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Quantum resonances and partial differential equations

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Abstract

Resonances, or scattering poles, are complex numbers which mathematically describe meta-stable states: the real part of a resonance gives the rest energy, and its imaginary part, the rate of decay of a meta-stable state. This description emphasizes the quantum mechanical aspects of this concept but similar models appear in many branches of physics, chemistry and mathematics, from molecular dynamics to automorphic forms.

In this article we will will describe the recent progress in the study of resonances based on the theory of partial differential equations.

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1. Introduction

Eigenvalues of self-adjoint operators appear naturally in quantum mechanics and are in fact what we observe experimentally in many situations. To explain the need for the more subtle notion of *quantum resonances* we consider the following simple example.

Let $V(x)$ be a potential on a bounded interval, as shown in Fig.1. a). If ξ denotes the classical momentum, then the classical energy is given by

$$E = \xi^2 + V(x)\,, \tag{1.1}$$

and the motion of a classical particle can deduced from this equation by considering E as the Hamiltonian. The quantized Hamiltonian is given by

$$P(h) = (hD_x)^2 + V(x)\,, \quad \xi \mapsto hD_x\,, \quad D_x = \frac{1}{i}\partial_x\,. \tag{1.2}$$

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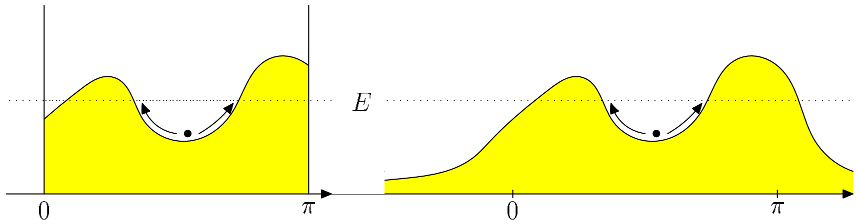
The operator $P(h)$ considered as an unbounded operator on L^2 of a bounded interval (with, say, Dirichlet boundary conditions) has a discrete spectrum, which gets denser and denser as $h \to 0$, which corresponds to getting closer to classical mechanics:

$$P(h)u(h) = E(h)u(h) \,, \quad E(h) \in \mathbf{R} \,, \quad \int |u(h)|^2 < \infty \,, \quad u(h)(\pm\pi) = 0 \,. \tag{1.3}$$

The eigenvalues, $E(h)$, are what we (in principle) observe, and the square-integrable eigenfunctions, $u(h)$, are the wave functions.

Now, consider the same example but with a potential $V(x)$ on $\mathbf{R}$, as shown in Fig.1. b). At the energy E, and inside the well created by the potential, the classical motion is the same as in the previous case. Hence, we expect that (at least for h very small) there should exist a quantum state corresponding to the classical one. It is clear in dimension one that for the potential shown in the figure, $P(h)$ given by (1.2) has *no* square integrable eigenfunctions (1.3).



(a) (b)

Figure 1: (a) A potential well on a finite interval. (b) A potential on the whole line the same classical picture but a very different quantum picture.

A non-obvious remedy for this is to think of eigevalues (in the case of Fig.1.a) as the poles of the resolvent of $P(h)$:

$$R(z,h) = (P(h) - z)^{-1} \,.$$

In the case of Fig1.b), the resolvent is not bounded on $L^2(\mathbf{R})$ for $z > 0$, which corresponds to free motion or scattering. However, under suitable assumptions on $V(x)$ near infinity we have a meromorphic continuation of $R(z,h)$ from $\mathrm{Im} z > 0$ to the lower half-plane:

$$R(z,h) \;:\; L^2_{\mathrm{comp}}(\mathbf{R}) \longrightarrow L^2_{\mathrm{loc}}(\mathbf{R}) \,.$$

The complex poles of $R(z,h)$ are the replacement for eigenvalues, are called *resonances*. For a recent presentation of these in the physical literature and for examples of current interest see for instance [7].

In this review, we will restrict ourselves to the case of

$$P(h) = -h^2\Delta + V(x) \,, \quad x \in \mathbf{R}^n \,,$$

where the potential $V(x)$ satisfies some decay and analyticity assumptions near infinity, or is simply compactly supported. Then our discussion above applies and resonances are defined as the poles of $R(z,h)$ – see [9] for an attractive new presentation of the meromorphic continuation properties and references. In our convention the resonances are located in the lower half-plane.

