

Microlocal scattering matrix for coupled Schrödinger operators and applications to semiclassical resonances

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Abstract. We consider a one-dimensional Schrödinger operator with matrix-valued potential. For such an operator, the WKB construction breaks down, not only at the turning points, but also at the crossing points where the potential has multiple eigenvalues. We study the connection problem at the crossing points and compute the semiclassical asymptotics of what we call microlocal scattering matrix. We apply this result to the semiclassical resonance width arising from the molecule predissociation in quantum chemistry.

1. Introduction

The one-dimensional motion of quantum particles with mass m and energy λ under the potential $V(x)$ is described by the Schrödinger equation

$$(hD)^2u(x) + V(x)u(x) = \lambda u(x),$$

where $D = -id/dx$, $h = \hbar/\sqrt{2m}$, and $\hbar$ is the Planck constant. In the semiclassical mechanics, h is regarded as a small parameter in view of the Bohr correspondence principle.

The so-called WKB solution or WKB approximation is a power series solution in h :

$$u(x, h) = e^{\frac{i}{h}\phi(x)} \sum_{k=0}^{\infty} a_k(x)h^k. \quad (1.1)$$

The phase function should be $\phi(x) = \pm \int^x \sqrt{\lambda - V(t)}dt$, and the first coefficient of the symbol should be $a_0(x) = (\lambda - V(x))^{-1/4}$ up to a multiplicative constant. The other coefficients are determined inductively by the so-called transport equations. A problem in this construction is that the infinite series diverge in general. Nevertheless, it was known before the birth of WKB theory that a finite partial sum gives a good approximation to a solution as Liouville–Green approximation, provided x is away from the zeros of $\lambda - V(x)$. Such exceptional points are called *turning points* since they are endpoints of the classically

allowed and forbidden regions. At these points, the phase and symbol functions of the WKB solution have singularities. The expression (1.1) should be regarded as an asymptotic expansion of a true solution $u(x, h)$ away from turning points. It is known as Stokes phenomenon that this asymptotic expression of a solution changes in a discontinuous way when we go beyond a turning point. Therefore, in order to know the global behavior of a solution, it is necessary to know the connection formula between WKB solutions at each turning point.

The WKB method applies to more general semiclassical equations. Here, we consider, among others, a system of equations

$$\mathcal{P}\mathbf{u} = \lambda\mathbf{u}, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad (1.2)$$

for a 2×2 matrix-valued operator

$$\mathcal{P} = \begin{pmatrix} P_1 & hW \\ hW^* & P_2 \end{pmatrix} = \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix} + h \begin{pmatrix} 0 & W \\ W^* & 0 \end{pmatrix}. \quad (1.3)$$

The diagonal entries P_1 and P_2 are Schrödinger operators with real smooth potentials V_1 and V_2 , respectively. The off-diagonal entries are interactions between P_1 and P_2 , which we assume to be small in h . For simplicity, W is supposed to be a multiplication operator by a real smooth function $W(x)$. Such a matrix-valued operator $\mathcal{P}$ appears in the quantum chemistry as the Born–Oppenheimer approximation (see [19]). The semiclassical parameter corresponds to the square root of the ratio of the mass of the nuclear and the electron.

In such a matrix-valued case arises an interesting problem called *energy-level crossing*. When the two potentials cross each other at a point $x = x_0$; $V_1(x_0) = V_2(x_0)$, the WKB construction

$$\mathbf{u}(x, h) = e^{\frac{i}{h}\phi(x)} \sum_{k=0}^{\infty} h^k \begin{pmatrix} a_{1,k}(x) \\ a_{2,k}(x) \end{pmatrix}$$

fails at this point, in addition to the turning points of each P_j (Section 2). Such a point is also called turning point in the general 1D WKB theory, but here we call it *crossing point*.

In this manuscript, we study the connection problem at a crossing point of the solutions to the system (1.2). More precisely, we define a *microlocal scattering matrix* at a *microlocal crossing point* and compute its asymptotic expansion in the semiclassical limit. Let

$$p_j(x, \xi) = \xi^2 + V_j(x), \quad H_{p_j} = \partial_\xi p_j \partial_x - \partial_x p_j \partial_\xi$$

be, respectively, the classical Hamiltonian and the Hamiltonian vector field corresponding to the Schrödinger operator P_j . Microlocal crossing points are the intersection $\Gamma_1(\lambda) \cap \Gamma_2(\lambda)$ of the characteristic sets $\Gamma_j(\lambda) := \{(x, \xi); p_j(x, \xi) = \lambda\}$. If (x_0, ξ_0) is a microlocal crossing point, then x_0 is a crossing point.

Let (x_0, ξ_0) be a microlocal crossing point, i.e., $p_j(x_0, \xi_0) = \lambda$ for $j = 1, 2$. Suppose $dp_j(x_0, \xi_0) \neq 0$ for $j = 1, 2$. Then, for each $j = 1, 2$ and for small enough $\varepsilon > 0$, the

curve $\gamma_j^\# = \bigcup_{0 < t < \varepsilon} \exp tH_{p_j}(x_0, \xi_0)$ is an outgoing classical trajectory (integral curve of H_{p_j}) starting from (x_0, ξ_0) , and $\gamma_j^b = \bigcup_{-\varepsilon < t < 0} \exp tH_{p_j}(x_0, \xi_0)$ is an incoming classical trajectory ending at (x_0, ξ_0) . To each $\gamma_j^{\#,b}$, $j = 1, 2$, we associate a suitably normalized WKB solution $\mathbf{f}_j^{\#,b}$ modulo $\mathcal{O}(h)$. The space of microlocal solutions on $\gamma_j^{\#,b}$ is a one-dimensional linear vector space generated by $\mathbf{f}_j^{\#,b}$ in the germ sense (Proposition 3.1), whereas the space of microlocal solutions in a neighborhood of (x_0, ξ_0) is two dimensional generated by $\mathbf{f}_1^\#$ and $\mathbf{f}_2^\#$ or by $\mathbf{f}_1^b$ and $\mathbf{f}_2^b$. The microlocal scattering matrix is defined as the 2×2 matrix associated with the change of these two bases (Proposition 4.2).

We suppose $V_1(x)$ and $V_2(x)$ cross at $x = 0$ with value 0: $V_1(0) = V_2(0) = 0$. We allow a tangential crossing to a finite order $V_1^{(k)}(0) = V_2^{(k)}(0)$ for $0 \leq k \leq n-1$, $V_1^{(n)}(0) \neq V_2^{(n)}(0)$. When $\lambda > 0$, $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$ intersect at two points $(0, \sqrt{\lambda})$, $(0, -\sqrt{\lambda})$ with contact order $m = n$, whereas when $\lambda = 0$, they intersect at one point $(0, 0)$ with contact order $m = 2n$ (see Figures 1 and 2 in Section 4).

Theorems 4.1 and 4.2 give the two-term asymptotic expansion of the microlocal scattering matrix at a crossing point for λ near a fixed energy λ_0 . Theorem 4.1 concerns the case $\lambda_0 > 0$ and Theorem 4.2 the case $\lambda_0 = 0$, where the crossing point is at the same time a turning point. The first term is the identity matrix (multiplied by the Maslov correction $-i$ in the turning-crossing point case $\lambda_0 = 0$), which implies that the quantum particles do not change trajectory at the principal level. The second term is off-diagonal and hence gives the change of trajectories from γ_1^b to $\gamma_2^\#$ and γ_2^b to $\gamma_1^\#$ at the crossing point. It is of order $h^{\frac{1}{m+1}}$, and the coefficient is explicitly computed. This coefficient is non-vanishing near λ_0 in the case $\lambda_0 > 0$, but presents an interesting behavior in the case $\lambda_0 = 0$, reflecting the fact that the intersection of $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$ splits to two points when λ becomes positive, while it disappears when λ becomes negative. It is expressed by a generalized Airy function.

To obtain these asymptotic formulas of the microlocal scattering matrix at a crossing point (x_0, ξ_0) , we compare the microlocal WKB solutions with the local exact solutions near x_0 , constructed in [8] (Lemma 5.2), and deduce the microlocal scattering matrix from the connection formula of the local exact solutions. They are infinite series solutions inductively determined by solving the inhomogenous equations for the operators $P_1 - \lambda$ and $P_2 - \lambda$ one after the other, which are convergent for sufficiently small h (Lemma 5.1). We construct two bases of local exact solutions whose asymptotic behaviors are known modulo $\mathcal{O}(h)$ on the left and the right of x_0 , respectively, and compute the Wronskian between these bases at x_0 . It turns out that the subprincipal terms, which determine the subprincipal terms of the microlocal scattering matrix, are given by an integral of the form

$$\int a_1(x, h)e^{\pm i\phi_1(x)/h} a_2(x, h)e^{\pm i\phi_2(x)/h} W(x) dx,$$

where $a_j(x, h)e^{\pm i\phi_j(x)/h}$ are the WKB solutions to the scalar Schrödinger equation $P_j u = \lambda u$. This is an oscillatory integral over an interval containing x_0 with a phase function of

the form with four patterns of signs:

$$\pm\phi_1(x) \pm \phi_2(x) = \pm \int (\lambda - V_1(t))^{\frac{1}{2}} dt \pm \int (\lambda - V_2(t))^{\frac{1}{2}} dt.$$

It has a critical point at the crossing point x_0 when the two signs are different, and the (degenerate) stationary phase method gives the asymptotic expansion of this oscillatory integral.

The last part of this manuscript (Sections 6 and 7) is devoted to an application of the microlocal scattering matrices at crossing points to a global scattering problem. We study the semiclassical distribution of the quantum resonances of the operator $\mathcal{P}$, assuming that P_1 has eigenvalues created by a simple well potential and that P_2 has continuous spectrum near the energy $\lambda_0 \in \mathbb{R}$ in question. Due to the presence of the interaction, the matrix-valued operator $\mathcal{P}$ may have resonances close to the eigenvalues of P_1 (Fermi's golden rule). We prove the existence of such resonances and compute the asymptotic formula of the imaginary part of these resonances (Theorem 6.1), which describes the lifetime of the corresponding semibound resonant states. Starting from the fact that the resonant state is microlocally infinitely small on the incoming (from infinity) classical trajectory, we can compute, using the microlocal scattering matrices at crossing points, the microlocal asymptotic behavior on all the classical trajectories on $\Gamma_1(\lambda) \cup \Gamma_2(\lambda)$. In particular, we deduce the resonance widths from the microlocal asymptotics on the outgoing (to infinity) classical trajectory (Proposition 7.1).

2. Construction of WKB solutions

We formally construct a WKB solution $\mathbf{u} = {}^t(u_1, u_2)$ to the system (1.2) in the WKB form

$$\mathbf{u}(x, h) = e^{i\phi(x)/h} \mathbf{a}(x, h), \quad \mathbf{a}(x, h) = \begin{pmatrix} a_1(x, h) \\ a_2(x, h) \end{pmatrix} \sim \sum_{k=0}^{\infty} h^k \begin{pmatrix} a_{1,k}(x) \\ a_{2,k}(x) \end{pmatrix}. \quad (2.1)$$

Since $e^{-\frac{i}{h}\phi(x)}(P_j - \lambda)(e^{\frac{i}{h}\phi(x)}a_j) = ((\phi')^2 + V_j - \lambda)a_j + \frac{h}{i}La_j - h^2a_j''$, where L is the first-order differential operator $L = 2\phi' \frac{d}{dx} + \phi''$, equation (1.2) with (2.1) requires the coefficients $a_{j,k}$ to satisfy

$$\begin{pmatrix} (\phi')^2 + V_1 - \lambda & 0 \\ 0 & (\phi')^2 + V_2 - \lambda \end{pmatrix} \mathbf{a}_k + \begin{pmatrix} -iL & W \\ W & -iL \end{pmatrix} \mathbf{a}_{k-1} + \frac{d^2}{dx^2} \mathbf{a}_{k-2} = 0, \quad (2.2)$$

for all $k = 0, 1, 2, \dots$, with the convention that $a_{j,-2} \equiv a_{j,-1} \equiv 0$. In particular, when $k = 0$, one has

$$\begin{pmatrix} (\phi')^2 + V_1 - \lambda & 0 \\ 0 & (\phi')^2 + V_2 - \lambda \end{pmatrix} \mathbf{a}_0 = 0. \quad (2.3)$$

In order to obtain a non-trivial sequence of coefficients, we should require either $(\phi')^2 + V_1 - \lambda = 0$ or $(\phi')^2 + V_2 - \lambda = 0$. Let ϕ satisfy the first one,

$$(\phi')^2 + V_1(x) - \lambda = 0. \quad (2.4)$$

This is the eikonal equation for the WKB solution to the single equation $(P_1 - \lambda)u_1 = 0$. It determines the phase function ϕ_1 up to an additive constant. If x is in the classically allowed region $\{x; V_1(x) \leq \lambda\}$, then the solution of (2.4) is written as $\phi(x) = \pm\phi_1(x)$, where

$$\phi_j(x, x_0) = \int_{x_0}^x \sqrt{\lambda - V_j(t)} dt, \quad j = 1, 2. \quad (2.5)$$

Here, x_0 is an arbitrary point in the classically allowed region. We will usually take as this point a turning point.

