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Resonances created by a conical intersection

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1 Introduction

We consider the semiclassical Schrödinger operator

$$P = -h^2\Delta_x + V(x), \tag{1}$$

where h is a small parameter, and consider the equation

$$Pu = zu, \tag{2}$$

where z is a spectral parameter. In this report, we restrict ourselves to a model of two-dimensional and two-level Schrödinger operator whose potential is given by

$$V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix} \quad x = (x_1, x_2), \tag{3}$$

and study the semicalssical distribution of the resonances of P (see [2] for more details).

A typical potential which generates resonances is a *well in an island*. This potential has a well in a compact set but decays to 0 at infinity. Then the operator P has no positive eigenvalues, but instead, it has resonances close to the eigenvalues of the corresponding simple well operator, i.e. the operator with $V(x)$ modified suitably out of the compact set. In particular the resonances at the non-degenerate minimum of the potential well are exponentially close to the real axis with respect to h ([6]) and called *shape resonances* .

Another typical potential is a matrix valued potential. Suppose $V(x)$ is a 2×2 matrix and let $v_1(x)$, $v_2(x)$ be its eigenvalues (which we often call eigenpotentials) with $v_1(x) \leq v_2(x)$. Suppose $v_2(x)$ has a well so that the scalar operator $P_2 = -h^2\Delta + v_2(x)$ has eigenvalues, while $v_1(x)$ decays, say to $-\infty$ at infinity. Then P has no eigenvalues but resonances. In case where $v_1(x) < v_2(x)$ for all x, these resonances are exponentially close to the real axis with respect to h ([7], [8], [1]).

Our potential (3) has eigen-potentials $v_1(x) = -|x|$ and $v_2(x) = |x|$, *intersecting conically* at the origin $x = 0$. The spectrum of the single Schrödinger operator $P_2 = -h^2\Delta_x + |x|$ consists of countably many eigenvalues (of finite multiplicity) tending to $+\infty$, while the spectrum of P, however, does not have any eigenvalue.

In this report, we fix a positive interval on the real axis of the complex z-plane and look for resonances of P near this interval.

Let us consider the motion of the classical particle whose Hamiltonian is $p_2(x,\xi) = |\xi|^2 + |x|$. It is realized by a small ball on a table (x-plane) connected by a string to another ball on the other extremity which is pendent through a small hall ($x = 0$) of the table. If the ball has a small but positive angular momentum, then it moves along an ellipse-like periodic orbit, while the other ball moves up and down. The smaller the angular momentum is, the closer to the hall the ball passes.

The quantum ball, however, falls down through the hall with some positive probability by a quantum effect. The imaginary part of resonances represents the inverse of the life span for the quantum ball to be on the table.

This situation is similar to the one-dimensional well in an island but at the top of the lower barrier top, in the sense that a trapped classical trajectory is connected to a non-trapped one through a stationary point. At the top of the lower barrier top, the corresponding classical mechanics defined by the classical Hamiltonian $p(x,\xi) = |\xi|^2 + V(x)$ has a homoclinic trajectory ([3]). Also in our case, we will see in the next section that the reduced Hamiltonian $p_l(r,\rho,h)$ (5) for each angular momentum has a homoclinic orbit. The resonances are created by this homoclinic orbit and, in particular, thier imaginary part, which we expect to be no longer exponentially small, is governed by the behavior of solutions near the stationary point.

2 Results

Making use of the particularity of the operator P, (2) can be reduced to a sequence of one-dimensional first order systems. Let

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

be the semiclassical Fourier transform of u, and using the polar coordinate $(\xi_1,\xi_2) = r(\cos\phi,\sin\phi)$, we develop $\hat{u}$ to the Fourier series with respect to ϕ:

$$\hat{u}(\xi) = r^{-1/2}\begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}\sum_{l\in\mathbb{Z}} e^{-i(l+1/2)\phi}w_l(r).$$

Then (2) is reduced to

$$P_l(r,hD_r,h)w_l = z\ w_l \quad (l \in \mathbb{N}), \tag{4}$$

where the symbol p_l of the operator P_l is

$$p_l(r,\rho,h) = \begin{pmatrix} r^2-\rho & h(l-\frac{1}{2})/r \\ h(l-\frac{1}{2})/r & r^2+\rho \end{pmatrix}. \tag{5}$$

(4) is also written in the form

$$\frac{h}{i}\frac{d}{dr}u = A(r,h)u, \quad A(r,h) = \begin{pmatrix} r^2-z & h(l-\frac{1}{2})/r \\ -h(l-\frac{1}{2})/r & z-r^2 \end{pmatrix}. \tag{6}$$

In this system, the origin $r = 0$ is a regular singular point of indices $\pm(l - \frac{1}{2})$, and $r = \infty$ is a irregular singular point.

