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Bounds on resolvents of dilated Schrödinger operators with non trapping potentials

BOUNDS ON RESOLVENTS OF DILATED SCHRODINGER OPERATORS WITH NON TRAPPING POTENTIALS

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ABSTRACT :

We provide bounds on resolvents of dilated Schrödinger operators via an exterior scaling. It is done under a non trapping condition on the potential which has a clear interpretation in classical mechanics. These bounds are a powerful tool to prove absence of resonances due to the tail of the potential in the shape resonance problem.

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In the following we consider the Schrödinger operator

$$H = -k^4 \Delta + V$$

on $L^2(\mathbb{R}^n \setminus K)$, $K = \{ x \in \mathbb{R}^n, |x| \le r_0 \}$, $r_0 > 0$

with a Dirichlet boundary condition on ∂K in the classical limit $k \downarrow 0$.

The precise conditions on V are given below. Most important is a suitable "non trapping condition" which allows to prove the absence of resonances for H in a k-independent neighbourhood of some fixed energy $E > 0$. To define the physically intuitive though vague notion of resonances, we use the concept of "Dilation-analicity", [AC] , (more precisely, the method of exterior complex scaling).
This consists in associating to H a 1-parameter family of "dilated Hamiltonians" H(θ) for θ belonging to some strip $|Im\,\theta| < \alpha$. This complex deformation will rotate the essential spectrum of H

by an angle $-2\,Im\,\theta$ and eigenvalues of H(θ) appearing in the sector

$$\{ -2\,Im\,\theta < Arg\,z < 0 \}$$

will be called resonances of H. They correspond to poles of the analytic continuation of expectations values of the resolvent (H-z) to "the second sheet".

Our interest in proving absence of resonances for the Dirichlet operator in $\mathbb{R}^n \setminus K$ comes from investigating the shape resonance problem [CDS2],[CDKS] .

Consider a potential V on $\mathbb{R}^n$ tending to zero at infinity with an absolute minimum $v_0 \ge 0$ within $K = \{ x \in \mathbb{R}^n, |x| \le r_0 \}$. Assume V strictly bigger than v_0 on ∂K.

It is physical folklore that a particle with energy E near v_0 and initially localized within K will penetrate the barrier around K and tunnel to infinity thus representing a resonance for H.

To render this precise it is convenient to decouple the potential well within K from the exterior domain by a fictitious Dirichlet boundary condition on ∂K. The associated Dirichlet Hamiltonian has point spectrum (due to the interior) embedded in the continuum (due to the exterior). Let E be an eigenvalue of the interior Dirichlet operator.

Rotating the essential spectrum by $-2\,Im\,\theta$ using the exterior scaling allows to remove perturbatively the Dirichlet condition on ∂K and a convergent "tunneling expansion",[CDS1], for the complex resonance near E can be obtained provided the exterior part of the potential in $\mathbb{R}^n \setminus K$ does not produce itself resonances in a sufficiently big complex neighbourhood of the energy E under consideration.

It is possible to prove absence of resonances due to the exterior by investigating the numerical range of H(θ) leading to global results holding for all energies in $\mathbb{R}^+$ [CDS 3] .

Here we sketch a local method which gives much stronger results near some fixed energy E [DK].

To start with, let us briefly recall definition and basic properties of exterior complex scaling [S] ,[GY] .

For $\theta \in \mathbb{R}$ consider the 1-parameter group of transformations

$$S(\theta) x = (r_0 + e^{\theta}(|x| - r_0)) \frac{x}{|x|} \qquad (x \in \mathbb{R}^n \setminus K) \qquad (1)$$

$$= r_\theta \, \omega$$

$S(\theta)$ induces in $L^2(\mathbb{R}^n \setminus K)$ an unitary mapping $U(\theta)$. Changing to polar coordinates

$$r = |x| \quad , \quad \omega = \frac{x}{|x|} \qquad \text{via}$$

$$\vartheta : L^2(\mathbb{R}^n \setminus K) \to L^2([r_0, \infty[\times S^{n-1})$$

$$(\vartheta f)(r, \omega) = r^{\frac{n-1}{2}} f(r\omega)$$

one finds for the dilated Laplacian

$$H_0(\theta) = U(\theta)(-\Delta) U^{-1}(\theta)$$

$$= -e^{-2\theta} D^2 + \frac{\Lambda}{r_0^2} \qquad (2)$$

where $D = \vartheta^{-1} \frac{d}{dr} \vartheta$, r_θ are defined by (1) and Λ corresponds to the Laplace Beltrami on S^{n-1}.

