:

**Proposition 4.1** *The energy  $E \in \mathbb{C}$  is a resonance of  $P$  if and only if there exists  $\nu \in (\mathbb{N} - \frac{1}{2})$  with  $c^+(E, h) = 0$ .*

To calculate the coefficients  $c^\pm(E, h)$ , which connect the solution  $u_0$  defined at the origin with the Jost solutions  $f^\pm$  defined at infinity, we need some intermediate solutions, which we will construct as exact WKB solutions. Let us recall the WKB construction of §3 in this case. Note that  $\text{tr } A = 0$  and so  $m = 1$ . Exact WKB solutions are of the form

$$u_\pm(x; x_0, \tilde{x}) = e^{\pm z(x)/h} T_\pm(z(x)) \begin{pmatrix} w_\pm^{\text{even}}(x) \\ w_\pm^{\text{odd}}(x) \end{pmatrix}, \quad (24)$$

where the phase function  $z(x)$  is defined by

$$z(x) = z(x; x_0) = \int_{x_0}^x \sqrt{g_+(t)g_-(t)} dt, \quad g_\pm(x) = \frac{h\nu}{x} \mp E \pm x^2$$

for a phase base point  $x_0$ ,  $T_\pm(z(x))$  is a  $2 \times 2$  matrix defined by (15) with

$$H(z(x)) = \left( \frac{g_-(x)}{g_+(x)} \right)^{1/4} = \left( \frac{h\nu + Ex - x^3}{h\nu - Ex + x^3} \right)^{1/4},$$

and  $w_\pm^{\text{even}}(x, h) = \sum_{n \geq 0} w_{2n, \pm}(z(x))$ ,  $w_\pm^{\text{odd}}(x, h) = \sum_{n \geq 0} w_{2n+1, \pm}(z(x))$  are constructed by recursive integrations with an amplitude base point  $\tilde{x}$ .

There are at most six turning points, the zeros of  $x \mapsto g_+(x)g_-(x)$ , in the whole complex plane  $\mathbb{C}_x$ . They are point-symmetric with respect to the origin and denoted by  $\{\pm r_j\}_{j=0}^2$ . For  $E > 0$  fixed and  $h\nu > 0$  sufficiently small, they are real and satisfy

$$0 < r_0 < r_1 < \sqrt{E} < r_2.$$

As  $h\nu \rightarrow 0$ ,  $r_0$  tends to 0, while  $r_1$  and  $r_2$  tend to  $\sqrt{E}$ , where  $\sqrt{E}$  denotes the square root of  $E \in \mathbb{C}$  in the right half-plane. Notice that  $r_0$  and  $r_1$  are zeros of  $g_+(x)$ , while  $r_2$  is a zero of  $g_-(x)$ .

We put branch cuts as in Figure 3 for the multi-valued functions

$$\sqrt{g_+(x)g_-(x)} = \frac{\sqrt{h^2\nu^2 - x^2(E - x^2)^2}}{x}, \quad H(z(x)) = \left( \frac{h\nu + Ex - x^3}{h\nu - Ex + x^3} \right)^{1/4},$$

and suppose that

$$\sqrt{h^2\nu^2 - x^2(E - x^2)^2}|_{x=0} = h\nu, \quad \left( \frac{h\nu + Ex - x^3}{h\nu - Ex + x^3} \right)^{1/4} \Big|_{x=0} = 1.$$

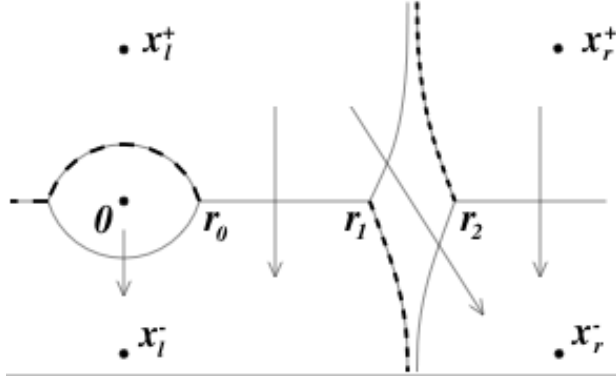


Figure 3: The Stokes curves, that is the level curves of  $x \mapsto \operatorname{Re} z(x)$ , which emanate from the turning points  $r_0, r_1, r_2$ . The arrows indicate the directions along which  $\operatorname{Re} z(x)$  increases. The dashed lines show the branch cuts.  $x_l^\pm$  and  $x_r^\pm$  are the amplitude base points for the constructed exact WKB solutions.

Let  $E > 0$  be positive, and let  $h\nu > 0$  be sufficiently small. Then, for example,  $\sqrt{g_+(x)g_-(x)} \in i\mathbb{R}^+$  for  $r_0 < x < r_1$  and  $r_2 < x$ , and  $H(z(x)) \in e^{-i\pi/4}\mathbb{R}^+$  for  $r_0 < x < r_1$ , while  $H(z(x)) \in e^{i\pi/4}\mathbb{R}^+$  for  $r_2 < x$ .

Choosing amplitude base points  $x_l^\pm, x_r^\pm$  as in Figure 3 ( $x_l^\pm$  are supposed to be purely imaginary for a technical reason in the proof of Lemma 6), we define the following six exact WKB solutions

$$\begin{aligned} u_0^\pm(x) &= u_\pm(x; r_0, x_l^\pm), \\ u_l^\pm(x) &= u_\pm(x; r_1, x_l^\pm), \\ u_r^\pm(x) &= u_\pm(x; r_2, x_r^\pm) \end{aligned}$$

with the turning points  $r_0, r_1, r_2$  as phase base points.

The three pairs  $(u_0^+(x), u_0^-(x)), (u_l^+(x), u_l^-(x)), (u_r^+(x), u_r^-(x))$  are all linearly independent and they are connected with  $u_0$  and  $(f^+, f^-)$  by transfer matrices  ${}^t(c_0^+(E, h), c_0^-(E, h)), T_1(E, h), T_2(E, h)$ , and  $T_3(E, h)$ :

$$u_0(x) = (u_0^+(x), u_0^-(x)) \begin{pmatrix} c_0^+(E, h) \\ c_0^-(E, h) \end{pmatrix}, \quad (25)$$

$$(u_0^+(x), u_0^-(x)) = (u_l^+(x), u_l^-(x))T_1(E, h), \quad (26)$$

$$(u_l^+(x), u_l^-(x)) = (u_r^+(x), u_r^-(x))T_2(E, h), \quad (27)$$

$$(u_r^+(x), u_r^-(x)) = (f^+(x), f^-(x))T_3(E, h). \quad (28)$$

Then, the coefficients  $c^+(E, h), c^-(E, h)$  in (23) are given by

$$\begin{pmatrix} c^+ \\ c^- \end{pmatrix} = T_3T_2T_1 \begin{pmatrix} c_0^+ \\ c_0^- \end{pmatrix}. \quad (29)$$

Now we can describe the strategy for the remainder of this article: The matrix  $T_3$  for the transfer at infinity is computed in §5, the coefficients  $c_0^\pm$  for the connection at the origin in §6, and the matrix  $T_2$  for the transfer near  $x = \sqrt{E}$  in §7. The matrix  $T_1$  is the easiest one, and can be determined right away



using Lemma 3.4. As  $u_0^\pm$  and  $u_l^\pm$  differ only in the base point of the phase, one uses (16) and (17) for  $x = x_l^\pm$  to obtain

$$T_1 = \begin{pmatrix} e^{S_{01}/h} & 0 \\ 0 & e^{-S_{01}/h} \end{pmatrix}, \quad (30)$$

where

$$S_{01}(E, h) = \int_{r_0}^{r_1} \sqrt{g_+(x)g_-(x)} dx = \int_{r_0}^{r_1} \frac{\sqrt{h^2\nu^2 - x^2(E - x^2)^2}}{x} dx.$$

Recalling the branch of the square root, we have

$$S_{01}(E, h) = \frac{i}{2} A(E, h). \quad (31)$$

## 5 Jost solutions

The Jost solutions of  $P_\nu u = Eu$  are characterised by their behavior (22) at infinity. They can be expressed as exact WKB solutions with base points of both phase and amplitude placed at infinity. This fact allows us to calculate  $T_3$ .

First we define the phase function with base point at infinity,

$$z(x, \infty) = \int_{+\infty}^x \left( \sqrt{h^2\nu^2 - t^2(E - t^2)^2}/t - i(t^2 - E) \right) dt + \frac{i}{3}(x^3 - 3Ex).$$

Taking the branch of the square root into account, we see that the integral converges absolutely, hence

$$z(x, \infty) = \frac{i}{3}(x^3 - 3Ex) + o(1) \quad (x \rightarrow +\infty).$$

Next, one notices, that the Stokes curves are asymptotically like horizontal lines  $\{\text{Im}x = \text{const.}\}$ , see Figure 3, and that

$$\frac{H'(x)}{H(x)} = \frac{h\nu}{2} \frac{E - 3x^2}{(h\nu - Ex + x^3)^2} = O(x^{-4}) \quad (x \rightarrow +\infty).$$

Hence, proceeding as in Section 3 of [26], one can construct well-defined exact WKB solutions  $u_\infty^\pm(x)$  with base points at infinity. Up to a constant prefactor,  $u_\infty^\pm(x)$  are the previously defined Jost solutions:

**Lemma 5.1** *Let  $u_\infty^\pm$  be the exact WKB solutions with phase and amplitude base point at infinity,  $f^\pm$  the Jost solutions defined in (22). Then,*

$$f^\pm(x) = \pm \frac{1}{2} e^{\pi i/4} u_\infty^\pm(x), \quad x > 0.$$

*Proof:* We just check the asymptotics of  $u_\infty^\pm$  at infinity. Since  $H(z(x)) \rightarrow e^{\pi i/4}$  as  $x \rightarrow +\infty$ , we get by an elementary calculation

$$u_\infty^\pm(x) \sim e^{\pm i(x^3 - 3Ex)/3h} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} e^{-\pi i/4} & e^{-\pi i/4} \\ \mp i e^{\pi i/4} & \pm i e^{\pi i/4} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

that is,

$$u_{\infty}^{+}(x) \sim 2e^{-\pi i/4} e^{i(x^3-3Ex)/3h} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad u_{\infty}^{-}(x) \sim -2e^{-\pi i/4} e^{-i(x^3-3Ex)/3h} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as  $x \rightarrow +\infty$ . □

**Remark 5.2** As an immediate consequence of the behaviour of the solutions  $u_{\infty}^{\pm}(x)$  for  $x \rightarrow +\infty$ , one observes the discrete spectrum of the full operator  $P = -h^2\Delta + V$  is empty.  $\diamond$

The main result of this section is the following proposition.

