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 $L_2(\mathbb{R}^n)$ (where
$\Delta$ is the Laplacian operator and $V$ is the operation of multiplication
by a real function which approaches 0 at $\infty$) 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 $n = 1, 2, 3$, 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 $H = L_2(\mathbb{R}^n)$ (with $n \leq 3$) with the inner product
$$\langle \phi, \psi \rangle = \int \phi(x)\psi(x)^* dx.$$ 

Let $s \subset H$ be the subset of infinitely differentiable functions whose
partial derivatives of all orders approach 0 at $\infty$ faster than $|x|^{-k}$
for all $k$. Let $P_j$ be the unique self adjoint operator in $H$ given by
$$P_j\psi = -i\partial\psi/\partial x_j \quad \text{for } \psi \in s.$$ 

Let $H_0$ be the unique selfadjoint operator which is equal to $P_1^2 + P_2^2$
$+ \cdots + P_n^2$ on $s$. If $g$ is a measurable function on $\mathbb{R}^n$, we shall also
use $g$, or even $g(x)$, to denote the operation of multiplication by $g$. If
$T$ is an operator in $H$, 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
$$[P_j, g]\psi = -i(\partial g/\partial x_j)\psi \quad \text{for } \psi \in D(P_j).$$ 

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

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

If $T$ is a selfadjoint operator in $H$, and $F$ is a measurable subset of $R$, let $E_F(T)$ be the associated spectral projection. Denote by $H_\alpha(T)$ the subspace of vectors $\psi$ such that the measure $F \to \|E_F(T)\psi\|^2$ is absolutely continuous with respect to Lebesgue measure. Then $H_\alpha(T)$ is a closed subspace which reduces $T$. Let $T_\alpha$ denote $T$ restricted to $H_\alpha(T)$. If $T = T_\alpha$ 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 $(\|H_0\phi\|^2 + ||\phi||^2)^{1/2}$ 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 $-\text{sgn}(x)V'(x) \geq 0$. Assume also that

$$-\text{sgn}(x)V'(x) \geq a |x|^{-3+e} \quad \text{for} \quad |x| \geq b$$

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

**Proof.** We shall find a bounded operator $A$ such that on $D(H)$, $i[H, A] \geq 0$, $i[H, A]$ 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

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

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 $H$ into $D(H)$, $P g(H+i)^{-1}$ is bounded. Therefore $A$ is a bounded map of $H$ into $D(H)$ which implies that $HA$ and $AH$ are both defined on $D(H)$ and bounded in the $H$-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 $H$, so it is sufficient to calculate its values for a dense set of $\phi$'s. Let $(H+i)^{-1}\phi \in \mathcal{S}$. Then
\[ B(\phi, \psi) = i \{ \langle \langle H - i \rangle^{-1} H(gP + Pg)(H + i) \rangle^{-1} \phi, \psi \} \]
\[ = i \{ [H(gP + Pg) - (gP + Pg)H](H + i) \rangle^{-1} \phi, (H + i) \rangle^{-1} \psi \} \]
\[ = \langle \{ i[H_0, g]P + iP[H_0, g] + ig[V, P] + i[V, P]g \} \times (H + i) \rangle^{-1} \phi, (H + i) \rangle^{-1} \psi \}
\[ = \langle (g'P^2 + 2Pg'P + P^2g' - 2gV')(H + i) \rangle^{-1} \phi, (H + i) \rangle^{-1} \psi \} \]

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

This gives, for all \( \phi \in D(H) \),
\[ i[H, A] \phi = 4(\langle H - i \rangle^{-1} Pg'P(H + i) \rangle^{-1} \phi \]
\[ = 2Pg'P + [P, [P, g']] = 2Pg'P - g''' \]

Now let us make the choice of \( g \) more specific; let
\[ g(x) = \left( \frac{2}{\pi} \right) \tan^{-1} cx. \]
Then
\[ g'(x) = 2c/\pi(1 + (cx)^2) \]
and
\[ g'''(x) = 4c^3[3(cx)^2 - 1]/\pi[1 + (cx)^2]^3. \]

Since \( g'(x) > 0 \), the first term of (2) is a positive operator, so we turn attention to the second term of (2). If \( |cx| \leq 3^{1/2} \), we have
\[ -2g(x)V'(x) \geq 0 \quad \text{and} \quad -g'''(x) \geq 0. \]

On the other hand if \( |cx| > 3^{1/2} \), \( |g(x)| > \frac{3}{2} \), so that
\[ -2g(x)V'(x) > -\frac{3}{2} \text{sgn}(x)V'(x). \]

Now let us choose \( c \) so that
\[ \sqrt{3}c \leq \min \{ b^{-1}, (\pi a/18\sqrt{3})^{1/4} \} \]
Then by (1) and (5),
\[ -2g(x)V'(x) \geq \frac{3}{4} a |x|^{-3+\epsilon} \quad \text{for} \quad |x| > 1/\sqrt{3}c \geq b. \]

On the other hand, from (4) we have
Thus for $|x| > 1/\sqrt{3c}$

$$-2g(x)V'(x) - g''''(x) \geq \left| x^{-4} \left( \frac{3a}{x} | x |^{1+\epsilon} - 12/\pi c \right) \right| > \left| x^{-4} \left( 2.3^{-(3+\epsilon)/2a/c} - 12/\pi c \right) \right| \geq 0.$$

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

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

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

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

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

which is positive if $\text{sgn}(x) V'(x) \leq 0$ 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 $-\text{sgn}(x) V'(x) \geq |x|^{-1+\epsilon}$ for $|x| > b$, $V$ locally square integrable, and

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

Then if $H = H_0 + V$, the spectrum of $H_0$ 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 $\text{sp}(H_{1a}) = [0, \infty)$. But since $V_2 \subseteq L_2(E) \cap L_2(E)$, $H_a = (H_1 + V_2)_a$ 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

\[
-|x|^{-1}|x \cdot \nabla V(x)| \geq a|x|^{-4+\epsilon} \text{ for } |x| \geq b \text{ for some positive } a \text{ and } b.
\]

Then \( H_0 + V \) is absolutely continuous.

**Proof.** As in the proof of Theorem 1, we shall define a bounded operator \( A \) such that \( i[A, A] \leq 0 \) on \( D(H) \), \( A \) maps \( H \) 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 \( H \). 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 \( r, \theta, \) and \( \phi \) 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 \( -i \frac{d}{dr} \) in \( L_2([0, \infty); L_2(S^2)) \) transforms to \( D_r = U^*(-i \frac{d}{dr})U \) where

\[
D(D_r) = D(P_1) \cap D(P_2) \cap D(P_3). \quad \text{Note that if } f \text{ is a boundedly differentiable function,}
\]

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

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

\[
A = (H - i)^{-1}(gD_r + D_3g)(H + i)^{-1}
\]

where \( g(r) = (2/\pi) \tan^{-1} cr \) with \( \sqrt{3e} \leq \min \{ b^{-1}, (\pi a/18\sqrt{13})^{1/4} \} \). From (10) it is clear that \( gD_r (H + i)^{-1} \) and \( D_r g (H + i)^{-1} \) are bounded, and so \( A \) maps \( H \) into \( D(H) \). \( A \) is selfadjoint, since \( g \) and \( D_r \) are symmetric.

Note that

\[
UH_0U^* = -\frac{d^2}{dr^2} + r^{-3}B
\]
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 $\psi \in S$

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

For such $\psi$, by (11),

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

and the argument of Theorem 1 applies.

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

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

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

The proof is the same as in Corollary 1.

**References**


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