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On the Absence of Resonances for Schrödinger Operators with Non-Trapping Potentials in the Classical Limit

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Abstract. We provide bounds on resolvents of dilated Schrödinger operators via exterior scaling. This depends crucially on a non-trapping condition on the potential which has a clear interpretation in classical mechanics. These bounds imply absence of resonances due to the tail of the potential in the shape resonance problem.

1. Introduction

This paper is motivated by recent work on the shape resonance problem [CDS 2], [CDKS] for Schrödinger operators $H=-k^4\Delta+V$ in the classical limit $k\downarrow 0$ and a related treatment of the predissociation problem for molecules given by a system of coupled Schrödinger equations [K].

In the analysis of the shape resonance and predissociation it is crucial to know that the operator H in the exterior of some suitably chosen ball with Dirichlet condition on its boundary $K=\{|x|=r_0\}$ does not possess any resonances in a sufficiently big neighborhood of some fixed energy $E>0$, resonances being defined by exterior complex scaling introduced by Simon [S] (see also [GY]). Furthermore a bound on the dilated resolvent $(H(\vartheta)-z)^{-1}$ is needed for z near E. We refer to [CDKS] for further details on the shape resonance problem and all motivation concerning the specific choice of the boundary sphere K and the energy E under consideration.

In this paper we prove absence of resonances by an *a priori* estimate via a simple inequality which was used in the work of Mourre [M 1, M 2] to discuss the propagation properties of quantum states for fixed Planck's constant $k=1$. The method allows us to handle potentials which are not $-\Delta$-compact. It depends crucially on negativity of the commutator $i[A,H]$ localized in energy, where A denotes the infinitesimal generator of the exterior scaling group. Classically this corresponds to negativity of the Poisson bracket $\{h,a\}$ between the principal symbols of H and A at some fixed energy E and is to be interpreted as a non-trapping condition on the potential [see (C3) below].

We remark that conditions involving more general "escape functions" $a(x, \xi)$ have been used in the approach of Helffer/Sjostrand [HS] to the problem of resonances in the classical limit.

With $a(x, \xi)=(|x|-r_0)\frac{x}{|x|}\cdot\xi$, a simple computation gives ($|x|=r$)

$$\{h, a\}|_{E=h(x,\xi)}=(r-r_0)\frac{\partial V}{\partial r}+2(V-E)\frac{r-r_0}{r}-2\frac{r_0}{r}k^4\frac{(\xi\cdot x)^2}{r^2}\bigg|_{E=h(x,\xi)}. \quad (1.1)$$

Our non-trapping condition (C3) requires the first two terms on the right-hand side of (1.1) to be negative. Thus a increases strictly along the integral curves of the Hamilton field X_h, and these will eventually leave each compact set in $h^{-1}(E)$. For Quantum Mechanics in the classical limit this is shown to imply absence of resonances for the Dirichlet operator in the exterior domain.

The plan of this paper is as follows. In Sect. 2 we review exterior complex scaling and introduce the assumptions imposed on the potential V. In Sect. 3 we prove our main result, Theorem 1, granted a linearized version in Theorem 2. The proof of Theorem 2 is given in Sect. 4 using a simultaneous localization in energy and space. This is possible in the classical limit since, roughly speaking "each commutator term occurring in the proof is of order k^2 when restricted to a subspace of finite energy." Estimates of the latter type are contained in the Appendix.

2. Exterior Complex Scaling and Basic Definitions

In $L^2(\Omega_e)$, $\Omega_e=\{x\in\mathbb{R}^n\colon |x|>r_0\}$, we transform to polar coordinates $r=|x|$, $\omega=\frac{x}{|x|}$ via the unitary map

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

The radial derivative $\frac{d}{dr}$ in $L^2([r_0,\infty)\times S^{n-1})$ is mapped into $D=\frac{n-1}{2r}+\omega\nabla$, and we have $-\Delta=-D^2+\frac{\Lambda}{r^2}$, where Λ corresponds to $B+\frac{1}{4}(n-1)(n-3)$, $B\geqq 0$ being the Laplace-Beltrami operator on S^{n-1}.

