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Resonances and complex absorbing potential method for the Wigner-von Neumann type Hamiltonian

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1 Introduction

1.1 Overview

In this talk, we study the Wigner-von Neumann type Hamiltonian P, which has a slowly decaying oscillatory potential.

A typical example is

$$P = -\frac{d^2}{dx^2} + a\frac{\sin 2x}{x} \quad \text{on} \quad L^2(\mathbb{R}),$$

where $a \in \mathbb{R}$.

We define the set of resonances $\mathrm{Res}(P)$ by a new complex distortion.

Moreover, we characterize resonances by the complex absorbing potential method:

$$\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon) = \mathrm{Res}(P),$$

where $P_\varepsilon = P - i\varepsilon x^2$ with $\varepsilon > 0$.

1.2 Basic spectral properties of Schrödinger operators

We take $V \in C(\mathbb{R}; \mathbb{R})$ such that $\lim_{|x| \to \infty} V(x) = 0$ and consider

$$P = -\frac{d^2}{dx^2} + V(x) \quad \text{on} \quad L^2(\mathbb{R}).$$

Then we have $\sigma_d(P) \subset (-\infty, 0)$ and $\sigma_{\mathrm{ess}}(P) = [0, \infty)$.

In this setting $\sigma_d(P)$ and $\sigma_{\mathrm{ess}}(P)$ basically correspond to bound states and scattering states, respectively.

A naive reasoning is that even if there exist classical bound states at positive energy, quantum states at positive energy will scatter to the infinity by the tunneling effect.

• There may be a positive eigenvalue; Wigner-von Neumann Hamiltonian.

• Classical bound states at positive energy create "hidden complex eigenvalues"; resonances.

1.3 Wigner-von Neumann Hamiltonian

Wigner and von Neumann(1929) constructed a Hamiltonian

$$P = -\frac{d^2}{dx^2} + V_{\mathrm{WvN}}(x) \quad \text{on} \quad L^2(\mathbb{R})$$

with $V_{\mathrm{WvN}}(x) = -8\frac{\sin 2x}{x} + \mathcal{O}(|x|^{-2})$ when $|x| \to \infty$ such that 1 is an eigenvalue of P (or its spherically symmetric three dimensional analogue).

The slow decay and oscillation are essential for the existence of positive eigenvalue: Kato(1959), Simon(1967).

Hamiltonians with slowly decaying oscillatory potentials (Wigner-von Neumann type Hamiltonian) have been investigated by many authors.

Problem 1: How about complex resonances?

1.4 What is resonance?

Resonances are the poles of meromorphic continuations of certain matrix elements of the resolvent or cutoff resolvent. They are analogous to discrete eigenvalues, which are poles of the original resolvent. Resonances represent quasi-steady states and they are also closely related to scattering theory (cf. Breit-Wigner formula).

For instance, assume $V(x)$ is analytic and decaying in $\{z = x + iy \in \mathbb{C}^d | |x| > R_0, |y| < K|x|\}$ for some $R_0 > 0$ and $K > 0$ (exterior dilation analyticity). Then for any $0 \not\equiv \chi \in C_c^\infty(\mathbb{R}^d)$, the cutoff resolvent $\chi(z - P)^{-1}\chi$ has a meromorphic continuation from the upper half plane to $\{z \in \mathbb{C} | -2\arctan K < \arg z < \pi\}$. The poles are called resonances of P and the set of resonances are denoted by $\mathrm{Res}(P)$.

1.5 Complex absorbing potential method

Zworski(2018) proved that for $P = -\Delta + V$ with $V \in L^\infty_{\mathrm{comp}}(\mathbb{R}^d)$ and $P_\varepsilon = P - i\varepsilon x^2$ with $\varepsilon > 0$,

$$\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon) = \mathrm{Res}(P)$$

in $\left\{ z \in \mathbb{C} \,\middle|\, -\frac{\pi}{4} < \arg z \le 0 \right\}$.