We should stress that most of the results hold for very general *black box perturbations* of Sjöstrand-Zworski [22] which allow for a study of diverse problems without going into their specific natures – see [20] for definitions. Also, despite the fact that the motivation presented here came from molecular dynamics, similar issues arise in other settings, from automorpic scattering to electromagnetic (obstacle) scattering – see [8], and [23] respectively.

We suggest the the surveys [12],[20],[31],[33], and [36] for the review of earlier results, and we concentrate on the progress achieved in the last few years. For an account of work based on other methods and motivated by different physical phenomena we refer to [13].

2. Trace formulæ for resonances

Trace formulæ provide one of the most elegant descriptions of the classical-quantum correspondence. One side of a formula is given by a trace of a quantum object, typically derived from a quantum Hamiltonian, and the other side is described in terms of closed orbits of the corresponding classical Hamiltonian. A new general approach based on *quantum monodromy operator* which quantizes the Poincaré map in a natural way was recently given in [24].

In general the spectral (or scattering) side of the formula is given in terms of the trace of a function of the quantum Hamiltonian $f(P(h))$. In the case of self-adjoint problems with discrete sets of eigenvalues the spectral theorem readily provides an expression for tr $f(P(h))$ but the problem becomes subtle for resonances. It has been studied by Lax-Phillips, Bardos-Guillot-Ralston, Melrose, Sjöstrand-Zworski, Guillopé-Zworski – see [34] and references given there.

More recently Sjöstrand [20],[21] introduced *local trace formulæ* for resonances, and that concept was developed further in [18] and [3]. For $P(h)$ given by (1.2) with $V(x)$ decaying sufficiently fast at infinity it can be stated as follows.

Let Ω be an open, simply connected, pre-compact subset of $\{\mathrm{Re}\, z > 0\} \subset \mathbf{C}$, such that $\Omega \cap \mathbf{R}$ is connected. Suppose that f is holomorphic in a neighbourhood of Ω and that $\psi \in C^\infty_c(\mathbf{R})$ is equal to 1 in $\Omega \cap \mathbf{R}$ and supported in a neighbourhood of $\Omega \cap \mathbf{R}$. Then, denoting the resonance set of $P(h)$ by $\mathrm{Res}(P(h))$,

$$\begin{gathered} \mathrm{tr}\; \big((f\psi)(P(h)) - (f\psi)(-h^2\Delta) \big) = \sum_{z \in \mathrm{Res}(P(h)) \cap \Omega} f(z) + E_{f,\psi}(h)\,, \\ |E_{f,\psi}(h)| \leq h^{-n} C_{\Omega,\psi} \max\{ |f(z)| \;:\; z \in \overline{\Omega}_1 \setminus \Omega\,,\ \mathrm{Im}\, z \leq 0 \}\,, \end{gathered} \tag{2.1}$$

where Ω_1 is a neighbourhood of Ω (see [3] and [18] for more precise versions).

The basic upper bound on the number of resonances is given as follows:

$$\sharp\, \mathrm{Res}(P(h)) \cap \Omega = \mathcal{O}(h^{-n})\,, \tag{2.2}$$

see [12],[19],[20],[33]. It would consequently appear that the error term in (2.1) is of the same order as the sum over the resonances. However, by choosing the function

f so that it is small in $\Omega_1 \setminus \Omega \cap \{\mathrm{Im}\, z \leq 0\}$, the sum of $f(z)$ can dominate the left hand side of (2.1). Doing that, Sjöstrand has shown that an analytic singularity of $E \mapsto |\{x \; : \; V(x) \geq E\}|$ at E_0 gives a lower bound in (2.2) for Ω a neighbourhood of E_0 – see [21] and references given there.

Another application of local trace formulæ techniques is in analysing resonances for *bottles*, that is perturbations of the Euclidean space in which the "size" of the perturbation may grow but which are connected to the euclidean infinity through a fixed "neck of the bottle" – see [21],[18].

3. Breit-Wigner approximations

In a scattering experiment the physical data is mathematically encoded in the scattering matrix, $S(\lambda, h)$. It is in the behaviour of objects derived from the scattering matrix that we see physical manifestations of abstractly defined resonances. The classical and still central Breit-Wigner approximation provides this connection. The most mathematically tractable case is provided by the *scattering phase* $\sigma(\lambda, h) = \log\det S(\lambda, h)/(2\pi i)$, which is defined for V's with sufficient decay (otherwise relative phase shifts have to be used, see [3]). When λ is close to a resonance $E - i\Gamma$, the Breit-Wigner approximation says that

$$\sigma'(\lambda, h) \sim \frac{1}{\pi} \frac{\Gamma}{(\lambda - E)^2 + \Gamma^2}\,, \tag{3.1}$$

that is, if Γ is small, $\sigma(\lambda)$ should change by approximately 1 as λ crosses E. This has been justified rigorously in some situations in whch a given resonance, close to the real axis, is isolated.