$H_0(\theta)$ extends analytically to a strip $|\text{Im } \theta| < \pi$ as a selfadjoint family of type A in the sense of Kato [K] with domain $H_0^2(\mathbb{R}^n \setminus K)$.

The spectrum of $H_0(\theta)$ is equal to $e^{-2\theta} \mathbb{R}^+$.

We assume that the potential V satisfies :

C1 : The multiplication operator in $L^2(\mathbb{R}^n \setminus K)$
$$V_\theta(x) = V(S(\theta)x) \, , \quad \theta \in \mathbb{R}$$
possesses an analytic continuation as a bounded operator to some strip

C2 : V is a positive C^3 function on $\mathbb{R}^n \setminus K$ with bounded derivatives $|\partial^\alpha V|$, $(|\alpha| \leq 3)$ and $\limsup\limits_{|x| \to +\infty} V(x) < E$ (for some $E \in \mathbb{R}^+$).

C3 : V is non-trapping at energy E i.e. :

There is an open set $\Omega \supset K$ with $\bar{\Omega}$ contained in the interior of $\{x \in \mathbb{R}^n, V(x) \geqslant E\}$ such that

(NTa) $\quad 2 \dfrac{r-r_0}{r} (V-E) + (r-r_0) \dfrac{\partial V}{\partial r} \leqslant -S$

on $\mathbb{R}^n \setminus \Omega$ for some $S > 0$

and

(NTb) $\quad V(x) \geqslant \min \{V(x), x \in \partial\Omega\}$, $\quad (x \in \Omega \setminus K)$

Our basic result on absence of resonances is

Theorem 1 :

Let V satisfy C1 – C3 . Let $H(\theta) = H_0(\theta) + V(\theta)$ be defined by exterior scaling ($|\text{Im}\,\theta| < \alpha$). Then

$\exists \alpha_0 > 0$, $\forall\, 0 < \text{Im}\,\theta < \alpha_0$, $\exists\, k_\theta > 0$,

$\exists$ a complex ngbh $W_\theta \ni E$ in the resolvent set of $H(\theta)$ such that

$$\| (H(\theta)-z)^{-1} \| \leqslant C\, |\text{Im}\,\theta|^{-1} \, , \quad (z \in W_\theta \, , \; k < k_\theta) \qquad (3)$$

Remark :

Writing $z = E + w_1 + i w_2$, $\quad w_1, w_2 \in \mathbb{R}$

W_θ can be taken to be of size

$$|w_2| < \tfrac{1}{20} S \; , \quad -\text{Im}\,\theta\, \tfrac{1}{10} S < w_2 < \tfrac{1}{40} S\, (\text{Im}\,\theta)^{-1} \, , \quad (\text{Im}\,\theta > 0)$$

(provided $\min \{V(x), x \in \partial\Omega\} \geqslant E + \tfrac{1}{5} S$).

Furthermore, the constant C in (3) is inversely proportional to S. W_θ and C thus depend on the potential only via the Non-trapping condition (NT).

Theorem 1 is proved by an a priori estimate via a Mourre's inequality [M] :

Lemma :

Let H be selfadjoint with domain $D(H)$ and $B \geqslant 0$ be bounded. then

$$\| (H-z \mp iB)\, f \| \geqslant |\text{Im}\,z|\, \| f \| \, , \quad (f \in D(H), \; \text{Im}\,z \gtrless 0) \qquad (4)$$

It suffices to consider purely imaginary $\theta = i\beta \in i\mathbb{R}^+$. To motivate our condition (NT) and to clarify the idea behind the proof of Theorem 1, we make the following heuristic argument :

denoting the infinitesimal generator of $U(\theta)$ by A, formal linearization of $H(\theta)$ gives $H + \theta i [A, H]$.

Comparing with (4) we expect an a priori estimate for small θ if $i [A, H]$ is strictly negative.