**Proposition 5.3** *There exists a positive  $\delta > 0$  independent of  $E \in \mathbb{C}$  and  $h > 0$ , such that the transfer matrix  $T_3$  defined in (28) satisfies*

$$T_3(E, h) = 2e^{-\pi i/4} \begin{pmatrix} e^{S_{2\infty}(E, h)/h} (1 + O(h)) & O(e^{-\delta/h}) \\ O(e^{-\delta/h}) & e^{-S_{2\infty}(E, h)/h} (1 + O(h)) \end{pmatrix}$$

as  $h \rightarrow 0$ , where  $S_{2\infty}(E, h)$  is the action between  $r_2$  and  $+\infty$ ,

$$S_{2\infty}(E, h) = \int_{r_2}^{+\infty} \left( \sqrt{h^2\nu^2 - x^2(E - x^2)^2}/x - i(x^2 - E) \right) dx + \frac{i}{3}(r_2^3 - 3Er_2).$$

*Proof:* We use the Wronskian formulas of Lemma 3.4 and the asymptotic expansions of Proposition 3.3 to calculate  $T_3$ . Setting

$$(u_r^+, u_r^-) =: (u_{\infty}^+, u_{\infty}^-) \tilde{T}_3,$$

the previous Lemma 5.1 gives

$$T_3 = \begin{pmatrix} 2e^{-\pi i/4} & 0 \\ 0 & -2e^{-\pi i/4} \end{pmatrix} \tilde{T}_3.$$

The difference of the phases  $z(x; r_2)$  and  $z(x; +\infty)$  is the action  $S_{2\infty}(E, h)$ , and we have

$$\mathcal{W}(u_r^{\pm}, u_{\infty}^{\mp}) = \pm 2i e^{\pm S_{2\infty}/h} (1 + O(h)), \quad \mathcal{W}(u_{\infty}^{\pm}, u_{\infty}^{\mp}) = \pm 2i (1 + O(h)).$$

Since there exists  $\delta > 0$  with

$$\mathcal{W}(u_r^{\pm}, u_{\infty}^{\pm}) = O(e^{-\delta/h}),$$

one obtains

$$\tilde{T}_3 = \begin{pmatrix} e^{S_{2\infty}/h} (1 + O(h)) & O(e^{-\delta/h}) \\ O(e^{-\delta/h}) & -e^{-S_{2\infty}/h} (1 + O(h)) \end{pmatrix}.$$

□

## 6 Asymptotics of the solution near the origin

We recall that the origin is a regular singular point of  $P_\nu$  with Fuchs indices  $\pm\nu$ , and that  $u_0$  is a solution corresponding to  $+\nu$ , which is unique up to a constant multiple. The purpose of this section is to calculate the connection coefficients  $c_0^\pm(E, h)$  in (25), that is to connect  $u_0$  with the exact WKB solutions  $u_0^+(x)$  and  $u_0^-(x)$ .

Let us look at the asymptotic behavior of the phase  $z(x) = z(x; r_0)$  as  $x \rightarrow 0$  for a fixed  $h > 0$ . Since  $\sqrt{h^2\nu^2 - x^2(E - x^2)^2} = h\nu + x\phi(x)$  with  $\phi(x)$  holomorphic near  $x = 0$ ,

$$e^{z(x)/h} = \exp\left(\int_{r_0}^x (h\nu/t + \phi(t)) dt/h\right) = C_{E,h} x^\nu \exp\left(\int_0^x \phi(t) dt/h\right)$$

where  $C_{E,h} := r_0^{-\nu} \exp(-\int_0^{r_0} \phi(t) dt/h) > 0$  is a positive constant. Moreover,  $H(x)$  is a holomorphic function at  $x = 0$  with  $H(0) = 1$ . Thus,

$$e^{z(x)/h} T_+(z(x)) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \sim C_{E,h} x^\nu \begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad x \rightarrow 0, \quad (32)$$

while  $h > 0$  fixed. This suggests, that  $u_0$  is collinear to an exact WKB solution of the type  $+$ . However, the amplitude base point  $\tilde{x}$  of the WKB solution should be placed at the origin to have

$$\begin{pmatrix} w_+^{\text{even}}(x) \\ w_+^{\text{odd}}(x) \end{pmatrix} \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad x \rightarrow 0,$$

since  $x \mapsto \text{Re } z(x)$  is decreasing as  $x$  tends to 0 in radial directions (see Figure 3). Moreover, the origin is a singular point for the equation and we need to check that the exact WKB solution  $u_+(x; r_0, 0)$  is well defined, i.e. the recurrence equations (11), (12) with initial value  $w_{0,+}^0 \equiv 1$ ,  $w_{n,+}^0(0) = 0$ ,  $n \geq 1$ , define a sequence of holomorphic functions  $\{w_{n,+}^0\}_{n \geq 0}$ , and the series  $\sum_{n \geq 0} w_{2n,+}^0(x)$  and  $\sum_{n \geq 0} w_{2n+1,+}^0(x)$  converge in a neighborhood of the origin. We rewrite (11), (12) with respect to  $x$ :

$$\left(\frac{d}{dx} + \frac{2}{h} \sqrt{g_+(x)g_-(x)}\right) w_{2n+1,+}^0(x) = \frac{H'_x(x)}{H(x)} w_{2n,+}^0(x), \quad (33)$$

$$\frac{d}{dx} w_{2n+2,+}^0(x) = \frac{H'_x(x)}{H(x)} w_{2n+1,+}^0(x), \quad (34)$$

where  $H'_x$  stands for the derivative of  $H$  with respect to  $x$ .

These equations are of the form

$$\frac{dw}{dx} + \frac{b(x)}{x} w = f(x), \quad w(0) = 0$$

with  $b(x)$  and  $f(x)$  given holomorphic functions at the origin. In our case,  $b \equiv 0$  for (34) or  $b(x) = 2x\sqrt{g_+(x)g_-(x)}/h$ ,  $b(0) = 2\nu$  for (33). This Cauchy problem has a unique holomorphic solution if  $\text{Re } b(0) > -1$ , and the solution is given by

$$w(x) = x \int_0^1 t^{b(0)} \exp\left(-x \int_t^1 \frac{b(xs) - b(0)}{xs} ds\right) f(xt) dt. \quad (35)$$

Hence,  $\{w_{n,+}^0\}$  are uniquely determined and given by the recursive integrals

$$w_{2n+2,+}^0 = I_0(w_{2n+1,+}^0), \quad w_{2n+1,+}^0 = I_1(w_{2n,+}^0),$$

where

$$\begin{aligned} I_0(f) &= \int_0^x \frac{H'_\xi(\xi)}{H(\xi)} f(\xi) d\xi = \frac{1}{2} \int_0^x \frac{h\nu(E - 3\xi^2)}{h^2\nu^2 - \xi^2(E - \xi^2)^2} f(\xi) d\xi, \\ I_1(f) &= \int_0^x e^{-\frac{2}{h} \int_\xi^x \sqrt{g_+(t)g_-(t)} dt} \frac{H'_\xi(\xi)}{H(\xi)} f(\xi) d\xi \\ &= \frac{1}{2} \int_0^x e^{-\frac{2}{h} \int_\xi^x \sqrt{h^2\nu^2/t^2 - (E-t^2)^2} dt} \frac{h\nu(E - 3\xi^2)}{h^2\nu^2 - \xi^2(E - \xi^2)^2} f(\xi) d\xi. \end{aligned}$$

It is not difficult to see that for any fixed positive  $h > 0$ , the series

$$w_{+,0}^{\text{even}}(x, h) = \sum_{n=0}^{\infty} w_{2n,+}^0(x), \quad w_{+,0}^{\text{odd}}(x, h) = \sum_{n=0}^{\infty} w_{2n+1,+}^0(x).$$

are absolutely convergent in a sufficiently small neighborhood of the origin. Hence, the function

$$\tilde{u}_0(x) := e^{z(x)/h} T_+(z(x)) \begin{pmatrix} w_{+,0}^{\text{even}}(x) \\ w_{+,0}^{\text{odd}}(x) \end{pmatrix}$$

defines a solution to (21). Next, we study the asymptotic behavior of the connection coefficients  $c_0^\pm(E, h)$  as  $h \rightarrow 0$ , using the exact WKB solution  $\tilde{u}_0$ . For that purpose we will need some bounds on  $w_{+,0}^{\text{even}}(x, h)$  and  $w_{+,0}^{\text{odd}}(x, h)$ . Since we will finally use those in the Wronskian formulas, it is enough to deal with the case when  $x$  is purely imaginary,  $x = iR$  with  $R > 0$ . We start by the following elementary estimate.

**Lemma 6.1** *For any  $\kappa \geq 0$ ,  $m > 0$  and  $\tau > 0$ , one has*

$$\int_0^\tau e^{\kappa(r-\tau)} \frac{r^{m-1}}{(1+r)^{m+1}} dr \leq \frac{1}{m} \left( \frac{\tau}{1+\tau} \right)^m.$$

*Proof:* One integrates by parts,

$$\begin{aligned} \int_0^\tau e^{\kappa(r-\tau)} \frac{r^{m-1}}{(1+r)^{m+1}} dr &= \frac{\tau^m}{m(1+\tau)^{m+1}} - \frac{1}{m} \int_0^\tau r^m \frac{d}{dr} \left( \frac{e^{\kappa(r-\tau)}}{(1+r)^{m+1}} \right) dr \\ &\leq \frac{1}{m} \left( \frac{\tau}{1+\tau} \right)^m. \end{aligned}$$

□

**Lemma 6.2** *For any  $E > 0$ ,  $\tau > 0$ , and  $n \in \mathbb{N}_0$ , one has*

$$|w_{n,+}^0(ih\nu\tau/E)| \leq \frac{K(\tau)^n}{n!} \left( \frac{\tau}{1+\tau} \right)^n, \quad (36)$$

where  $K(\tau) = 1 + 3h^2\nu^2\tau^2/E^3$ .

*Proof:* For  $x = iR$ ,  $R > 0$ , we have by the changes of variables  $t = is$ ,  $\xi = i\rho$ ,

$$I_0(f)|_{x=iR} = \frac{1}{2i} \int_0^R \frac{h\nu(E + 3\rho^2)}{h^2\nu^2 + \rho^2(E + \rho^2)^2} f(i\rho) d\rho,$$

$$I_1(f)|_{x=iR} = \frac{1}{2i} \int_0^R e^{-\frac{2}{h} \int_\rho^R \frac{\sqrt{h^2\nu^2 + s^2(E+s^2)^2}}{s} ds} \frac{h\nu(E + 3\rho^2)}{h^2\nu^2 + \rho^2(E + \rho^2)^2} d\rho.$$

Since

$$h^2\nu^2 + s^2(E + s^2)^2 > E^2 s^2, \quad \frac{h\nu(E + 3\rho^2)}{h^2\nu^2 + \rho^2(E + \rho^2)^2} \leq \frac{h\nu(E + 3R^2)}{h^2\nu^2 + \rho^2 E^2},$$

we have for  $R = \nu\tau/E$ ,

$$|I_0(f)|_{x=i\nu\tau/E} \leq \frac{K(\tau)}{2} \int_0^\tau \frac{1}{1+r^2} |f(ih\nu r/E)| dr, \quad (37)$$

$$|I_1(f)|_{x=i\nu\tau/E} \leq \frac{K(\tau)}{2} \int_0^\tau e^{2\nu(r-\tau)} \frac{1}{1+r^2} |f(ih\nu r/E)| dr. \quad (38)$$

We now proceed by induction over  $n \in \mathbb{N}_0$ . Since  $w_{0,+}^0 \equiv 1$ , inequality (36) is trivially satisfied for  $n = 0$ . Next, we assume that (36) holds for  $n = 2k$ . Then, from (38) and Lemma 6.1, one has

$$\begin{aligned} |w_{2k+1,+}^0(ih\nu\tau/E)| &= |I_1(w_{2k,+}^0)|_{x=i\nu\tau/E}| \\ &\leq \frac{K(\tau)}{2} \int_0^\tau e^{2\nu(r-\tau)} \frac{1}{1+r^2} |w_{2k,+}^0(ih\nu r/E)| dr \\ &\leq \frac{K(\tau)^{2k+1}}{2k!} \int_0^\tau e^{2\nu(r-\tau)} \frac{r^{2k}}{(1+r)^{2k+2}} dr \\ &\leq \frac{K(\tau)^{2k+1}}{(2k+1)!} \left( \frac{\tau}{1+\tau} \right)^{2k+1}. \end{aligned}$$

Thus (36) holds for  $n = 2k + 1$ . In the same way, we can show that it holds for  $n = 2k + 2$ .  $\square$

**Proposition 6.3** *There exists a non-zero constant  $a(E, h) \neq 0$  such that*

$$u_0(x) = a(E, h) \tilde{u}_0(x).$$

The connection coefficients  $c_0^\pm(E, h)$  in (25) are analytic in  $E$  near  $E_0 > 0$  and behave as

$$c_0^+(E, h) = a(E, h)(1 + o(1)), \quad c_0^-(E, h) = -i a(E, h)(1 + o(1))$$

uniformly for  $E$  near  $E_0 > 0$  as  $h \rightarrow 0$ .