Let u_0^l, $f_\pm^l$ be the solutions to (4) defined by the following asymptotic conditions respectively:

$$u_0^l(r,h) \sim r^{l-1/2} \begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad (r \to 0),$$

$$f_+^l(r,h) \sim e^{i(r^3-3zr)/3h} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad f_-^l(r,h) \sim e^{-i(r^3-3zr)/3h} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (r \to +\infty).$$

u_0^l can be expressed as linear combination of f_+^l and f_-^l:

$$u_0^l = c_+^l(z,h) f_+^l + c_-^l(z,h) f_-^l.$$

Then the resonances of P are characterized as follows:

Proposition 2.1 *$z \in \mathbb{C}$ is a resonance if and only if there exists $l \in \mathbb{N}$ such that $c_+^l(z,h) = 0$.*

Let us fix a positive interval $I = [a,b], a > 0$. For $z \in I$ and sufficiently small h, the Hamilton vector field H_{p_l} on the energy surface $\{(r,\rho); \det(p_l(r,\rho) - z) = 0\}$ has a periodic orbit $\gamma^l(z,h)$. Indeed, the Hamilton flow $\exp tH_{p_l}$ coincides, as a set , with the energy surface itself, and it is given by

$$\left\{ (r,\rho); \rho = \pm\sqrt{(r^2 - z)^2 - \frac{h^2(l-\frac{1}{2})^2}{r^2}} \right\}.$$

Hence the periodic orbit exists inside the domain bounded by $\rho = r^2 - z$, $\rho = -r^2 + z$ and the ρ-axis, and it converges to the boundary in the limit $h \to 0$.

This orbit generates the resonances. Let $S^l(z,h) = \int_\gamma \rho dr$ be the action integral for this orbit. By Stokes theorem, it is given by

$$S^l(z,h) = 2\int_{r_0}^{r_1} \sqrt{r^2(r^2-z)^2 - h^2(l-\frac{1}{2})^2} \frac{dr}{r},$$

where r_0 and r_1 $(0 < r_0 < r_1)$ are the first two zeros of the function in the square root, i.e. the intersections of the orbit with the r-axis. $S^l(z,h)$ has the following asymptotic property:

Lemma 2.2 *One has*

$$S^l(z,h) = \frac{4}{3}z^{3/2} + \pi(l - \frac{1}{2})h + O(h^2|\log h|) \tag{7}$$

as $h \to 0$ uniformly with respect to $z \in I$.

The following theorem is a Bohr-Sommerfeld type quantization condition of resonances:

Theorem 2.3 *Given $z_0 \in I$ and $l \in \mathbb{N}$, there exist $\epsilon > 0$, $h_0 > 0$ and a function $\delta(z,h)$ defined in $\{(z,h) \in \mathbb{C} \times \mathbb{R}_+; |z - z_0| < \epsilon, 0 < h < h_0\}$ and tending to 0 as $h \to 0$, such that the following equivalence holds for sufficiently small h:*

$$c_+^l(z,h) = 0 \quad \Leftrightarrow \quad e^{-i\pi/4}\sqrt{\frac{\pi h}{2}}\,(l+\frac{1}{2})z^{-3/4}e^{iS^l(z,h)/h} + 1 = \delta(z,h). \tag{8}$$

The right hand side of (8) can be written, roughly speaking, in the form of the generalized Bohr-Sommerfeld quantization condition

$$c(z,h)e^{iS(z)/h} = 1, \quad c(z,h) \sim c_0(z)e^{i\pi\theta}h^{\alpha},$$

where $S(z)$, $c_0(z)$ are real-valued functions and θ, α are real numbers. Let us look for roots of this equation near a real point $z = z_0$. Supposing that $S(z)$ is analytic near $z = z_0$, we replace $S(z)$ by $S_0 + S_1(z - z_0)$. Then by an easy calculation, we see that the roots z satisfy

$$z - z_0 \sim \frac{-S_0 + (2k - \theta)\pi h}{S_1} - i\frac{\alpha}{S_1}h\log\frac{1}{h}$$

for some integer k. The set of roots make a complex sequence pararell to the real axis, and the interval of the succesive roots is $2\pi h/S_1$ and the imaginary part is $-\frac{\alpha}{S_1}h\log\frac{1}{h}$. θ is called *Maslov index*. In the usual Bohr-Sommerfeld condition for a simple perodic trajectory, S_0 is the action, S_1 is the period and $c(z,h) = -1$, i.e. $\theta = 1$ and $\alpha = 0$.

