Resonance free regions for systems of semiclassical Schrödinger operators and applications

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Abstract

We consider an $N \times N$ system of semiclassical differential operators with N Schrödinger operators in the diagonal part and small interactions of order h^ν, where h is a semiclassical parameter and ν is a constant larger than one. We study the absence of resonance near a non-trapping energy for each Schrödinger operators. The width of resonances is estimated from below by $Mh\log(1/h)$ and the coefficient M can be taken propotional to $\nu - 1$.

1 Introduction

We are interested in the resonance free domain for the semiclassical $N \times N$ matrix Schrödinger operator

$$\mathcal{P}(h) = \mathcal{P}_0(h) + h^\nu W, \quad \mathcal{P}_0(h) = \operatorname{diag}(P_1(h), P_2(h), \dots, P_N(h)) \tag{1.1}$$

where

$$P_j(h) = -h^2 \triangle + V_j(x),\ x \in \mathbb{R}^n,\ (h \searrow 0),$$

is the semiclassical Schrödinger operator, and $\nu \geq 1$. Here $W = W(x, hD_x)$ is a symmetric $N \times N$-matrix valued first-order semiclassical differential operator. Such an operator appears in the Born-Oppenheimer approximation of molecules, after reduction to an effective Hamiltonian (see e.g. [KMSW]). For each semiclassical Schrödinger operator $P_j(h)$ $(j = 1, 2, \dots, N)$ with C^∞ potential $V_j(x)$, it is well known that there are no resonances with imaginary part of order $h\log(1/h)$ around an energy level E_0 satisfying the non-trapping condition (see [Ma1, SjZw]). We recall that an energy E_0 is said to be non-trapping if for all compact $K \subset p_j^{-1}(E_0)$ there exists $T_K > 0$ such that

$$(x, \xi) \in K \Longrightarrow \exp(tH_{p_j})(x, \xi) \notin K,\ |t| > T_K, \tag{1.2}$$

where $p_j(x,\xi)=|\xi|^2+V_j(x)$ is the classical Hamiltonian corresponding to $P_j(h)$. Here $H_{p_j}=2\xi\cdot\partial_x-(\partial V_j)(x)\cdot\partial_\xi$ denotes the Hamiltonian vector field, and $\exp(tH_{p_j})(x,\xi)$ the corresponding Hamiltonian flow. It is well-known that (see [GeMa]) the non-trapping condition (1.2) is equivalent to the existence of an escape function $G_j(x,\xi)$ in a neighborhood of $p_j^{-1}(E_0)$, that is, a function $G_j\in C^\infty(\mathbb{R}^{2n};\mathbb{R})$ satisfying

$$H_{p_j}(G_j)\geq\delta \text{ on } \{|p_j(x,\xi)-E_0|\leq\varepsilon\} \tag{1.3}$$

for some δ, $\varepsilon>0$.

Assume that (1.3) holds for $j=1,\cdots,N$. It follows from the Martinez' result that for all integer M there are no resonances with imaginary part of order $h\log(1/h)$ for the non perturbed operator $\mathcal{P}_0(h)$ (see also [SjZw]). The aim of this note is to study the stability of this resonance free domain under the perturbation $h^\nu W$. Recall that the real part and the negative imaginary part of a resonance respectively give the frequency and the exponential decay rate of the associate resonant state. In particular, resonance close to the real axis give information about the long term behavior of the solution of the wave equation $\left(\partial_t^2+\mathcal{P}(h)\right)u=0$. Thus, it is of interest to study semiclassical resonance free regions. On the other hand, it is well known that the scattering phase (or the spectral shift function, see (2.5)) has a meromorphic extension and its poles are the resonances. Using this facts, we will deduce an asymptotic expansion of the spectral shift function with remainder depending on the resonance free region from our main results (Corollary 2.2 and Theorem 2.1).