*Proof:* The first part is a direct consequence of (32) and the construction of the solution  $\tilde{u}_0(x)$ .

The second part is an Airy type connection formula at least at the level of the principal term. Let us review briefly how to derive this by the Wronskian formulas (18) and (19). The coefficients  $c_0^+$ ,  $c_0^-$  are given by

$$c_0^+ = a \frac{\mathcal{W}(\tilde{u}_0, u_0^-)}{\mathcal{W}(u_0^+, u_0^-)}, \quad c_0^- = -a \frac{\mathcal{W}(\tilde{u}_0, u_0^+)}{\mathcal{W}(u_0^+, u_0^-)}.$$

Since all the solutions involved just differ in the choice of the amplitude base point, we can apply formulas (18) and (19) to get

$$\mathcal{W}(u_0^+, u_0^-) = 2i w_+^{\text{even}}(x_l^-; r_0, x_l^+), \quad \mathcal{W}(\tilde{u}_0, u_0^-) = 2i w_+^{\text{even}}(x_l^-; r_0, 0).$$

The Wronskian  $\mathcal{W}(\tilde{u}_0, u_0^+)$  is more delicate, since there is a branch cut between the origin and  $x_l^+$ , see Figure 2. Hence,  $u_0^+$  should be considered on the other Riemann surface. Let us denote by  $\hat{x}$  the point on the Riemann surface continued from  $x$  to the same point turning around  $r_0$  by the angle  $-2\pi$ . Since  $g_+(x)^{1/2} = -g_+(\hat{x})^{1/2}$  and  $g_+(x)^{1/4} = ig_+(\hat{x})^{1/4}$ , we have

$$z(x, r_0) = -z(\hat{x}, r_0), \quad H(x) = -iH(\hat{x}), \quad T_+(x) = iT_-(\hat{x}),$$

and for the series summands we get  $w_{n,\pm}(\hat{x}) = w_{n,\mp}(x)$ . Consequently, we have

$$u_0^+(x_l^+, r_0, 0) = iu_-(\hat{x}_l^+, r_0, 0),$$

which yields

$$\mathcal{W}(\tilde{u}_0, u_0^+) = -2w_+^{\text{even}}(\hat{x}_l^+, r_0, 0).$$

On the other hand, we know that

$$w_+^{\text{even}}(x_l^-; r_0; x_l^+) = 1 + O(h),$$

because we can take a path from  $x_l^+$  to  $x_l^-$ , along which  $x \mapsto \text{Re } z(x)$  increases and which passes far away to the right from the turning point  $r_0$ . Hence

$$c_0^+ = a w_+^{\text{even}}(x_l^-; r_0; 0) (1 + O(h)), \quad c_0^- = -ia w_+^{\text{even}}(\hat{x}_l^+; r_0; 0) (1 + O(h)),$$

and it is enough for the proof to show

$$\lim_{h \rightarrow 0} w_+^{\text{even}}(x_l^-; r_0; 0) = \lim_{h \rightarrow 0} w_+^{\text{even}}(\hat{x}_l^+; r_0; 0) = 1. \quad (39)$$

Let  $E > 0$ . Recall that  $w_{+,0}^{\text{even}} = \sum_{n=0}^{\infty} (I_0 \circ I_1)^n(1)$ . Hence, if we write  $x_l^+ = iR$ , then

$$\begin{aligned} w_+^{\text{even}}(\hat{x}_l^+; r_0; 0) &= w_{+,0}^{\text{even}}(iR) = 1 + (I_0 \circ I_1)(w_{+,0}^{\text{even}})|_{x=iR} \\ &= 1 + \frac{1}{2iE} \int_0^{\infty} \chi_{(0, \frac{ER}{h\nu})}(r) \frac{E + 3h^2\nu^2r^2/E^2}{1 + r^2(1 + h^2\nu^2r^2/E^3)^2} I_1(w_{+,0}^{\text{even}})|_{x=ih\nu r/E} dr, \end{aligned}$$

where  $\chi_{(0, \frac{ER}{h\nu})}$  is the characteristic function of the interval  $(0, \frac{ER}{h\nu})$ . The integrand is dominated by an integrable function: indeed, Lemma 6.2 gives for  $r \in (0, \frac{ER}{h\nu})$

$$|w_{+,0}^{\text{even}}(ih\nu r/E)| \leq \sum_{n \geq 0} |w_{+,0}^{2n}(ih\nu E/r)| \leq \sum_{n \geq 0} \frac{K(r)^{2n}}{(2n)!} \left( \frac{r}{1+r} \right)^{2n} \leq \cosh \tilde{K},$$

$$|I_1(w_{+,0}^{\text{even}})(ih\nu r/E)| \leq \tilde{K} \cosh \tilde{K},$$

with  $\tilde{K} = 1 + 3R^2/E$ , and

$$0 \leq \chi_{(0, \frac{ER}{h\nu})}(r) \frac{E + 3h^2\nu^2r^2/E^2}{1 + r^2(1 + h^2\nu^2r^2/E^3)^2} \leq \frac{E\tilde{K}}{1 + r^2}.$$

On the other hand, the integrand tends to 0 as  $h \rightarrow 0$  for any fixed  $r > 0$ , since  $I_1(w_{+,0}^{\text{even}})|_{x=0} = 0$ . By Lebesgue's dominated convergence theorem, we obtain the second identity of (39) for  $E > 0$  and by analyticity for  $E$  near  $E_0 > 0$ . The first identity of (39) is proven just in the same way.  $\square$

## 7 Connection formula near the critical point

In this section, we compute the transfer matrix  $T_2$ , which connects  $u_l^\pm(x) = u^\pm(x; r_1, x_l^\pm)$  with  $u_r^\pm(x) = u^\pm(x; r_2, x_r^\pm)$ ,

$$(u_l^+(x), u_l^-(x)) = (u_r^+(x), u_r^-(x))T_2(E, h),$$

see (27). We will show

**Proposition 7.1** For all  $E \in \mathbb{C}$  near  $E_0 > 0$ , the transfer matrix  $T_2$  is of the form

$$T_2(E, h) = \begin{pmatrix} t(E, h) & s(E, h) \\ -\overline{s(E, h)} & -\overline{t(E, h)} \end{pmatrix}, \quad (40)$$

and the asymptotics of  $t(E, h)$  and  $s(E, h)$  for  $h \rightarrow 0$  are given by

$$t(E, h) = -\sqrt{\frac{\pi h}{2}} \nu E^{-3/4} e^{-i\pi/4} + O(h|\ln h|), \quad s(E, h) = i + O(h).$$

The proof of Proposition 7.1 is given in Section 7.5.

**Remark 7.2** From the symmetry properties

$$u_r^+ = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{u_r^-}, \quad u_l^- = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{u_l^+}, \quad (41)$$

we know *a priori* that  $T_2$  is indeed of the claimed form (40). Hence, it remains to prove the asymptotic behaviour of  $t(E, h)$  and  $s(E, h)$  as  $h \rightarrow 0$ .  $\diamond$

The exact WKB method is not enough to compute the  $h$ -asymptotics of  $T_2(E, h)$ , because the two turning points  $r_1$  and  $r_2$  coalesce at  $x = \sqrt{E}$  as  $h \rightarrow 0$ . In other words: The Wronskian of two exact WKB solutions, say  $u_l^+$  and  $u_r^-$ , is given in terms of  $w_+^{\text{even}}$  computed along a path from  $x_l^+$  to  $x_r^-$  passing between  $r_1$  and  $r_2$ , but the  $h$ -asymptotic formula for  $w_+^{\text{even}}$  (Proposition 3.3) does not hold because of the singularity of the function  $H$  at  $r_1$  and  $r_2$ .

Hence, one resorts to a microlocal study of the equation  $P_\nu u = Eu$  near the point  $(x, \xi) = (\sqrt{E}, \xi)$  for  $E > 0$ , where  $\xi$  is the dual variable of  $x$ . The equation  $P_\nu u = Eu$  is reduced to a simple microlocal normal form  $Qw = 0$  (see Section 7.1), whose solutions are well studied. From these solutions we obtain two basis sets of microlocal solutions  $(\tilde{f}^+, \tilde{f}^-)$ ,  $(\tilde{g}^+, \tilde{g}^-)$  of  $P_\nu u = Eu$ , which are related via a constant matrix  $R$ :

$$(\tilde{f}^+, \tilde{f}^-)R = (\tilde{g}^+, \tilde{g}^-), \quad R = \begin{pmatrix} p & q \\ -q & -p \end{pmatrix},$$

see Section 7.2. The exact WKB solutions  $u_l^\pm, u_r^\pm$  are expressed in terms of these basis sets by

$$\begin{aligned} (u_l^+, u_l^-) &= (\tilde{f}^+, \tilde{f}^-)A_l = (\tilde{g}^+, \tilde{g}^-)B_l, \\ (u_r^+, u_r^-) &= (\tilde{f}^+, \tilde{f}^-)A_r = (\tilde{g}^+, \tilde{g}^-)B_r, \end{aligned}$$

where the constant matrices  $A_{l,r}$  and  $B_{l,r}$  satisfy

$$A_l = RB_l, \quad A_r = RB_r. \quad (42)$$

Then, the matrix  $T_2$  is given by

$$T_2 = A_r^{-1} A_l = B_r^{-1} B_l. \quad (43)$$

Hence, the  $h$ -asymptotics of  $t(E, h)$  and  $s(E, h)$  can be obtained from the study of the connection matrices  $A_{l,r}$  and  $B_{l,r}$  (see Sections 7.3 and 7.4).

## 7.1 Normal form

We now transform the equation  $(P_\nu - E)u = 0$  near  $(x, \xi) = (\sqrt{E}, \xi)$ ,  $E > 0$ , to a simple microlocal normal form  $Qw = 0$ . As an intermediate step, the reduction will pass by the famous Landau-Zener system (46), the prototypic ordinary differential problem for non-adiabatic transitions due to an avoided eigenvalue crossing.

**Theorem 7.3** *Let  $E > 0$  and  $u(x, h)$  be a solution of  $(P_\nu - E)u = 0$ . Let  $V$  be the metaplectic operator associated with the  $\frac{\pi}{4}$ -rotation in phase space*

$$\kappa_{\frac{\pi}{4}} : T^*\mathbb{R} \rightarrow T^*\mathbb{R}, \quad (x, \xi) \mapsto \frac{1}{\sqrt{2}}(x - \xi, x + \xi).$$

*There exists a locally diffeomorphic change of coordinates  $x \mapsto \phi(x) = y$ ,  $x > 0$ , with  $\phi(\sqrt{E}) = 0$  and a matrix-valued  $C^\infty$ -symbol  $M(y, h) = \text{Id} + O(h)$  such that for any cut-off function  $\chi \in C_c^\infty(\mathbb{R})$  identically equal to 1 in an interval around  $y = 0$*

$$w(y, h) = V(\chi(y)M(y, h)u(\phi^{-1}(y), h))$$

*satisfies  $Qw = r$ , where*

$$Q = \begin{pmatrix} y & \frac{\gamma}{\sqrt{2}} \\ -\frac{\gamma}{\sqrt{2}} & -hD_y \end{pmatrix},$$

*$\gamma = \gamma(E, h)$  is a constant with  $\gamma(E, h) = \frac{\nu}{\sqrt{2}}E^{-3/4}h + O(h^2)$ , and  $r(y, h) = O(h^\infty)$  uniformly in an interval around  $y = 0$  together with all its derivatives.*

*Proof:* We proceed in three steps to reduce the equation  $P_\nu u = Eu$ , that is

$$hD_x u(x) = A(x)u(x), \quad A(x) = \begin{pmatrix} x^2 - E & h\nu/x \\ -h\nu/x & E - x^2 \end{pmatrix}. \quad (44)$$

