ABSOLUTE CONTINUITY OF HAMILTONIAN OPERATORS WITH REPULSIVE POTENTIAL

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Introduction. One expects that the absolutely continuous part of the spectrum of a Hamiltonian operator $H=-\Delta+V$ in $L_2(E^n)$ (where Δ is the Laplacian operator and V is the operation of multiplication by a real function which approaches 0 at ∞) will be the interval $[0, \infty)$. That this is the essential spectrum has been shown under very weak assumptions on V [**7**], but the absolute continuity has been demonstrated only under much stronger assumptions [**1**], [**2**], [**3**], [**8**].

In this paper we prove that for smooth positive potentials V which are sufficiently repulsive outside some bounded set, the operator $-\Delta+V$ is absolutely continuous. Our conditions are similar to those in the previous work of Odeh [**5**]. We use results of Putnam [**6**] on commutators of pairs of selfadjoint operators. Our method works for dimensions $n=1$, 2, or 3, though we consider only two cases, $n=1$ (because of its simplicity) and $n=3$ (because of its importance for applications). Only partial results seem possible in higher dimensions.

1. **Notation.** Let $\boldsymbol{H}=L_2(E^n)$ (with $n\leqq 3$) with the inner product

$$\langle \phi, \psi \rangle = \int \phi(x)\psi(x)^* dx.$$

Let $\mathcal{S}\subset\boldsymbol{H}$ be the subset of infinitely differentiable functions whose partial derivatives of all orders approach 0 at ∞ faster than $|x|^{-k}$ for all k. Let P_j be the unique self adjoint operator in $\boldsymbol{H}$ given by

$$P_j\psi = -i\partial\psi/\partial x_j \qquad \text{for } \psi \in \mathcal{S}.$$

Let H_0 be the unique selfadjoint operator which is equal to $P_1^2+P_2^2+\cdots+P_n^2$ on $\mathcal{S}$. If g is a measurable function on E^n, we shall also use g, or even $g(x)$, to denote the operation of multiplication by g. If T is an operator in $\boldsymbol{H}$, we write $D(T)$ for the domain of T.

Let us note here a few facts about commutators $[A, B]=AB-BA$ of such operators.

(1) If g is differentiable, and g and all partial derivatives of g are bounded, then

$$[P_j, g]\psi = -i(\partial g/\partial x_j)\psi \qquad \text{for } \psi \in D(P_j).$$

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(2) If g is twice differentiable, and the first and second partial derivatives of g are bounded,

$$i[H_0, g] \subset \sum_{j=1}^{n} (P_j \partial g/\partial x_j + \partial g/\partial x_j P_j).$$

If T is a selfadjoint operator in $\boldsymbol{H}$, and F is a measurable subset of $\boldsymbol{R}$, let $E_F(T)$ be the associated spectral projection. Denote by $\boldsymbol{H}_a(T)$ the subspace of vectors ψ such that the measure $F \mapsto \|E_F(T)\psi\|^2$ is absolutely continuous with respect to Lebesgue measure. Then $\boldsymbol{H}_a(T)$ is a closed subspace which reduces T. Let T_a denote T restricted to $\boldsymbol{H}_a(T)$. If $T = T_a$ we say T is absolutely continuous.

If V is the sum of a square integrable function and a bounded function then $H_0 + V$ defines a selfadjoint operator on $D(H) = D(H_0)$, and the graph norms $(\|H\psi\|^2 + \|\psi\|^2)^{1/2}$ and $(\|H_0\psi\|^2 + \|\psi\|^2)^{1/2}$ are equivalent for $\psi \in D(H)$ [**4**, V. 5.3]. We shall consider such operators in the following sections.

2. **Hamiltonian operators in** $L_2(E)$. Let $n = 1$ in the above definitions, and call $P_1 = P$.

THEOREM 1. *Let V be differentiable, V and V' bounded, and $-\operatorname{sgn}(x) V'(x) \geqq 0$. Assume also that*

$$(1) \qquad -\operatorname{sgn}(x) V'(x) \geqq a|x|^{-3+\epsilon} \qquad \textit{for } |x| \geqq b$$

for some positive ϵ, a and b. Then $H_0 + V$ is absolutely continuous.

PROOF. We shall find a bounded operator A such that on $D(H)$, $i[H, A] \geqq 0$, $i[H, A]$ is bounded, and 0 is not in the point spectrum of $i[H, A]$. Then, by a theorem of Putnam [**6**, Theorem 2.13.2], H is absolutely continuous. We shall set

$$A = (H - i)^{-1}(gP + Pg)(H + i)^{-1}$$

where g is real valued and infinitely differentiable, and all derivatives of g are bounded. Since $D(H) = D(H_0) \subset D(P)$, $gP(H+i)^{-1}$ is bounded. Since $g(H+i)^{-1}$ is a bounded map of $\boldsymbol{H}$ into $D(H)$, $Pg(H+i)^{-1}$ is bounded. Therefore A is a bounded map of $\boldsymbol{H}$ into $D(H)$ which implies that HA and AH are both defined on $D(H)$ and bounded in the $\boldsymbol{H}$-norm, so that $i[H, A]$ is bounded. If