2 Main Result

Let $\mathcal{H}_N$ be the space of Hermitian $N\times N$ matrices endowed with the norm $\|\cdot\|_{N\times N}$, where for $A\in\mathcal{H}_N$, $\|A\|_{N\times N}:=\sup_{\{v\in\mathbb{R}^N;|v|\leq1\}}|Av|$. Here, we recall some basic notions of semiclassical and mirolocal analysis, referring to the books [DiSj, Iv, Ma2, Zw] for more details. Let $S^m(\mathbb{R}^{2n};\mathcal{H}_N)$ $(m\in\mathbb{N})$ be the space of symbols $a\in C^\infty(\mathbb{R}^{2n};\mathcal{H}_N)$ satisfying the inequality

$$\left\|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)\right\|_{N\times N}\leq C_{k,l}\langle\xi\rangle^{(m-|\beta|)/2}$$

on whole $(x,\xi)\in\mathbb{R}^{2n}$ for any multiindices $\alpha,\beta\in\mathbb{N}^n$ with $\mathbb{N}=\{0,1,2,\ldots\}$, $\langle\xi\rangle=(1+|\xi|^2)^{1/2}$. The h-pseudodifferential operator corresponding to a symbol $a\in S^m(\mathbb{R}^{2n};\mathcal{H}_N)$ denoted $a^w(x,hD)$ is defined on Sobolev space $H^m(\mathbb{R}^n;\mathbb{C}^N)$ by

$$a^w(x,hD)u(x):=\frac{1}{(2\pi h)^n}\iint_{\mathbb{R}^{2n}}e^{i(x-y)\cdot\xi/h}a\left(\frac{x+y}{2},\xi\right)u(y)dyd\xi \tag{2.1}$$

for $u = u(x) \in H^m(\mathbb{R}^n; \mathbb{C}^N)$.

We study the absence of resonances in the semiclassical limit $h \to 0_+$ in a neighborhood of an energy $E_0 \in \mathbb{R}$. For that, let us introduce the following assumptions :

(A1) For $j = 1, \dots, N$, $V_j(x)$ is a real-valued smooth function on $\mathbb{R}^n$, satisfying following conditions:

1. It extends to a holomorphic function in an angular complex domain near infinity $\mathcal{S}^n$, where $\mathcal{S}$ is given by

$$\mathcal{S} = \left\{z \in \mathbb{C}\,;\ |\mathrm{Im}\, z| < (\tan\theta_0)|\mathrm{Re}\, z|,\ \ |\mathrm{Re}\, z| > R_0\right\}$$

for some constants $0 < \theta_0 < \pi/2$, $R_0 > 0$.

2. It admits a limit different from E_0 as $x \to \infty$ in $\mathcal{S}^n$.

(A2) For any $j \in \{1, \cdots, N\}$ there exists $G_j \in C^\infty(\mathbb{R}^{2n}; \mathbb{R})$ such that (1.3) holds.

(A3) $W = W^w(x, hD_x)$ is a symmetric $N \times N$-matrix valued first-order semiclassical differential operator, where $W(x,\xi) = (a_{i,j}(x)\xi + b_{i,j}(x)))_{1 \le i,j \le N}$. We assume that $x \mapsto a_{i,j}(x), b_{i,j}(x)$ are bounded with all their derivatives, and extends to a bounded analytic function on $\mathcal{S}^n$.

Under the above assumptions, $\mathcal{P}(h)$ is self-adjoint with domain $H^2(\mathbb{R}^n; \mathbb{C}^N)$, and the resonances of $\mathcal{P}(h)$ can be defined, e.g., as the values $E \in \mathbb{C}_- = \{\mathrm{Im}\, z < 0\}$ such that the equation $\mathcal{P}(h)u = Eu$ has a non trivial outgoing solution u, that is, a non identically vanishing solution such that, for some small positive (probably h-dependent constant) $\varepsilon > 0$, the function $u \circ \zeta_\varepsilon$ is in $L^2(\mathbb{R}; \mathbb{C}^N)$ where $\zeta_\varepsilon(x) = x + i\varepsilon\zeta_0(x)$ with $\zeta_0 \in C^\infty(\mathbb{R})$ satisfies $\zeta_0(x) = 0$ for $|x| \le R_0$ and $\zeta_0(x) = x$ for $|x| \ge 2R_0$ (see, e.g., [AgCo, DyZw, ReSi]). Equivalently, the resonances are the eigenvalues of the operator $\mathcal{P}_\varepsilon(h) = U_\varepsilon \mathcal{P}(h) U_\varepsilon^{-1}$ acting on $L^2(\mathbb{R}^n; \mathbb{C}^N)$, where $U_\varepsilon u = |\zeta_\varepsilon'(x)|^{n/2}\, u \circ (\zeta_\varepsilon \otimes I_N)$ (see, e.g., [HeMa]). Note that there is no essential spectrum in some complex neighborhood (depending only on ε) of E_0 due to the assumption that the limit of V_j is not equal to E_0 for any $j = 1, 2, \dots, N$. We denote by $\mathrm{Res}(\mathcal{P}(h))$ the set of these resonances.