The proof employed the dilation analytic method.

Complex absorbing potential method is used in physical chemistry.

In the Fourier space, this is analogous to the viscosity limit for 1st order PDEs.

Zworski proposed a problem of finding V such that $\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon)$ is not discrete and took $V = \frac{\sin 2x}{x}$ as a candidate.

Problem 2: Study $\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon)$ for the Wigner-von Neumann type Hamiltonian P.

2 Results

2.1 Assumption

Assumption 1. The potential $V(x)$ has the following form:

$$V(x) = \sum_{j=1}^{J} s_j(x) W_j(x),$$

where $J \in \mathbb{N}$, $s_j \in C(\mathbb{R};\mathbb{R})$ are periodic functions with period π whose Fourier series converge absolutely, and $W_j \in C^\infty(\mathbb{R};\mathbb{R})$ have analytic continuations to the region $\{z = x + iy \in \mathbb{C} \mid |x| > R_0, |y| < K|x|\}$ for some $R_0 > 0$ and $K > 0$ with the bound $|W_j(z)| \le C|z|^{-\mu}$ for some $\mu > 0$ in this region.

- A typical example is $V(x) = a\frac{\sin 2x}{x}$ for $a \in \mathbb{R}$.
- By taking $s_j(x) = 1$, dilation analytic potentials are included.
- We work in one space dimension. How about the spherically symmetric

higher dimensional case?

- Unfortunately, the original Wigner-von Neumann potential

$$V_{\mathrm{WvN}}(x) = (1+g(x)^2)^{-2}(-32\sin x)(g(x)^3\cos x - 3g(x)^2\sin^3 x + g(x)\cos x + \sin^3 x),$$

where $g(x) = 2x - \sin 2x$, does not seem to satisfy the analyticity condition of Assumption 1.

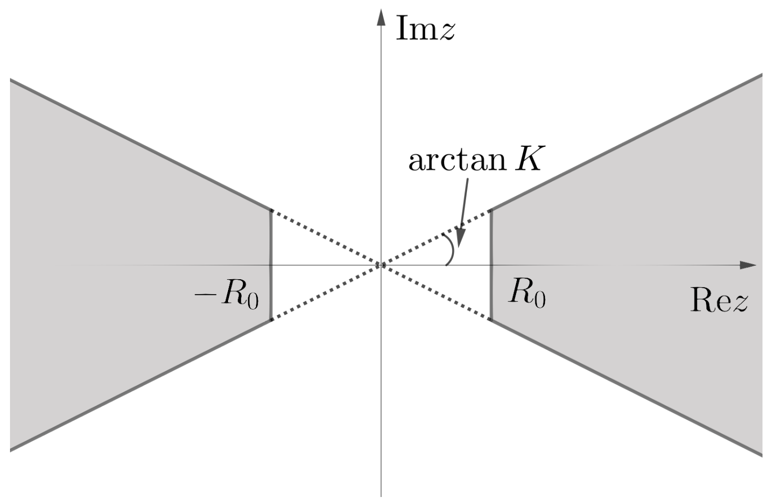

Figure 1 The domain of analyticity

2.2 Result 1

We set $R_+(z) = (z - P)^{-1}$ for $\mathrm{Im} z > 0$. We write the set of thresholds by $\mathcal{T} = \{n^2 \mid n \in \mathbb{N} \cup \{0\}\}$.