Letting $r_\vartheta=r_0+e^\vartheta(r-r_0)$, ($r>r_0$, $\vartheta\in\mathbb{R}$) one defines the exterior scaling group in polar coordinates by

$$(U(\vartheta)f)(r,\omega)=e^{\vartheta/2}f(r_\vartheta,\omega), \quad (2.1)$$

and obtains for the scaled Laplace operator

$$-\Delta(\vartheta)=U(\vartheta)(-\Delta)U(\vartheta)^{-1}=-e^{-2\vartheta}D^2+\frac{\Lambda}{r_\vartheta^2}. \quad (2.2)$$

We consider Schrödinger operators $H=-k^4\Delta+V$ on $L^2(\Omega_e)$ with a Dirichlet boundary condition on $K=\{|x|=r_0\}$, where V is supposed to satisfy the following conditions:

(C1):

$V(\vartheta)=U(\vartheta)VU(\vartheta)^{-1}$ possesses an analytic continuation as a bounded operator to some strip $S_\alpha=\left\{|\mathrm{Im}\,\vartheta|<\alpha<\frac{\pi}{4}\right\}$.

(C2):

V is a positive C^3-function on Ω_e with bounded derivatives $\partial^\alpha V$ ($|\alpha|\leqq 3$) and $\overline{\lim_{x\to\infty}}\, V(x)<E$ for some $E>0$.

(C3):

"The constant E in (C2) is a non-trapping energy for V," i.e.

(NT1):

$K\subset J_E=\{x\in\bar{\Omega}_e\colon V(x)>E\}$.

(NT2):

There is $S>0$ such that

$$2\frac{r-r_0}{r}(V(x)-E)+(r-r_0)\frac{\partial V}{\partial r}(x)<-S \qquad (x\in\Omega_e\backslash J_E). \tag{2.3}$$

Assuming (C1) the operator $H(\vartheta)=U(\vartheta)HU(\vartheta)^{-1}$ with Dirichlet condition on K extends analytically to the strip S_α as a self-adjoint family of type A [Ka] with domain $D(-\Delta^D)=H^2(\Omega_e)\cap H_0^1(\Omega_e)$.

Note that we require (NT2) outside the region J_E forbidden for classical particles with energy E. J_E is stable under small variations in E and (NT2) actually holds on some slightly larger set. This will be convenient when we consider quantum states with energy near E, and we state it as

Lemma 2.1. *The energy $E>\overline{\lim_{x\to\infty}}\, V(x)$ is non-trapping if and only if there is $S>0$ and a compact set $\Omega\subset\mathbb{R}^n$ such that*

(NT1′):

$K\subset\mathring{\Omega}$ *and* $\Omega\subset J_E\cup\{|x|<r_0\}$.

(NT2′):

$\operatorname*{Min}_{\partial\Omega\cap\Omega_e} V\leqq V|_{\Omega\cap\Omega_e}$.

(NT3′):

$$2\frac{r-r_0}{r}(V-E)+(r-r_0)\frac{\partial V}{\partial r}<-S\ (x\in\Omega_e\backslash\Omega).$$

Proof. It suffices to show (NT) $\Rightarrow$ (NT′). Since the left-hand side of (NT2) is continuous in x and ∂J_E is compact by (C2) we can find $\delta>0$ such that (2.3) holds for $x\in\Omega_e\backslash M_\delta$, where

$$M_\delta=\{x\in J_E\colon \operatorname{dist}(x,\partial J_E)\geqq\delta\}.$$

For sufficiently small δ, we have $K \subset M_\delta$ and furthermore $V_\delta := \underset{x \in M_\delta}{\mathrm{Min}}\, V(x) > E$ by definition of M_δ. Choosing $\tilde{E}$ such that $E < \tilde{E} < V_\delta$ the set $\Omega = J_{\tilde{E}} \cup \{|x| < r_0\}$ satisfies (NT′).