*First step.* One turns the quadratic diagonal entries of  $A(x)$  into linear ones. Let  $y = \phi(x)$  with

$$\phi(x) = (x - \sqrt{E}) \left( \frac{2}{3}(x - \sqrt{E}) + 2\sqrt{E} \right)^{1/2}.$$

In the right half-plane, the function  $\phi(x)$  is a biholomorphic map with  $\phi(\sqrt{E}) = 0$  and  $\phi(x)\phi'(x) = x^2 - E$ . The function

$$\psi(y) = \psi(\phi(x)) = \frac{(\frac{2}{3}(x - \sqrt{E}) + 2\sqrt{E})^{1/2}}{x(x + \sqrt{E})} \quad (45)$$

is analytic in a neighborhood of  $y = 0$ , satisfying  $\psi(0) = E^{-3/4}/\sqrt{2}$  and  $\psi(\phi(x))\phi'(x) = 1/x$ . Moreover, if  $u(x)$  satisfies (44), then  $v(y) = v(\phi(x)) = u(x)$  satisfies

$$hD_y v(y) = \begin{pmatrix} y & h\nu\psi(y) \\ -h\nu\psi(y) & -y \end{pmatrix} v(y).$$



*Second step.* The second step makes the off-diagonal entries constant modulo  $O(h^\infty)$  by a change of the unknown function

$$\tilde{w}(y, h) = M(y, h)v(y, h).$$

Lemma B.1 constructs a matrix-valued  $\mathcal{C}^\infty$ -symbol  $M(y, h) = \text{Id} + O(h)$  such that  $\tilde{w}(y, h)$  satisfies

$$\begin{pmatrix} hD_y - y & -\gamma \\ \bar{\gamma} & hD_y + y \end{pmatrix} \tilde{w}(y, h) = r(y, h)\tilde{w}(y, h) \quad (46)$$

where  $\gamma = \frac{\nu}{\sqrt{2}}E^{-3/4}h + O(h^2)$  and  $r(y, h) = O(h^\infty)$  uniformly in an interval around  $y = 0$  together with all its derivatives.

*Third step.* Multiplying a cut off function  $\chi$  and then operating the metaplectic operator  $V$  from the left to equation (46), we obtain by Lemma B.2

$$Qw(y, h) = -\frac{1}{\sqrt{2}}V(\chi(y)r(y, h)\tilde{w}(y, h) - ih\chi'(y)\tilde{w}(y, h)).$$

The right hand side is of  $O(h^\infty)$  uniformly in interval around  $y = 0$  together with its all derivatives.  $\square$

**Remark 7.4** The proof of Theorem 7.3 shows, that  $\gamma$ ,  $\phi$ , and  $M$  depend analytically on  $E$  for  $E \in \mathbb{C}$  near some  $E_0 > 0$ .  $\diamond$

## 7.2 Solutions of the normal form

Here we compute the solutions of the normal form. The equation

$$Qw = 0, \quad w = {}^t(w_1, w_2)$$

is equivalent to

$$w_1 = -\frac{\gamma}{\sqrt{2}y}w_2, \quad \frac{h}{i}yw_2' = \frac{|\gamma|^2}{2}w_2. \quad (47)$$

This is a well-studied saddle point problem (see for example [17], [6], or section 5 in [26]). The system (47) has two maximal solutions

$$f^\pm(y) = {}^t(f_1^\pm(y), f_2^\pm(y)),$$

with

$$f_1^\pm(y) = -\frac{\gamma}{\sqrt{2}y}\chi_{(0, \infty)}(\pm y)|y|^{\frac{i}{2k}|\gamma|^2},$$

$$f_2^\pm(y) = \chi_{(0, \infty)}(\pm y)|y|^{\frac{i}{2k}|\gamma|^2},$$

where  $\chi_{(0, \infty)}$  is the characteristic function of the interval  $(0, \infty)$ . Moreover, we have two additional solutions

$$g^\pm(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_h f^\pm(y), \quad (48)$$

where  $\mathcal{F}_h u(\eta) = \frac{1}{\sqrt{2\pi h}} \int_{\mathbb{R}} e^{-iy\eta/h} u(y) dy$  is the  $h$ -Fourier transform and  $\mathcal{C}u = \bar{u}$  is the complex conjugate. Indeed, we have the following identity:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_h Q = -Q \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_h.$$

Since  $\mathcal{CF}_h = \mathcal{F}_h^{-1}\mathcal{C}$ , we also have

$$f^\pm(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{CF}_h g^\pm(y). \quad (49)$$

These four solutions are linearly dependent, and as in Proposition 5.5 in [26] one obtains the following connection formula.

**Proposition 7.5** *The solutions  $f^\pm$  and  $g^\pm$  of  $Qw = 0$  are connected by*

$$(g^+, g^-) = (f^+, f^-)R, \quad R = \begin{pmatrix} p & q \\ -q & -p \end{pmatrix}, \quad (50)$$

where

$$\begin{aligned} p &= \frac{h^{\frac{1}{2} - \frac{i}{2k}|\gamma|^2}}{i\gamma\sqrt{\pi}} \Gamma\left(1 - \frac{i}{2h}|\gamma|^2\right) \exp\left(\frac{\pi}{4h}|\gamma|^2\right), \\ q &= \frac{h^{\frac{1}{2} - \frac{i}{2k}|\gamma|^2}}{i\gamma\sqrt{\pi}} \Gamma\left(1 - \frac{i}{2h}|\gamma|^2\right) \exp\left(-\frac{\pi}{4h}|\gamma|^2\right). \end{aligned}$$

**Remark 7.6** In view of the relations (48) and (49), the matrix  $R$  satisfies  $R\bar{R} = \text{Id}$ , that is  $|p|^2 - |q|^2 = 1$  and  $p\bar{q} = \bar{p}q$ .  $\diamond$

### 7.3 Frequency sets of the microlocal and WKB solutions

Let us study the frequency set of the microlocal solutions  $f^\pm$ ,  $g^\pm$  and the exact WKB solutions  $u_\pm^l$ ,  $u_\pm^r$ .

First, the frequency set of the microlocal solutions are subsets of  $\mathbb{R}_y \times \mathbb{R}_\eta$  as follows:

$$\begin{aligned} \text{FS}(f_1^\pm) &\subset \{y = 0\} \cup \{\eta = 0, \pm y > 0\}, \\ \text{FS}(g_1^\pm) &\subset \{\eta = 0\} \cup \{y = 0, \pm \eta > 0\}. \end{aligned}$$

Second, let  $\sigma_{r,l}^\pm \subset \mathbb{R}_x \times \mathbb{R}_\xi$  be the Lagrangian manifolds defined by

$$\sigma_l^\pm = \{r_0 < x < r_1, \xi = \pm(E - x^2)\}, \quad \sigma_r^\pm = \{r_2 < x, \xi = \pm(x^2 - E)\}. \quad (51)$$

Since  $z'(x) = \sqrt{h^2\nu^2 - x^2(E - x^2)^2}/x$ , one has

$$\text{FS}(u_l^\pm) \cap \{r_0 < x < r_1\} \subset \sigma_l^\pm, \quad \text{FS}(u_r^\pm) \cap \{x > r_2\} \subset \sigma_r^\pm.$$

Now we transform to the normal form of Theorem 7.3, that is operate  $N$  to the exact WKB solutions  $u_{l,r}^\pm$ , where

$$Nu(y, h) = V(\chi(y)M(y, h)u(\phi^{-1}(y), h)).$$

Since  $u_{l,r}^\pm$  are solutions of the equation  $(P_\nu - E)u = 0$ , we see that for any  $k \geq 0$

$$D_y^k Q(Nu_{l,r}^\pm) = O(h^\infty).$$

Hence,  $Nu_{l,r}^\pm$  are microlocal solutions of  $Qw = 0$  near  $(0, 0)$ . Since the vector space of such solutions is two-dimensional, see Proposition 17 of [6], there exist matrix-valued  $\mathcal{C}^\infty$ -symbols

$$A_l = (\alpha_{jk}^l), \quad A_r = (\alpha_{jk}^r), \quad B_l = (\beta_{jk}^l), \quad B_r = (\beta_{jk}^r), \quad (52)$$

such that microlocally near  $(0, 0)$

$$\begin{aligned} (Nu_l^+, Nu_l^-) &= (f^+, f^-)A_l = (g^+, g^-)B_l, \\ (Nu_r^+, Nu_r^-) &= (f^+, f^-)A_r = (g^+, g^-)B_r. \end{aligned}$$

Returning back to the  $(x, \xi)$  variables, i.e. operating  $N^{-1}$  from the left, we have microlocally near  $(\sqrt{E}, 0)$ ,

$$\begin{aligned} (u_l^+, u_l^-) &= (\tilde{f}^+, \tilde{f}^-)A_l = (\tilde{g}^+, \tilde{g}^-)B_l, \\ (u_r^+, u_r^-) &= (\tilde{f}^+, \tilde{f}^-)A_r = (\tilde{g}^+, \tilde{g}^-)B_r, \end{aligned}$$

where

$$\tilde{f}^\pm = N^{-1}(\tilde{\chi}f^\pm), \quad \tilde{g}^\pm = N^{-1}(\tilde{\chi}g^\pm) \quad (53)$$

and  $\tilde{\chi} \in \mathcal{C}_c^\infty(\mathbb{R})$  a cut-off function, which is identically equal to 1 near  $y = 0$  and satisfies  $\text{supp}(\tilde{\chi}) \subset \text{supp}(\chi)$ . By Lemma B.2, we have

$$\text{FS}(\tilde{f}^\pm) = \kappa_\phi^{-1}(\kappa_{\frac{\pi}{4}}\text{FS}(\tilde{\chi}f^\pm)), \quad \text{FS}(\tilde{g}^\pm) = \kappa_\phi^{-1}(\kappa_{\frac{\pi}{4}}\text{FS}(\tilde{\chi}g^\pm)),$$

where

$$\kappa_\phi^{-1} : T^*\mathbb{R} \rightarrow T^*\mathbb{R}, \quad (x, \xi) \mapsto (\phi^{-1}(x), \xi \phi'(\phi^{-1}(x)))$$

is the inverse of the canonical transformation  $\kappa_\phi(x, \xi) = (\phi(x), \xi/\phi'(x))$  associated with  $\phi$ . Clearly,

$$\begin{aligned} \kappa_{\frac{\pi}{4}}\text{FS}(f_1^\pm) &\subset \{\eta = -y\} \cup \{\eta = y, \pm y > 0\}, \\ \kappa_{\frac{\pi}{4}}\text{FS}(g_1^\pm) &\subset \{\eta = y\} \cup \{\eta = -y, \mp y > 0\}. \end{aligned}$$

Since  $\phi(x)\phi'(x) = x^2 - E$ , this yields

$$\begin{aligned} \text{FS}(\tilde{f}^+) \cap U &\subset \sigma_l^- \cup \sigma_r^+ \cup \sigma_r^-, & \text{FS}(\tilde{f}^-) \cap U &\subset \sigma_l^+ \cup \sigma_l^- \cup \sigma_r^+, \\ \text{FS}(\tilde{g}^+) \cap U &\subset \sigma_l^+ \cup \sigma_r^+ \cup \sigma_r^-, & \text{FS}(\tilde{g}^-) \cap U &\subset \sigma_l^+ \cup \sigma_l^- \cup \sigma_r^- \end{aligned}$$

with  $U = \{r_0 < x < r_1 \text{ or } x > r_2\}$ , see Figure 4.  $\sigma_l^+$  is neither contained in  $\text{FS}(u_l^-)$  nor in  $\text{FS}(\tilde{f}^+)$ , while it is contained in  $\text{FS}(\tilde{f}^-)$ . Hence,  $\alpha_{22}^l = 0$ . Analogously one obtains

$$\alpha_{11}^r = \alpha_{22}^l = \beta_{12}^r = \beta_{21}^l = 0. \quad (54)$$

## 7.4 Connection between microlocal and exact WKB solutions

We now compute the remaining coefficients of the matrices  $A_{l,r}$  and  $B_{l,r}$  connecting the microlocal solutions  $\tilde{f}^\pm, \tilde{g}^\pm$  with the WKB solutions  $u_l^\pm, u_r^\pm$  of  $P_\nu u = Eu, E > 0$ . As a first step, the stationary phase method gives the following formulae for the microlocal solutions, whose proof is to be found in Appendix C.