Theorem 1. *Under Assumption 1, there exists a complex neighborhood $\Omega \subset \mathbb{C}$ of $[0, \infty) \setminus \mathcal{T}$ such that the following holds: For any $f, g \in L^2_{\mathrm{comp}}(\mathbb{R})$, the matrix element $(f, R_+(z)g)$ has a meromorphic continuation to Ω.*

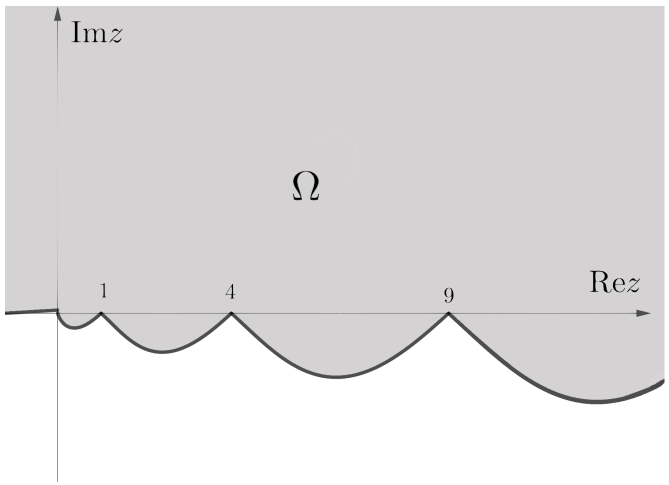

Figure 2 The domain Ω in theorems

2.3 Definition of resonances

We define resonances of P using Theorem 1.

Definition 1. A complex number $z \in \Omega$ is called a resonance if z is a pole of $(f, R_+(z)g)$ for some $f, g \in L^2_{\mathrm{comp}}(\mathbb{R})$. The multiplicity m_z is defined as the maximal number m such that there exist $f_1, \dots, f_m, g_1, \dots, g_m \in L^2_{\mathrm{comp}}(\mathbb{R})$ with $\det\bigl(\frac{1}{2\pi i}\oint_{C(z)}(f_i, R_+(\zeta)g_j)d\zeta\bigr)_{i,j=1}^{m} \neq 0$, where $C(z)$ is a small circle around z. The set of resonances is denoted by $\mathrm{Res}(P)$.

Remark 2.1. $\mathrm{Res}(P)$ is discrete in Ω and $m_z < \infty$ for any $z \in \Omega$.

- If z is not a resonance, we set $m_z = 0$.

2.4 Result 2

We recall $P_\varepsilon = P - i\varepsilon x^2$, where $\varepsilon > 0$. We easily see that P_ε, $\varepsilon > 0$, has purely discrete spectrum on $L^2(\mathbb{R})$.

Theorem 2. *Under Assumption 1, there exists a complex neighborhood $\Omega \subset \mathbb{C}$ of $[0, \infty) \setminus \mathcal{T}$ such that $\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon) = \mathrm{Res}(P)$ in Ω including multiplicities. In particular, $\lim_{\varepsilon \to 0} \sigma_d(P_\varepsilon)$ is discrete in Ω. More precisely, for any $z \in \Omega$ there exists $\rho_0 > 0$ such that for any $0 < \rho < \rho_0$ there exists $\varepsilon_0 > 0$ such that for any $0 < \varepsilon < \varepsilon_0$,*

$$\#\sigma_d(P_\varepsilon) \cap B(z, \rho) = m_z,$$

where $B(z, \rho) = \{w \in \mathbb{C} \mid |w - z| \leq \rho\}$.

- In particular, this disproves the conjecture by M. Zworski outside the thresholds.

3 Idea of the proofs

3.1 Review of complex distortion

Global dilation analyticity: Aguilar-Combes(1971).

We set $A = \frac{1}{2}(x \cdot D + D \cdot x)$ with $D = \frac{1}{i}\partial$. Then the unitary group $U_\theta = e^{i\theta A}$ generated by A is

$$U_\theta f = e^{i\theta A} f(x) = (\det \Phi_\theta'(x))^{\frac{1}{2}} f(\Phi_\theta(x)) = e^{d\theta/2} f(e^\theta x)$$

for $f \in L^2(\mathbb{R}^d)$. Here the dilation $\Phi_\theta(x) = e^\theta x$ is the flow of the vector field $v(x) = x$.

Consider the Schrödinger operator $P = -\Delta + V$ and define $P_\theta = U_\theta P U_\theta^{-1}$ for $\theta \in \mathbb{R}$. Note that $U_\theta(-\Delta)U_\theta^{-1} = e^{-2\theta}(-\Delta)$ has an analytic continuation with respect to θ.