3. Bounds on the Dilated Resolvent

This section contains our main result concerning the absence of resonances [defined as eigenvalues of $H(\vartheta)$] in some k-independent neighborhood of a non-trapping energy E and an explicit bound on the resolvent of $H(\vartheta)$:

Theorem 3.1. *Let V satisfy* (C1)...(C3). *Let $H(\vartheta)$ be defined by exterior scaling* $(0 \leqq \mathrm{Im}\,\vartheta < \alpha)$. *Let*

$$W_\vartheta = \{z \in \mathbb{C} : |\mathrm{Re}(z-E)| < C_1,\ -C_2 \,\mathrm{Im}\,\vartheta < \mathrm{Im}\, z < C_3 (\mathrm{Im}\,\vartheta)^{-1}\},$$

with suitably chosen constants $C_i > 0$ independent of ϑ and k. Then there is $\alpha_0 > 0$ and $C \in \mathbb{R}$ such that for $0 < \mathrm{Im}\,\vartheta < \alpha_0$ we can find $k_\vartheta > 0$ such that

$$\|(H(\vartheta) - z)^{-1}\| \leqq C |\mathrm{Im}\,\vartheta|^{-1} \qquad (z \in W_\vartheta,\ k < k_\vartheta). \tag{3.1}$$

Remark. One can take $C_1 = \frac{S}{20}$, $C_2 = \frac{S}{10}$, $C_3 = \frac{S}{40}$ provided $\min_{\partial\Omega \cap \Omega_e} V \geqq E + \frac{2}{5} S$, where Ω is the set appearing in (NT′). In [CDKS] ϑ is taken as a function of k. Then a slight variant of Theorem 1 is applicable. The bound (3.1) remains true for $\vartheta = C_N k^N$ $(N \in \mathbb{N})$, $z \in W_{\vartheta(k)}$ and k small enough. This follows from inserting $\vartheta \sim k^N$ in our proof below and keeping track of the k-dependence (see the remark following Lemma 4.2). In the form stated above Theorem 1 has been used in [K]. □

Let us indicate briefly the main idea of our proof while introducing some notation needed later on. It clearly suffices to consider imaginary $\vartheta = i\beta$ and in a first step we look at the linearization in ϑ of

$$e^{2\vartheta}(H(\vartheta) - z), z = E + w_1 + i w_2,$$

with w_1, w_2 real and small. This leads to

$$\tilde{H}(\vartheta, k, z) = H_r + i\beta H_i, \tag{3.2}$$

where

$$H_r = -k^4 \Delta + V - E - w_1 + 2\beta w_2,$$

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

The main difficulty in proving an a priori estimate for $\tilde{H}(\vartheta, k, z)$ which then leads to (3.1) comes from states φ with energy near E, since then $H_r \varphi$ is approximately zero. For such states H_i plays the crucial role. In fact for states φ with energy near E the rotational energy $k^4 \frac{\Lambda}{r^2}$ will be approximately $E - V$. Inserting this into H_i (see

Lemma 4.1) it follows from (NT) that H_i is a strictly negative operator outside the classically forbidden region J_E, for $|z-E|$ small. Since in the classical limit quantum states with energy near E are localized outside J_E (Lemma 4.2) the following well known inequality can still successfully be applied.

Lemma 3.2. *Let A be self-adjoint with domain $D(A)$ and $B \geqq C > 0$ be bounded. Then*

$$\|(A \mp iB)\varphi\| \geqq C\|\varphi\| \qquad (\varphi \in D(A)). \tag{3.3}$$

This leads then to:

Theorem 3.3. *Let $\tilde{H}(\vartheta, k, z)$ $(\vartheta \in i\mathbb{R})$ be given by (3.2). Then there is an interval $I = [E-\delta, E+\delta]$ such that the following holds: Let $P = P_I(H)$ be the spectral projection for H on I and let $Q = 1-P$. Then there are constants $a, b, \alpha_0 > 0$ such that for $0 < \operatorname{Im}\vartheta < \alpha_0$ and W_ϑ as in Theorem 3.1 there is $k_\vartheta > 0$ such that*

$$\|\tilde{H}(\vartheta, k, z)P\varphi\| \geqq a|\vartheta|\,\|P\varphi\| \qquad (k < k_\vartheta,\ z \in W_\vartheta), \tag{3.4}$$

$$\|\tilde{H}(\vartheta, k, z)Q\varphi\| \geqq b\|Q\varphi\| \qquad (\varphi \in D(H),\ k < k_\vartheta,\ z \in W_\vartheta). \tag{3.5}$$