With this $\phi = \phi_1$, the second condition in (2.3) becomes

$$\begin{pmatrix} 0 & 0 \\ 0 & V_2 - V_1 \end{pmatrix} \mathbf{a}_0 = 0,$$

and hence, we have

$$a_{2,0}(x) = 0, \quad (2.6)$$

unless $V_1(x) - V_2(x)$ vanishes identically.

The recurrence equation (2.2) becomes

$$L_1 a_{1,k-1} = i a''_{1,k-2} - i W a_{2,k-1}, \quad (2.7)$$

$$(V_2(x) - V_1(x)) a_{2,k} = i L_1 a_{2,k-1} + a''_{2,k-2} - W a_{1,k-1}, \quad (2.8)$$

for $k \geq 1$, where $L_j = 2\phi'_j \frac{d}{dx} + \phi''_j$ for $j = 1, 2$.

The transport equation (2.7) with $k = 1$ gives $L_1 a_{1,0} = 0$, which is the first transport equation for the single equation $(P_1 - \lambda)u_1 = 0$, and the solution is given up to a multiplicative constant by

$$a_{1,0}(x) = \frac{1}{(\lambda - V_1(x))^{\frac{1}{4}}}.$$

Next, the transport equation (2.8) with $k = 1$ yields, with (2.6),

$$a_{2,1}(x) = \frac{W(x)}{(V_1(x) - V_2(x))(\lambda - V_1(x))^{\frac{1}{4}}}.$$

The second coefficient $a_{1,1}$ of the first entry satisfies

$$L_1 a_{1,1} = i a''_{1,0} - i W a_{2,1} = \left(\frac{i}{(\lambda - V_1(x))^{\frac{1}{4}}} \right)' - i \frac{W(x)^2}{(V_1(x) - V_2(x))(\lambda - V_1(x))^{\frac{1}{4}}}.$$

This is a first-order linear differential equation and is uniquely solved in any interval in the classically allowed region for p_1 free from turning point and crossing point when an initial condition $a_{1,1}(x_1) = 0$ is imposed at some point x_1 in this interval.

In the same way, we inductively determine $a_{1,k}$ by (2.7), and $a_{2,k}$ by (2.8) one after the other. Thus, we obtain formal a power series solutions of the form

$$\begin{aligned} \mathbf{u}_1^\pm(x, h) &= e^{\pm \frac{i}{h} \phi_1(x)} \sum_{k=0}^{\infty} h^k \begin{pmatrix} a_{1,k}(x) \\ a_{2,k}(x) \end{pmatrix} \\ &= \frac{e^{\pm \frac{i}{h} \phi_1(x)}}{(\lambda - V_1(x))^{\frac{1}{4}}} \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + h \begin{pmatrix} * \\ \frac{W(x)}{V_1(x) - V_2(x)} \end{pmatrix} + \dots \right), \end{aligned} \quad (2.9)$$

where we omit the computation of $*$ = $(\lambda - V_1(x))^{\frac{1}{4}} a_{1,1}$.

Similarly, starting from the eikonal equation $(\phi_2')^2 + V_2(x) - \lambda = 0$, we get other formal solutions:

$$\mathbf{u}_2^\pm(x, h) = \frac{e^{\pm \frac{i}{h} \phi_2(x)}}{(\lambda - V_2(x))^{\frac{1}{4}}} \left(\begin{pmatrix} 0 \\ 1 \end{pmatrix} + h \begin{pmatrix} \frac{W(x)}{V_2(x) - V_1(x)} \\ * \end{pmatrix} + \dots \right). \quad (2.10)$$

As in the usual single Schrödinger equation case, these expressions of solutions have singularities at the turning points, i.e., the zeros of $\lambda - V_j(x)$. In our matrix case, moreover, they have additional singularities at the zeros of $V_1(x) - V_2(x)$, which we will call *crossing points*.

These apparent singularities are due to the divergence of the infinite series. To give a sense to these divergent series, we take a Borel sum. Namely, we construct functions $\mathbf{u}_j^\pm(x, h)$ which have the infinite series as their asymptotic expansions as $h \rightarrow 0$. We denote them again by the same notations $\mathbf{u}_j^\pm(x, h)$. They are no longer solutions to our system (1.2), but are only quasi-modes; i.e., they satisfy

$$(\mathcal{P} - \lambda) \mathbf{u}_j^\pm = \mathcal{O}(h^\infty),$$

uniformly in an interval contained in the classically allowed region away from turning points and crossing points. We see in the next section that they can be regarded as *microlocal solutions* when restricted to the characteristic set in the phase space.

We finally recall, before ending this section, that our construction of WKB solutions of the form (2.9) and (2.10) depends on the choice of the base point x_0 of the phase function and the base point x_1 of the symbol function. In the following, we specify the choice of x_0 , but we do not specify x_1 . The change of x_1 results in an error of order h since this choice first appears for $a_{1,1}$, as we saw above.

3. Microlocal WKB solutions

We now introduce a notion of *microlocal solution*. Let ξ be the dual variable of the position variable x , which stands for the momentum. The phase space is the product space $\mathbb{R}_x \times \mathbb{R}_\xi$, which is a symplectic manifold equipped with the 2-form $dx \wedge d\xi$.

Let (x_0, ξ_0) be a point in the phase space. We say that an h -dependent function $u(x, h) \in L^2(\mathbb{R}; \mathbb{C})$ with $\|u\|_{L^2(\mathbb{R})}$ is *microlocally infinitely small* (see [23]) at (x_0, ξ_0) , and write

$$u \equiv 0 \quad \text{at } (x_0, \xi_0),$$

if there exists a smooth function $\chi_0(x, \xi)$ bounded with all its derivatives satisfying

$$\chi_0(x_0, \xi_0) = 1$$

such that

$$\|\chi_0^W u\|_{L^2(\mathbb{R})} = \mathcal{O}(h^\infty)$$

as h tends to 0. Here, χ_0^W is the Weyl quantization of the symbol $\chi_0(x, \xi)$, namely, the semiclassical pseudodifferential operator defined by

$$[\chi_0^W u](x, h) = \frac{1}{2\pi h} \iint_{\mathbb{R}^2} e^{\frac{i}{h}(x-y)\xi} \chi_0\left(\frac{x+y}{2}, \xi\right) u(y) dy d\xi. \quad (3.1)$$

A vector-valued function is said to be microlocally infinitely small at a point in the phase space if each element is microlocally infinitely small there. The complement in the phase space of such points is called *frequency set* and denoted by $\text{FS}(\mathbf{u})$.

We also say that $\mathbf{u}$ is a *microlocal solution* to the system $(\mathcal{P} - \lambda)\mathbf{u} = 0$ at (x_0, ξ_0) if $(\mathcal{P} - \lambda)\mathbf{u} \equiv 0$ at (x_0, ξ_0) .

Let

$$p_j(x, \xi) := \xi^2 + V_j(x), \quad j = 1, 2,$$

be the classical Hamiltonians associated with the Schrödinger operator P_j . The characteristic set of $\mathcal{P} - \lambda$ is defined as the union of the characteristic sets $\Gamma_j(\lambda)$ of P_j , $j = 1, 2$:

$$\Gamma(\lambda) = \Gamma_1(\lambda) \cup \Gamma_2(\lambda), \quad \Gamma_j(\lambda) = \{(x, \xi); p_j(x, \xi) = \lambda\}.$$

Each characteristic set $\Gamma_j(\lambda)$ consists of curves symmetric with respect to the x -axis; i.e., if $(x, \xi) \in \Gamma_j(\lambda)$, then $(x, -\xi) \in \Gamma_j(\lambda)$. The intersection points $(x, 0)$ of $\Gamma_j(\lambda)$ with the x -axis are called *turning points*.

We call *microlocal crossing points* the intersection of $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$, i.e., the points (x, ξ) such that $p_1(x, \xi) = p_2(x, \xi) = \lambda$. Recall that we also called crossing points the zeros of $V_1(x) - V_2(x)$. Let us call these points *crossing points* and those points *microlocal crossing points*. Then, if (x, ξ) is a microlocal crossing point, x is a crossing point. But if x is a crossing point, the microlocal crossing points exist only when λ is greater than or equal to the crossing value $V_1(x) = V_2(x) =: \lambda_c$. The microlocal crossing points associated with the crossing point x are $(x, \pm\sqrt{\lambda - \lambda_c})$.

It is well known in the theory of semiclassical and microlocal analysis (see, for example, [7, 23, 30]) that the frequency set of a solution to a scalar semiclassical pseudodifferential equation is included in the characteristic set and that it propagates along the integral curve of the Hamiltonian vector field (we call such a curve *classical trajectory* in what follows) of the real principal-type symbol (propagation of frequency sets).

These facts also hold in our matrix case in the following sense: if $\mathbf{u} \in L^2(\mathbb{R}; \mathbb{C}^2)$ with $\|\mathbf{u}\| \leq 1$ satisfies $\|(\mathcal{P} - \lambda)\mathbf{u}\|_{L^2} = \mathcal{O}(h^\infty)$, then $\mathbf{u} \equiv \mathbf{0}$ outside $\Gamma(\lambda)$.

If, moreover, $\mathbf{u}$ is microlocally infinitely small at a point on a connected classical trajectory $\gamma_1 \subset \Gamma_1(\lambda) \setminus \Gamma_2(\lambda)$ of p_1 [resp., $\gamma_2 \subset \Gamma_2(\lambda) \setminus \Gamma_1(\lambda)$ of p_2] where p_1 [resp., p_2] is real principal type, then $\mathbf{u}$ is microlocally infinitely small at any point on γ_1 [resp., γ_2]. Remark that the propagation of frequency set does not hold beyond a microlocal crossing point. As we will see later, the frequency set on one of $\Gamma_j(\lambda)$, $j = 1, 2$, may propagate to the other one after the microlocal crossing point.