Assume that $V_\theta = U_\theta V U_\theta^{-1}$ also has an analytic continuation with respect to θ (and $-\Delta$-compact). Then P_θ is well-defined for complex θ and $\sigma_{\mathrm{ess}}(P_\theta) = e^{-2i\mathrm{Im}\theta}[0, \infty)$.

The simple formula

$$(f, R_+(z)g) = (U_{\overline{\theta}}f, (z - P_\theta)^{-1}U_\theta g)$$

is valid for complex θ if f, g are analytic vectors for A. We consider $\mathrm{Im}\theta > 0$. This implies that $(f, R_+(z)g)$ has a meromorphic continuation and resonances are defined in $\{z \in \mathbb{C} | -2\mathrm{Im}\theta < \arg z \leq 0\}$. Moreover, resonances coincide with discrete eigenvalues of P_θ.

Hunziker-type distortion: Hunziker(1986).

Take a vector field v on $\mathbb{R}^d$ such that $v(x) = x$ for $|x| \gg 1$ and $v(x) = 0$ for $|x| \leq R_0 + 1$, and set $\Phi_\theta(x) = x + \theta v(x)$ rather than the flow of v. Set $U_\theta f(x) = (\det \Phi'_\theta(x))^{\frac{1}{2}} f(\Phi_\theta(x))$ and $P_\theta = U_\theta P U_\theta^{-1}$.

Then the resonance theory can be constructed under the assumption that $V(x)$ is analytic and decaying in $\{x \in \mathbb{C}^d || \mathrm{Re}x| > R_0, |\mathrm{Im}x| < K|\mathrm{Re}x|\}$ for some $R_0 > 0$ and $K > 0$. Then P_θ has an analytic continuation with respect to θ and resonances coincide with its eigenvalues.

There are other distortions;

Momentum distortion: Sigal(1984), Cycon(1989), Nakamura(1990).
Complex distortion on the Fourier space for exponentially decaying or dilation analytic potentials.

Microlocal distortion: Helffer-Sjöstrand(1986).
Based on microlocal and geometric viewpoints. Powerful but difficult.

Geometric complex scaling: Sjöstrand-Zworski(1991).
Distortion on the configuration space. Based on more geometric viewpoint than Hunziker. This enables us to study resonances in a larger angle in the complex plane.

3.2 Relation with Mourre inequality

General idea Let P and A be self adjoint operators.
Formally speaking, analyticity of $P_\theta = e^{i\theta A} P e^{-i\theta A}$would mean that

$$\sum_{j=0}^{\infty} \frac{1}{j!} \mathrm{ad}(i\theta A)^j P$$

converges for complex θ. If $\theta = i\delta$ with $\delta > 0$, the leading part of the imaginary part of P_θ is $-\delta[P, iA]$. Thus, to define the resonances, it will be enough to find A such that

1. $[P, iA]$ is positive for some energy interval I of P, that is the Mourre inequality with a compact remainder K holds;
$$E_I(P)[P, iA]E_I(P) \geq cE_I(P) + K$$
in the quadratic form sense.
2. The repeated commutators $\mathrm{ad}(iA)^j P$ are well-behaved for $j \geq 0$.
This does not hold for our P with $A = \frac{1}{2}(x \cdot D + D \cdot x)$ since $D^j V(x)$ does not decay faster than $V(x)$.