Remark. Given S and Ω in (NT′) and assuming $\min\limits_{\partial\Omega \cap \Omega_e} V > E + \frac{2}{5}S$, we may choose $\delta = \dfrac{S}{5}$, $a = \dfrac{S}{20}$, $b = \dfrac{S}{20}$. δ, a, b depend on V only via S and Ω. □

Granted Theorem 3.3, we complete the

Proof of Theorem 3.1. We start deriving an a priori estimate for $\tilde{H}(\vartheta, k, z)$. From now on we suppress the explicit dependence on ϑ, k, z in $\tilde{H}$. For $\varphi \in D(H)$ we have

$$\|\tilde{H}\varphi\|^2 \geqq \|\tilde{H}P\varphi\|^2 + \|\tilde{H}Q\varphi\|^2 - 2|\langle Q\varphi, \tilde{H}^*\tilde{H}P\varphi\rangle|, \tag{3.6}$$

where

$$\tilde{H}^*\tilde{H} = H_r^2 + |\vartheta|^2 H_i^2 + \vartheta[H, H_i].$$

Since $H_i - 2\dfrac{r_0}{r^3}k^4 \Lambda$ is multiplication by a C^2-function with bounded derivatives, it follows readily from Lemma A2 in our appendix that $[H, H_i]P$ is of order k^2 and that $H_i^2 P$ is bounded uniformly in k.

Thus we obtain from (3.6) applying Schwarz inequality and using Theorem 3.3

$$\|\tilde{H}\varphi\| \geqq \tfrac{1}{2}a|\vartheta|\,\|\varphi\| \tag{3.7}$$

for $|\vartheta|$, $k < k_\vartheta$ sufficiently small. The Taylor expansion in ϑ is controlled by

$$\begin{aligned}\|\{e^{2\vartheta}(H(\vartheta)-z) - \tilde{H}\}\varphi\| &\leqq \left\|\left\{e^{2\vartheta}\frac{r^2}{r_\vartheta^2} - 1 - 2\vartheta\frac{r_0}{r}\right\}k^4\frac{\Lambda}{r^2}\varphi\right\| + |\vartheta|^2 C\|\varphi\| \\ &\leqq C|\vartheta|^2\{\|\varphi\| + \|H\varphi\|\} \end{aligned}\tag{3.8}$$

for some constant C independent of ϑ and k. Using Lemma A2 it is easy to see that

$$\|H\varphi\| \leqq 2\|\tilde{H}\varphi\| + C\|\varphi\| \tag{3.9}$$

for $|\vartheta|$ sufficiently small, and combining (3.7), (3.8), (3.9) we obtain

$$\|(H(\vartheta)-z)\varphi\| \geqq (1-C|\vartheta|^2)\|\tilde{H}\varphi\| - C|\vartheta|^2\|\varphi\| \geqq \tfrac{1}{4}a|\vartheta|\,\|\varphi\| \tag{3.10}$$

for $|\vartheta|$ sufficiently small. Now it follows from standard arguments that $(H(\vartheta)-z)^{-1}$ exists and obeys (3.1).

4. Localization in Energy and Space

We prove two lemmata employed in the subsequent proof of Theorem 3.3 as outlined in Sect. 3.

Lemma 4.1. *Let $F\in C_0^\infty(\mathbb{R})$ and let F_H be the operator associated by the spectral theorem. Let $E_+ > \sup\operatorname{supp} F$ and let $g\in C^2(\mathbb{R}^n)$ be nonnegative with bounded derivatives. Then there is $C\in\mathbb{R}$ such that*

$$F_H g k^4 \frac{\Lambda}{r^2} g F_H \leqq F_H g^2 (E_+ - V) F_H + Ck^2 . \tag{4.1}$$

Proof. Let P be the spectral projection for H associated to $\operatorname{supp} F$. Then $[g, F_H]P$ is $O(k^2)$ by Lemma A3 and so is $P\left[k^4\frac{\Lambda}{r^2}, g\right]$. Thus we have computing $\operatorname{mod} O(k^2)$

$$F_H k^4 \frac{\Lambda}{r^2} g^2 F_H = PgF_H k^4 \frac{\Lambda}{r^2} F_H g P \leqq PgF_H(H-V)F_H g P . \tag{4.2}$$

Commuting g with F_H proves (4.1). $\square$

Next we show that in the classical limit quantum states with energy near E have very low probability of being within the classically forbidden region J_E.