In our case, we see from Lemma 2.2 and Theorem 2.3 that $S(z) = \frac{4}{3}z^{3/2}$, $\theta = l + \frac{1}{4}$ and $\alpha = \frac{1}{2}$. More precisely, we obtain the following corollary about the semiclassical distribution of resonances. Here, we take $\lambda = z^{3/2}$ as spectral parameter and, putting $\tilde{I} = I^{3/2}$, look for resonances in $\{\lambda \in \mathbb{C}_-; \operatorname{Re}\lambda \in \tilde{I},\ \operatorname{Im}\lambda = o(1) \text{ as } h \to 0\}$. For each $k, l \in \mathbb{N}$, we put $\lambda_{kl} = \frac{3\pi}{8}(8k - 4l - 1)$ and

$$\Gamma_l(h) = \{\lambda_{kl}h - \frac{3}{8}i(h\log\frac{1}{h} - h\log\frac{\pi(l+\frac{1}{2})^2}{\lambda_{kl}h}); k \in \mathbb{Z} \text{ s.t. } \lambda_{kl}h \in \tilde{I}\}.$$

Corollary 2.4 *For any $N \in \mathbb{N}$, there exists $h_0(N) > 0$ such that for any $h \in (0, h_0(N))$ and $\lambda \in \bigcup_{l \le N}\Gamma_l(h)$ there is a resonance z of the operator P with $\lambda - z^{3/2} = o(h)$ uniformly for all $\lambda \in \bigcup_{l \le N}\Gamma_l(h)$*

Notice that $\lambda_{kl}h \in \tilde{I}$, and hence the second term of the imaginary part of $\lambda \in \Gamma_l(h)$ is of $O(h)$ and smaller than the first term. Thus, $\Gamma_l(h)$ is an almost horizontal sequence of complex points in the λ-plane, and $\bigcup_{l\leq N}\Gamma_l(h)$ is a lattice which consists of N horizontal sequences. Theorem 2.4 means that for a fixed positive interval I, we can find as many horizontal sequences of resonances as we want for sufficiently small h, whose imaginary part increases as the angular momentum number does.

3 Methods

The resonances are created by the periodic orbit $\gamma^l(z,h)$ and roughly speaking, the quantization condition (8) is the condition that any WKB solution *microlocally defined* on a point on γ^l coincides with the one obtained after a continuation along this orbit.

In this section, we briefly review two technical elements.

One is the exact WKB method for 2×2 systems, which is a natural extension of the method of Gérard and Grigis [4] applied to single Schrödinger operators.

The other is the microlocal reduction to a normal form of our operator at the point $(r,\rho)=(\sqrt{z},0)$, which is a hyperbolic stationary point of $\det p_l$ in the limit $h\to 0$.

In the following subsections, we will use the notation (x,ξ) instead of (r,ρ).

3.1 Exact WKB solution

Here, the WKB solution is the solution of (6), which is of the form

$$u(x,h)=e^{i\phi(x,h)/h}Q(x)w(x,h), \tag{9}$$

$$w(x,h)\sim\begin{pmatrix}1\\0\end{pmatrix}\quad (h\to 0),$$

where the phase function $\phi(x,h)$ is a primitive of an eigenvalue of A, and the principal symbol $Q(x,h)$ is a matrix which diagonalize A. In our case, $\mathrm{tr}A=0$ and hence

$$\phi(x)=\pm\int^x\sqrt{\det A(t)}\,dt. \tag{10}$$

Let us take, say, the plus one here. Moreover, we can choose Q such that $Q^{-1}MQ$ is off-diagonal (this choice is unique up to multiplication by a diagonal constant matrix):

$$Q^{-1}AQ=\begin{pmatrix}\sqrt{\det A} & 0\\ 0 & -\sqrt{\det A}\end{pmatrix}, \tag{11}$$

$$Q^{-1}Q'=-\begin{pmatrix}0 & c_+(x)\\ c_-(x) & 0\end{pmatrix}. \tag{12}$$

Then the function w in (9) satisfies

$$\frac{dw}{dx} + \begin{pmatrix} 0 & 0 \\ 0 & 2i\phi'/h \end{pmatrix} w = \begin{pmatrix} 0 & c^- \\ c^+ & 0 \end{pmatrix} w. \tag{13}$$