Writing $a = (|x| - r_0) \frac{x}{|x|} \cdot \xi$, $h = k^4 \xi^2 + V$

for the principal symbols of A and H, we compute the Poisson bracket $\{h, a\}$ at energy $E = k^4 \xi^2 + V(x)$ and find

$$\{h, a\}\Big|_{E = k^4 \xi^2 + V} = (r - r_0) \frac{\partial V}{\partial r} + 2(V - E)(r - r_0) - 2 \frac{r_0}{r} k^4 \frac{(\xi \cdot x)^2}{r^2}\Big|_{E = k^4 \xi^2 + V} \quad (5)$$

Negativity of $\{h, a\}$ at energy E implies the absence of closed trajectories for the hamilton field X_h in $h^{-1}(E)$. Since a attains its maximum on each compact set and a increases strictly along the integral curves of X_h these will eventually leave each compact set in $h^{-1}(E)$. The last term on the r.h.s. of (5) representing a radial kinetic energy becomes zero for ξ orthogonal to x. This corresponds to purely rotational motion and is the worst case to consider if one tries to prove absence of resonances. Neglecting therefore this term in (5) we found (NTa).

Note that (NTb) forbids tunneling from $\mathbb{R}^n \setminus \Omega$ to Ω .

In order to exploit this classical ideas in the limit $k \searrow 0$ we choose a small intervall $J = [E - \delta, E + \delta]$ with $\min\{V(x), x \in \partial \Omega\} > E + \delta$ We denote by $P = P_J(H)$ the spectral projection for H associated to J and let $Q = 1 - P$.

For purely algebrical reasons we prefer to cancel the factor $e^{-2\theta}$ in (2) and we denote by $\tilde{H}(\theta, z)$ the formal linearization of $e^{2\theta}(H(\theta) - z)$ in $\theta \in i\mathbb{R}^+$.

It is explicitly given by ($z = E + w_1 + i w_2$)

$$\tilde{H}(\theta, z) = H_r + i \beta H_i \quad \text{where} \quad (6)$$

$$H_r = H - w_1 + 2 \beta w_2$$

$$H_i = 2(V - E) + (r - r_0) \frac{\partial V}{\partial r} + 2 \frac{r_0}{r} k^4 \frac{\Lambda}{r^2} - 2 w_1 - \beta^{-1} w_2$$

We proceed by giving an a priori extimate for different ranges of energy.

<u>Theorem 2</u> :

$\exists\ a, b, d_o > 0\ ,\ \forall\ 0 < \text{Im}\ \theta < d_o\ ,$ $\exists$ a complex

neighbourhood $W_\theta \ni E\ ,\ \exists\ k_\theta > 0$

$$\|\ \tilde{H}(\theta, z)\ P\ \mathcal{L}\ \| \geqslant\ a\ |\theta|\ \|P\mathcal{L}\|$$ (7a)

$$(k < k_\theta\ ,\ z \in W_\theta\ ,\ \mathcal{L} \in D(H))$$

$$\|\ \tilde{H}(\theta, z)\ Q\ \mathcal{L}\ \| \geqslant\ b\ \|Q\mathcal{L}\|$$ (7b)

(7b) is essentially a consequence of the spectral theorem and some control on the imaginary part of H. From now on we stop writing the explicit dependance on θ , z .

The difficult part of Theorem 2 is (7a). Here it is essential to use that for $k \searrow 0$ $P\mathcal{L}$ is strongly localized outside the region which is classically forbidden for particles with energy within J. More precisely, let $\chi \in C_o^\infty (\mathbb{R}^n)$ be a cut off function supported outside a neighbourhood of

$$\{ x \in \mathbb{R}^n\ ,\ V(x) \leqslant E + \delta\ \}$$. Then

$$\|\ \chi P \mathcal{L}\ \| \leqslant\ C_p\ k^p\ \|P\mathcal{L}\|\ ,\ (p \in \mathbb{N})$$ (8)

This result can be proved by smoothing out the characteristic function of J to some C_o^∞ function F supported in a slightly enlarged interval and doing some commutator estimates on

$$\chi\ F(H)\ =\ \chi \int_\mathbb{R}\ \hat{F}(t)\ e^{-itH}\ dt\ .$$

Alternatively one can use bounds on

$$\|\ \chi\ (H - z - i k^p)\ \mathcal{L}\ \|\qquad (z \in J)$$

and Stone's formula [COKS] .