Theorem 2.1 *Under the assumptions* (A1-3), *there exists a positive constant M (independent of ν and h) such that*

$$\mathrm{Res}(\mathcal{P}(h)) \cap \{z \in \mathbb{C}_-;\ |z - E_0| < M(\nu - 1)h\log(1/h)\} = \emptyset \tag{2.2}$$

holds for $\nu > 1$ and for h small enough.

Corollary 2.2 *Fix* $\nu \geq 1$. *Assume* (A1), (A3), *and suppose that there exists an escape function* $G \in C^{\infty}(\mathbb{R}^{2n};\mathbb{R})$ (*independent of* j) *such that* (1.3) *holds for all* p_j, $j = 1, \cdots, N$. *Then for any* $M > 0$, *there exists* $h_0(M) > 0$ *such that for* $0 < h < h_0(M)$ *we have*

$$\mathrm{Res}(\mathcal{P}(h)) \cap \{z \in \mathbb{C}_-;\ |z - E_0| < Mh\log(1/h)\} = \emptyset. \tag{2.3}$$

2.1 Comments and applications

Here, as in [Di] and [DyG] we give an asymptotic expansion of the spectral shift function with remainder depending on the resonance free regions given in Corollary 2.2 and Theorem 2.1. The proofs are quite similar to those of [Di] and [DyG]. For this reason we omit the details.

First let us recall the notion of the spactral shift function (SSF for short). Let $V_{j,\infty}$ be the limit as $|x|$ tends to infinity of the potential $V_j(x)$, and put

$$\mathcal{P}_{\infty}(h) = \mathrm{diag}(P_{1,\infty}(h), P_{2,\infty}(h), \ldots, P_{N,\infty}(h)),$$

where $P_{j,\infty}(h) = -h^2\Delta + V_{j,\infty}$. We assume that there exists $\delta > n$ such that for all $\alpha \in \mathbb{N}^n$ there exists $C_\alpha > 0$ such that

$$\sum_{1\leq i,j\leq N} |\partial_x^\alpha a_{i,j}(x)| + |\partial_x^\alpha b_{i,j}(x)| + |\partial_x^\alpha (V_j(x) - V_{j,\infty})| \leq C_\alpha \langle x\rangle^{-\delta-|\alpha|}. \tag{2.4}$$

Inequality (2.4) enables us to define the SSF, $s(\lambda, h) \in \mathcal{D}'(\mathbb{R})$, related to operators $\mathcal{P}(h)$ and $\mathcal{P}_\infty(h)$ following the general theory (see [DyZw] and the references given there) by the equality

$$\mathrm{tr}\big[f(\mathcal{P}(h)) - f(\mathcal{P}_\infty(h))\big] = -\langle s'(\cdot;h), f(\cdot)\rangle = \int_{\mathbb{R}} s(\lambda;h) f'(\lambda)d\lambda, \tag{2.5}$$

for any $f \in C_0^\infty(\mathbb{R})$. In the scalar case $N = 1$, it is well known that $s'(\lambda;h)$ has a complete asymptotic expansion in powers of h near a non-trapping energy E_0. Under the assumption of Corollary 2.2, this result has been generalized in [ADF] for $\mathcal{P}(h)$ with $N > 1$. As indicated above, we will improve and generalize this result as a consequence of Corollary 2.2.