Now, let us observe the frequency set of the WKB solutions $\mathbf{u}_j^\pm$, $j = 1, 2$, that we constructed in the previous section. Let $\Gamma_t(\lambda)$ be the set of turning points and $\Gamma_c(\lambda)$ the set of microlocal crossing points:

$$\begin{aligned}\Gamma_t(\lambda) &= \Gamma_{1,t}(\lambda) \cup \Gamma_{2,t}(\lambda), \quad \Gamma_{j,t}(\lambda) := \{(x, 0); V_j(x) = \lambda\}, \\ \Gamma_c(\lambda) &:= \Gamma_1(\lambda) \cap \Gamma_2(\lambda) = \{(x, \xi); V_1(x) = V_2(x) \leq \lambda, \xi = \pm \sqrt{\lambda - V_1(x)}\}.\end{aligned}$$

To each function $\mathbf{u}_j^\pm$, there corresponds a connected component γ of the set $\Gamma(\lambda) \setminus (\Gamma_t(\lambda) \cup \Gamma_c(\lambda))$ in the phase space. This component γ is chosen in such a way that it belongs to $\Gamma_j^\pm(\lambda) := \Gamma_j(\lambda) \cap \{(x, \xi); \pm \xi > 0\}$ and $\mathbf{u}_j^\pm$ is defined in its x -projection $\pi(\gamma)$. According to this correspondence, we write $\mathbf{f}_\gamma := \mathbf{u}_j^\pm$ and call it *microlocal WKB solution* on γ . Recall that the WKB solution $\mathbf{u}_j^\pm$ depends on the choice of the base point $x_0 \in \pi(\gamma)$ for the phase function $\phi_j(x, x_0)$ (see (2.5)), and the base point x_1 of the symbol. When necessary, we will also denote $\mathbf{f}_\gamma = \mathbf{f}_{\gamma, \rho}$ specifying the point $\rho \in \mathbb{R}^2$ on γ such that

$$\pi(\rho) = x_0.$$

The microlocal WKB solution $\mathbf{f}_\gamma$ satisfies

$$(\mathcal{P} - \lambda)\mathbf{f}_\gamma = \mathcal{O}(h^\infty) \quad \text{in } \pi(\gamma),$$

as we saw in the previous section. Moreover, $\mathbf{f}_\gamma$ is microlocalized exactly on γ in the region $\pi(\gamma) \times \mathbb{R}_\xi$ of the phase space. In fact, the set γ is a Lagrangian manifold defined by

$$\xi = \pm \phi_j'(x) = \pm \sqrt{\lambda - V_j(x)}$$

for x in the classically allowed region for p_j , and the stationary phase method applied to the integral (3.1) for the WKB expression (2.9) or (2.10) of $\mathbf{u}_j^\pm$ gives a non-trivial asymptotic expansion only for (x, ξ) on γ . The phase function of this integral is $(x - y)\xi \pm \phi_j(y)$, and the critical point is given by $(y, \xi) = (x, \pm \phi_j'(x))$.

On the contrary, to each connected component γ of the set $\Gamma(\lambda) \setminus (\Gamma_t(\lambda) \cup \Gamma_c(\lambda))$ a microlocal WKB solution $\mathbf{f}_\gamma$ is associated. Moreover, the vector space of microlocal solutions on each γ is one dimensional. In fact, if $\gamma \subset \Gamma_1(\lambda) \setminus \Gamma_2(\lambda)$, say, the operator $P_1 - \lambda$ is reduced to the normal form hD_x while $P_2 - \lambda$ is elliptic there. Therefore, it is generated by $\mathbf{f}_\gamma$.

Summing up, we have the following proposition.

Proposition 3.1. *Let $\mathbf{u} \in L^2(\mathbb{R}; \mathbb{C}^2)$, $\|\mathbf{u}\|_{L^2} \leq 1$, be a solution to the system (1.2). Then, for each connected component γ of the set $\Gamma(\lambda) \setminus (\Gamma_t(\lambda) \cup \Gamma_c(\lambda))$, there exists a complex number α_γ such that*

$$\mathbf{u} \equiv \alpha_\gamma \mathbf{f}_\gamma \quad \text{on } \gamma.$$

Remark 3.2. The number α_γ is determined up to $\mathcal{O}(h^\infty)$ when the base points of the phase and the symbol are specified, but up to $\mathcal{O}(h)$ when only the base point of the phase is specified.

4. Microlocal scattering matrix at a crossing point

If we know the complex number α_γ for all the connected components γ of $\Gamma(\lambda) \setminus \Gamma_t(\lambda) \cap \Gamma_c(\lambda)$, we have all the microlocal information of $\mathbf{u}$ in the phase space since $\mathbf{u}$ is microlocally infinitely small outside the characteristic set $\Gamma(\lambda)$, as stated in the previous section. This permits us to know the global behavior of $\mathbf{u}$ modulo $\mathcal{O}(h^\infty)$, which leads to the asymptotic study of eigenvalues or resonances. In fact, it holds that if a solution $\mathbf{u} \in L^2(\mathbb{R}; \mathbb{C}^2)$, $\|\mathbf{u}\|_{L^2} \leq 1$, to the system (1.2) is microlocally infinitely small everywhere in $I \times \mathbb{R}_\xi$ for an interval $I \subset \mathbb{R}_x$, then $\|\mathbf{u}\|_{L^2(I)} = \mathcal{O}(h^\infty)$. Namely, the microlocal behavior in $I \times \mathbb{R}_\xi$ determines the local behavior in I modulo $\mathcal{O}(h^\infty)$.

Thus, the global study of solutions to the system (1.2) is reduced to the connection of the coefficients α_γ at each turning point and crossing point. The connection problem at a turning point is well known at least for the scalar case in general dimension as Maslov's theory (see [25]). In the system case also, similar formulas hold as long as the turning point is not a crossing point.

4.1. Connection at a turning point

Let $(x^*, 0) \in \Gamma_t \setminus \Gamma_c$. Suppose, for example, it is a turning point of p_1 : $(x^*, 0) \in \Gamma_{1,t}$. We assume that it is a simple turning point, i.e., $V_1'(x^*) \neq 0$. Then, there are exactly two connected components of $\Gamma(\lambda) \setminus \Gamma_t(\lambda) \cup \Gamma_c(\lambda)$ which have the turning point $(x^*, 0)$ as an extremity. Let γ^b be the one which has $(x^*, 0)$ as endpoint of the Hamiltonian flow $\exp tH_{p_1}$ on it and $\gamma^\#$ the other one. In other words, γ^b is the incoming classical trajectory to $(x^*, 0)$ and $\gamma^\#$ is the outgoing classical trajectory from $(x^*, 0)$.

Let $\mathbf{f}_b$ and $\mathbf{f}_\#$ be microlocal solutions defined on γ_b and $\gamma_\#$, respectively, with phase functions $\phi_1(x, x^*)$ based on the turning point x^* (see (2.5)), and let $\alpha_\# = \alpha_{\gamma_\#}$ and $\alpha_b = \alpha_{\gamma_b}$ for short where $\alpha_{\gamma_\#}$ and α_{γ_b} are defined by Proposition 3.1. Under this setting, the following asymptotic connection formula holds. For the proof, we refer, for example, to [9].

Proposition 4.1. *Let $\mathbf{u} \in L^2(\mathbb{R}; \mathbb{C}^2)$, $\|\mathbf{u}\|_{L^2} \leq 1$, be a solution to the system (1.2). If*

$$\mathbf{u} \equiv \alpha_b \mathbf{f}_b \quad \text{on } \gamma_b,$$

$$\mathbf{u} \equiv \alpha_\# \mathbf{f}_\# \quad \text{on } \gamma_\#,$$

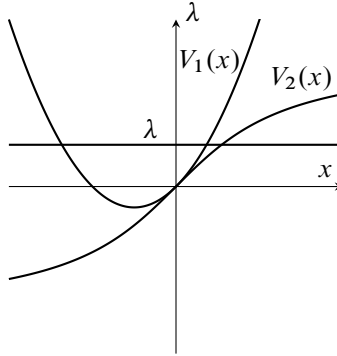


Figure 1. Potentials V_1 and V_2 .

then it holds modulo $\mathcal{O}(h)$ that

$$\alpha_{\sharp} = -i\alpha_{\flat} = e^{-i\frac{\pi}{2}}\alpha_{\flat}.$$

4.2. Connection at a microlocal crossing point

Now, we study the connection at a microlocal crossing point. Let $\rho := (x_0, \xi_0) \in \mathbb{R}_x \times \mathbb{R}_{\xi}$ be a microlocal crossing point $\rho \in \Gamma_c(\lambda) = \Gamma_1(\lambda) \cap \Gamma_2(\lambda)$. We assume without loss of generality that $x_0 = 0$ and

$$V_1(0) = V_2(0) = 0. \quad (4.1)$$

We, moreover, assume that $V_1(x)$ and $V_2(x)$ intersect at $x = 0$ at a finite order; i.e., there exists $n \in \mathbb{N}$ such that

$$V_1^{(k)}(0) - V_2^{(k)}(0) = 0 \quad (0 \leq k \leq n-1), \quad V_1^{(n)}(0) - V_2^{(n)}(0) \neq 0.$$

If $\lambda > 0$, one has $\xi_0 = \pm\sqrt{\lambda}$ and there are two crossing points $\rho_+ := (0, \sqrt{\lambda})$ and $\rho_- := (0, -\sqrt{\lambda})$ symmetric with respect to the x -axis. They are not turning points. If on the contrary $\lambda = 0$, one has $\xi_0 = 0$ and $\rho = (0, 0)$. This is not only a crossing point but also a turning point. This is the case we avoided in the previous subsection. In this case, we will assume that $x = 0$ is a simple zero of $V_1(x)$ and $V_2(x)$:

$$V_1'(0) \neq 0, \quad V_2'(0) \neq 0,$$

Above the crossing level $\lambda > 0$, $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$ intersect at two points $(0, \sqrt{\lambda})$ and $(0, -\sqrt{\lambda})$ and the contact order m at these points is both n :

$$H_{p_1}^k p_2(0, \pm\sqrt{\lambda}) = 0 \quad (0 \leq k \leq n-1), \quad H_{p_1}^n p_2(0, \pm\sqrt{\lambda}) \neq 0. \quad (4.2)$$

On the contrary, at the crossing level $\lambda = 0$, $\Gamma_1(0)$ and $\Gamma_2(0)$ intersect at one point $(0, 0)$ and the contact order m at this point is $2n$:

$$H_{p_1}^k p_2(0, 0) = 0 \quad (0 \leq k \leq 2n-1), \quad H_{p_1}^{2n} p_2(0, 0) \neq 0. \quad (4.3)$$

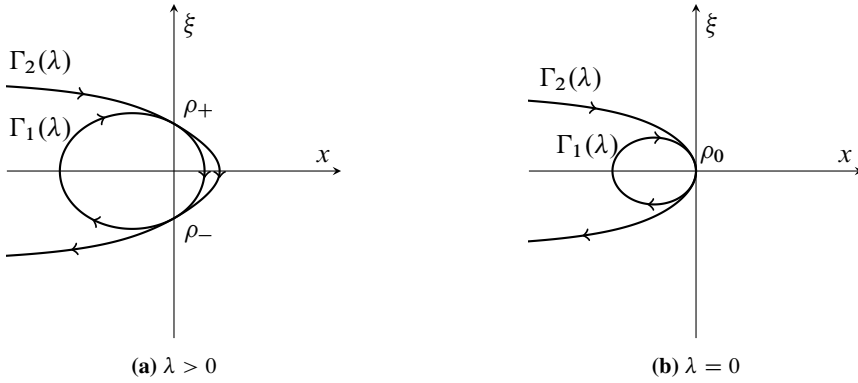


Figure 2. Characteristic sets $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$.

As in the previous case of a turning point, we denote $\gamma_{j,b}, \gamma_{j,\#}$ for each $j = 1, 2$ the incoming and the outgoing classical trajectories on $\Gamma_j(\lambda)$ having ρ as their extremity. We write also $\alpha_{j,b}, \alpha_{j,\#}$ as the coefficients $\alpha_{\gamma_{j,b}}, \alpha_{\gamma_{j,\#}}$ defined in Proposition 3.1.