In view of (2.2) the number of resonances in fixed regions can be very large and for h small clouds of resonances need to be considered to obtain a correct form of the Breit-Wigner approximation. A formalism for that was introduced by Petkov-Zworski [16],[18], and it was developed further by Bruneau-Petkov [3] and Bony-Sjöstrand [2]. It is closely related to extending the trace formula (2.1) to h dependent Ω's. To formulate it, let us introduce $\omega(z, E) = (1/\pi)\int_E (|\mathrm{Im}\, z|/|z-\lambda|^2) d\lambda$, $\mathrm{Im}\, z < 0$, the harmonic measure corresponding to the upper half-plane. Then, for non-critical λ's (that is for λ's for which $\xi^2 + V(x) = \lambda \Rightarrow d_{(x,\xi)}(\xi^2 + V(x)) \neq 0$)

$$\sigma(\lambda + \delta, h) - \sigma(\lambda - \delta, h) = \sum_{\substack{z \in \mathrm{Res}(P(h)) \\ |z - \lambda| < h}} \omega(z, [\lambda - \delta, \lambda + \delta]) + \mathcal{O}(\delta) h^{-n}\,, \tag{3.2}$$

$0 < \delta < h/C$. The main point is that δ can be made arbitrarily small and that we only need to include resonances close to λ. If we do not assume that λ is non-critical weaker, but still useful, results can be obtained from factorization of the scattering determinant [18], or more generally, from the the analysis of the phase shift function [3].

One of the consequencies of the development of the Breit-Wigner approximations for clouds of resonances were new estimates on the number of resonances in small regions, first in [16], and then in greater generality in [1],[3],[18]. If in place of (2.2) we had a Weyl law with a remainder $\mathcal{O}(h^{1-n})$, then, as for eigenvalues,

$$\sharp \{z \in \mathrm{Res}(P(h)) \; : \; |z-\lambda| < \delta\} = \mathcal{O}(\delta)h^{-n} \,, \quad Ch < \delta < 1/C \,. \tag{3.3}$$

It turns out that despite the lack of the Weyl law we still have this estimate for non-critical λ's.

4. Resonance expansions of propagators

In the case of discrete spectrum of a self-adjoint operator the propagator, $\exp(-itP(h)/h)$ can be expanded in terms of the eigenvalues. In fact, our understanding of "state specificity" often comes from such "Fourier decompositions" into modes. For problems in which decay or escape to infinity are possible such expansions are still expected but just as in the case of trace formulæ far from obvious. For non-trapping perturbations and in the context of the wave equation the expansions in terms of resonances were studied in late 60's by Lax-Phillips and Vainberg (see the references in [30]).

For trapping perturbations the expansions were investigated by Tang-Zworski [30], and then by Burq-Zworski [5], Christiansen-Zworski [6], Stefanov [26], and most recently by Nakamura-Stefanov-Zworski [14].

Here, we will recall the general expansion given in [5]: let $\chi \in C^\infty_{\rm c}(\mathbf{R}^n)$, $\psi \in C^\infty_{\rm c}((0,\infty))$, and let chsupp $\psi = [a,b]$. There exists $0 < \delta < c(h) < 2\delta$ and L, so that we have

$$\begin{aligned} \chi e^{-itP(h)/h} \chi \psi(P(h)) = & \sum_{z \in \Omega(h) \cap \mathrm{Res(P)}} \chi \mathrm{Res}(e^{-it\bullet/h} R(\bullet, h), z) \chi \psi(P(h)) \\ & + \; \mathcal{O}_{L^2 \to L^2}(h^\infty) \,, \quad \text{for} \;\; t > h^{-L} \,, \end{aligned} \tag{4.1}$$

$\Omega(h) = (a - c(h), b + c(h)) - i[0, 1/C)$, and where $\mathrm{Res}(f(\bullet), z)$ denotes the residue of a meromorphic family of operators, f, at z.