Formulas relating the scattering resonances and the SSF was considered by many authors. In [Me], Melrose has studied how the location of resonances is reflected in the asymptotic behavior at high energies of spectral shift function in obstacle scattering through the trace formula (2.5). A more general local trace formula relating the derivative of the SSF and the resonances has been established in [Sj] (see also [BP]). The case of a system of h-pseudodifferential operator was treated in [Ne]. In particular, under the conditions (A1) ,(A2) and (2.4), it follows from Theorem 4.1 in [Ne] and

Theorem in [BP] (see also [Di]) that if $E_0 \notin \{V_{1,\infty}, \cdots, V_{N,\infty}\}$ then there exist a simply connected complex (h-independent) neighborhood Ω of E_0, a holomorphic function g on Ω and a small positive constant h_0 such that for all $\lambda \in I := \mathbb{R} \cap \Omega$ and all $h \in]0, h_0]$ we have

$$s'(\lambda, h) = \operatorname{Im} g(\lambda, h) - \frac{1}{\pi} \sum_{\substack{\omega \in \operatorname{Res}(P(h)) \cap \Omega \\ \operatorname{Im} \omega < 0}} \frac{\operatorname{Im}\omega}{|\lambda - \omega|^2} + \sum_{\omega \in I \cap \operatorname{Res}(P(h))} \delta(\lambda - \omega), \tag{2.6}$$

$$|g(z, h)| \leq Ch^{-n}. \tag{2.7}$$

Combining this with Theorem 2.1 (resp. Corallary 2.2), we obtain

$$s'(\lambda, h) = \operatorname{Im} g(\lambda, h) - \frac{1}{\pi} \sum_{\substack{\omega \in \operatorname{Res}(P(h)) \cap \Omega \\ \operatorname{Im} \omega < \zeta h \log(h)}} \frac{\operatorname{Im}\omega}{|\lambda - \omega|^2} \tag{2.8}$$

with $\zeta = M(\nu - 1)$ (resp. $\zeta > 0$ arbitrary).

Now let $\theta \in C_0^\infty(] - \frac{1}{C}, \frac{1}{C}[; \mathbb{R})$ be equal to one on $] - \frac{1}{2C}, \frac{1}{2C}[$, and let $\mathcal{F}_h\theta$ be its semiclassical Fourier transform. Let $f \in C_0^\infty(\mathbb{R})$ be equal to one near E_0. Assuming (A1), (A2), (A3) and (2.4), it follows from (2.7), (2.8) and the fact that $\theta' = 0$ on $] - \frac{1}{2C}, \frac{1}{2C}[$ that

$$\mathcal{F}_h\theta * fs'(\lambda, h) = f(\lambda)s'(\lambda, h) + \mathcal{O}(h^{\frac{\zeta}{2C} - 1}). \tag{2.9}$$

On the other hand, it follows from Theorem 2.6 in [ADF] (see also [DiSj] and [Iv]) that $\mathcal{F}_h\theta * fs'(\lambda; h)$ has a complete asymptotic expansion in powers of h near $\lambda = E_0$ provided that E_0 satisfies (1.3) and $C \gg 1$. Combining this with (2.9), we obtain :

Theorem 2.3 *Fix $E_0 \notin \{V_{1,\infty}, V_{2,\infty}, \cdots, V_{N,\infty}\}$, and assume* (A1-3), (2.4), *and* (2.9). *There exits $\eta > 0$ (independent of ν and h) such that $s'(\cdot, h)$ has an asymptotic expansion of the form*

$$s'(\lambda, h) = (2\pi h)^{-n} \left(\sum_{j \geq 0} \gamma_{2j}(\lambda) h^{2j} + \mathcal{O}(h^{\frac{\zeta}{2C}}) \right), \quad \text{as } h \searrow 0, \tag{2.10}$$

uniformly for $\lambda \in]E_0 - \eta, E_0 + \eta[$. Here ζ is any arbitrary integer if (A2) *holds with $G_1 = \cdots = G_N$, and $\zeta = M(\nu - 1), \nu > 1$ for the general case where M is given in Theorem 2.1. The coefficients $\gamma_{2j}(\lambda)$ can be computed explicitly. In particular*

$$\gamma_0(\lambda) = \frac{\omega_n}{2} \sum_{k=1}^{N} \int_{\mathbb{R}^n} \left((\lambda - V_k(x))_+^{\frac{n-2}{2}} - (\lambda - V_{k,\infty})_+^{\frac{n-2}{2}} \right) dx, \tag{2.11}$$

where ω_n is the volume of the unit sphere $\mathbb{S}^{n-1}$ and $\lambda_+ := \max(\lambda, 0)$.