3.3 Mourre estimate with difference conjugate operator

Nakamura(2015) showed that the Mourre theory can be constructed using a difference conjugate operator

$$A' = \frac{1}{2}(x \cdot D' + D' \cdot x), \quad D'u(x) = \frac{1}{2\pi i}(u(x+\pi) - u(x-\pi))$$

under the assumption that $x\Delta^\pi V$ is $-\frac{d^2}{dx^2}$-compact and $x^2\Delta^\pi\Delta^\pi V$ is $-\frac{d^2}{dx^2}$-bounded, where $\Delta^\pi u(x) = \frac{1}{\pi}(u(x+\pi) - u(x))$.
In the Fourier space, A' is a differential operator

$$\widetilde{A'} = \frac{1}{2\pi}\big((i\partial_\xi) \cdot \sin(\pi\xi) + \sin(\pi\xi) \cdot (i\partial_\xi)\big).$$

Thus

$$[\xi^2, i\widetilde{A'}] = \frac{2}{\pi}\sin(\pi\xi)\xi$$

is positive or negative when $|\xi| \notin \mathbb{Z}_{\geq 0}$. Thus the Mourre inequality holds for $\pm A'$ in $[0,\infty) \setminus \mathcal{T}$. (In higher dimensional case, we can treat low energy regime $(0,1)$.)
Moreover, $\mathrm{ad}(iA')^j V$ is bounded any $j \geq 0$ if $V = a\frac{\sin 2x}{x}$.

3.4 Periodic Fourier complex distortion

The above considerations lead us to consider $e^{i\theta\widetilde{A'}}$, which is the pullback by the flow of $\sin(\pi\xi)$.

In place of $e^{i\theta\widetilde{A'}}$, we take Hunziker-type distortion in the Fourier space

$$\Phi_\theta(\xi) = \xi + \theta \sin(\pi\xi), \quad U_\theta f(\xi) = \Phi'_\theta(\xi)^{\frac{1}{2}} f(\Phi_\theta(\xi)),$$

where $\theta \in (-\pi^{-1}, \pi^{-1})$.

In the Fourier space, P has the form $\widetilde{P} = \xi^2 + \widetilde{V}$, where $\widetilde{V} = (2\pi)^{-1/2}\hat{V}*$ is a convolution operator and $\hat{V}$ is the Fourier transform $\hat{V}(\xi) = (2\pi)^{-1/2}\int V(x)e^{-ix\xi}dx$.

Then we define our distorted operator

$$\widetilde{P}_\theta := U_\theta \widetilde{P} U_\theta^{-1} = (\xi + \theta\sin(\pi\xi))^2 + \widetilde{V}_\theta, \quad \widetilde{V}_\theta = U_\theta \widetilde{V} U_\theta^{-1}.$$

This is our **periodic Fourier complex distortion.**

3.5 Analyticity of $\widetilde{V}_\theta$

Lemma 1. *Under Assumption 1, $\widetilde{V}_\theta$ is analytic with respect to θ and ξ^2-compact for θ in some complex neighborhood of $\{i\delta \mid -K\pi^{-1} < \delta < K\pi^{-1}\}$, where K is the constant in Assumption 1. Moreover, for any $\gamma > 0$ there is a decomposition $\widetilde{V}_\theta = \widetilde{V}_{\theta,1} + \widetilde{V}_{\theta,2}$ such that $\|\widetilde{V}_{\theta,1}\|_{H^{-N}\to H^N} < \infty$ for any $N > 0$ and $\|\widetilde{V}_{\theta,2}\|_{L^2\to L^2} < \gamma$.*

This is the most technical part of our arguments and we omit it. But for the model case $V(x) = a\frac{\sin 2x}{x}$, the proof is much simpler. In this case, one can show that $\widetilde{V}_\theta f(\xi) = (\Phi_\theta')^{\frac{1}{2}}\widetilde{V}(\Phi_\theta')^{\frac{1}{2}} f(\xi)$ by simple computations using the special form of $\widetilde{V} = \frac{a}{2}\chi_{[-2,2]}*$. Then the Lemma 1 for this case follows by an easy argument.

3.6 Essential spectrum of deformed operator

Lemma 1 implies that $\widetilde{P}_\theta$ is analytic with respect to θ and the essential spectrum of $\widetilde{P}_\theta$ is given by $\sigma_{\rm ess}(\widetilde{P}_\theta) = \left\{ (\xi + \theta \sin(\pi\xi))^2 \;\middle|\; \xi \in \mathbb{R} \right\}$.