By some simple commutator estimate the rotational energy operator

$$\mathcal{L}\ \frac{r_o}{r}\ k^4\ \Lambda\qquad$$ in the imaginary part of $\tilde{H}$ can be bounded on

the energy range J by $\mathcal{L}\ \frac{r_o}{r}\ (E + \delta - V)$ modulo a small error of order k^2 P.

Thus (NTa) guarantees negativity of H_i in the classically accessible region

$$\{ x \in \mathbb{R}^n,\ V(x) \leqslant E + \delta \}\quad .$$

Using (8) it is now possible to modify H_i (applied to $P\mathcal{L}$) to become a strictly negative bounded operator while making errors

of order $k^2\ \|P\mathcal{L}\|$ (this order of magnitude is determined by

some   commutators   which   behave   typically   like

$$k^4 \| \nabla P \underline{\ell} \| \leq C k^2 \| P \underline{\ell} \|$$).

Thus (7a) is a direct consequence of the Mourre inequality (4).

To give a proof of Theorem 1 observe that

$$\| \tilde{H} \underline{\ell} \|^2 \geq \| \tilde{H} P \underline{\ell} \|^2 + \| \tilde{H} Q \underline{\ell} \|^2 \tag{9}$$
$$- 2 | (Q \underline{\ell}, \tilde{H}^* \tilde{H} P \underline{\ell}) |$$
$$\geq C | \theta |^2 \| \underline{\ell} \|^2$$

for some $C > 0$ and $| \theta |$ small.
Here we used (7a) , (7b) and the fact that the mixed term

$$| (Q \underline{\ell}, \tilde{H}^* \tilde{H} P \underline{\ell}) |$$ is   small   compared   to   the   rest   which

involves agin some commutator analysis.

It remains to justify the linearisation procedure. Using (2) and
C1 this boils down to a remainder estimate in the Taylor
expansion of

$$e^{2\theta} \frac{r^2}{r_\theta^2}$$

An explicit calculation gives

$$\| (e^{2\theta} (H(\theta) - z) - \tilde{H}) \underline{\ell} \| \leq C | \theta |^2 \{ \| \underline{\ell} \| + \| \tilde{H} \underline{\ell} \| \} \tag{10}$$

$$(\underline{\ell} \in D(H))$$

and one obtains from (9)

$$\| (H(\theta) - z) \underline{\ell} \| \geq C | \theta | \| \underline{\ell} \| \quad , \quad (\underline{\ell} \in D(H)) \tag{11}$$

for z sufficiently close to E.

Now by a standard argument [M], the a priori estimate (11) and
the fact that H(θ) is a closed operator imply existence of the
resolvent for z near E. The explicit bound in (3) follows
directly from (11).

REFERENCES

[AC] J. AGUILAR, J.M. COMBES : A Class of Analytic Perturbation for One-body Schrödinger Hamiltonians. Comm. Math. Phys.22 269-279 (1971).

[CDKS] J.M. COMBES, P. DUCLOS, M. KLEIN and R. SEILER : On the shape resonance in the classical limit. To appear.

[CDS1] J.M. COMBES, P. DUCLOS, R. SEILER : Convergent Expansions for Tunneling. Comm. Math. Phys.92, 229-245 (1983).

[CDS2] J.M. COMBES, P. DUCLOS, R. SEILER : On the shape Resonance in "Resonances-Models and Phenomena", Springer Lecture notes in Physics,211, 64 (1984)

Resonances and scattering in the classical limit. Proceedings of "Méthode semi-classique en Mécanique Quantique". Publication de l'université de Nantes (1985).

[CDS3] J.M. COMBES, P. DUCLOS, R. SEILER : One dimensional shape resonances. CPT-85/P.? . To appear.

[DK] P. DUCLOS, M. KLEIN : On the absence of resonances for some Schrödinger in the classical limit. Preprint CPT-85/P.?. To appear.

[GY] S. GRAFFI, K. YAJIMA : Exterior scaling and the AC-stark effect in a Coulomb Field. Comm. Math. Phys.89, 277-301 (1983)

[K] T. KATO : Perturbation theory for linear operators. Berlin-Heidelberg-New York : Springer 66.

[M] E. MOURRE : Absence of Singular Continuous Spectrum for certain Self-Adjoint Operators. Comm. Math. Phys.78, 391-408 (1981).

[S] B. SIMON : The definition of Molecular Resonances Curves by the Method of Exterior Complex Scaling. Phys. Letters 71A, 211-214 (1979).