In general, the conclusion in the above theorem is of interest only when ν is small enough. If $G_1 = \cdots = G_N$, (2.10) was proved in [ADF].

3 Proof of Theorem 2.1 and Corollary 2.2

Throughout this section we fix $E_0 \in \mathbb{R}$, and we assume (A1-3). Let $\zeta_0(x)$, U_ε and P_ε be the function and the operators as introduced above. For simplicity of the notations we ignore the dependence of the operators $\mathcal{P}(h), \mathcal{P}_0(h), P_j(h)$, etc on h and we denote it $\mathcal{P}, \mathcal{P}_0, P_j$, etc.

For $M > 0$ (to be fixed later), we denote

$$\widetilde{U} := \operatorname{diag}(e^{-\varepsilon \widetilde{G}_1^w/h}, \ldots, e^{-\varepsilon \widetilde{G}_N^w/h}). \tag{3.1}$$

and

$$\widetilde{\mathcal{P}}_\varepsilon := \widetilde{\mathcal{P}}_{0,\varepsilon} + h^\nu \widetilde{W}_\varepsilon = \widetilde{U}\mathcal{P}_\varepsilon \widetilde{U}^{-1} \tag{3.2}$$

where $\varepsilon = Mh\log(1/h)$ and $\widetilde{G}_j = G_j - \zeta_0(x)\cdot\xi$. Notice that, by assumption **(A1)**-(2), the operator $P_j(h)$ tends to $-h^2\Delta + \text{Const.}$ when $|x|$ tends to infinity. Thus, we may assume that $G_j(x,\xi) = x\cdot\xi$ for $|x|$ large enough. Combining this with the fact that $\zeta_0(x)$ for $|x| > 2R_0$, we deduce that $\tilde{G}_j \in C_0^\infty(\mathbb{R}^{2n};\mathbb{R})$. This implies that the operator $e^{-\varepsilon \widetilde{G}_j^w/h}$ is well defined as an h-pseudodifferential one in an exotic class $S^\delta(\mathbb{R}^{2n})$ for some $\delta > 0$ (see chapter 7 and chapter 12 in [DiSj]). In particular, $e^{\pm\varepsilon \widetilde{G}_j^w/h}$ is a bounded linear operator from $L^2(\mathbb{R}^n)$ into $L^2(\mathbb{R}^n)$. Hence that $\tilde{U}$ and $\tilde{U}^{-1}$ are bounded from $L^2(\mathbb{R}^n;\mathbb{C}^N)$ into $L^2(\mathbb{R}^n;\mathbb{C}^N)$.

Let us now prove Theorem 2.1 and Corollary 2.2. Under the non-trapping condition (1.3), it follows from [SjZw] that $(\mathcal{P}_{0,\varepsilon} - E_0)^{-1}$ is well defined, and there exists $c_0 > 0$ (independent of M and h) such that

$$\left\| \left(\tilde{\mathcal{P}}_{0,\varepsilon} - E_0 \right)^{-1} \right\|_{\mathcal{L}(L^2)} \leq \frac{c_0}{\varepsilon}.$$

Therefore, for $E \in \mathcal{B}_h(M) = \{z \in \mathbb{C}_-;\ |z - E_0| < c_1\varepsilon\}$ with $c_1 < \frac{1}{c_0}$, the operator $(\mathcal{P}_{0,\varepsilon} - E)$ is invertible and

$$\left\| \left(\tilde{\mathcal{P}}_{0,\varepsilon} - E \right)^{-1} \right\|_{\mathcal{L}(L^2)} \leq \frac{c_0}{2\varepsilon}. \tag{3.3}$$