$$B(\phi, \psi) = i(\langle HA\phi, \psi\rangle - \langle \phi, HA\psi\rangle)$$

$B(\cdot\,,\cdot)$ is a bounded sesquilinear form on $\boldsymbol{H}$, so it is sufficient to calculate its values for a dense set of ϕ's. Let $(H+i)^{-1}\phi \in \mathcal{S}$. Then

$$B(\phi, \psi) = i\{\langle (H - i)^{-1}H(gP + Pg)(H + i)^{-1}\phi, \psi\rangle - \langle \phi, (H - i)^{-1}H(gP + Pg)(H + i)^{-1}\psi\rangle\}$$
$$= i\langle [H(gP + Pg) - (gP + Pg)H](H + i)^{-1}\phi, (H + i)^{-1}\psi\rangle$$
$$= \langle \{i[H_0, g]P + iP[H_0, g] + ig[V, P] + i[V, P]g\} \times (H + i)^{-1}\phi, (H + i)^{-1}\psi\rangle$$
$$= \langle (g'P^2 + 2Pg'P + P^2g' - 2gV')(H + i)^{-1}\phi, (H + i)^{-1}\psi\rangle.$$

Now

$$g'P^2 + P^2g' = Pg'P - [P, g']P + Pg'P + P[P, g'] = 2Pg'P + [P, [P, g']] = 2Pg'P - g'''.$$

This gives, for all $\phi \in D(H)$,

$$i[H, A]\phi = \{4(H - i)^{-1}Pg'P(H + i)^{-1} - (H - i)^{-1}[g''' + 2gV'](H + i)^{-1}\}\phi. \tag{2}$$

Now let us make the choice of g more specific; let

$$g(x) = (2/\pi) \tan^{-1} cx. \tag{3}$$

Then

$$g'(x) = 2c/\pi(1 + (cx)^2)$$

and

$$g'''(x) = 4c^3[3(cx)^2 - 1]/\pi[1 + (cx)^2]^3. \tag{4}$$

Since $g'(x) > 0$, the first term of (2) is a positive operator, so we turn attention to the second term of (2). If $|cx| \leqq 3^{-1/2}$, we have

$$-2g(x)V'(x) \geqq 0 \quad \text{and} \quad -g'''(x) \geqq 0.$$

On the other hand if $|cx| > 3^{-1/2}$, $|g(x)| > \frac{1}{3}$, so that

$$-2g(x)V'(x) > -\tfrac{2}{3} \operatorname{sgn}(x)V'(x). \tag{5}$$

Now let us choose c so that

$$\sqrt{3}c \leqq \min\{b^{-1}, (\pi a/18\sqrt{3})^{1/\epsilon}\} \tag{6}$$

Then by (1) and (5),

$$-2g(x)V'(x) \geqq \tfrac{2}{3}\, a\,|x|^{-3+\epsilon} \qquad \text{for } |x| > 1/\sqrt{3}c \geqq b. \tag{7}$$

On the other hand, from (4) we have

(8) $$g'''(x) \leqq 12/\pi c|x|^4.$$

Thus for $|x| > 1/\sqrt{3}c$

$$-2g(x)V'(x) - g'''(x) \geqq |x|^{-4}(\tfrac{2}{3}a|x|^{1+\epsilon} - 12/\pi c)$$
$$> |x|^{-4}(2\cdot 3^{-(3+\epsilon)/2}a/c^{\epsilon} - 12/\pi)/c \geqq 0.$$

(The first inequality follows from (7) and (8), the second from $|x| > 1/\sqrt{3}c$, and the third from (6).) This establishes that $i[H, A]$ is a positive operator.

If $i[H, A]\psi = 0$, one would have

$$0 = (i[H, A]\psi, \psi) \geqq \int (-2g(x)V'(x) - g'''(x))|(H+i)^{-1}\psi(x)|^2 dx$$

which would imply $(H+i)^{-1}\psi = 0$ since $-2g(x)V'(x) - g'''(x) > 0$ for all x. Since $(H+i)^{-1}$ is injective, we see that 0 is not in the point spectrum of $i[H, A]$. ∎

Let us add a few words in motivation of the choice of A. This operator may be regarded as a kind of quantum mechanical analogue to the function on classical mechanical phase space $f(p, q) = (2/\pi)p \tan^{-1} cq$, where p and q are respectively the momentum and position coordinates. The classical Poisson bracket of the Hamiltonian $p^2 + V(q)$ with f is

$$(\partial H/\partial p)(\partial f/\partial q) - (\partial H/\partial q)(\partial f/\partial p)$$
$$= 2/\pi\{p^2c/[1 + (cx)^2] - \tan^{-1}(cq)V'(q)\}$$

which is positive if $\operatorname{sgn}(x)V'(x) \leqq 0$ for all x. This leads to the conjecture that the quantum mechanical analogue $i[H, A]$ is also positive.