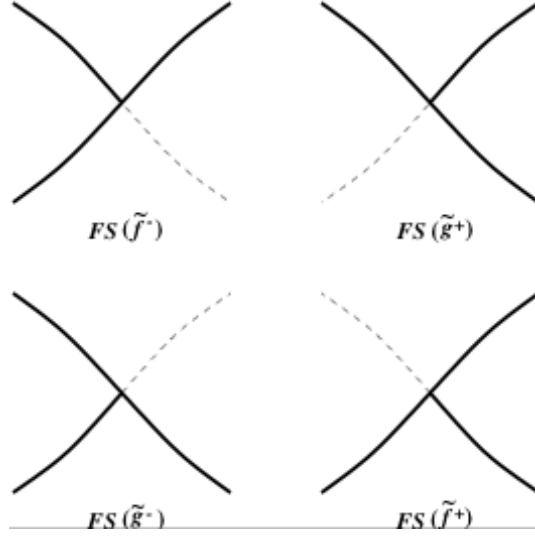


Figure 4: Frequency sets of the microlocal solutions  $\tilde{f}^\pm$  and  $\tilde{g}^\pm$  defined in (53).

**Lemma 7.7** For the microlocal solutions  $\tilde{f}^\pm$  of  $P_\nu u = Eu$ ,  $E > 0$ , defined in (53), one has microlocally near the Lagrangian manifolds  $\sigma_l^+$  and  $\sigma_r^-$  defined in (51) that

$$\tilde{f}^-(x) = e^{i\pi/8} 2^{1/4} e^{+z(x;r_1)/h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h)) \quad \text{near } \sigma_l^+, \quad (55)$$

$$\tilde{f}^+(x) = e^{i\pi/8} 2^{1/4} e^{-z(x;r_2)/h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h)) \quad \text{near } \sigma_r^-. \quad (56)$$

It remains to connect  $e^{\pm z(x;r_1)/h}$  and  $e^{\pm z(x;r_2)/h}$  to the WKB solutions  $u_l^\pm$  and  $u_r^\pm$ .

**Proposition 7.8** With the notation of Lemma 7.7, we have microlocally

$$u_l^+ = k_l^+ \tilde{f}^- \quad \text{near } \sigma_l^+, \quad u_r^+ = k_r^+ \tilde{g}^+ \quad \text{near } \sigma_r^+,$$

$$u_l^- = k_l^- \tilde{g}^- \quad \text{near } \sigma_l^-, \quad u_r^- = k_r^- \tilde{f}^+ \quad \text{near } \sigma_r^-,$$

where

$$k_l^+ = -2^{3/4} e^{i\pi/8} (1 + O(h)), \quad k_r^- = -2^{3/4} e^{-i3\pi/8} (1 + O(h)),$$

and

$$k_l^- = -i \overline{k_l^+}, \quad k_r^+ = i \overline{k_r^-}.$$

*Proof:* To prove these relations, say the first one, it is enough to calculate the asymptotic behavior of  $\tilde{f}^-$  and  $u_l^+$  near  $\sigma_l^+$ . First, recall the exact WKB formula

$$\begin{aligned} u_l^\pm(x) &= e^{\pm z(x;r_1)/h} T_\pm(z(x;r_1)) \begin{pmatrix} w_\pm^{\text{even}}(x) \\ w_\pm^{\text{odd}}(x) \end{pmatrix} \\ &= e^{\pm z(x;r_1)/h} T_\pm(z(x;r_1)) \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 + O(h)) \end{aligned}$$

with

$$T_\pm(z) = \begin{pmatrix} H^{-1}(z) \mp iH(z) & H^{-1}(z) \pm iH(z) \\ -H^{-1}(z) \mp iH(z) & -H^{-1}(z) \pm iH(z) \end{pmatrix}$$

and

$$H(z(x)) = \left( \frac{h\nu + Ex - x^3}{h\nu - Ex + x^3} \right)^{1/4}.$$

Let  $x \in ]r_0, r_1[$  be fixed. With the branches of the fourth root chosen in Section 4, one has  $H(z(x)) = e^{-i\pi/4} + O(h)$  as  $h \rightarrow 0$ . Hence,

$$\begin{aligned} T_+(z(x)) \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} H^{-1}(z(x)) - iH(z(x)) \\ -H^{-1}(z(x)) - iH(z(x)) \end{pmatrix} = -2e^{i\pi/4} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h)), \\ T_-(z(x)) \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} H^{-1}(z(x)) + iH(z(x)) \\ -H^{-1}(z(x)) + iH(z(x)) \end{pmatrix} = +2e^{i\pi/4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 + O(h)), \end{aligned}$$

and therefore

$$\begin{aligned} u_l^+(x) &= -2e^{i\pi/4} e^{+z(x;r_1)/h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h)), \\ u_l^-(x) &= +2e^{i\pi/4} e^{-z(x;r_1)/h} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 + O(h)). \end{aligned} \tag{57}$$

Comparing (57) and (55), we immediately obtain

$$k_l^+ = -2^{3/4} e^{i\pi/8} (1 + O(h)).$$

Similarly, for fixed  $x$  in the interval  $]r_2, \infty[$ ,  $H(z(x)) = e^{\pi i/4} + O(h)$  as  $h \rightarrow 0$ , and

$$\begin{aligned} u_r^+(x) &= +2e^{-i\pi/4} e^{+z(x;r_2)/h} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 + O(h)), \\ u_r^-(x) &= -2e^{-i\pi/4} e^{-z(x;r_2)/h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h)). \end{aligned} \tag{58}$$

Comparing (58) and (56), we immediately get

$$k_r^- = -2^{3/4} e^{-i3\pi/8} (1 + O(h)).$$

For the computation of  $k_r^+$  and  $k_l^-$  we use some symmetry properties. Recall that

$$g^\pm(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_h f^\pm(y),$$

and

$$\mathcal{C}\mathcal{F}_h = \mathcal{F}_h^{-1}\mathcal{C}, \quad \mathcal{C}V^{-1} = V\mathcal{C}, \quad V^{-1}\mathcal{F}_h^{-1} = V,$$

where the last identity comes from  $\mathcal{F}_h^{-1}$  being the metaplectic operator of the transformation  $(x, \xi) \mapsto (\xi, -x)$ , up to a normalizing constant. Hence,

$$V^{-1}g^\pm = V^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}\mathcal{F}_h f^\pm = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} V^{-1}\mathcal{F}_h^{-1}\mathcal{C}f^\pm = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{C}V^{-1}f^\pm$$

and

$$\tilde{g}^\pm = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{\tilde{f}^\pm}. \quad (59)$$

On the other hand,

$$u_r^+ = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{u_r^-}, \quad u_l^- = -i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{u_l^+},$$

which together with (59) yields

$$k_l^- = -i \overline{k_l^+}, \quad k_r^+ = i \overline{k_r^-}.$$

□

Proposition 7.8 yields for the entries of the connection matrices  $A_{l,r}$  and  $B_{l,r}$  defined in (52)

$$\alpha_{21}^l = k_l^+, \quad \alpha_{12}^r = k_r^-, \quad \beta_{22}^l = k_l^-, \quad \beta_{11}^r = k_r^+.$$

Combining these with the knowledge on the vanishing matrix elements (54) and the relations  $A_l = RB_l$ ,  $A_r = RB_r$ , one obtains

$$B_l = \begin{pmatrix} -\frac{1}{q}k_l^+ & -\frac{p}{q}k_l^- \\ 0 & k_l^- \end{pmatrix}, \quad B_r = \begin{pmatrix} k_r^+ & 0 \\ -\frac{p}{q}k_r^+ & \frac{1}{q}k_r^- \end{pmatrix}. \quad (60)$$

## 7.5 Computation of $T_2(E, h)$

Finally, we prove Proposition 7.1 calculating the asymptotic behavior of  $t(E, h)$  and  $s(E, h)$  as  $h \rightarrow 0$ . Let  $E > 0$ . By (43) and (60),

$$T_2 = B_r^{-1}B_l = \begin{pmatrix} -\frac{1}{q} \frac{k_l^+}{k_r^+} & -\frac{p}{q} \frac{k_l^-}{k_r^+} \\ \frac{p}{q} \frac{k_l^+}{k_r^-} & \frac{q^2 - p^2}{q} \frac{k_l^-}{k_r^-} \end{pmatrix}. \quad (61)$$

**Remark 7.9** The identity (61) is consistent with  $T_2 = \begin{pmatrix} t & s \\ -\bar{s} & -\bar{t} \end{pmatrix}$ , since

$$\overline{\left(\frac{k_l^+}{k_r^+}\right)} = -\frac{k_l^-}{k_r^-}, \quad \overline{\left(\frac{k_l^-}{k_r^-}\right)} = -\frac{k_l^+}{k_r^+}, \quad \overline{\left(\frac{p}{q}\right)} = \frac{p}{q}, \quad \frac{1}{\bar{q}} = \frac{p^2 - q^2}{q},$$

which is checked by direct calculation. ◇

By Proposition 7.5 and Proposition 7.8, we then get

$$t = -\frac{1}{q} \frac{k_l^+}{k_r^+} = -\frac{\sqrt{\pi} \gamma \exp\left(\frac{\pi}{4h} |\gamma|^2 + \frac{i}{2h} |\gamma|^2 \ln h\right)}{\sqrt{h} \Gamma\left(1 - \frac{i}{2h} |\gamma|^2\right) e^{i\pi/4}} (1 + O(h)).$$

Since  $\gamma = \frac{\nu}{\sqrt{2}} E^{-3/4} h + O(h^2)$  and

$$\Gamma\left(1 - \frac{i}{2h} |\gamma|^2\right) = \sqrt{\frac{\frac{\pi}{2h} |\gamma|^2}{\sin\left(\frac{\pi}{2h} |\gamma|^2\right)}} \left(1 + \frac{|\gamma|^2}{4h^2}\right) = 1 + O(h),$$

we have

$$t = -\sqrt{\frac{\pi h}{2}} \nu E^{-3/4} e^{-i\pi/4} + O(h |\ln h|)$$

and

$$s = -\frac{p}{q} \frac{k_l^-}{k_r^+} = -i \exp\left(\frac{\pi}{2h} |\gamma|^2\right) (1 + O(h)) = -i + O(h).$$

Since all the terms involved depend analytically on  $E$  for  $E \in \mathbb{C}$  near  $E_0 > 0$ , see Remark 7.4, we have proven Proposition 7.1.

## 8 Proof of the main results

In this section, we compute the Bohr-Sommerfeld type quantization condition of Theorem 1.4 and derive the semiclassical distribution of resonances given in Theorem 1.5.