Proposition 4.2. *Let $\mathbf{f}_{j,b}, \mathbf{f}_{j,\#}$ be the microlocal solutions to (1.2) defined on $\gamma_{j,b}, \gamma_{j,\#}$ for each $j = 1, 2$ with the phase base point at the microlocal crossing point ρ . Then, there exists an h -dependent constant 2×2 matrix T such that if $\mathbf{u} \in L^2(\mathbb{R}; \mathbb{C}^2)$, $\|\mathbf{u}\|_{L^2} \leq 1$ is a solution to the system (1.2), and if $\alpha_{j,b}, \alpha_{j,\#}$ are defined for each $j = 1, 2$ by*

$$\begin{aligned} \mathbf{u} &\equiv \alpha_{j,b} \mathbf{f}_{j,b} && \text{on } \gamma_{j,b}, \\ \mathbf{u} &\equiv \alpha_{j,\#} \mathbf{f}_{j,\#} && \text{on } \gamma_{j,\#}, \end{aligned}$$

then it holds modulo $\mathcal{O}(h)$ that

$$\begin{pmatrix} \alpha_{1,\#} \\ \alpha_{2,\#} \end{pmatrix} = T \begin{pmatrix} \alpha_{1,b} \\ \alpha_{2,b} \end{pmatrix}.$$

Remark 4.3. Here, we do not specify the symbol base point, and hence, the microlocal WKB solutions are defined up to $\mathcal{O}(h)$ only. That is why the microlocal scattering matrix is determined up to $\mathcal{O}(h)$.

We call the matrix $T = (t_{jk})_{j,k=1,2}$ *microlocal scattering matrix* here, since it describes the outgoing waves in terms of the incoming ones. The diagonal entries t_{jj} stand for the transmission of particles along $\Gamma_j(\lambda)$, while the anti-diagonal entries t_{jk} stand for the “change of trajectories” from $\Gamma_k(\lambda)$ to $\Gamma_j(\lambda)$ at the crossing point. Such a notion was first introduced by Colin de Verdière in [6], where he calls T *local scattering matrix*.

Proof. The two pairs $(\mathbf{f}_{1,b}, \mathbf{f}_{2,b})$ and $(\mathbf{f}_{1,\#}, \mathbf{f}_{2,\#})$ are bases of the vector space of the microlocal solutions in a neighborhood of ρ . In fact, it can be shown that if $\mathbf{u} \equiv 0$ on $\gamma_{1,b} \cup \gamma_{2,b}$, then $\mathbf{u} \equiv 0$ on $\gamma_{1,\#} \cup \gamma_{2,\#}$, and vice versa. ■

We are interested in the asymptotic behavior of the microlocal scattering matrix in the semiclassical limit $h \rightarrow 0$. For the sake of the application to the resonance asymptotics, we fix a real energy λ_0 and consider the microlocal scattering matrix for λ 's in a complex neighborhood of λ_0 : $\mathcal{R}_{\lambda_0}(\delta_1, \delta_2) := \{\lambda \in \mathbb{C}; |\operatorname{Re} \lambda - \lambda_0| < \delta_1, |\operatorname{Im} \lambda| < \delta_2\}$ for h -dependent small δ_1 and δ_2 .

Let us begin with the generic case where the crossing point in question is not a turning point.

Theorem 4.1. *Suppose $\lambda_0 > 0$ and let $T_{\pm}$ be the microlocal scattering matrices at the crossing points $\rho_{\pm} = (0, \pm\sqrt{\lambda_0})$. Then, there exist $C > 0$ and $\varepsilon > 0$ such that $T_{\pm}$ satisfy, for $\lambda \in \mathcal{R}_{\lambda_0}(Ch, Ch)$, the asymptotic formulas*

$$T_+ = \operatorname{Id} - ih^{\frac{1}{n+1}} \begin{pmatrix} 0 & \bar{\omega} \\ \omega & 0 \end{pmatrix} + \mathcal{O}(h^{\frac{1}{n+1}+\varepsilon}) \quad \text{as } h \rightarrow 0, \quad (4.4)$$

$$T_- = \operatorname{Id} - ih^{\frac{1}{n+1}} \begin{pmatrix} 0 & \omega \\ \bar{\omega} & 0 \end{pmatrix} + \mathcal{O}(h^{\frac{1}{n+1}+\varepsilon}) \quad \text{as } h \rightarrow 0, \quad (4.5)$$

where the constant $\omega \in \mathbb{C}$ is given by

$$\omega = \mu_n \left(\frac{2(n+1)!}{|V_1^{(n)}(0) - V_2^{(n)}(0)|} \right)^{\frac{1}{n+1}} \lambda_0^{-\frac{n}{2(n+1)}} \Gamma\left(\frac{n+2}{n+1}\right) W(0), \quad (4.6)$$

$$\mu_n = \begin{cases} \exp\left(\frac{i\pi}{2(n+1)} \operatorname{sgn}(V_2^{(n)}(0) - V_1^{(n)}(0))\right) & \text{when } n \text{ is odd,} \\ \cos\left(\frac{\pi}{2(n+1)}\right) & \text{when } n \text{ is even.} \end{cases}$$

Remark 4.4. The transversal case $n = 1$ was computed by Colin de Verdière in [6] using the Landau–Zener normal form reduction. We also mention the multiphase method due to Kucherenko [20]. It was also computed in [9] under the assumption that the interaction W is a first-order differential operator $W = r_0(x) + ir_1(x)hD_x$ with real-valued coefficients $r_0(x)$ and $r_1(x)$, elliptic at the crossing point, i.e., $r_0(0) \pm ir_1(0)\sqrt{\lambda_0} \neq 0$. In this work, the scalar normal form $x\xi$ (see [13, 28]) was used.

In the tangential case $n > 1$, the result is due to [2]. Notice in (4.6) that the second term in (4.4) and (4.5) vanishes when the interaction W vanished at the crossing point $x = 0$. In such cases, the precise second term was computed by Louatron in [21].

Recently, Higuchi, Louatron, and Taira have established a microlocal normal form for general 2×2 matrix-valued semiclassical pseudodifferential operators at a tangential crossing point. Using this normal form, the computation of the above formulas becomes much simpler [16].

Next, we consider the particular case where the crossing point is also a turning point. Notice that $\lambda_0 = 0$ is a transition energy in the sense that there are two microlocal crossing points near $(0, 0)$ for small positive energies λ above this level, whereas for small negative

energies below this level, there is no microlocal crossing point near $(0, 0)$. Such transition will be expressed in terms of a kind of generalized Airy function. It is defined by

$$A_n(\lambda) = \frac{1}{2\pi} \int_{\mathbb{R}} \exp\left(i \int_0^\eta (\lambda + \tau^2)^n d\tau\right) d\eta.$$

This coincides with the standard Airy function when $n = 1$:

$$A_1(\lambda) = \text{Ai}(\lambda) := \frac{1}{2\pi} \int_{\mathbb{R}} e^{i(\lambda\eta + \frac{\eta^3}{3})} d\eta.$$

As this standard one, the generalized Airy function $A_n(\lambda)$ has the following asymptotic properties as $\lambda \rightarrow \pm\infty$.

Proposition 4.5. *As $\lambda \rightarrow +\infty$, one has*

$$A_n(\lambda) = \frac{1}{\pi} \sin\left(\frac{\pi}{n+1}\right) \Gamma\left(\frac{n+2}{n+1}\right) \left(\frac{n+1}{2^n}\right)^{\frac{1}{n+1}} \lambda^{-\frac{n}{2(n+1)}} \exp(-c_n \lambda^{n+\frac{1}{2}}),$$

while as $\lambda \rightarrow -\infty$, one has

$$A_n(\lambda) = \frac{2}{\pi} \Gamma\left(\frac{n+2}{n+1}\right) \left(\frac{n+1}{2^n}\right)^{\frac{1}{n+1}} \alpha_n(\lambda) |\lambda|^{-\frac{n}{2(n+1)}}.$$

Here, the constant c_n and the function $\alpha_n(\lambda)$ are given by

$$c_n = \int_0^1 (1-t^2)^n dt = \frac{(2n)!!}{(2n+1)!!}, \quad \alpha_n(\lambda) = \begin{cases} \cos(c_n |\lambda|^{n+\frac{1}{2}} - \frac{\pi}{2(n+1)}) & \text{for even } n, \\ \cos \frac{\pi}{2(n+1)} \cos(c_n |\lambda|^{n+\frac{1}{2}}) & \text{for odd } n. \end{cases}$$

Using this function, the microlocal scattering matrix at a turning crossing point is expressed as in the following theorem [3].

Theorem 4.2. *Suppose $\lambda_0 = 0$ and let T be the microlocal scattering matrix at the crossing point $\rho_0 = (0, 0)$. Then, there exist $C > 0$ and $\varepsilon > 0$ such that T_0 satisfies the asymptotic formula*

$$iT_0 = \text{Id} - ih^{\frac{1}{2n+1}} \begin{pmatrix} 0 & \kappa \\ \kappa & 0 \end{pmatrix} + \mathcal{O}(h^{\frac{1+\varepsilon}{2n+1}}) \quad \text{as } h \rightarrow 0,$$

for $\lambda \in \mathcal{R}_{\lambda_0}(Ch^{\frac{2}{2n+1}}, Ch)$, where $\kappa = \kappa(\lambda, h)$ is given by

$$\kappa = \frac{2\pi W(0)}{|V_1'(0)V_2'(0)|^{\frac{1}{4}}} q_n^{-\frac{1}{2n+1}} A_n\left(-\frac{q_n^{\frac{2}{2n+1}}}{|V_1'(0)V_2'(0)|^{\frac{1}{2}}} \frac{\lambda}{h^{\frac{2}{2n+1}}}\right), \quad q_n = \frac{V_1^{(n)}(0) - V_2^{(n)}(0)}{n! |V_1'(0)V_2'(0)|^{\frac{1}{4}}}.$$

Remark that the quantity in the function A_n is in the form $-c\lambda/h^{\frac{2}{2n+1}}$ with a positive constant c , and is bounded in h when λ is in the complex rectangle $\mathcal{R}_{\lambda_0}(Ch^{\frac{2}{2n+1}}, Ch)$. But if we take C large enough, we see from this theorem and Proposition 4.5 that the number κ oscillates when $\lambda/h^{\frac{2}{2n+1}}$ is positive and large, and that κ is positive and small when $\lambda/h^{\frac{2}{2n+1}}$ is negative and large.

5. Local exact solutions and microlocal scattering matrix

Let ρ be a microlocal crossing point in the phase space. Recall that, under (4.1), $\rho = \rho_+ = (0, \sqrt{\lambda_0})$ or $\rho_- = (0, -\sqrt{\lambda_0})$ when $\lambda_0 > 0$ and $\rho = (0, 0)$ when $\lambda_0 = 0$. In order to compute the microlocal scattering matrix T at ρ , we construct local exact solutions to the system (1.2) in a small neighborhood I of $x = 0$.

Here, we study this only in the case $\lambda_0 > 0$. It is known that there exist exact solutions $u_j^\pm$ to the scalar Schrödinger equations $(P_j - \lambda)u = 0$ for each $j = 1, 2$ with the semiclassical asymptotic behavior

$$u_j^\pm \sim (\lambda - V_j(x))^{-\frac{1}{4}} \exp\left(\pm \frac{i}{h} \int_0^x \sqrt{\lambda - V_j(t)} dt\right), \quad \text{as } h \rightarrow 0,$$

in the classically allowed region for λ close to $\lambda_0 > 0$. We can assume without loss of generality that the Wronskian of u_j^+ and u_j^- is exactly given by

$$\mathcal{W}(u_j^+, u_j^-) = u_j^+(u_j^-)' - u_j^-(u_j^+)' = -\frac{2i}{h}.$$

We suppose here that the smooth function $W(x)$ has a compact support in I . Let $K_{j,L}$ and $K_{j,R}$ be the operators acting on functions f in $C^\infty(\mathbb{R})$ defined by

$$\begin{aligned} K_{j,L}f &:= \frac{i}{2} \int_{-\infty}^x (u_j^+(x)u_j^-(y) - u_j^-(x)u_j^+(y))W(y)f(y)dy, \\ K_{j,R}f &:= \frac{i}{2} \int_{\infty}^x (u_j^+(x)u_j^-(y) - u_j^-(x)u_j^+(y))W(y)f(y)dy. \end{aligned}$$

They satisfy

$$(P_j - \lambda)K_{j,L}f = -hWf, \quad (P_j - \lambda)K_{j,R}f = -hWf.$$

Using these operators, we construct exact solutions to the system (1.2) by a successive approximation. The following lemma can be proved using the same argument as the proof of the next Lemma 5.2.