Lemma 4.2. *Let $I=[0,E]$ for some $E\in\mathbb{R}$ and let $P=P_I(H)$ be the associated spectral projection. Let $\chi\in C_0^\infty(\bar{\Omega}_e)$ with $\operatorname{supp}\chi\subset J_E$. Then there is $C\in\mathbb{R}$ such that*

$$\|\chi P\| \leqq Ck^2 . \tag{4.3}$$

Proof. Let $E_\chi=\min\{V(x)\colon x\in\operatorname{supp}\chi\}$ and choose $E<E_+<E_\chi$. Then there is $\tilde{\chi}\in C^\infty(\Omega_e)$ equal to 1 on $\{V(x)\leqq E_+\}$, and such that $\operatorname{supp}\tilde{\chi}\cap\operatorname{supp}\chi=\phi$. Let $F\in C_0^\infty(\mathbb{R})$ be equal to 1 on I and supported within $(-\infty, E_+)$. Then $H_+ = H + E_+\tilde{\chi} \geqq E_+$ and thus $F_{H_+}=0$. This implies using $\chi\tilde{\chi}=0$,

$$\chi P = \chi \int_{\mathbb{R}} dt\hat{F}(t)\{e^{-iHt} - e^{-iH_+t}\}P = iE_+ \int dt\hat{F}(t)\int_0^t d\tau[\chi, e^{-iH_+(t-\tau)}]\tilde{\chi}e^{-iH\tau}P . \tag{4.4}$$

But

$$[\chi, e^{-iH_+t}] = \int_0^t ds e^{-iH_+(t-s)} i[-k^4\Delta, \chi]e^{-iH_+s} , \tag{4.5}$$

and

$$\|k^4 \nabla e^{-iH_+s}\tilde{\chi}e^{-iH\tau}P\| \leqq Ck^2 , \tag{4.6}$$

since commuting V through everything generates bounded terms and gives in leading order $k^4 VP = O(k^2)$. Inserting (4.5) into (4.4) and using (4.6) yields

$$\|\chi P\| \leqq Ck^2 \int dt |\hat{F}(t)|\, |q(t)| \tag{4.7}$$

for some polynomial $q(t)$ which proves (4.3).

Remark. Estimate (4.3) can be sharpened to

$$\|\chi P\| \leqq C_N k^N \qquad (N \in \mathbb{N}). \tag{4.8}$$

This may be proved continuing the commutation process of $[-k^4 \Delta, \chi]$ with e^{-iH+S} in (4.5) or using bounds on $\|\chi(H-z-ik^N)^{-1}\varphi\|$ $(z \in I)$ – see [CDKS] – and Stone's formula. We need (4.8) when generalizing Theorem 3.1 to the case $\vartheta = C_N k^N$ as indicated in the remark following Theorem 3.1. □

Proof of Theorem 3.3. We start proving estimate (3.4) which is the difficult part of the theorem. We assume the non-trapping condition in the form (NT′). Thus given Ω in (NT′) we fix the range of energy $I = [E-\delta, E+\delta]$ by requiring $E+\delta < V_\Omega = \operatorname*{Min}_{\partial\Omega \cap \Omega_e} V$. Let $F \in C_0^\infty(\mathbb{R})$ be equal to 1 on I and supported within $(-\delta, V_\Omega)$. Then we have using boundedness of $k^{-2}[H_i, H]P$ (which follows from Lemma A2) and Lemma A3

$$\|\tilde{H}P\varphi\| \geqq \|\{H_r + i\beta F_H H_i F_H\} P\varphi\| \qquad \bmod |\beta| k^2 \|P\varphi\|. \tag{4.9}$$