For the energy interval $((n-1)^2, n^2)$, we take $\theta = (-1)^n i\delta = \pm i\delta$. We set $\delta_0 = \min\{\pi^{-1}, K\pi^{-1}\}$ and consider $0 < \delta < \delta_0$. We set $\Omega_{n,\delta}$ as in Figure 4.

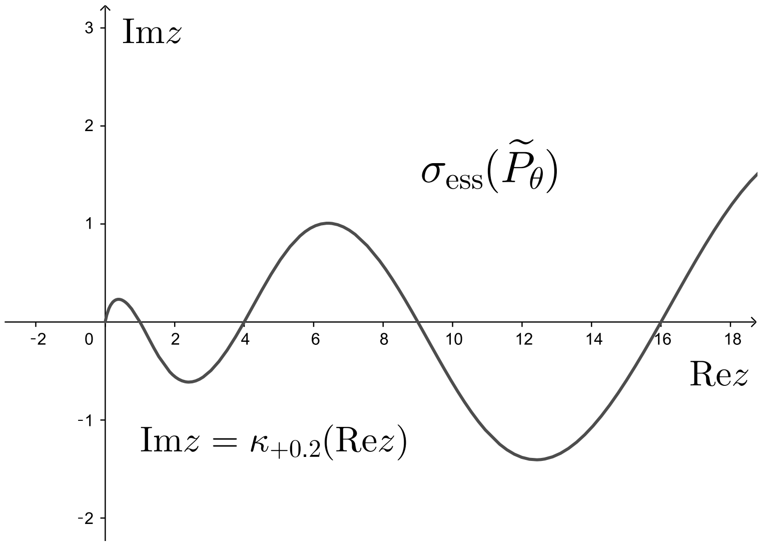

Figure 3 $\sigma_{\rm ess}(\widetilde{P}_\theta)$ for $\theta = 0.2i$.

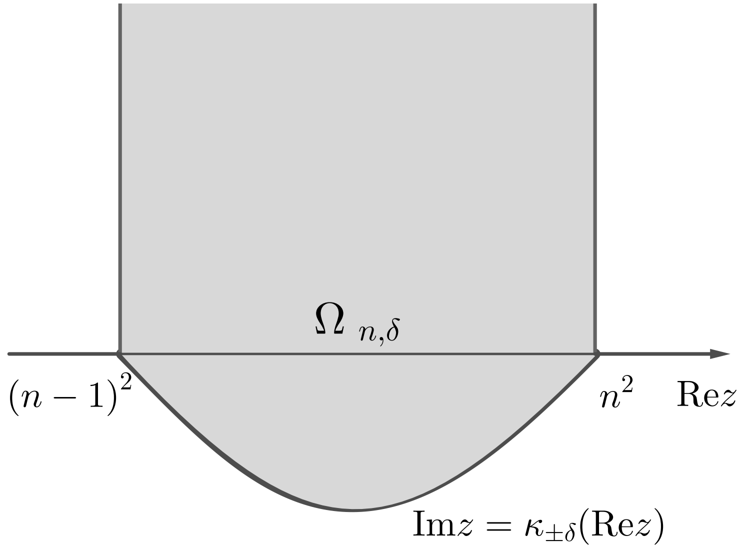

Figure 4 The region $\Omega_{n,\delta}$.

3.7 Definition of resonances

Then Theorem 1 is true for $\Omega = \bigcup_{n \in \mathbb{N}} \Omega_{n,\delta_0}$.

Basically, the proof of Theorem 1 follows the standard arguments of resonance theory once we prove the analyticity of $\widetilde{P}_\theta$.

Here are some remarks:

- For the set of analytic vectors, we take $\mathcal{A} = L^2_{\mathrm{comp}}(\mathbb{R})$. Since the Fourier transform of $f \in \mathcal{A}$ is analytic, $U_\theta \hat{f}$ is analytic with respect to θ.