We can construct a solution of this system in the form

$$w(x,h) = \sum_{n=0}^{\infty} \begin{pmatrix} w_{2n} \\ w_{2n-1} \end{pmatrix}, \tag{14}$$

by determining inductively the functions $w_n(z,h)$ by

$$w_{-1} \equiv 0, \quad w_0 \equiv 1, \tag{15}$$

and for $n \geq 1$,

$$\left\{ \begin{array}{rcl} \frac{d}{dx} w_{2n} & = & c^- \, w_{2n-1}, \\ \left(\frac{d}{dx} + \frac{2i\phi'}{h}\right) w_{2n-1} & = & c^+ \, w_{2n-2}, \end{array} \right. \tag{16}$$

Let x_0 be a point where A is holomorphic and regular (i.e. $\det A \neq 0$). Then c_+ and c_- are holomorphic at x_0 and the differential equations (16) with initial conditions at $x = x_0$

$$w_n|_{x=x_0} = 0 \quad (n \geq 1) \tag{17}$$

uniquely determine the sequence of holomorphic functions $\{w_n(x,h;x_0)\}_{n=-1}^{\infty}$ and the sum (14) converges in a neighborhood of x_0.

A WKB solution (9) is said to be *defined microlocally* on the Lagrangian manifold $\Lambda = \{(x,\xi); \xi = \phi'(x)\}$. In our case, γ^l consists of two Lagrangian manifolds and two points

$$\gamma^l = \Lambda_+ \cup \Lambda_- \cup \{(r_0,0)\} \cup \{(r_1,0)\},$$

where $\Lambda_\pm = \{(x,\xi); \xi = \pm\sqrt{\det A}\}$. $\{(r_0,0)\}$ and $\{(r_1,0)\}$ are the point which tends as $h \to 0$ to the singularity $(0,0)$ and the stationary point $(\sqrt{z},0)$ of p_l respectively.

The main problem reduces to the connection between the WKB solutions defined microlocally on Λ_+ and that defined of Λ_- at the points $(r_0,0)$ and $(r_1,0)$. In the next section, we focus to the study at $(r_1,0)$, which indeed governs the imaginary part of resonances (see Introduction).

3.2 Normal form

In this section, we reduce the operator P near $(r_1,0)$ to a simpler one. More precisely, we transform the equation (6) to a simple microlocal normal form

$$Qw = 0, \quad Q = \begin{pmatrix} y & \frac{\gamma}{\sqrt{2}} \\ -\frac{\gamma}{\sqrt{2}} & -hD_y \end{pmatrix},$$

microlocally near the point $(x, \xi) = (\sqrt{z}, 0)$, where $\gamma = \gamma(z, h)$ is a constant satisfying

$$\gamma(z, h) = \frac{l - 1/2}{\sqrt{2}} z^{-3/4} h + O(h^2). \tag{18}$$

This reduction is carried out in three steps.

First, by the change of variable $y = \phi(x)$ with

$$\phi(x) = (x - \sqrt{z}) \left(\tfrac{2}{3}(x - \sqrt{z}) + 2\sqrt{z}\right)^{1/2},$$

(6) becomes

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

where $v(y) = v(\phi(x)) = u(x)$ and

$$\psi(y) = \psi(\phi(x)) = (l - \frac{1}{2}) \frac{(\frac{2}{3}(x - \sqrt{z}) + 2\sqrt{z})^{1/2}}{x(x + \sqrt{z})}. \tag{19}$$

The second step makes the off-diagonal entries constant modulo $O(h^\infty)$. We can construct a matrix-valued C^∞-symbol satisfying $M(y, h) = \mathrm{Id} + O(h)$ such that

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

satisfies

$$\begin{pmatrix} hD_y - y & -\gamma \\ \overline{\gamma} & hD_y + y \end{pmatrix} \widetilde{w}(y, h) = r(y, h) \widetilde{w}(y, h) \tag{20}$$

where γ satisfies (18) and $r(y, h) = O(h^\infty)$ uniformly in an interval around $y = 0$ together with all its derivatives.

The last step is to rotate the operator by the angle $\pi/4$ in the phase space by the integral operator

$$Rg(y) = c \int_{\mathbb{R}} e^{-\frac{i}{2h}(y^2 - 2\sqrt{2}xy + x^2)} g(x) dx,$$

where $c = e^{i\pi/8} (\sqrt{2}\pi h)^{-1/2}$ is a normalizing constant. This operator satisfies the relations

$$R(hD_y - y) = -\sqrt{2} y R, \qquad R(hD_y + y) = \sqrt{2}\, hD_y R. \tag{21}$$

Multiplying a cut off function χ and then operating R from the left to equation (20), we obtain from (21)

$$Qw(y, h) = -\frac{1}{\sqrt{2}} R \left(\chi(y) r(y, h) \widetilde{w}(y, h) - ih\chi'(y) \widetilde{w}(y, h)\right).$$

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

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