Lemma 5.1. *For $S = L, R$, we have*

$$\|K_{1,S}K_{2,S}\|_{\mathcal{B}(C(I))} = \mathcal{O}(h^{\frac{1}{m+1}}), \quad \|K_{2,S}K_{1,S}\|_{\mathcal{B}(C(I))} = \mathcal{O}(h^{\frac{1}{m+1}}),$$

where $\mathcal{B}(C(I))$ is the space of bounded linear operators on the space of continuous functions $C(I)$ on I , equipped with the usual operator norm.

This lemma implies that the infinite sums

$$J_{12,S} := \sum_{k=0}^{\infty} (K_{1,S}K_{2,S})^k, \quad J_{21,S} := \sum_{k=0}^{\infty} (K_{2,S}K_{1,S})^k$$

converge for sufficiently small h in the space $\mathcal{B}(C(I))$ of bounded operators on $C(I)$.

For $S = L, R$, we set

$$\begin{aligned}\mathbf{w}_{1,S}^{\pm} &:= \begin{pmatrix} J_{12,S} u_1^{\pm} \\ K_{2,S} J_{12,S} u_1^{\pm} \end{pmatrix} = \begin{pmatrix} u_1^{\pm} \\ K_{2,S} u_1^{\pm} \end{pmatrix} + \mathcal{O}(h^{\frac{1}{m+1}}), \\ \mathbf{w}_{2,S}^{\pm} &:= \begin{pmatrix} K_{1,S} J_{21,S} u_2^{\pm} \\ J_{21,S} u_2^{\pm} \end{pmatrix} = \begin{pmatrix} K_{1,S} u_2^{\pm} \\ u_2^{\pm} \end{pmatrix} + \mathcal{O}(h^{\frac{1}{m+1}}).\end{aligned}$$

We see that these 8 functions $\mathbf{w}_{j,S}^{\varepsilon}$ for $j = 1, 2$, $S = R, L$, and $\varepsilon = +, -$ are all exact solutions to the system (1.2) in the interval I .

Let $\gamma_{j,b}^{\pm}$ be the incoming trajectories to the crossing point $\rho_{\pm}$ and $\gamma_{j,\#}^{\pm}$ the outgoing ones from $\rho_{\pm}$ along $\Gamma_j(\lambda_0)$ in $I \times \mathbb{R}_{\xi}$:

$$\begin{aligned}\gamma_{j,b}^{+} &= \Gamma_j(\lambda_0) \cap \{(x, \xi) \in I \times \mathbb{R}; x < 0, \xi > 0\}, \\ \gamma_{j,\#}^{+} &= \Gamma_j(\lambda_0) \cap \{(x, \xi) \in I \times \mathbb{R}; x > 0, \xi > 0\}, \\ \gamma_{j,b}^{-} &= \Gamma_j(\lambda_0) \cap \{(x, \xi) \in I \times \mathbb{R}; x > 0, \xi < 0\}, \\ \gamma_{j,\#}^{-} &= \Gamma_j(\lambda_0) \cap \{(x, \xi) \in I \times \mathbb{R}; x < 0, \xi < 0\},\end{aligned}$$

and let $\mathbf{f}_{j,b}^{\pm}$ and $\mathbf{f}_{j,\#}^{\pm}$ be the microlocal WKB solutions on $\gamma_{j,b}^{\pm}$ and $\gamma_{j,\#}^{\pm}$, respectively, with phase base point at $\rho_{\pm}$.

We easily see the asymptotic behavior of $\mathbf{w}_{j,L}^{\pm}$ on the left of the origin $I \cap \{x < 0\}$ and that of $\mathbf{w}_{j,R}^{\pm}$ on the right of the origin $I \cap \{x > 0\}$.

Lemma 5.2. *The exact solution $\mathbf{w}_{1,L}^{+}$ microlocally behaves like*

$$\mathbf{w}_{1,L}^{+} \equiv \begin{cases} \mathbf{f}_{1,b}^{+} & \text{on } \gamma_{1,b}^{+}, \\ \mathbf{0} & \text{on } \gamma_{1,\#}^{-} \cup \gamma_{2,b}^{+} \cup \gamma_{2,\#}^{-}, \end{cases} \quad (5.1)$$

modulo $\mathcal{O}(h)$ as $h \rightarrow 0$. Similarly, the other solutions $\mathbf{w}_{j,L}^{\pm}$ and $\mathbf{w}_{j,R}^{\pm}$ behave microlocally like

$$\begin{aligned}\mathbf{w}_{j,L}^{+} &\equiv \begin{cases} \mathbf{f}_{j,b}^{+} & \text{on } \gamma_{j,b}^{+}, \\ \mathbf{0} & \text{on } \gamma_{j,\#}^{-} \cup \gamma_{\hat{j},b}^{+} \cup \gamma_{\hat{j},\#}^{-}, \end{cases} & \mathbf{w}_{j,R}^{+} &\equiv \begin{cases} \mathbf{f}_{j,\#}^{+} & \text{on } \gamma_{j,\#}^{+}, \\ \mathbf{0} & \text{on } \gamma_{j,b}^{-} \cup \gamma_{\hat{j},\#}^{+} \cup \gamma_{\hat{j},b}^{-}, \end{cases} \\ \mathbf{w}_{j,L}^{-} &\equiv \begin{cases} \mathbf{f}_{j,\#}^{-} & \text{on } \gamma_{j,\#}^{-}, \\ \mathbf{0} & \text{on } \gamma_{j,b}^{+} \cup \gamma_{\hat{j},\#}^{-} \cup \gamma_{\hat{j},b}^{+}, \end{cases} & \mathbf{w}_{j,R}^{-} &\equiv \begin{cases} \mathbf{f}_{j,b}^{-} & \text{on } \gamma_{j,b}^{-}, \\ \mathbf{0} & \text{on } \gamma_{j,\#}^{+} \cup \gamma_{\hat{j},b}^{-} \cup \gamma_{\hat{j},\#}^{+}, \end{cases}\end{aligned}$$

modulo $\mathcal{O}(h)$ as $h \rightarrow 0$ for $j = 1, 2$.

Proof. We only prove (5.1). Recall that, modulo $\mathcal{O}(h^{\frac{2}{m+1}})$, we have

$$\mathbf{w}_{1,L}^{+} = {}^t(u_1^{+}, K_{2,L}u_1^{+}),$$

and

$$\begin{aligned} K_{2,L}u_1^+(x) &= \frac{i}{2} \int_{-\infty}^x (u_2^+(x)u_2^-(y) - u_2^-(x)u_2^+(y))W(y)u_1^+(y)dy \\ &= \frac{i}{2}u_2^+(x) \int_{-\infty}^x u_2^-(y)u_1^+(y)W(y)dy - \frac{i}{2}u_2^-(x) \int_{-\infty}^x u_2^+(y)u_1^+(y)W(y)dy. \end{aligned}$$

The last two integrals are oscillatory integrals with integrand

$$u_2^-u_1^+W = \frac{W}{(E-V_1)^{\frac{1}{4}}(E-V_2)^{\frac{1}{4}}} \exp\left(\frac{i}{h} \int_0^y (E-V_1(t))^{\frac{1}{2}} - (E-V_2(t))^{\frac{1}{2}} dt\right), \quad (5.2)$$

$$u_2^+u_1^+W = \frac{W}{(E-V_1)^{\frac{1}{4}}(E-V_2)^{\frac{1}{4}}} \exp\left(\frac{i}{h} \int_0^y (E-V_1(t))^{\frac{1}{2}} + (E-V_2(t))^{\frac{1}{2}} dt\right). \quad (5.3)$$

The first integrand has a critical point at the crossing point $y = 0$, but it is outside the integration range when $x < 0$, and the second one no critical point. Therefore, the integrals are both $\mathcal{O}(h)$. This ends the proof. ■

The 4 solutions $(\mathbf{w}_{1,L}^+, \mathbf{w}_{2,L}^+, \mathbf{w}_{1,L}^-, \mathbf{w}_{2,L}^-)$ as well as the 4 solutions $(\mathbf{w}_{1,R}^+, \mathbf{w}_{2,R}^+, \mathbf{w}_{1,R}^-, \mathbf{w}_{2,R}^-)$ make two bases of exact solutions to the system $\mathcal{P}\mathbf{u} = \mathbf{0}$ in I . Therefore, there exists a constant 4×4 matrix A such that

$$(\mathbf{w}_{1,L}^+, \mathbf{w}_{2,L}^+, \mathbf{w}_{1,L}^-, \mathbf{w}_{2,L}^-) = (\mathbf{w}_{1,R}^+, \mathbf{w}_{2,R}^+, \mathbf{w}_{1,R}^-, \mathbf{w}_{2,R}^-)A. \quad (5.4)$$

According to the previous lemma, we find the following lemma.

Lemma 5.3. *The microlocal scattering matrix T at the crossing point $\rho_+ = (0, \sqrt{\lambda_0})$ is equal modulo $\mathcal{O}(h)$ to the 2×2 block matrix A_{11} of*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

defined by (5.4).

We are now going to compute A at the principal level modulo $\mathcal{O}(h^{\frac{2}{m+1}})$ in the semi-classical limit. We rewrite the definition (5.4) of A in the form

$$\begin{pmatrix} \mathbf{w}_{1,L}^+ & \mathbf{w}_{2,L}^+ & \mathbf{w}_{1,L}^- & \mathbf{w}_{2,L}^- \\ (\mathbf{w}_{1,L}^+)' & (\mathbf{w}_{2,L}^+)' & (\mathbf{w}_{1,L}^-)' & (\mathbf{w}_{2,L}^-)' \end{pmatrix} = \begin{pmatrix} \mathbf{w}_{1,R}^+ & \mathbf{w}_{2,R}^+ & \mathbf{w}_{1,R}^- & \mathbf{w}_{2,R}^- \\ (\mathbf{w}_{1,R}^+)' & (\mathbf{w}_{2,R}^+)' & (\mathbf{w}_{1,R}^-)' & (\mathbf{w}_{2,R}^-)' \end{pmatrix} A,$$

and look at this identity at $x = 0$. Here, $'$ stands for the derivative with respect to x . Notice that both sides are 4×4 matrices. The first column vector on the left-hand side is

$${}^t(u_1^+(0), (K_{2,L}u_1^+)(0), (u_1^+)'(0), (K_{2,L}u_1^+)'(0)).$$

The term $(K_{2,L}u_1^+)(0)$ is expressed in a linear combination of $u_2^+(0)$ and $u_2^-(0)$:

$$\begin{aligned}(K_{2,L}u_1^+)(0) &= \frac{i}{2} \int_{-\infty}^x (u_2^+(x)u_2^-(y) - u_2^-(x)u_2^+(y))W(y)u_1^+(y)dy|_{x=0} \\ &= \frac{i}{2} \int_{-\infty}^0 (u_2^+(0)u_2^-(y) - u_2^-(0)u_2^+(y))W(y)u_1^+(y)dy \\ &= c_{1L}^+u_2^+(0) + c_{1L}^-u_2^-(0),\end{aligned}$$

with

$$c_{1L}^+ = \frac{i}{2} \int_{-\infty}^0 u_2^-(y)u_1^+(y)W(y)dy, \quad c_{1L}^- = -\frac{i}{2} \int_{-\infty}^0 u_2^+(y)u_1^+(y)W(y)dy.$$