### 8.1 Quantization condition

Recall that Proposition 4.1 gives the quantization condition of resonances as  $c^+(E, h) = 0$ , where  $c^\pm(E, h)$  is the product of three transfer matrices  $T_1, T_2, T_3$  and the connection coefficients  $c_0^\pm$ ,

$$\begin{pmatrix} c^+ \\ c^- \end{pmatrix} = T_3 T_2 T_1 \begin{pmatrix} c_0^+ \\ c_0^- \end{pmatrix},$$

see identity (29). On the other hand, we have calculated the following asymptotics:

$$\begin{aligned} T_1 &= \begin{pmatrix} e^{S_{01}/h} & 0 \\ 0 & e^{-S_{01}/h} \end{pmatrix}, \\ T_2 &= \begin{pmatrix} t & -i + O(h) \\ -i + O(h) & -\bar{t} \end{pmatrix}, \\ t &= -\sqrt{\frac{\pi h}{2}} e^{-i\pi/4} \nu E^{-3/4} + O(h |\ln h|), \\ T_3 &= 2e^{-i\pi/4} \begin{pmatrix} e^{S_{2\infty}/h} (1 + O(h)) & O(e^{-\delta/h}) \\ O(e^{-\delta/h}) & e^{-S_{2\infty}/h} (1 + O(h)) \end{pmatrix}, \\ \begin{pmatrix} c_0^+ \\ c_0^- \end{pmatrix} &= a \begin{pmatrix} 1 + o(1) \\ -i + o(1) \end{pmatrix}, \end{aligned}$$

see (30), Proposition 7.1, Proposition 5.3, and Proposition 6.3, respectively. Then,

$$c^+ = 2a e^{-\pi i/4} e^{S_{2\infty}/h} (1 + O(h)) \times \\ \times \left( t e^{S_{01}/h} (1 + o(1)) - e^{-S_{01}/h} (1 + o(1)) \right) + O(e^{-\delta/h}).$$

Hence,  $c^+(E, h) = 0$  if and only if

$$\sqrt{\frac{\pi h}{2}} \nu e^{-i\pi/4} E^{-3/4} e^{2S_{01}(E, h)/h} + 1 = o(1) \quad (62)$$

as  $h \rightarrow 0$ , which, together with (31), proves Theorem 1.4.

## 8.2 Distribution of resonances

We now study the asymptotic behavior of the function  $A(E, h) = \frac{2}{i} S_{01}(E, h)$  as  $h \rightarrow 0$ , where

$$A(E, h) = 2 \int_{r_0}^{r_1} \frac{\sqrt{r^2(E - r^2)^2 - h^2 \nu^2}}{r} dr.$$

Recall that if  $E > 0$ , then  $r^2(E - r^2)^2 - h^2 \nu^2 > 0$  for  $r \in (r_0, r_1)$ , and that the square root in the formula for  $A(E, h)$  is taken to be positive. Substituting  $y = r^2/E$ , one gets

$$A(E, h) = 2E^{3/2} \int_{y_0}^{y_1} \frac{\sqrt{y(1-y)^2 - h^2 \nu^2/E^3}}{2y} dy$$

with  $y_0 = r_0^2/E$  and  $y_1 = r_1^2/E$ .  $y_0$  and  $y_1$  are zeros of the cubic polynomial  $y(1-y)^2 - \mu^2$  with  $\mu = h\nu E^{-3/2}$ . If  $\mu > 0$  is small and positive, then  $y(1-y)^2 - \mu^2$  has three zeros  $0 < y_0(\mu) < y_1(\mu) < 1 < y_2(\mu)$  with  $y_0(\mu) \rightarrow 0$  and  $y_{1,2}(\mu) \rightarrow 1$  as  $\mu \rightarrow 0$ . We define

$$I(\mu) = \int_{y_0(\mu)}^{y_1(\mu)} \frac{\sqrt{y(1-y)^2 - \mu^2}}{2y} dy,$$

where the square root is taken to be positive for  $0 < \mu \ll 1$ . Since

$$A(E, h) = 2E^{3/2} I(\mu), \quad \mu = \frac{h\nu}{E^{3/2}},$$

we study the asymptotic behavior of the function  $I(\mu)$  as  $\mu \rightarrow 0$ . For this, we have to understand the  $\mu$ -dependence of  $y_0(\mu)$  and  $y_1(\mu)$ . When  $\mu^2$  turns around 0 once in the positive sense (i.e.  $\mu$  becomes  $e^{\pi i} \mu$ ), then  $y_0(\mu)$  turns around 0 in the positive sense and  $y_1(\mu)$  and  $y_2(\mu)$  exchange their position turning half around 1 in the positive sense. As a consequence, taking the branch into account,

$$I(e^{\pi i} \mu) = I(\mu) + R(\mu) + T(\mu) \quad (63)$$

with

$$R(\mu) = -i \int_{\Gamma_0} \frac{\sqrt{\mu^2 - y(1-y)^2}}{2y} dy, \quad T(\mu) = -i \int_{y_1(\mu)}^{y_2(\mu)} \frac{\sqrt{\mu^2 - y(1-y)^2}}{2y} dy,$$



where  $\Gamma_0$  is a contour around 0. These functions have the following properties:

**Lemma 8.1**  $T(\mu)$  is a holomorphic function of  $\mu^2$  at  $\mu = 0$ , and

$$R(\mu) = -\pi\mu, \quad T(\mu) = \frac{\pi i \mu^2}{4}(1 + O(\mu^2)).$$

In particular,  $R(e^{\pi i} \mu) = -R(\mu)$  and  $T(e^{\pi i} \mu) = T(\mu)$ .

*Proof:* By the residue theorem,  $R(\mu) = \pi\sqrt{\mu^2} = -\pi\mu$ . For the study of  $T(\mu)$ , we move by the locally biholomorphic change of variables  $v = \sqrt{y}(y-1)$  from a neighborhood of  $y = 1$  to a neighborhood of  $v = 0$ ,

$$T(\mu) = -i \int_{-\mu}^{\mu} \sqrt{\mu^2 - v^2} f(v) dv$$

where  $f(v) = (2y(v))^{-1} \frac{d}{dv} y(v)$  is holomorphic in a neighborhood of  $v = 0$  and satisfies  $f(v) = \frac{1}{2} + f'(0)v + O(v^2)$ . Hence,

$$T(\mu) = i\mu^2 \int_{-1}^1 \sqrt{1-w^2} f(\mu w) dw = i\mu^2 \left( \frac{1}{2} \int_{-1}^1 \sqrt{1-w^2} dw + O(\mu^2) \right),$$

since  $\int_{-1}^1 \sqrt{1-w^2} w dw = 0$ . □

**Proposition 8.2**  $I(\mu)$  is ramified at  $\mu = 0$  and satisfies

$$I(\mu) = \frac{2}{3} + \frac{\pi}{2}\mu + O(\mu^2 |\ln \mu|) \quad (\mu \rightarrow 0).$$

*Proof:* By Lemma 8.1, we have from (63)

$$\begin{aligned} I(e^{2\pi i} \mu) &= I(e^{\pi i} \mu) + R(e^{\pi i} \mu) + T(e^{\pi i} \mu) \\ &= (I(\mu) + R(\mu) + T(\mu)) - R(\mu) + T(\mu) = I(\mu) + 2T(\mu). \end{aligned}$$

Since  $\ln(e^{2\pi i} \mu) = \ln \mu + 2\pi i$ , this means that the function

$$B(\mu) = I(\mu) - \frac{1}{\pi i} T(\mu) \ln \mu$$

is single-valued around  $\mu = 0$ . Moreover, since  $T(\mu)$  behaves quadratically in  $\mu$  near  $\mu = 0$ ,  $B(\mu)$  is holomorphic near  $\mu = 0$  with

$$B(\mu) \xrightarrow{\mu \rightarrow 0} B(0) = I(0) = \int_0^1 (1-x^2) dx = \frac{2}{3}.$$

Differentiating equation (63), one gets  $B'(0) = I'(0) = \frac{\pi}{2}$ . Hence,

$$\begin{aligned} I(\mu) &= B(0) + B'(0)\mu + \frac{1}{\pi i} T(\mu) \ln \mu + O(\mu^2) \\ &= \frac{2}{3} + \frac{1}{\pi i} T(\mu) \ln \mu + \frac{\pi}{2}\mu + O(\mu^2) = \frac{2}{3} + \frac{\pi}{2}\mu + O(\mu^2 |\ln \mu|). \end{aligned}$$

□

*Proof of Theorem 1.5:* The quantization condition (62) is satisfied, if and only if there exists an integer  $k \in \mathbb{Z}$  such that

$$iA(E, h) - \frac{1}{2} h \ln E^{3/2} + \frac{1}{2} h \ln \left( \frac{\pi}{2} \nu^2 h \right) = \left( 2k + \frac{5}{4} \right) i\pi h + o(h). \quad (64)$$

Setting  $\lambda = E^{3/2}$ , Proposition 8.2 implies

$$A(E, h) = 2\lambda I(\nu h/\lambda) = \frac{4}{3} \lambda + \pi \nu h + O(h^2 |\ln h|),$$

and the quantization condition (64) becomes

$$\frac{4}{3} i\lambda - \frac{1}{2} h \ln \lambda + \frac{1}{2} h \ln \left( \frac{\pi}{2} \nu^2 h \right) = \left( 2k - \nu + \frac{5}{4} \right) i\pi h + o(h).$$

Writing  $\lambda = \lambda_1 + i\lambda_2$  with  $\lambda_1, \lambda_2 \in \mathbb{R}$ , the real and imaginary part of the above condition read as

$$\frac{4}{3} \lambda_1 - \frac{1}{2} h \arg \lambda = \left( 2k - \nu + \frac{5}{4} \right) \pi h + o(h), \quad (65)$$

$$-\frac{4}{3} \lambda_2 - \frac{1}{2} h \ln |\lambda| + \frac{1}{2} h \ln \left( \frac{\pi}{2} \nu^2 h \right) = o(h). \quad (66)$$

Now, we assume that  $a < \lambda_1 < b$  and  $\lambda_2 = o(1)$  as  $h \rightarrow 0$ . Then,

$$\arg \lambda = \arctan(\lambda_2/\lambda_1) = o(1), \quad \ln |\lambda| = \ln \lambda_1 + \frac{1}{2} \ln(1 + \lambda_2^2/\lambda_1^2) = \ln \lambda_1 + o(1).$$

Setting  $\lambda_{k\nu} = \frac{3\pi}{16}(8k - 4\nu + 5)$ , equations (65) and (66) become

$$\lambda_1 = \frac{3\pi}{16}(8k - 4\nu + 5)h + o(h) = \lambda_{k\nu}h + o(h),$$

$$\lambda_2 = -\frac{3}{8} \left( h \ln \frac{1}{h} - h \ln \frac{\pi \nu^2}{2\lambda_{k\nu}h} \right) + o(h).$$

□

## A Spectrum of $P^+ = -\hbar^2 \Delta + |x|$

The Schrödinger operator  $P^+$  has a locally bounded positive potential, which increases to infinity as  $|x| \rightarrow \infty$ . Hence,  $P^+$  is essentially self-adjoint on  $C_0^\infty(\mathbb{R}^2)$  and has purely discrete spectrum. We are looking for eigenvalues  $E \in ]a, b[$  in a bounded positive interval  $]a, b[ \subset \mathbb{R}^+$ . In polar coordinates  $x = r(\cos \theta, \sin \theta)$ ,  $r > 0$ ,  $\theta \in \mathbb{T}$  the differential expression  $-\hbar^2 \Delta_x + |x|$  reads as

$$-\hbar^2 \left( \partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_\theta^2 \right) + r.$$

Hence,  $E$  is a *formal* solution of the eigenvalue problem  $(P^+ - E)\psi = 0$  if and only if there exists  $l \in \mathbb{N}_0$  such that

$$-\hbar^2 \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{l^2}{r^2} \right) w_l(r) + (r - E)w_l(r) = 0.$$

Substituting  $w_l(r) = r^{-1/2} u_l(r)$ , this is equivalent to

$$-\hbar^2 \left( \frac{d^2}{dr^2} + \frac{\frac{1}{4} - l^2}{r^2} \right) u_l(r) + (r - E)u_l(r) = 0. \quad (67)$$

The ordinary differential equation (67) has  $r = 0$  as a regular singular point with indices  $\frac{1}{2} \pm l$ , while  $r = \infty$  is an irregular singular point of rank two. There are two linearly independent solutions, which behave as  $r^{1/2}$  and  $r^{1/2} \ln r$  (for  $l = 0$ ) or  $r^{1/2+l}$  and  $r^{1/2-l}$  (for  $l \neq 0$ ) near  $r = 0$ .