The function $c(h)$ depends on the distribution of resonances: roughly speaking we cannot "cut" through a dense cloud of resonances. Even in the very well understood case of the modular surface [6, Theorem 1] there is, currently at least, a need for some non-explicit grouping of terms. This is eliminated by the separation condition [30, (4.4)] which however is hard to verify.

The unpleasant feature of (4.1) is the need for very large times $\sim h^{-L}$ and the presence of a non-universal parameter, $c(h)$. The former is necessary in this formulation as one sees by considering the free case $P(h) = -h^2\Delta$. However an expansion valid for all times is possible in the case when a part of V constitutes a *barrier* separating the trapped set in $\{(x,\xi) \; : \; \xi^2 + V(x) \in \mathrm{supp}\, \psi\}$ from infinity [14]. The example shown in Fig.1. b) is of that type. By the trapped set in $\Sigma \subset T^*\mathbf{R}^n$ we mean the set

$$K \cap \Sigma = \{(x,\xi) \in \Sigma \; : \; |\exp(tH_p)(x,\xi)| \not\longrightarrow \infty \,, \; t \longrightarrow \pm\infty\} \,, \tag{4.2}$$

where H_p is the Hamilton vectorfield of $p = \xi^2 + V(x)$. One of the components comes from the work of Stefanov [27] on making estimates (2.2) more quantitative with constants related to the volume of the trapped set (for yet finer results of that type see Section.6).

5. Separation from the real axis

One of the most striking applications of PDE techniques in the study of resonances is the work of Burq (see [4] and references given there) on the separation of resonances from the real axis, estimates of the cut-off resolvent on the real axis, and the consequent estimates on the time decay of energy.

For non-trapping perturbations we have the following estimate on the truncated meromorphically continued resolvent

$$\|\chi R(z,h)\chi\|_{L^2\to L^2} \leq C\frac{\exp(C|\mathrm{Im}\, z|/h)}{h}\,, \quad \mathrm{Im}\, z > -Mh\log\frac{1}{h}\,, \quad \chi \in C_{\rm c}^\infty(\mathbf{R}^n)\,, \tag{5.1}$$

for any M, see [11] for the absence of resonances (implicit in (5.1)), and [14] for the (easily derived) estimate.

Since the work of Stefanov-Vodev and Tang-Zworski (see [27],[29],[31] and references given there) we know that in many trapping situations[1], there exist many resonances converging to the real axis[2]. The question then is how close could the resonances approach the real axis or, as it turns out equivalently, how big can the truncated resolvent be on the real axis. Heuristically, tunneling should prevent arbitrary closeness to the real axis, and the separation should be universally given by at least $\exp(-S/h)$.

Tunneling of solutions is made quantitative in PDEs through *Carleman estimates* used classically to show unique continuation of solutions of second order equations. Following the work of Robbiano, and Lebeau-Robbiano, Burq succeeded in applying Carleman estimates to a wide range of resonance problems – see [4] and references given there. In the setting described here his basic result says that if Ω is as in (2.1) then

$$\begin{gathered} \exists\, S_1, S_2\,, \quad z \in \mathrm{Res}(P(h))\cap\Omega \implies \mathrm{Im}\, z > -\exp(-S_1/h)\,, \\ \|\chi R(z,h)\chi\|_{L^2\to L^2} \leq \exp(S_2/h)\,, \quad z\in\Omega\cap\mathbf{R}\,, \quad \chi\in C_{\rm c}^\infty(\mathbf{R}^n)\,. \end{gathered} \tag{5.2}$$

In addition, improved estimates are possible if χ is assumed to have support outside the projection of the trapped set:

$$\|\chi R(z,h)\chi\|_{L^2\to L^2} \leq C/h\,, \quad z\in\Omega\cap\mathbf{R}\,, \quad \chi\in C_{\rm c}^\infty(\mathbf{R}^n\setminus\pi(K))\,. \tag{5.3}$$

That means that away from the interaction region $\pi(K)$ we have, on the real axis, the same estimates as in the non-trapping case (5.1) and that has immediate applications in scattering theory [28].

[1] roughly speaking, whenever there exists an elliptic orbit of the H_p-flow

[2] That in specific trapping situations there exist resonances whose distance to the real axis is of order $\exp(-S/h)$ is classical in physics with the most precise mathematical results given by Helffer-Sjöstrand – see [9]. Here we concentrate on very general existence results which guarantee lower bounds on the number of resonances.