Similarly, $(K_{2,L}u_1^+)'(0)$ is written in linear combination of $(u_2^+)'(0)$ and $(u_2^-)'(0)$:

$$(K_{2,L}u_1^+)'(0) = c_{1L}^+(u_2^+)'(0) + c_{1L}^-(u_2^-)'(0).$$

We define a matrix B by

$$B = \begin{pmatrix} u_1^+(0) & 0 & u_1^-(0) & 0 \\ 0 & u_2^+(0) & 0 & u_2^-(0) \\ (u_1^+)'(0) & 0 & (u_1^-)'(0) & 0 \\ 0 & (u_2^+)'(0) & 0 & (u_2^-)'(0) \end{pmatrix}.$$

Then, we have

$$\begin{aligned}\begin{pmatrix} \mathbf{w}_{1,L}^+ & \mathbf{w}_{2,L}^+ & \mathbf{w}_{1,L}^- & \mathbf{w}_{2,L}^- \\ (\mathbf{w}_{1,L}^+)' & (\mathbf{w}_{2,L}^+)' & (\mathbf{w}_{1,L}^-)' & (\mathbf{w}_{2,L}^-)' \end{pmatrix} \Big|_{x=0} &= B(I + C_L), \\ \begin{pmatrix} \mathbf{w}_{1,R}^+ & \mathbf{w}_{2,R}^+ & \mathbf{w}_{1,R}^- & \mathbf{w}_{2,R}^- \\ (\mathbf{w}_{1,R}^+)' & (\mathbf{w}_{2,R}^+)' & (\mathbf{w}_{1,R}^-)' & (\mathbf{w}_{2,R}^-)' \end{pmatrix} \Big|_{x=0} &= B(I + C_R),\end{aligned}$$

where C_S , $S = L, R$ are 4×4 matrices of the form

$$C_S = \begin{pmatrix} 0 & c_{2S}^+ & 0 & c_{4S}^+ \\ c_{1S}^+ & 0 & c_{3S}^+ & 0 \\ 0 & c_{2S}^- & 0 & c_{4S}^- \\ c_{1S}^- & 0 & c_{3S}^- & 0 \end{pmatrix}.$$

The entries $c_{jL}^\pm$ are given by

$$\begin{aligned}c_{2L}^+ &= \frac{i}{2} \int_{-\infty}^0 u_1^-(y)u_2^+(y)W(y)dy, & c_{2L}^- &= -\frac{i}{2} \int_{-\infty}^0 u_1^+(y)u_2^+(y)W(y)dy, \\ c_{3L}^+ &= \frac{i}{2} \int_{-\infty}^0 u_2^-(y)u_1^-(y)W(y)dy, & c_{3L}^- &= -\frac{i}{2} \int_{-\infty}^0 u_2^+(y)u_1^-(y)W(y)dy, \\ c_{4L}^+ &= \frac{i}{2} \int_{-\infty}^0 u_1^-(y)u_2^-(y)W(y)dy, & c_{4L}^- &= -\frac{i}{2} \int_{-\infty}^0 u_1^+(y)u_2^-(y)W(y)dy,\end{aligned}$$

and $c_{jR}^\pm$ are given similarly with the lower endpoint of the integral replaced by $+\infty$.

Remark here that C_L, C_R are of $\mathcal{O}(h^{\frac{1}{m+1}})$. In fact, as in the proof of Lemma 5.2, the entries $c_{jS}^{\pm}$ are oscillatory integrals possibly with a critical point at the origin. The order of this critical point is the contact order $n = m$ of the two potentials, and hence by the degenerate stationary phase method, we see that it is of order $h^{\frac{1}{m+1}}$.

Then, we obtain, for h small enough,

$$\begin{aligned} A &= (I + C_R)^{-1}(I + C_L) = I + C_L - C_R + \mathcal{O}(h^{\frac{2}{m+1}}) \\ &= I + \begin{pmatrix} 0 & c_2^+ & 0 & c_4^+ \\ c_1^+ & 0 & c_3^+ & 0 \\ 0 & c_2^- & 0 & c_4^- \\ c_1^- & 0 & c_3^- & 0 \end{pmatrix} + \mathcal{O}(h^{\frac{2}{m+1}}), \end{aligned}$$

where

$$\begin{aligned} c_1^+ &= \frac{i}{2} \int_{-\infty}^{\infty} u_1^+(y) u_2^-(y) W(y) dy, & c_1^- &= -\frac{i}{2} \int_{-\infty}^{\infty} u_1^+(y) u_2^+(y) W(y) dy, \\ c_2^+ &= \frac{i}{2} \int_{-\infty}^{\infty} u_1^-(y) u_2^+(y) W(y) dy, & c_2^- &= -\frac{i}{2} \int_{-\infty}^{\infty} u_1^+(y) u_2^+(y) W(y) dy, \\ c_3^+ &= \frac{i}{2} \int_{-\infty}^{\infty} u_1^-(y) u_2^-(y) W(y) dy, & c_3^- &= -\frac{i}{2} \int_{-\infty}^{\infty} u_1^-(y) u_2^+(y) W(y) dy, \\ c_4^+ &= \frac{i}{2} \int_{-\infty}^{\infty} u_1^-(y) u_2^-(y) W(y) dy, & c_4^- &= -\frac{i}{2} \int_{-\infty}^{\infty} u_1^+(y) u_2^-(y) W(y) dy. \end{aligned}$$

The semiclassical asymptotics of these entries are obtained by the stationary phase method again as in the proof of Lemma 5.2. Remark that the off-diagonal entries c_1^+ , c_2^+ of the block A_{11} , which are the second terms of the microlocal scattering matrix T_+ , include as integrand the product of two WKB solutions with different signs like (5.2). The phases of these oscillatory integrals have a critical point at the crossing point $y = 0$. Contrary to the case of Lemma 5.2, the critical point is in the range of integration, and the stationary phase method gives the asymptotics of these integrals. Notice that the critical point is degenerated in the general case $n \geq 2$, but in our one-dimensional setting, it is not difficult to compute it (see, e.g., [17])

More precisely, we have the following asymptotic formula, which gives Theorem 4.1:

$$c_1^+ = -i\omega h^{\frac{1}{m+1}} + \mathcal{O}(h^{\frac{2}{m+1}}), \quad c_2^+ = -i\bar{\omega} h^{\frac{1}{m+1}} + \mathcal{O}(h^{\frac{2}{m+1}}),$$

where ω is given by (4.6).

6. Application to the semiclassical distribution of resonances

As an application of the results of Theorems 4.1 and 4.2 in the previous section, we study the resonance asymptotics of the matrix-valued operator $\mathcal{P}$ defined by (1.3). The following microlocal strategy for the resonances of a matrix Schrödinger operator was also used in [9, 14, 15].

6.1. Fermi's golden rule

We assume that the functions $V_1(x)$, $V_2(x)$, and $W(x)$ appearing in the operator (1.3) are all real-valued on $\mathbb{R}$ and analytic in an angular complex neighborhood of $\mathbb{R}$,

$$\mathcal{S} := \{x \in \mathbb{C}; |\operatorname{Im} x| < (\tan \theta_0)(1 + |\operatorname{Re} x|)\},$$

for some positive constant $\theta_0 < \pi/2$. Moreover, $V_1(x)$, $V_2(x)$ have limits as $\operatorname{Re} x \rightarrow \pm\infty$ in this domain; for $j = 1, 2$,

$$V_j(x) \rightarrow V_j^\pm \quad \text{as } \operatorname{Re} x \rightarrow \pm\infty \text{ in } \mathcal{S}.$$

For $W(x)$, we assume that it is bounded there.

We fix a real energy $\lambda_0 \in \mathbb{R}$, near which we will study the distribution of resonances. We assume that $V_1(x)$ is a simple well-type potential with respect to this energy level λ_0 and that $V_2(x)$ is non-trapping type. In the terminology of quantum chemistry, V_1 is bonding while V_2 is anti-bonding. More precisely, we assume the following assumptions.

For V_1 , we assume $V_1^+, V_1^- > \lambda_0$ and there exist $a_0 < b_0$ such that

$$\frac{V_1(x) - \lambda_0}{(x - a_0)(x - b_0)} > 0 \quad \forall x \in \mathbb{R}.$$

Remark that a_0 and b_0 are simple zeros of $V_1(x) - \lambda_0$, called simple turning points. The characteristic set $\Gamma_1(\lambda_0)$ is a simple closed curve, and the classical trajectory is periodic along this curve.

For V_2 , we assume $V_2^- < \lambda_0 < V_2^+$ and there exists $c_0 \in \mathbb{R}$ such that

$$\frac{V_2(x) - \lambda_0}{x - c_0} > 0, \quad \forall x \in \mathbb{R}.$$

Remark that c_0 is also a simple zero of $V_2(x) - \lambda_0$. The characteristic set $\Gamma_2(\lambda_0)$ is an unbounded curve. The classical trajectory $(x(t), \xi(t))$ along this curve tends to

$$(-\infty, \mp \sqrt{\lambda_0}) \quad \text{as } t \rightarrow \pm\infty$$

(see Figure 1 in Section 4).

Under the above assumptions, the spectrum of P_1 near λ_0 consists of (simple) eigenvalues. In the semiclassical limit $h \rightarrow +0$, they are approximated by the energies satisfying the so-called *Bohr–Sommerfeld quantization rule* (see [18, 27, 29]):

$$-e^{i\mathcal{A}(\lambda)/h} = 1, \tag{6.1}$$

where $\mathcal{A}(\lambda)$ is the action of the classical Hamiltonian $p_1(x, \xi)$ defined as line integral of the one form ξdx along this curve:

$$\mathcal{A}(\lambda) := \int_{\Gamma_1(\lambda)} \xi dx.$$

It is a smooth function of λ with $\mathcal{A}'(\lambda) > 0$, and the derivative $\mathcal{A}'(\lambda)$ is the period of the classical trajectory on $\Gamma_1(\lambda)$. The condition (6.1) can be rewritten as

$$\mathcal{A}(\lambda) = (2k + 1)\pi h, \quad k \in \mathbb{Z},$$

and hence, the eigenvalues near λ_0 are a sequence with interval $\sim 2\pi h/\mathcal{A}'(\lambda_0)$.

On the other hand, the spectrum of P_2 near λ_0 consists of continuous spectrum. It is also known by [12] that there is no resonance in an h -independent small complex neighborhood of λ_0 for h sufficiently small. (In the case of only C^∞ potential, the resonance free zone is smaller with imaginary part of order $h|\log h|$, see [24].)

The matrix-valued operator $\mathcal{P}$ is self-adjoint in $L^2(\mathbb{R}; \mathbb{C}^2)$ with domain $H^2(\mathbb{R}; \mathbb{C}^2)$. Its spectrum near λ_0 consists of essential spectrum. In the trivial case where the interaction is absent, i.e., $W(x) \equiv 0$, the spectrum of $\mathcal{P}$ near λ_0 is of course the union of the spectrum of P_1 and P_2 , i.e., the continuous spectrum with embedded eigenvalues. In the general case with non-trivial interaction, it is expected that the eigenvalues shift in the lower complex plane as resonances (Fermi's golden rule).