Let $\tilde{w}_{j,k,\varepsilon}(x, hD_x) = e^{-\varepsilon \tilde{G}_j^w/h} U_\varepsilon w_{j,k}(x, hD_x) U_\varepsilon^{-1} e^{\varepsilon \tilde{G}_k^w/h}$ be the (j,k)-element of the operator $\tilde{W}_\varepsilon$. A standard result on h-pseudodifferential calculus yields

$$\begin{aligned} \|\tilde{w}_{j,k,\varepsilon}(x, hD_x)\|_{\mathcal{L}(H^2 \to L^2)} &\leq C_{j,k} e^{M\|\tilde{G}_k - \tilde{G}_j\|_\infty \log(1/h)} \\ &= C_{j,k} h^{-M\|\tilde{G}_k - \tilde{G}_j\|_\infty}. \end{aligned} \tag{3.4}$$

On the other hand, for $\lambda \ll -1$, standard elliptic estimates and the above inequality yield

$$\left\| \tilde{W}_\varepsilon \left(\mathcal{P}_{0,\varepsilon} - \lambda\right)^{-1} \right\|_{\mathcal{L}(L^2)} \leq \tilde{C} h^{-\kappa M}$$

where $\kappa := \max_{1\leq j,k\leq N} \|\tilde{G}_k - \tilde{G}_j\|_\infty$. Consequently

$$h^\nu \left\| \tilde{\mathcal{W}}_\varepsilon \left(P_{0,\varepsilon} - E\right)^{-1} \right\|_{\mathcal{L}(L^2)} \tag{3.5}$$

$$\leq h^\nu \left\| \tilde{\mathcal{W}}_\varepsilon \left(\left(\tilde{\mathcal{P}}_{0,\varepsilon} - \lambda \right)^{-1} + (E - E_1) \left(\mathcal{P}_{0,\varepsilon} - \lambda\right)^{-1} \left(\tilde{\mathcal{P}}_{0,\varepsilon} - E \right)^{-1} \right) \right\|_{\mathcal{L}(L^2)}$$

$$\leq C_3 h^{\nu - \kappa M} + C_4 \frac{h^{\nu - 1 - \kappa M}}{\log(1/h)},$$

uniformly for $E \in \mathcal{B}_h(M)$. Therefore, if $\nu - 1 - \kappa M \geq 0$ then

$$h^\nu \left\| \tilde{\mathcal{W}}_\varepsilon \left(P_{0,\varepsilon} - E\right)^{-1} \right\|_{\mathcal{L}(L^2)} = o(1).$$

Combining this with the obvious equality

$$(\tilde{\mathcal{P}}_\varepsilon - E) = \left(I + h^\nu \tilde{\mathcal{W}}_\varepsilon (\tilde{\mathcal{P}}_{0,\varepsilon} - E)^{-1} \right) (\tilde{\mathcal{P}}_{0,\varepsilon} - E), \tag{3.6}$$

we deduce that $(\tilde{\mathcal{P}}_\varepsilon - E)$ is invertible for $E \in \mathcal{B}_h(M)$, and hence that $(\mathcal{P}_\varepsilon - E)$ is bijective, since $(\tilde{\mathcal{P}}_\varepsilon - E) = \tilde{U}(\mathcal{P}_\varepsilon - E)\tilde{U}^{-1}$ and $\tilde{U}, \tilde{U}^{-1}$ are bounded. This ends the proof of Theorem 2.1.

To prove Corollary 2.2, assume that $G_j = G_k$ holds for all $j, k \in \{1, \cdots, N\}$. Since $\tilde{G}_j - \tilde{G}_k = G_j - G_k$, it follows that $\kappa = 0$. Therefore, from (3.5) we deduce that for all $M > 0$ and all $\nu \geq 1$, we have

$$h^\nu \left\| \tilde{\mathcal{W}}_\varepsilon \left(P_{0,\varepsilon} - E\right)^{-1} \right\|_{\mathcal{L}(L^2)} = o(1), \tag{3.7}$$

uniformly for $E \in \mathcal{B}_h(M)$. Now, as in the proof of Theorem 2.1, Corollary 2.2 follows from (3.6) and (3.7).

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