Next we choose a C^∞-partition of unity on Ω_e, $1 = \chi^2 + \tilde{\chi}^2$, with $\chi = 1$ on $\Omega \cap \Omega_e$ and $\operatorname{supp}\chi \subset J_{E+\delta}$. Lemma 4.2 combined with a simple commutator estimate yields

$$\|\{H_r + i\beta F_H H_i F_H\}\chi^2 P\| \leqq Ck^2. \tag{4.10}$$

Thus we get, letting $B = F_H \tilde{\chi} H_i \tilde{\chi} F_H$,

$$\|\tilde{H}P\varphi\| \geqq \|\{H_r \tilde{\chi}^2 + i\beta B\} P\varphi\| \qquad \bmod(|\vartheta| k^2 \|P\varphi\|, k^2 \|P\varphi\|). \tag{4.11}$$

Applying Lemma 4.1 with $g = \left(2\frac{r_0}{r}\right)^{1/2} \tilde{\chi}$ and observing $\operatorname{supp}\tilde{\chi} \subset \overline{\Omega_e \backslash \Omega}$ we get from (3.2) $\bmod(Ck^2)$,

$$B \leqq \sup_{x \in \Omega_e \backslash \Omega} 2(V-E) + (r-r_0)\frac{\partial V}{\partial r} - 2w_1 - \beta^{-1} w_2 + 2\frac{r_0}{r}(E_+ - V), \tag{4.12}$$

where we may choose $\sup \operatorname{supp} F < E_+ < E + \frac{3}{2}\delta$. Assuming

$$|2w_1| < \frac{\delta}{2}, \qquad w_2 > -\frac{\delta}{2}\beta, \qquad \delta = \frac{S}{5}, \tag{4.13}$$

which can be achieved decreasing our previous choice either for δ or for S, we find from (4.12) and (NT3′),

$$B \leqq -\frac{S}{5} \quad (k \text{ sufficiently small}). \tag{4.14}$$

Thus (3.4) follows from (4.11) using (4.14) and Lemma 3.2. To prove (3.5) let $\{E_\lambda\}$ be the resolution of the identity associated with H and let $\psi = Q\varphi$. Then $\langle \psi, E_\lambda \psi \rangle$ is constant in $\lambda \in I$ and with $H_r = H - (E + w_1 + 2\beta w_2) = H - \tilde{E}$ one obtains

$$\|H_r \psi\|^2 = \int_{\sigma(H)\setminus I} (\lambda - \tilde{E})^2 d\langle \psi, E_\lambda \psi \rangle \geqq \left(\frac{\delta}{2}\right)^2 \|\psi\|^2 \tag{4.15}$$

for $|w_1| < \frac{\delta}{4}$, $|w_2| < |\vartheta|^{-1} \frac{\delta}{8}$. Combining this constraint with (4.13) defines a region W_ϑ as fixed in Theorem 1. Our specific choice $\delta = \frac{S}{5}$ corresponds to the remarks following Theorems 3.1, 3.3. Since using Lemma A2

$$\|H_i Q \varphi\| \leqq 2 \|H_r Q \varphi\| + C \|Q \varphi\|, \tag{4.16}$$

estimate (4.3) follows from (4.15) for $|\vartheta|$ sufficiently small.

Appendix

We prove some technical estimates needed in Sect. 3.4. Throughout the Appendix we let $H = -k^4 \Delta + V$, where V is supposed to satisfy (C2). We let I be any finite interval and denote by $P = P_I(H)$ the associated spectral projection.

First we prove a quadratic inequality which will imply H-boundedness of the radial and rotational kinetic energy operator.

Lemma A1. *In the sense of quadratic forms on $H_0^1(\Omega_e) \cap H^2(\Omega_e) = D(H)$:*

$$D^4 + \left(\frac{\Lambda}{r^2}\right)^2 \leqq \Delta^2 + \frac{2}{r^4} \Lambda \qquad (n \neq 2), \tag{A1}$$

$$D^4 + \left(\frac{\Lambda + \frac{1}{4}}{r^2}\right)^2 \leqq (\Delta + \tfrac{1}{4})^2 + \frac{2}{r^4} (\Lambda + \tfrac{1}{4}) \qquad (n = 2). \tag{A2}$$