The resonances of $\mathcal{P}$ in a sufficiently small complex neighborhood of λ_0 are defined as the values $\lambda \in \mathbb{C}$ such that the equation

$$\mathcal{P}\mathbf{u} = \lambda\mathbf{u}$$

has a non-trivial “outgoing” solution $\mathbf{u}$. A solution $\mathbf{u}$ is said to be *outgoing* if the complex dilation $\mathbf{u}(xe^{i\theta})$ with a small enough $0 < \theta < \theta_0$ is in $L^2(\mathbb{R}; \mathbb{C}^2)$. Remark here that $\mathbf{u}(xe^{i\theta})$ is well defined for $0 < \theta < \theta_0$ thanks to the analyticity of the coefficients of the operator $\mathcal{P}$ in the angular domain $\mathcal{S}$. Equivalently, the resonances are the eigenvalues of the non-self-adjoint operator

$$\mathcal{P}_\theta := U_\theta \mathcal{P} U_{-\theta},$$

where U_θ is the dilation operator $U_\theta \mathbf{u}(x) := \mathbf{u}(xe^{i\theta})$. The spectrum of this non-self-adjoint operator $\mathcal{P}_\theta$ consists of the essential spectrum $\bigcup_{j=1,2,\varepsilon=\pm} (V_j^\varepsilon + \bar{\mathbb{R}}_+ e^{-2i\theta})$ and complex eigenvalues, i.e., resonances, possibly appearing in

$$(V_2^- + \bar{\mathbb{R}}_+ e^{-2i(0,\theta]}) \setminus \bigcup_{j=1,2,\varepsilon=\pm} (V_j^\varepsilon + \bar{\mathbb{R}}_+ e^{-2i\theta}).$$

We denote by $\text{Res}(\mathcal{P})$ the set of resonances of $\mathcal{P}$. The rectangular domain $\mathcal{R}_{\lambda_0}(\delta_1, \delta_2)$ does not contain the essential spectrum of $\mathcal{P}_\theta$ for $V_2^- < \lambda_0 < \min(V_2^+, V_1^\pm)$ and for sufficiently small (depending on θ) δ_1 and δ_2 .

The imaginary part of the resonances (resonance width), interpreted as the reciprocal of the lifespan of the semibound state, should be closely related with the interaction between the two classical dynamics of p_1 and p_2 . Intuitively, particles trapped in the periodic trajectory Γ_1 may change the trajectory to Γ_2 thanks to the interaction and escape to the infinity. We naturally expect that the “probability” of this change of trajectory from Γ_1 to Γ_2 should govern the resonance width in the semiclassical limit, and the higher is this probability, the wider is the resonance width.

6.2. Resonance asymptotics in the presence of crossings

In the case where the two potentials have a gap $\inf_{x \in \mathbb{R}} |V_1(x) - V_2(x)| > 0$, the two trajectories $\Gamma_1(\lambda_0)$ and $\Gamma_2(\lambda_0)$ are disjoint. Even in this case, an exponentially small in h interaction exists (called *phase space tunneling*), and it has been shown that the resonance width is exponentially small (e.g., [4, 10, 11, 22, 26]).

We are interested in the case where

$$\Gamma_1(\lambda_0) \cap \Gamma_2(\lambda_0) \neq \emptyset. \quad (6.2)$$

This implies that the two potentials V_1 and V_2 cross at least at one point. We assume for simplicity that the origin $x = 0$ is the unique potential crossing point with crossing value 0

$$V_1(0) = V_2(0) = 0. \quad (6.3)$$

We allow that the crossing be tangential, but assume that the contact is of finite order:

$$V_1^{(k)}(0) - V_2^{(k)}(0) = 0 \quad (0 \leq k \leq n-1), \quad V_1^{(n)}(0) - V_2^{(n)}(0) \neq 0.$$

See Figure 1 for the shape of potentials. Remark again that the crossing of the potentials (6.3) does not imply the intersection (6.2) of $\Gamma_1(\lambda_0)$ and $\Gamma_2(\lambda_0)$. If λ_0 is below the crossing level 0, then $\Gamma_1(\lambda_0)$ and $\Gamma_2(\lambda_0)$ are disjoint. Ashida [1] gave the exponentially small asymptotics of the resonance width in such a case. The condition (6.2) implies that λ_0 is above the crossing level $\lambda_0 > 0$, or at the crossing level $\lambda_0 = 0$. The configurations in the phase space of the characteristic sets $\Gamma_1(\lambda_0)$ and $\Gamma_2(\lambda_0)$ are like Figure 2 (a) when $\lambda_0 > 0$ and like Figure 2 (b) when $\lambda_0 = 0$. Above the crossing level, $\Gamma_1(\lambda_0)$ and $\Gamma_2(\lambda_0)$ intersect at two points $(0, \sqrt{\lambda_0})$ and $(0, -\sqrt{\lambda_0})$ and the contact order m at these points is both n , whereas at the crossing level $\lambda_0 = 0$, $\Gamma_1(0)$ and $\Gamma_2(0)$ intersect at one point $(0, 0)$ and the contact order m at this point is $2n$ (see (4.2), (4.3)).

Let $\text{BS}(P_1)$ be the discrete set of the approximated eigenvalues of P_1 in $[\lambda_0 - \delta_1, \lambda_0 + \delta_1]$ satisfying the Bohr–Sommerfeld quantization rule (6.1):

$$\text{BS}(P_1) = \text{BS}_{\delta_1}(P_1) := \{\lambda \in [\lambda_0 - \delta_1, \lambda_0 + \delta_1]; -e^{i\mathcal{A}(\lambda)/h} = 1\}.$$

In what follows, the scales δ_1, δ_2 are

$$\delta_1 = \begin{cases} \delta, & \text{when } \lambda_0 > 0, \\ Lh^{\frac{2}{2n+1}}, & \text{when } \lambda_0 = 0, \end{cases} \quad \delta_2 = Lh$$

for a small enough h -independent $\delta > 0$ and an arbitrary large fixed constant L .

Suppose that the interaction does not vanish at $x = 0$: $W(0) \neq 0$. Then, we have the following theorem (see [21] for the case of vanishing interaction $W(0) = 0$).

Theorem 6.1. *There exists a bijective map*

$$z_h : \text{BS}(P_1) \rightarrow \text{Res}(\mathcal{P}) \cap \mathcal{R}$$

for sufficiently small h such that

$$|z_h(\lambda) - \lambda| = \mathcal{O}(h^{\frac{m+3}{m+1}}).$$

Moreover, the imaginary part of $z_h(\lambda)$ has the following asymptotic formula as $h \rightarrow 0^+$ for any $E \in \mathfrak{B}_h$:

$$\operatorname{Im} z_h(\lambda) = -\mathcal{D}(\lambda)h^{\frac{m+3}{m+1}} + \mathcal{O}(h^{\frac{m+3}{m+1}+\varepsilon}),$$

for some $\varepsilon > 0$, where the coefficient $\mathcal{D}(\lambda)$ is given in terms of ω in Theorem 4.1 and κ in Theorem 4.2 by

$$\begin{aligned} \mathcal{D}(\lambda) &= \frac{2|\omega|^2}{\mathcal{A}'(\lambda)} \sin^2\left(\frac{\mathcal{S}(\lambda)}{2h} + \arg \omega\right) & \text{when } \lambda_0 > 0, \\ \mathcal{D}(\lambda) &= \frac{\kappa^2}{\mathcal{A}'(\lambda)} & \text{when } \lambda_0 = 0. \end{aligned}$$

Here, the function $\mathcal{S}(\lambda)$ is the volume of the domain bounded by the classical trajectory $\gamma_{2\downarrow}$ from ρ_+ to ρ_- along $\Gamma_2(\lambda)$ and the classical trajectory $\gamma_{1\uparrow}$ from ρ_- to ρ_+ along $\Gamma_1(\lambda)$:

$$\mathcal{S}(\lambda) = \int_{\gamma_{2\downarrow} \cup \gamma_{1\uparrow}} \xi dx. \quad (6.4)$$

7. From microlocal scattering matrix to resonances

In this section, we prove Theorem 6.1 using the formulas in Theorem 4.1 of the microlocal scattering matrix at a crossing point that we studied in Section 4. The main strategy is the same for the two cases $\lambda_0 > 0$ and $\lambda_0 = 0$, and we sketch the proof only in the case $\lambda_0 > 0$.

Let $\lambda \in (\lambda_0 - \delta_1, \lambda_0 + \delta_1)$ be a real energy sufficiently close to λ_0 . Under the assumptions on the potentials V_1 and V_2 , the characteristic sets $\Gamma_1(\lambda)$ and $\Gamma_2(\lambda)$ intersect at two points $\rho_{\pm} = (0, \pm\sqrt{\lambda})$. The set $\Gamma(\lambda) \setminus (\Gamma_c(\lambda) \cup \Gamma_t(\lambda))$ consists of 8 connected components: 2 unbounded components $\gamma_{2,b}^+, \gamma_{2,\#}^- \in \Gamma_2(\lambda)$ and 6 bounded components $\gamma_{1,b}^{\pm}$, $\gamma_{1,\#}^{\pm} \subset \Gamma_1^{\pm}(\lambda)$ and $\gamma_{2,\#}^+ \subset \Gamma_2^+(\lambda)$, $\gamma_{2,b}^- \subset \Gamma_2^-(\lambda)$. Along $\gamma_{2,b}^+$, the classical trajectory of p_2 goes to infinity as time goes to $-\infty$ and along $\gamma_{2,\#}^-$, the classical trajectory of p_2 goes to infinity as time goes to $+\infty$. The trajectories $\gamma_{1,b}^-, \gamma_{2,b}^-$ end at ρ_- , and $\gamma_{1,b}^+$ end at ρ_+ , while $\gamma_{1,\#}^+, \gamma_{2,\#}^+$ start from ρ_+ and $\gamma_{1,\#}^-$ start from ρ_- .

Suppose that $\mathbf{w} = {}^t(w_1, w_2)$ satisfies $\mathcal{P}\mathbf{w} = \lambda\mathbf{w}$. Let us compute the microlocal asymptotics on the above 8 trajectories using the connection formulas in Section 4, starting from the following two initial data:

$$\mathbf{w} \equiv 0 \quad \text{on } \gamma_{2,b}^+, \quad (7.1)$$

$$\mathbf{w} \equiv \mathbf{f}_{\gamma_{1,b}^+, \rho_+} \quad \text{on } \gamma_{1,b}^+, \quad (7.2)$$

where $\mathbf{f}_{\gamma_{1,b}^+, \rho_+}$ is the microlocal WKB solution defined on $\gamma_{1,b}^+$ with the base point ρ_+ for the phase function (see Section 3). The initial condition (7.1) is concerned with the fact that the resonant state is microlocally infinitely small in the incoming trajectory from infinity. The condition (7.2) is just a normalization of $\mathbf{w}$; i.e., the coefficient $\alpha_{\gamma_{1,b}^+, \rho_+}$ defined in Proposition 3.1 is equal to 1. The two microlocal data (7.1) and (7.2) will determine the microlocal information of $\mathbf{w}$ everywhere in the phase space.

By (7.1) and (7.2), the two microlocal data on the incoming trajectories are given near ρ_+ , and hence, the microlocal scattering matrix $T_+ = (t_{jk}^+)$ at ρ_+ gives the two microlocal data on the outgoing trajectories $\gamma_{1,\#}^+$ and $\gamma_{2,\#}^+$:

$$\begin{aligned}\mathbf{w} &\equiv t_{11}^+ \mathbf{f}_{\gamma_{1,\#}^+, \rho_+} && \text{on } \gamma_{1,\#}^+, \\ \mathbf{w} &\equiv t_{21}^+ \mathbf{f}_{\gamma_{2,\#}^+, \rho_+} && \text{on } \gamma_{2,\#}^+, \end{aligned}$$

where $\mathbf{f}_{\gamma_{j,\#}^+, \rho_+}$, $j = 1, 2$, are the microlocal WKB solutions with phase base point at ρ_+ .