Looking at the irregular singularity at infinity, there is a fundamental system  $u_\infty^\pm(r)$ , which behaves as  $(r - E)^{-1/4} \exp(\pm(r - E)^{3/2}/h)$  near  $r = \infty$ . Hence, a necessary and sufficient condition for  $E$  being an eigenvalue of  $P^+$  reads as follows.

**Lemma A.1**  *$E \in \sigma_{\text{disc}}(P^+)$  if and only if there exists  $l \in \mathbb{N}_0$  such that  $\mathcal{W}(u^0, u_\infty^-) = 0$ , where  $\mathcal{W}(u^0, u_\infty^-) = u^0 (u_\infty^-)' - (u^0)' u_\infty^-$  is the Wronskian of the two solutions to (67),*

$$\begin{aligned} u^0(r) &\sim r^{1/2+l}, & r \rightarrow 0, \\ u_\infty^-(r) &\sim (r - E)^{-1/4} e^{-(r-E)^{3/2}/h}, & r \rightarrow \infty. \end{aligned}$$

Let us have a closer look at the potential of equation (67)

$$Q(r) = r - E + h^2(l^2 - 1/4)/r^2$$

for the case  $l > 0$ . If  $h > 0$  is sufficiently small, then the potential  $Q$  has three distinct simple turning points: they are zeros of the cubic polynomial  $r^3 - Er^2 + h^2(l^2 - 1/4)$ . Two of them are at a distance  $O(h)$  from  $r = 0$ , while the third is at a distance  $O(h)$  from  $r = E$ . All three turning points are real. The first one is negative, while the other two are positive. We denote these two by  $\alpha_1, \alpha_2 > 0$ . The strategy for characterizing the quantization condition  $\mathcal{W}(u^0, u_\infty^-) = 0$  is the following. We connect

1.  $u^0$  with two exact WKB solutions  $\tilde{u}^\pm$  built with the Langer-modified potential  $\tilde{Q}(r) = r - E + h^2 l^2 / r^2$  defined for  $r \in ]\alpha_1, \alpha_2[$  with the phase base point at  $\alpha_1$ , see [12];
2.  $\tilde{u}^\pm$  with two exact WKB solutions  $u_l^\pm$  defined for  $r \in ]\alpha_1, \alpha_2[$  with the phase base point at  $\alpha_2$ ;
3.  $u_l^\pm$  with an exact WKB solution  $u_r^-$  defined for  $r > \alpha_2$ , which is collinear to  $u_\infty^-$ .

Proceeding along the indicated three steps, one proves the following quantization condition.

**Proposition A.2** *Assume  $l > 0$ . Then,*

$$\mathcal{W}(u^0, u_\infty^-) = 0 \implies e^{iA^+(E, h)/h} + 1 = o(1), \quad h \rightarrow 0,$$

with

$$A^+(E, h) = 2 \int_{\alpha_1}^{\alpha_2} \sqrt{E - r - h^2(l^2 - \frac{1}{4})/r^2} \, dr.$$

An asymptotic study of the action  $A^+(E, h)$  analogous to that in §8.2 reveals a parallel structure between the resonant set of the full operator  $P$  and the upper level operator  $P^+$ . A resonance  $E$  of  $P$  is characterized by a Bohr-Sommerfeld type condition

$$\tilde{t} e^{iA(E, h)/h} + 1 = o(1) \quad (h \rightarrow 0),$$

where  $\tilde{t}$  is related to non-adiabatic transitions, and  $A(E, h)$  is an action integral. An eigenvalue  $E$  of  $P^+$  is characterized by a Bohr-Sommerfeld condition

$$e^{iA^+(E, h)/h} + 1 = o(1) \quad (h \rightarrow 0),$$

where  $A^+(E, h)$  is an action integral. The actions can be expressed as

$$\begin{aligned} A(E, h) &= 2E^{3/2}I(\mu), & \mu &= h\nu E^{-3/2}, & \nu &\in \mathbb{N} - \frac{1}{2}, \\ A^+(E, h) &= iE^{3/2}I^+(\mu), & \mu &= h\sqrt{l^2 - \frac{1}{4}}E^{-3/2}, & l &\in \mathbb{N}, \end{aligned}$$

where  $I(\mu)$  and  $I^+(\mu)$  share the same  $\mu$ -asymptotics for  $\mu \rightarrow 0$ .

## B Proof of Theorem 7.3

**Lemma B.1** *Let  $\nu \in \mathbb{N} - \frac{1}{2}$ ,  $y \mapsto \psi(y)$  the function defined in (45) with  $\psi(0) = \frac{E^{-3/4}}{\sqrt{2}}$ ,  $E > 0$ , and  $v(y) = v(y, h)$  a solution of*

$$hD_y v(y) = \begin{pmatrix} y & h\nu\psi(y) \\ -h\nu\psi(y) & -y \end{pmatrix} v(y). \quad (68)$$

*Then, there exists a matrix-valued  $C^\infty$ -symbol  $M(y, h) = \text{Id} + O(h)$ , such that  $w(y, h) = M(y, h)v(y, h)$  satisfies*

$$\begin{pmatrix} hD_y - y & -\gamma \\ \bar{\gamma} & hD_y + y \end{pmatrix} w(y, h) = r(y, h)w(y, h), \quad (69)$$

*where  $\gamma = \frac{\nu}{\sqrt{2}}E^{-3/4}h + O(h^2)$  and  $r(y, h) = O(h^\infty)$  uniformly in an interval around  $y = 0$  together with all its derivatives.*

*Proof:* We rewrite equation (68) as  $hD_y v(y, h) = B(y, h)v(y, h)$  with

$$B(y, h) = B_0(y) + hB_1(y) = \begin{pmatrix} y & 0 \\ 0 & -y \end{pmatrix} + h \begin{pmatrix} 0 & \nu\psi(y) \\ -\nu\psi(y) & 0 \end{pmatrix}$$

and equation (69) as  $(hD_y - G(y, h))w(y, h) = r(y, h)w(y, h)$  with

$$G(y, h) \sim \sum_{n=0}^{\infty} G_n(y)h^n, \quad G_0(y) = B_0(y), \quad G_n(y) \equiv \begin{pmatrix} 0 & \gamma_n \\ -\bar{\gamma}_n & 0 \end{pmatrix} \quad (n \geq 1).$$

We are looking for

$$M(y, h) \sim \sum_{n=0}^{\infty} M_n(y)h^n, \quad M_n(y) = \begin{pmatrix} m_n(y) & q_n(y) \\ \bar{q}_n(y) & \bar{m}_n(y) \end{pmatrix} \quad (n \geq 0)$$

such that

$$hD_y M = GM - MB$$

or equivalently for all  $n \geq 0$

$$D_y M_{n-1} = \sum_{j=0}^n (G_j M_{n-j} - M_j B_{n-j}) \quad (70)$$

with convention  $M_{-1} = 0$ ,  $B_n = 0$  for  $n \geq 2$ .

Equation (70) is satisfied for  $n = 0$ , if we take  $M_0(y) \equiv \text{Id}$ , i. e.  $m_0(y) \equiv 1$  and  $q_0(y) \equiv 0$ . Then, we have for  $n \geq 1$

$$\begin{aligned} G_n &= -iM'_{n-1} - \sum_{j=0}^{n-1} G_j M_{n-j} + M_{n-1} B_1 + M_n B_0 \\ &= -iM'_{n-1} - \sum_{j=1}^{n-1} G_j M_{n-j} + M_{n-1} B_1 - 2y \begin{pmatrix} 0 & q_n \\ -\bar{q}_n & 0 \end{pmatrix}. \end{aligned}$$

Since  $\psi(y) \in \mathbb{R}$  for  $y \in \mathbb{R}$ , the previous equation is equivalent to

$$\gamma_n = -iq'_{n-1}(y) - \sum_{j=1}^{n-1} \gamma_j \bar{m}_{n-j}(y) + \nu\psi(y)m_{n-1}(y) - 2yq_n(y), \quad (71)$$

$$0 = -im'_{n-1}(y) - \sum_{j=1}^{n-1} \gamma_j \bar{q}_{n-j}(y) - \nu\psi(y)q_{n-1}(y). \quad (72)$$

Let us start with  $n = 1$ . Substituting  $y = 0$  in (71) yields

$$\gamma_1 = \nu\psi(0),$$

and we automatically obtain

$$q_1(y) = -\frac{1}{2y} (\gamma_1 - \nu\psi(y)),$$

which is smooth (even analytic) near  $y = 0$ . Setting  $m_1(0) = 0$ , equation (72) gives

$$m_1(y) = i \int_0^y (\gamma_1 \bar{q}_1(y') + \nu\psi(y')q_1(y')) dy'.$$

If  $\gamma_j, m_j, q_j$  with  $m_j(0) = 0$  are determined for  $1 \leq j \leq n$ , then (71) yields

$$\gamma_{n+1} = -iq'_n(0)$$

and

$$q_{n+1}(y) = -\frac{1}{2y} (\gamma_n + iq'_n(y) + \sum_{j=1}^n \gamma_j \bar{m}_{n+1-j}(y) - \nu\psi(y)m_n(y)),$$

which is smooth (even analytic) near  $y = 0$ . Setting  $m_{n+1}(0) = 0$ , equation (72) then gives

$$m_{n+1}(y) = i \int_0^y \left( \sum_{j=1}^{n+1} \gamma_j \bar{q}_{n+2-j}(y') + \nu\psi(y')q_{n+1}(y') \right) dy'.$$

Since  $m_n(y)$  and  $q_n(y)$ ,  $n \geq 0$ , are smooth functions near  $y = 0$ , there exists a matrix-valued  $\mathcal{C}^\infty$ -symbol  $M(y, h)$  with  $M(y, h) \sim \sum_{n \geq 0} M_n(y)h^n$  such that (69) holds.  $\square$

Theorem 2.15 in [10] yields the following result about the  $\frac{\pi}{4}$ -rotation.

**Lemma B.2** Let  $\kappa_{\frac{\pi}{4}}(y, \eta) = \frac{1}{\sqrt{2}}(y - \eta, y + \eta)$  be the  $\frac{\pi}{4}$ -rotation in phase space  $T^*\mathbb{R}$ . The metaplectic operator  $V$  of the transpose linear canonical transformation  $\kappa_{\frac{\pi}{4}}^* = \kappa_{-\frac{\pi}{4}}$  satisfies

$$V(hD_y - y) = -\sqrt{2}yV, \quad V(hD_y + y) = \sqrt{2}hD_yV.$$

Moreover,  $\text{FS}(Vu) = \kappa_{-\frac{\pi}{4}}\text{FS}(u)$  for  $u \in \mathcal{S}'$ .

**Remark B.3** A formula for  $V$  in terms of oscillatory integrals is given by

$$Vg(y) = e^{i\pi/8}(\sqrt{2\pi h})^{-1/2} \int_{\mathbb{R}} e^{-\frac{i}{2h}(y^2 - 2\sqrt{2}xy + x^2)} g(x) dx,$$

see Theorem 4.53 in [10] or Proposition 5.3 in [26].  $\diamond$

## C Proof of Lemma 7.7

In this appendix, we prove one of the two formulae of Lemma 7.7, i.e. compute the asymptotic expansion of  $\tilde{f}^+$  microlocally near  $\sigma_r^-$ .