- Resonances coincide with the discrete eigenvalues of $\widetilde{P_\theta}$ including multiplicities using the formula

$$(f, R_+(z)g) = (U_{\overline{\theta}} \hat{f}, (z - \widetilde{P_\theta})^{-1} U_\theta \hat{g}).$$

In particular, $\mathrm{Res}(P)$ is discrete and $m_z < \infty$ for any $z \in \Omega$.

3.8 Viscosity limit

The proof follows the strategy of Zworski(2018) replacing complex dilation by our periodic Fourier complex distortion.

In the Fourier space, P_ε has the following form:

$$\widetilde{P}_\varepsilon = \xi^2 + \widetilde{V} + i\varepsilon\partial_\xi^2.$$

We set $\widetilde{P}_{\varepsilon,\theta} = U_\theta \widetilde{P}_\varepsilon U_\theta^{-1}$. Then $\sigma_d(\widetilde{P}_{\varepsilon,\theta}) = \sigma_d(\widetilde{P}_\varepsilon)$ including multiplicities by the analyticity with respect to θ.

Thus it is enough to show $\lim_{\varepsilon\to 0} \sigma_d(\widetilde{P}_{\varepsilon,\theta}) = \sigma_d(\widetilde{P}_\theta)$. We prove this by Gohberg-Sigal theory and their operator valued Rouché's theorem.

We first consider the distorted free Hamiltonian ($\widetilde{P}_{\varepsilon,\theta}$ with $V = 0$)

$$\widetilde{Q}_{\varepsilon,\theta} = (\xi + \theta\sin(\pi\xi))^2 - i\varepsilon D_\xi (1 + \pi\theta\cos(\pi\xi))^{-2} D_\xi - i\varepsilon r_\theta(\xi), \quad \varepsilon \geq 0.$$

We employ the semiclassical microlocal analysis in the Fourier space with the semiclassical parameter $h = \sqrt{\varepsilon}$ to obtain a resolvent estimate

$$\|(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}\|_{L^2 \to L^2} \leq C$$

for small $\varepsilon > 0$. The semiclassical limit corresponds to the viscosity limit.

By a perturbation argument and operator valued Rouché's theorem, it suffices to show

$$\lim_{\varepsilon \to 0} \|\widetilde{V}_\theta(\widetilde{Q}_{0,\theta} - w)^{-1} - \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}\|_{L^2 \to L^2} = 0. \tag{1}$$

By the second part of Lemma 1, we can replace $\widetilde{V}_\theta$ by a smoothing $\widetilde{V}_{\theta,1}$. By the resolvent equation, we also learn

$$\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta} - w)^{-1} - \widetilde{V}_{\theta,1}(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$$

$$= -i\varepsilon \widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta} - w)^{-1}(D_\xi(1 + \pi\theta\cos(\pi\xi))^{-2}D_\xi + r_\theta(\xi))(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}.$$

Since $\widetilde{V}_{\theta,1} : H^{-2} \to L^2$,

$$\|\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta} - w)^{-1} - \widetilde{V}_{\theta,1}(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}\|_{L^2 \to L^2} \leq C\varepsilon,$$

which completes the proof. We can take $\Omega = \bigcup_{n \in \mathbb{N}} \Omega_{n,\delta_1}$ with $\delta_1 = \min\{(\sqrt{2} - 1)\pi^{-1}, K\pi^{-1}\}$.

4 Summary

• We defined the resonances for the Wigner-von Neumann type Hamiltonian by introducing periodic complex distortion in the Fourier space.

• We also characterized resonances as limit points of discrete eigenvalues in the viscosity-type limit.

Problems

- Relation with quasi-steady states.
- Relation with scattering theory.
- Spherically symmetric higher dimensional case.
- Resonances for the original Wigner-von Neumann Hamiltonian.
- Structure of resolvent near threshold.

Thank you for listening!