Semiclassical resonances for matrix Schrödinger operators with vanishing interactions at crossings of classical trajectories

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1 Framework and assumptions

We investigate spectral properties in the semiclassical limit of the matrix-valued Schrödinger operator

$$P := \begin{pmatrix} P_1 & hU \\ hU^* & P_2 \end{pmatrix} \tag{1}$$

where $P_j := (hD_x)^2 + V_j(x)$, $j \in \{1,2\}$ are the scalar Schrödinger operators, D_x is $-i\partial_x$ and $h > 0$ denotes the usual semiclassical parameter. Here U is a multiplication operator by a smooth, real-valued function $r(x)$. This model arises in the framework of the Born-Oppenheimer approximation, motivated for example by the study of the molecular predissociation phenomena in quantum chemistry (see [GM14] for an history). In this context, the imaginary part of the resonances of P is proportional to the inverse of the half-life of the particle described by P. The aim of this talk is to give an h-asymptotic expansion of the imaginary part of the resonances.

We consider potentials V_j that are analytic outside of a compact set, and we fix an energy $E_0 \in \mathbb{R}$ for which V_1 has a "simple well" and V_2 is "non-trapping". In the absence of the interaction U, P_2 has an essential spectrum, P_1 has eigenvalues that can be approximated by a Bohr-Sommerfeld quantification condition **(B-S)** and locally around E_0 we have $\sigma(P) = \sigma(P_1) \cup \sigma(P_2)$. However in the presence of the interaction term U, the eigenvalues of P_1 can shift under the real line and become *resonances* for the operator P (Fermi's golden rule). In this talk, we assume that the set $\{x \in \mathbb{R}, V_1(x) = V_2(x)\}$ is reduced to $\{0\}$ and that $V_2 - V_1$ vanish at $x = 0$ at a finite order $m \in \mathbb{N}^*$:

$$(V_2 - V_1)^{(j)}(0) = 0 \text{ for all } j \in \{0, \dots, m-1\}, \quad \text{and} \quad (V_2 - V_1)^{(m)}(0) \neq 0.$$

Moreover, we assume $E_0 > V_1(0) = V_2(0)$.

In this setting, authors in [AFH22] computed an asymptotic expansion of the imaginary part of the resonances for P. However they also assumed an elliptic condition on U, that is to say $r(0) \neq 0$ (independently of h). In this talk, we generalize the results obtained in [AFH22] by relaxing this elliptic condition. More specifically, we assume that the function r can vanish at $x = 0$ at a finite order $k \in \mathbb{N}$ satisfying $k < m$.

2 Main result

Theorem 2.1 ([Lou23]). *Consider a complex box $\mathcal{R}_h := [E_0 - Lh, E_0 + Lh] + i[-Lh, Lh]$ with $L > 0$. We note $\mathfrak{B}_h$ the set of $E \in \mathcal{R}_h$ satisfying **(B-S)**. Then for all small $h > 0$, there exist a* *one-to-one correspondance* $z_h : \mathfrak{B}_h \to \mathrm{Res}(P) \cap \mathcal{R}_h$ *satisfying* $|z_h(E) - E| = O\left(h^{1+2\frac{k+1}{m+1}}\right)$ *and, for all* $E \in \mathfrak{B}_h$*,*

$$\operatorname{Im} z_h(E) = -h^{1+2\frac{k+1}{m+1}} \frac{2\sqrt{2}|\omega_k|^2}{\sqrt{\mathcal{A}'(E_0)}} \left|\sin\left(\arg(\omega_k) + \frac{\mathcal{B}(E)}{2h}\right)\right|^2 + O\left(h^{1+2\frac{k+1}{m+1}+s}\right). \tag{2}$$

When both k *and* m *are odd and satisfy* $k+1 < m$*, then* $|z_h(E) - E| = O\left(h^{1+2\frac{k+2}{m+1}}\right)$ *and*

$$\operatorname{Im} z_h(E) = -h^{1+2\frac{k+2}{m+1}} \frac{2\sqrt{2}|\omega_{k,odd}|^2}{\sqrt{\mathcal{A}'(E_0)}} \left|\sin\left(\arg(\omega_{k,odd}) + \frac{\mathcal{B}(E)}{2h}\right)\right|^2 + O\left(h^{1+2\frac{k+2}{m+1}+s}\right). \tag{3}$$

Here, $\omega_k, \omega_{k,odd} \in \mathbb{C}$ *are constants independent of* E *and* h*,* $\quad s := \min(1/3, 1/(m+1))$*,* $\mathcal{B}(E) := 2\left(\int_{a(E)}^{0} \sqrt{E - V_1(x)}dx + \int_0^{b(E)} \sqrt{E - V_2(x)}dx\right)$ *and* $\mathcal{A}(E) := 2\int_{a(E)}^{a'(E)} \sqrt{E - V_1(x)}dx$*.*

3 Difficulties and key ideas

The study revolves around the analysis of the microlocal solutions of $(P - E)u = 0$, called *resonant states*. Ideally, we would construct these microlocal solutions via usual WKB constructions as in the scalar case. It is possible to construct them *away* from crossing points (the construction can be brought to the scalar case). However this is not possible at the crossing points of the two classical trajectories $\Gamma_j(E_0) := \{(x, \xi) \in \mathbb{R}^2,\ \xi^2 + V_j(x) = E_0\}$.

This difficulty can be overcome by proving a **microlocal connection formula**. This formula states that the space of microlocal solutions at crossing points is two dimensional, and it states the existence of a *transfer matrix* (or microlocal scattering matrix) that describes the microlocal behavior of resonant states at the crossing points. We will give an h-asymptotic expansion of this matrix.

One way to prove this is to construct *exact* solutions in a neighborhood of the crossing points (it is possible only locally). Essentially, the h-asymptotic behavior of the transfer matrix is given by the h-asymptotic behavior of those exact solutions. Those solutions are integrals of functions of the form $\sigma(x)e^{\frac{i}{h}\phi(x)}$ whose phase ϕ has a critical point at $x = 0$ corresponding to the $x-$coordinate of the crossing points. In our case, $r(x)$ appears as a multiplicative factor in $\sigma(x)$ and also vanishes at $x = 0$ which is why we need a **stationary phase estimate** for this **degenerate case**.

References

[AFH22] M. Assal, S. Fujiié, and K. Higuchi. Semiclassical resonance asymptotics for systems with degenerate crossings of classical trajectories. *arXiv:2211.11651*, 2022.

[GM14] A. Grigis and A. Martinez. Resonance widths for the molecular predissociation. *Analysis and PDE*, 7(5):1027–1055, 2014.

[Lou23] Vincent Louatron. Semiclassical resonances for matrix schrödinger operators with vanishing interactions at crossings of classical trajectories. *arXiv:2306.02350*, 2023.