Now, we continue $\mathbf{f}_{\gamma_{1,\#}^+, \rho_+}$ from $\gamma_{1,\#}^+$ to $\gamma_{1,b}^-$ beyond the turning point $(b_0, 0)$, and $\mathbf{f}_{\gamma_{2,\#}^+, \rho_+}$ from $\gamma_{2,\#}^+$ to $\gamma_{2,b}^-$ beyond the turning point $(c_0, 0)$. Let $\mathbf{f}_{\gamma_{1,b}^-, \rho_-}$ and $\mathbf{f}_{\gamma_{2,b}^-, \rho_-}$ be the microlocal WKB solutions defined, respectively, on $\gamma_{1,b}^-$ and $\gamma_{2,b}^-$ with phase base point at ρ_- . Then, Proposition 4.1 tells us that, modulo $\mathcal{O}(h)$,

$$\begin{aligned}\mathbf{w} &\equiv -it_{11}^+ \exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx\right) \mathbf{f}_{\gamma_{1,b}^-, \rho_-} && \text{on } \gamma_{1,b}^-, \\ \mathbf{w} &\equiv -it_{21}^+ \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx\right) \mathbf{f}_{\gamma_{2,b}^-, \rho_-} && \text{on } \gamma_{2,b}^-, \end{aligned}$$

where

$$\gamma_{1\downarrow} := \gamma_{1,\#}^+ \cup \gamma_{1,b}^-, \quad \gamma_{2\downarrow} := \gamma_{2,\#}^+ \cup \gamma_{2,b}^-.$$

Here, the exponential terms come from the change of base points of the microlocal WKB solutions from ρ_+ to ρ_- .

Finally, we go through the crossing point ρ_- using the microlocal scattering matrix $T_- = (t_{jk}^-)$ at ρ_- . We then obtain

$$\mathbf{w} \equiv -i \left(t_{11}^+ t_{11}^- \exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx\right) + t_{21}^+ t_{12}^- \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx\right) \right) \mathbf{f}_{\gamma_{1,\#}^-, \rho_-} \quad \text{on } \gamma_{1,\#}^-, \quad (7.3)$$

$$\mathbf{w} \equiv -i \left(t_{11}^+ t_{21}^- \exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx\right) + t_{21}^+ t_{22}^- \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx\right) \right) \mathbf{f}_{\gamma_{2,\#}^-, \rho_-} \quad \text{on } \gamma_{2,\#}^-. \quad (7.4)$$

Further continuing (7.3) from $\gamma_{1,\#}^-$ to $\gamma_{1,b}^+$ passing through the turning point $(a_0, 0)$ using Proposition 4.1, we have

$$\mathbf{w} \equiv - \left(t_{11}^+ t_{11}^- \exp\left(\frac{i}{h} \mathcal{A}(\lambda)\right) + t_{21}^+ t_{12}^- \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow} \cup \gamma_{1\uparrow}} \xi dx\right) \right) \mathbf{f}_{\gamma_{1,b}^+, \rho_+} \quad \text{on } \gamma_{1,b}^+, \quad (7.5)$$

where $\gamma_{1\uparrow} := \gamma_{1,\#}^- \cup \gamma_{1,b}^+$.

This microlocal expression of $\mathbf{w}$ on $\gamma_{1,b}^+$ should coincide with (7.2). Recall now that

$$t_{11}^\pm = 1, \quad t_{22}^\pm = 1 \quad \text{mod } \mathcal{O}(h^{\frac{1}{m+1}}), \quad (7.6)$$

$$t_{21}^+ = -i\omega h^{\frac{1}{m+1}}, \quad t_{12}^+ = -i\bar{\omega} h^{\frac{1}{m+1}}, \quad t_{21}^- = -i\bar{\omega} h^{\frac{1}{m+1}}, \quad t_{12}^- = -i\omega h^{\frac{1}{m+1}} \quad \text{mod } \mathcal{O}(h^{\frac{1+\varepsilon}{m+1}}),$$

for some $\varepsilon > 0$. Then, the coefficient of $\mathbf{f}_{\gamma_{1,b}^+, \rho_+}$ on the RHS of (7.5) is $-\exp(\frac{i}{h}\mathcal{A}(\lambda)) + \mathcal{O}(h^{\frac{2}{m+1}})$. The compatibility condition between (7.2) and (7.5) reads

$$1 + \exp\left(\frac{i}{h}\mathcal{A}(\lambda)\right) = \mathcal{O}(h^{\frac{1}{m+1}}). \quad (7.7)$$

This is nothing but the Bohr–Sommerfeld quantization rule modulo $\mathcal{O}(h^{\frac{1}{m+1}})$ for the operator P_1 . The existence of the bijection z_h from $\text{BS}(P_1)$ to the set of resonances $\text{Res}(\mathcal{P})$ in the complex neighborhood $\mathcal{R}$ is justified by a contradiction argument used in [5], which guarantees the non-existence of resonances away from $\text{BS}(P_1)$, and by the Kato–Rellich theorem, which shows the one-to-one correspondence.

On the other hand, let $\alpha_{2,\#}^-$ be the constant such that

$$\mathbf{w} \equiv \alpha_{2,\#}^- \mathbf{f}_{\gamma_{2,\#}^-, \rho_-} \quad \text{on } \gamma_{2,\#}^-, \quad (7.8)$$

where $\mathbf{f}_{\gamma_{2,\#}^-, \rho_-}$ is the microlocal WKB solution defined on $\gamma_{2,\#}^-$ with the phase base point at the crossing point $\rho_- = (0, -\sqrt{\lambda})$. Then, (7.4) compared with (7.8) implies

$$\alpha_{2,\#}^- = -it_{11}^+ t_{21}^- \exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx\right) - it_{21}^+ t_{22}^- \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx\right).$$

Using again (7.6), we obtain, modulo $\mathcal{O}(h^{\frac{1+\varepsilon}{m+1}})$,

$$\begin{aligned} \alpha_{2,\#}^- &= -\left(\bar{\omega} \exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx\right) + \omega \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx\right)\right) h^{\frac{1}{m+1}} \\ &= -|\omega| \left(\exp\left(\frac{i}{h} \int_{\gamma_{1\downarrow}} \xi dx - \arg \omega\right) + \exp\left(\frac{i}{h} \int_{\gamma_{2\downarrow}} \xi dx + \arg \omega\right) \right) h^{\frac{1}{m+1}}. \end{aligned}$$

Recall the definition of $\mathcal{S}(\lambda)$ (see (6.4)). Then, we have

$$\int_{\gamma_{1\downarrow}} \xi dx - \int_{\gamma_{2\downarrow}} \xi dx = \mathcal{A}(\lambda) - \mathcal{S}(\lambda).$$

Thus, we obtain

$$|\alpha_{2,\#}^-| = 2|\omega| \left| \cos\left(\frac{\mathcal{A}(\lambda) - \mathcal{S}(\lambda)}{2h} - \arg \omega\right) \right| h^{\frac{1}{m+1}}. \quad (7.9)$$

The fact that λ satisfies the Bohr–Sommerfeld quantization rule (7.7) implies $\cos \frac{\mathcal{A}(\lambda)}{2h} = 0$, $|\sin \frac{\mathcal{A}(\lambda)}{2h}| = 1$ modulo $\mathcal{O}(h^{\frac{2}{m+1}})$, and hence,

$$\left| \cos\left(\frac{\mathcal{A}(\lambda) - \mathcal{S}(\lambda)}{2h} - \arg \omega\right) \right| = \left| \sin\left(\frac{\mathcal{S}(\lambda)}{2h} + \arg \omega\right) \right|. \quad (7.10)$$

Then, Theorem 6.1 in the case $\lambda_0 > 0$ follows from (7.7), (7.9), (7.10) and the following proposition which express the imaginary part of the resonances in terms of the microlocal data $|\alpha_{2,\#}^-|$ on the outgoing tail $\gamma_{2,\#}^-$ (see [12] for the scalar but more general operator case).

Proposition 7.1. *Suppose that z is a resonance in $\mathcal{R}_{\lambda_0}$ and $\mathbf{w} = {}^t(w_1, w_2)$ a corresponding resonant state normalized by (7.2): $\mathcal{P}\mathbf{w} = z\mathbf{w}$. Let $\alpha_{2,\#}^- = \alpha_{2,\#}^-(z, h)$ be the constant determined by (7.8) for the resonant state $\mathbf{w}$. Then, the resonance width $\text{Im } z$ is asymptotically given by*

$$\text{Im } z = -\frac{h|\alpha_{2,\#}^-|^2}{2\mathcal{A}'(\lambda)} + \mathcal{O}(h^{\frac{4}{3}} + h^{\frac{m+2}{m+1}}). \quad (7.11)$$

Proof. The resonant state $\mathbf{w}$ is outgoing. In our setting, it implies that $\mathbf{w}$ is exponentially decaying as $x \rightarrow \infty$ because large x is in the classically forbidden region for both p_1 and p_2 . This means that $\mathbf{w} \in L^2([\hat{x}, +\infty))$ for any $\hat{x} \in \mathbb{R}$. On the other hand, negative large x is in the classically forbidden region for p_1 but in the classically allowed region for p_2 . We take $\hat{x}$ on the left of the leftmost turning point of p_1 for any $\lambda \in \mathcal{R}_{\lambda_0}$, which implies in particular $V_2(\hat{x}) < \lambda < V_1(\hat{x})$. Then, the vertical line $\{(x, \xi); x = \hat{x}\}$ in the phase space intersects with $\Gamma_2(\lambda)$ at two points $(\hat{x}, \pm\hat{\xi})$ with $\hat{\xi} = \sqrt{\lambda - V_2(\hat{x})} > 0$, and has no intersection with $\Gamma_1(\lambda)$. The point $(\hat{x}, \hat{\xi})$ is on $\gamma_{2,b}^+$, and $(\hat{x}, -\hat{\xi})$ is on $\gamma_{2,\#}^-$.

We compute the scalar product in $L^2([\hat{x}, +\infty))$ of $\mathbf{w}$ with $(\mathcal{P} - z)\mathbf{w} = 0$ to have

$$\begin{aligned} 0 &= \langle (\mathcal{P} - z)\mathbf{w}, \mathbf{w} \rangle_{L^2([\hat{x}, +\infty))} \\ &= \|hD_x \mathbf{w}\|_{L^2([\hat{x}, +\infty))}^2 - z\|\mathbf{w}\|_{L^2([\hat{x}, +\infty))}^2 - h^2 \langle \mathbf{w}'(\hat{x}), \mathbf{w}(\hat{x}) \rangle. \end{aligned}$$

Taking the imaginary part of this identity, we obtain an expression of the resonance width in terms of the values of the normalized resonant state $\mathbf{w}$ and its derivative at the point $\hat{x}$:

$$\text{Im } z \cdot \|\mathbf{w}\|_{L^2([\hat{x}, +\infty))}^2 = -h^2(w_1'(\hat{x})\overline{w_1(\hat{x})} + w_2'(\hat{x})\overline{w_2(\hat{x})}). \quad (7.12)$$

First, it turns out from (7.1), (7.2) and the fact that the microlocal scattering matrices are diagonal modulo $\mathcal{O}(h^{\frac{1}{m+1}})$ that, at the principal level, it is microlocalized only on $\Gamma_1(\lambda_0)$. It follows (see [2, 9]) that

$$\|\mathbf{w}\|_{L^2([\hat{x}, +\infty))}^2 = 2\mathcal{A}'(\lambda) + \mathcal{O}(h^{\frac{1}{3}} + h^{\frac{1}{m+1}}). \quad (7.13)$$

The error $h^{\frac{1}{3}}$ comes from the turning point and $h^{\frac{1}{m+1}}$ from the crossing point.

Second, we deduce from (7.1) and (7.8) the following asymptotics at $x = \hat{x}$:

$$\begin{aligned} w_1(\hat{x}) &= \mathcal{O}(h), \quad w_2(\hat{x}) = \frac{\alpha_{2,\#}^-}{(\lambda - V_2(x))^{\frac{1}{4}}} \exp\left(-\frac{i}{h} \int_0^x \sqrt{\lambda - V_2(t)} dy\right) (1 + \mathcal{O}(h)), \\ w_1'(\hat{x}) &= \mathcal{O}(1), \quad \overline{w_2'}(\hat{x}) = \frac{i}{h} \overline{\alpha_{2,\#}^-} (\lambda - V_2(x))^{\frac{1}{4}} \exp\left(\frac{i}{h} \int_0^x \sqrt{\lambda - V_2(t)} dy\right) (1 + \mathcal{O}(h)). \end{aligned}$$

The formula (7.11) is obtained from (7.12), (7.13) and these asymptotics. ■

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