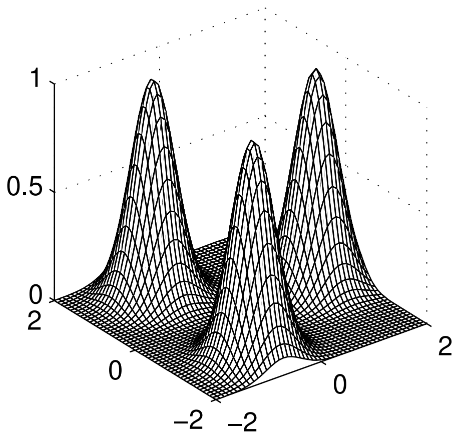


Figure 2: Graph of a potential $V(x)$, for which the classical flow of the Hamiltonian $\xi^2 + V(x)$ is hyperbolic for energies close to 0.5.

6. Resonances in chaotic scaterring

Since the work of Sjöstrand [19] on geometric upper bounds for the number of resonances, it has been expected that for chaotic scattering systems the density of resonances near the real axis can be approximately given by a power law with the power equal to half of the dimension of the trapped set (see (6.1) below). Upper bounds in geometric situations have been obtained in [32] and [35].

An example of a potential in $V \in C^\infty_{\rm c}(\mathbf{R}^2)$ for which the flow of H_p, $p = \xi^2 + V(x)$, is hyperbolic (and hence scattering exhibits chaotic features) is shown in Fig.6.

A recent numerical study [10] for that potential indicates that the density of resonances satisfies a lower bound related to the dimension of the trapped set – see Fig.6. In a complicated semi-classical situation studied in [10], the dimension is a delicate concept and it may be that different notions of dimension have to be used for upper and lower bounds. That point is emphasized in [25] where numerical data for semi-classical zeta function for several convex obstacles is analyzed.

In the case of *convex co-compact hyperbolic quotients*, $X = \Gamma \backslash \mathbf{H}^2$, studied in [35] the situation is particularly simple as the quantum resonances coincide with the zeros of the zeta-function – see [15]. The notion of the dimension of the trapped set is also clear as it is given by $2(1+\delta)$. Here $\delta = \dim \Lambda(\Gamma)$ is the dimension of the limit set of Γ, that is the set of accumulation points of the elements of Γ (they are all hyperbolic), $\Lambda(\Gamma) \subset \partial \mathbf{H}^2$.

Hence we expect that

$$\sum_{|\mathrm{Im}\, s| \leq r\,,\ \mathrm{Re}\, s > -C} m_\Gamma(s) \sim r^{1+\delta}\,, \tag{6.1}$$

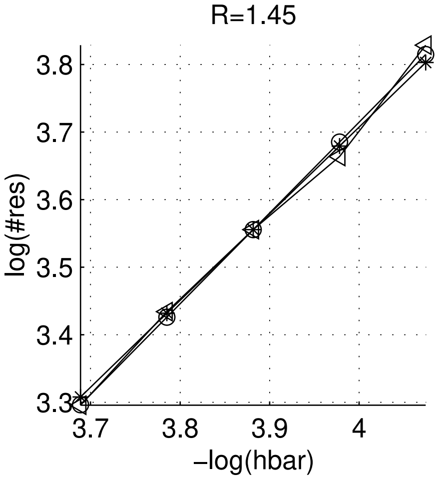


Figure 3: A plot of $\log(N_{res})$ as a function for $-\log(\hbar)$ for the potential shown in in Fig. 6. The value of $\hbar$ ranges from 0.025 to 0.017. Triangles represent numerical data, circles least squares regression, and stars the slope predicted by the conjecture.

where $m_\Gamma(s)$ is the multiplicity of the zero of the zeta function of Γ at s. We also changed the traditional convention: here $h^2 s(1-s) = z$ in the notation of previous sections, and $h(\text{Re } s - 1/2)$, $h\text{Im } s$ correspond to $\text{Im } z$, $\text{Re } z$ respectively.

An upper bound of this form was established in [35] but a simpler method giving improved upper bounds has been recently presented in [37]. The new method is based on zeta function techniques. What we obtain is a bound in the case of convex co-compact Schottky groups

$$\sum \{ m_\Gamma(s) \ : \ r \leq \text{Im } s \leq r+1 \,, \quad \text{Re } s > -C_0 \} \leq C_1 r^\delta \,, \tag{6.2}$$

where $\delta = \dim \Lambda(\Gamma)$. This improved estimate is a "fractal" version of (3.3): $1+\delta$ now plays the rôle of n. It is clear that the method works in greater generality and implementing it is part of an ongoing project.

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