Proof. $-D^2$ and Λ are positive operators in dimension $n \neq 2$ while $\Lambda \geqq -\frac{1}{4}$ for $n = 2$. First consider $n \neq 2$. Then

$$D^4 + \left(\frac{\Lambda}{r^2}\right)^2 = \Delta^2 + D^2 \frac{\Lambda}{r^2} + \frac{\Lambda}{r^2} D^2, \tag{A3}$$

where

$$D^2 \frac{\Lambda}{r^2} + \frac{\Lambda}{r^2} D^2 = \Lambda^{1/2} \left\{ 2 \frac{1}{r} D^2 \frac{1}{r} + \left[\left[D^2, \frac{1}{r}\right], \frac{1}{r}\right] \right\} \Lambda^{1/2} \leqq \frac{2}{r^4} \Lambda, \tag{A4}$$

since the first term is negative and $\left[\left[D^2, \frac{1}{r}\right], \frac{1}{r}\right] = 2\left[D, \frac{1}{r}\right]^2 = \frac{2}{r^4}$.

(A2) follows replacing Λ by $\Lambda + \frac{1}{4}$ and Δ by $\Delta + \frac{1}{4}$ in (A3). □

We use Lemma A1 to prove

Lemma A2. *For $\varphi \in D(H)$ we have*

$$\left\| k^4 \frac{\Lambda}{r^2} \varphi \right\| \leqq \|H \varphi\| + C \|\varphi\|. \tag{A5a}$$

Furthermore for any $g \in C^2(\Omega_e)$ with bounded derivatives the following commutators are bounded uniformly in k:

b) $[H, D]P$,

c) $k^2[H, D^2]P$,

d) $k^2\left[H, \frac{\Delta}{r^2}\right]P$,

e) $[H, g]k^2\frac{\Delta}{r^2}P$,

f) $k^2\left[H, g\frac{\Delta}{r^2}\right]P$.

Proof. Taking expectation values in (A1) we get from Schwarz inequality

$$\left(\left\|\frac{\Delta}{r^2}\varphi\right\| - r_0^{-2}\|\varphi\|\right)^2 \leqq \|\Delta\varphi\|^2 + r_0^{-4}\|\varphi\|^2. \tag{A6}$$

Since V is bounded this proves (A5a) for $n \neq 2$. For $n=2$ (A5a) follows from (A2). (b) follows from (A5a) since

$$[H, D] = -\frac{\partial V}{\partial r} + \frac{2}{r}k^4\frac{\Delta}{r^2}. \tag{A7}$$

For (c) we only treat the first term in $[H, D^2] = [H, D]D + D[H, D]$. Using (A7) and neglecting bounded operators appearing to the left of derivatives estimating $k^2[H, D^2]P$ is reduced to estimating

$$k^2DP + k^6\frac{\Delta}{r^2}DP. \tag{A8}$$

Clearly the first term is bounded and

$$\left\|k^6\frac{\Delta}{r^2}DP\varphi\right\| \leqq k^2\|HDP\varphi\| + Ck^2\|DP\varphi\|, \tag{A9}$$

using (A5a) and $DP\varphi \in D(H)$. But

$$\|HDP\varphi\| \leqq \|DPHP\varphi\| + \|[H, D]P\varphi\| \leqq Ck^{-2}\|P\varphi\|, \tag{A10}$$

using (b) which proves (c). (d) follows from (c) since $\left[\frac{\Delta}{r^2}, H\right] = [D^2, H] + [V, \Delta]$. As in (A9) one proves boundedness of $k^6V\frac{\Delta}{r^2}P$ which implies (e). (f) follows immediately from (e) and (d).

Lemma A3. *Let $F \in C_0^\infty(\mathbb{R})$ and F_H be the associated operator. Let W be a linear operator in $L^2(\Omega_e)$ such that $[W, H]P$ is uniformly bounded in k. Then $[W, F_H]P$ is uniformly bounded.*

Proof. We use the formula $F_H = \int \hat{F}(t)e^{-iHt}dt$ to obtain

$$[W, F_H]P = \int dt\hat{F}(t)\int_0^t ds e^{-iH(t-s)}[H, W]e^{-iHs}P. \tag{A11}$$

Since P commutes with e^{-iHs} the assertion follows from the rapid decrease of $\hat{F}$. $\square$

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