COROLLARY 1. *Let V be differentiable for $|x| > b$ and* $-\operatorname{sgn}(x)V'(x) \geqq |x|^{-3+\epsilon}$ *for $|x| > b$, V locally square integrable, and*

(9) $$\lim_{x\to\infty} \int_{|x-y|<1} |V(y)|^2 dy = 0.$$

Then if $H = H_0 + V$, the spectrum of H_a is $[0, \infty)$.

PROOF. $V = V_1 + V_2$ where V_1 satisfies (9) and the conditions of Theorem 1, and V_2 is a square integrable function with compact support. Because of (9), the essential spectrum of $H_1 = H_0 + V_1$ is $[0, \infty)$ [**7**], and by Theorem 1, $H_1 = H_{1a}$ so that $\operatorname{sp}(H_{1a}) = [0, \infty)$. But since $V_2 \in L_1(E) \cap L_2(E)$, $H_a = (H_1 + V_2)_a$ is unitarily equivalent to $H_{1a} = H_1$.

(See [4, p. 546]. $V_2 = V_2' V_2''$ where $V_2'(H_0+i)^{-1}$ and $V_2''(H_0+i)^{-1}$ are in the Schmidt class. But $(H_1+i)^{-1} = (H_0+i)^{-1}(I - V_1(H_1+i)^{-1})$, where $I - V_1(H_1+i)^{-1}$ is a bounded operator [7], which implies that $V_2'(H_1+i)^{-1}$ and $V_2''(H_1+i)^{-1}$ are Schmidt class.) ■

3. **Hamiltonian operators in three dimensions.** Let $n=3$ in the definitions of §1.

THEOREM 2. *Let V be differentiable, V and $|\nabla V|$ bounded, and $-|x|^{-1}x\cdot\nabla V(x) \geqq a|x|^{-3+\epsilon}$ for $|x| \geqq b$ for some positive a and b. Then $H_0 + V$ is absolutely continuous.*

PROOF. As in the proof of Theorem 1, we shall define a bounded operator A such that $i[H, A] \geqq 0$ on $D(H)$, A maps $\boldsymbol{H}$ into $D(H)$, and $i[H, A]$ does not have 0 in its point spectrum. It will be convenient to use a different representation of $\boldsymbol{H}$. Let U be the unitary transformation $U: L_2(E^3) \to L_2([0, \infty); L_2(S^2))$ (where S^2 is the unit sphere in E^3), defined for functions $\psi(r, \theta, \phi) = f(r)g(\theta, \phi)$ by

$$U\psi(r) = rf(r)g$$

(where r, θ, and ϕ are the usual spherical coordinates on E^3). The multiplication operator h on $L_2([0, \infty); L_2(S^2))$ defined by $(hf)(r) = h(r)f(r)$, transforms to

$$U^*hU\psi(r, \theta, \phi) = h(r)\psi(r, \theta, \phi).$$

On the other hand the symmetric operator $-i\ d/dr$ in $L_2([0, \infty); L_2(S^2))$ transforms to $D_r = U^*(-i\ d/dr)U$ where

$$D_r = \sum_j (x_j/r)P_j - (i/r); \tag{10}$$

$D(D_r) = D(P_1) \cap D(P_2) \cap D(P_3)$. Note that if f is a boundedly differentiable function,

$$[f, D_r] = (i/r)x\cdot\nabla f \qquad \text{on } D(H). \tag{11}$$

We define A on $L_2(E^3)$ by

$$A = (H - i)^{-1}(gD_r + D_r g)(H + i)^{-1}$$

where $g(r) = (2/\pi)\tan^{-1} cr$ with $\sqrt{3}c \leqq \min\{b^{-1}, (\pi a/18\sqrt{13})^{1/\epsilon}\}$. From (10) it is clear that $g\,D_r(H+i)^{-1}$ and $D_r\,g(H+i)^{-1}$ are bounded, and so A maps $\boldsymbol{H}$ into $D(H)$. A is selfadjoint, since g and D_r are symmetric.

Note that

$$UH_0U^* = -d^2/dr^2 + r^{-2}B$$

where B is a positive operator in $L_2(S^2)$.

Calculations in $L_2([0, \infty); L_2(S^2))$ similar to those in the proof of Theorem 1 yield, for $\psi \in \mathcal{S}$

$$i[H_0, gD_r + D_r g]\psi = 4D_r g' D_r - g''' + 4gr^{-3}B.$$

For such ψ, by (11),

$$i[V, gD_r + D_r g]\psi = -2r^{-1}g(x \cdot \nabla V)\psi,$$

and the argument of Theorem 1 applies. ■

COROLLARY 2. *Let V be differentiable for $|x| > b$, and $-r^{-1}x \cdot \nabla V(x) \geqq |x|^{-3+\epsilon}$, V locally square integrable, and*

$$\lim_{x \to \infty} \int_{|x-y|<1} |V(y)|^2 dy = 0.$$

Then if $H = H_0 + V$, the spectrum of H_a is $[0, \infty)$.

The proof is the same as in Corollary 1.

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