Recall that near  $y = 0$

$$\tilde{f}^+(\phi^{-1}(y)) = M(y, h)^{-1}V^{-1}f^+(y)$$

where the inverse of the metaplectic operator is given by

$$V^{-1}f^+(y) = e^{i\pi/8}(\sqrt{2\pi h})^{-1/2} \int_{\mathbb{R}} e^{i(y^2 + z^2 - 2\sqrt{2}yz)/(2h)} f^+(z) dz,$$

and that

$$f^+ = {}^t(f_1^+, f_2^+), \quad f_1^+ = -\frac{\gamma}{\sqrt{2}y} \chi_{(0, \infty)}(y) |y|^{\frac{i}{2h}|\gamma|^2}, \quad f_2^+ = \chi_{(0, \infty)}(y) |y|^{\frac{i}{2h}|\gamma|^2}.$$

Let us compute the asymptotic expansion of

$$\begin{aligned} V^{-1}f_2^+(y) &= e^{i\pi/8}(\sqrt{2\pi h})^{-1/2} \int_0^\infty e^{i\varphi(y, z)/h} dz, \\ \varphi(y, z) &= \frac{1}{2}(y^2 + z^2 - 2\sqrt{2}yz + |\gamma|^2 \ln z). \end{aligned}$$

Since  $\gamma = O(h)$ , the phase function  $\varphi(y, z)$  has two real critical points

$$z_c^\pm(y) = (y \pm \sqrt{y^2 - |\gamma|^2})/\sqrt{2},$$

which are the roots of  $\frac{\partial \varphi}{\partial z}(y, z) = z - \sqrt{2}y + \frac{|\gamma|^2}{2z}$ . The phase of the asymptotic expansion will be given by  $\varphi(y, z_c^\pm(y))$ . Since we are on  $\sigma_r^-$ , we can assume  $x > \sqrt{E}$ , i.e.  $y > 0$  and independently from  $h$ . Then,

$$z_c^+(y) = \sqrt{2}y + O(h^2), \quad z_c^-(y) = \frac{|\gamma|^2}{2\sqrt{2}y} + O(h^2)$$

and

$$\varphi(y, z_c^\pm(y)) = \mp \frac{1}{2}y^2 + O(h^2).$$

This means that the critical points  $z_c^+(y)$  and  $z_c^-(y)$  will contribute on  $\sigma_r^-$  and  $\sigma_r^+$ , respectively. Hence, we have only to compute the contribution from  $z_c^+(y)$ . Since  $\frac{\partial^2 \varphi}{\partial z_c^2}(y, z_c^+(y)) = 1 - \frac{|\gamma|^2}{2z_c^+(y)^2} = 1 + O(h^2)$ ,  $z_c^+(y)$  is a non-degenerate critical point, and the stationary phase theorem says that

$$V^{-1} f_2^+(y) = e^{i\pi/8} 2^{1/4} e^{i\varphi(y, z_c^+(y))/h} + O(h)$$

microlocally near  $\sigma_r^-$ . Comparing  $i\varphi(\phi(x), z_c^+(\phi(x))) = -\frac{i}{2}\phi(x)^2 + O(h^2)$  with

$$z(x; r_2) = \int_{r_2}^x \sqrt{h^2 \nu^2 - t^2(E - t^2)} / t dt,$$

we observe for  $x > r_2$

$$\begin{aligned} -\frac{d}{dx} z(x; r_2) &= -\sqrt{h^2 \nu^2 - x^2(E - x^2)} / x = -i(x^2 - E) + O(h^2) \\ &= \frac{d}{dx} \left(-\frac{i}{2}\phi(x)^2\right) + O(h^2), \end{aligned}$$

since  $\phi(x)\phi'(x) = x^2 - E$ . Because of  $z(r_2; r_2) = 0$ , one obtains

$$-z(x; r_2) = -\frac{i}{2}\phi(x)^2 - \frac{i}{2}\phi(r_2)^2 + O(h^2).$$

If  $\phi(r_2)^2 = O(h^2)$ , then  $i\varphi(\phi(x), z_c^+(\phi(x))) = -z(x; r_2) + O(h^2)$ . Consequently,

$$V^{-1} f_2^+(\phi(x)) = e^{i\pi/8} 2^{1/4} e^{-z(x; r_2)/h} (1 + O(h))$$

and

$$\tilde{f}^+(x) = e^{i\pi/8} 2^{1/4} e^{-z(x; r_2)/h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 + O(h))$$

microlocally near  $\sigma_r^-$ , since  $M(\phi(x), h) = \text{Id} + O(h)$ .

It remains to prove  $\phi(r_2)^2 = O(h^2)$ . The turning point  $r_2$  is a zero of the function  $x \mapsto h^2 \nu^2 / x^2 - (E - x^2)^2$ . This is equivalent to  $\det(a(r_2, 0)) = 0$  with

$$a(x, \xi) = \begin{pmatrix} -\xi + x^2 - E & \frac{h\nu}{x} \\ -\frac{h\nu}{x} & -\xi - x^2 + E \end{pmatrix}$$

the symbol of the operator  $A(x) - hD_x$ . The first step of the normal form transformation of Theorem 7.3 reads on the symbol level as

$$a(x, \xi) = \phi'(x) \tilde{a}(\phi(x), \xi / \phi'(x))$$

with

$$\tilde{a}(x, \xi) = \begin{pmatrix} -\xi + x & h\nu\psi(x) \\ -h\nu\psi(x) & -\xi - x \end{pmatrix}.$$

Since  $\phi'(r_2) \neq 0$ , one has  $\det(a(r_2, 0)) = 0$  if and only if  $\det(\tilde{a}(\phi(r_2), 0)) = 0$ . The rest of the normal form transformation is

$$\sqrt{2} q \circ \kappa_{\frac{\pi}{4}} = M \#_h \tilde{a} \#_h M^{-1}$$

with

$$q(y, \eta) = \begin{pmatrix} y & \frac{\gamma}{\sqrt{2}} \\ -\frac{\gamma}{\sqrt{2}} & -\eta \end{pmatrix}$$

the symbol of the normal form operator  $Q$ , and  $\sharp_h$  the Moyal product of semiclassical Weyl calculus. The  $h$ -asymptotics of  $\sharp_h$  together with the linear  $\xi$ -dependance of  $\tilde{a}(x, \xi)$  yield

$$M \sharp_h \tilde{a} \sharp_h M^{-1} = M \tilde{a} M^{-1} - i h M' M^{-1} = M \tilde{a} M^{-1} + O(h^2).$$

Hence,  $\tilde{a} = \sqrt{2} M^{-1} (q \circ \kappa_{\frac{\pi}{4}}) M + O(h^2)$  and

$$\det(a(r_2, 0)) = 0 \Leftrightarrow \det(q \circ \kappa_{\frac{\pi}{4}}(r_2, 0)) = O(h^2) \Leftrightarrow \phi(r_2)^2 = O(h^2).$$

## References

- [1] J. Aguilar and J.M. Combes. A class of analytic perturbations for one body Schrödinger Hamiltonians *Commun. Math. Phys.*, 22: 269–279, 1971.
- [2] J. Avron and A. Gordon. Born-Oppenheimer approximation near level crossing. *Phys. Rev. Lett.*, 85(1): 34–37, 2000.
- [3] J. Avron and A. Gordon. Born-Oppenheimer wave function near level crossing. *Phys. Rev. A*, 62: 062504-1–062504-9, 2000.
- [4] H. Baklouti. Asymptotique des largeurs de résonances pour un modèle d’effet tunnel microlocal. *Ann. Inst. Henri Poincaré, Phys. Théor.* 68(2): 179–228, 1998.
- [5] L. Cederbaum, R. Friedman, V. Ryaboy, and N. Moiseyev. Conical intersections and bound molecular states embedded in the continuum. *Phys. Rev. Lett.*, 90(1): 013001-1–013001-4, 2003.
- [6] Y. Colin de Verdière and B. Parisse. Équilibre instable en régime semi-classique. I. Concentration microlocale. *Comm. Partial Differential Equations*, 19(9&10): 1535–1563, 1994.
- [7] J.M. Combes, P. Duclos, and R. Seiler. The Born Oppenheimer approximation. *Rigorous Atomic and molecular Physics*, 185–212, 1981.
- [8] W. Domcke, D. Yarkony, and H. Köppel (eds.). *Conical intersections*. World Scientific Publishing, Advanced Series in Physical Chemistry, Vol. 15, 2004.
- [9] C. Fermanian-Kammerer and P. Gérard. Mesures semi-classiques et croisements de mode. *Bull. S.M.F.*, 130(1): 123–168, 2002.
- [10] G. Folland. *Harmonic analysis in phase space*. Annals of mathematics studies, 122, Princeton University Press, Princeton, 1989.
- [11] S. Fujiié and T. Ramond Matrice de scattering et résonances associées à une orbite hétérocline. *Ann. Inst. Henri Poincaré, Phys. Théor.*, 69(1): 31–82, 1998.
- [12] S. Fujiié and T. Ramond. Exact WKB analysis and the Langer modification with application to barrier top resonances. C. Howls (ed.), *Toward the exact WKB analysis of differential equations, linear or non-linear*, Kyoto University Press, 15–31, 2000.



- [13] C. Gérard and A. Grigis. Precise estimates of tunneling and eigenvalues near a potential barrier. *J. Differ. Equations*, 72(1): 149-177, 1988.
- [14] G.A. Hagedorn. A time dependent Born-Oppenheimer approximation. *Commun. Math. Phys.*, 77: 1-19, 1980.
- [15] G.A. Hagedorn. Molecular propagation through electron energy level crossings. *Memoirs A.M.S.* 536, 111, 1994.
- [16] G.A. Hagedorn and A. Joye. A time-dependent Born-Oppenheimer approximation with exponentially small error estimates. *Commun. Math. Phys.*, 223(3): 583-626, 2001.
- [17] B. Helffer and J. Sjöstrand. Semiclassical analysis for Harper's equation III. *Mém. Soc. Math. France (N.S.)*, 39, 1989.
- [18] I. Herbst. Dilation analyticity in constant electric field I. The two body problem. *Commun. Math. Phys.* 64:279-298, 1979.
- [19] M. Klein, A. Martinez, R. Seiler, and X.P. Wang. On the Born-Oppenheimer expansion for polyatomic molecules. *Comm. Math. Phys.*, 143: 607-639, 1992.
- [20] K. Koike. On a regular singular point in the exact WKB analysis. C. Howls (ed.), *Toward the exact WKB analysis of differential equations, linear or non-linear*, Kyoto Univ. Press, 9-10, 39-53, 2000.
- [21] C. Lasser and C. Fermanian-Kammerer. Wigner measures and codimension two crossings. *J. Math. Phys.*, 44(2): 507-527, 2003.
- [22] C. Lasser and S. Teufel. Propagation through conical crossings: an asymptotic semigroup. *Commun. Pure Appl. Math.* 58: 1188-1230, 2005.
- [23] A. Martinez. Estimates on complex interactions in phase space. *Math. Nachr.* 167: 203-254, 1994.
- [24] S. Nakamura. On an example of phase space tunneling. *Ann. Inst. Henri Poincaré, Phys. Théor.* 63(2): 211-229, 1995.
- [25] L. Nédélec. Résonances semi-classique pour l'opérateur de Schrödinger matriciel en dimension deux. *Ann. Inst. Henri Poincaré Phys. Théor.*, 65(2): 129-162, 1996.
- [26] T. Ramond. Semiclassical study of quantum scattering on the line. *Commun. Math. Phys.*, 177: 221-254, 1996.
- [27] F. Rellich. Störungstheorie der Spektralzerlegung. I. *Math. Ann.*, 113: 600-619, 1937.
- [28] J. Sjöstrand and M. Zworski. Complex scaling and the distribution of scattering poles. *J. Amer. Math. Soc.*, 4: 729-769, 1991.
- [29] H. Spohn and S. Teufel. Adiabatic decoupling and time-dependent Born-Oppenheimer theory. *Commun. Math. Phys.*, 224(1): 113-132, 2001.
- [30] C. Zener. Non-adiabatic crossing of energy levels. *Proc. Royal Soc. London Ser. A*, 137: 696-702, 1932.
- [31] M. Zworski. Resonances in physics and geometry. *Notices Amer. Math. Soc.*, 46(3), 1999.



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