Finiteness of Bound States of General N-Body Operators

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Consider the \((N+1)\)-body Schrödinger operator of atomic type,

\[ P_N = \sum_{j=1}^{N} (-\Delta_i - \frac{Z}{|x^i|}) + \sum_{1 \leq i < j \leq N} \frac{1}{|x^i - x^j|}. \]

This is the Hamiltonian of an atom with an infinitely heavy nucleus of charge \(Z\) and \(N\) electrons of charge 1 and mass \(1/2\). Here \(x^i \in \mathbb{R}^3\) is the coordinate of the \(i\)th electron and \(\Delta_i\) denotes the Laplacian in \(\mathbb{R}^3\) with respect to the variable \(x^i\). For the operator \(P_N\) the next theorem gives a classic result. (For the appropriate references we refer the reader to the extensive reference list in [4].)

**Theorem 1.** (Zhizlin (1960, 1969, 1971), Uchiyama (1969) and others) The operator \(P_N\) given by (1) has at most a finite number of bound states if and only if \(Z \leq N - 1\).

In this paper we work towards a theory for general \(N\)-body operators which would include the results in Theorem 1 for atoms as well as results for molecules. A portion of this task has been accomplished in [2] for general atomic-type operators of the form

\[ P = -\sum_{i=1}^{N} (2m_i)^{-1} \Delta_i + \sum_{i=1}^{N} v_{oi}(x^i) + \sum_{1 \leq i < j \leq N} v_{ij}(x^i - x^j) \]

where \(m_i\) is the mass of the \(i\)th electron. As in [2] we proceed from the foundation laid by Agmon[1]. Define

\[ H = -\sum_{i,j=1}^{n} \partial_i a^{ij} \partial_j + q(x), \quad x \in \mathbb{R}^n \]

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where $H$ satisfies the following (3)(i)-(iv):

(i) Each $a_{ij}$ is a bounded, continuous, real-valued function on $\mathbb{R}^n$.
(ii) The matrix $A(x) = [a_{ij}(x)]$ is symmetric and its smallest eigenvalue $\mu(x)$ is a positive continuous function on $\mathbb{R}^n$.

(3)

(iii) $q \in L^1(\mathbb{R}^n)_{\text{loc}}$.
(iv) $q_- = \max(-q, 0) \in M_{\text{loc}}(\mathbb{R}^n)$, where $M(\mathbb{R}^n) = M_0(\mathbb{R}^n)$ is the Sturmian class of functions.

The sesquilinear form which gives rise to $H$ is

(4) $\rho[\varphi, \psi] = \int_{\mathbb{R}^n} \{ \langle \nabla_A \varphi, \nabla_A \psi \rangle + q \varphi \bar{\psi} \} \, dx$ \quad ($\varphi, \psi \in C^\infty_0(\mathbb{R}^n)$),

where $\rho[\varphi] := \rho[\varphi, \varphi]$ and

(5) $\langle \nabla_A \varphi, \nabla_A \psi \rangle = \sum_{i,j=1}^n a_{ij} \nabla \varphi \nabla \bar{\psi}$.

Define

(6) $\Lambda(H) = \inf \{ \rho[\varphi] : \varphi \in C^\infty_0(\mathbb{R}^n), \|\varphi\| = 1 \}$.

If $\Lambda(H) > -\infty$, the sesquilinear form $\rho[\varphi, \psi]$ on $C^\infty_0(\mathbb{R}^n) \times C^\infty_0(\mathbb{R}^n)$ is proved to be a densely defined symmetric form which is bounded below and closable in $L^2(\mathbb{R}^n)$ - see Agmon[1] and [2].

Henceforth, let $H$ denote the self-adjoint operator in $L^2(\mathbb{R}^n)$ associated with the form $\rho[\varphi, \psi]$. Then, the least point of the essential spectrum of $H$ is given by

(7) $\Sigma(H) = \sup_{K: \text{compact}} \left[ \inf \{ \rho[\varphi] : \varphi \in C^\infty_0(\mathbb{R}^n - K), \|\varphi\| = 1 \} \right]$.

Agmon [1] gave an interesting, alternative expression for $\Sigma(P)$ which is related to the celebrated HVZ Theorem of quantum physics - see the references in Sigal[3] or [4].

Let $B(0; R) := \{ x \in \mathbb{R}^n : \|x\| < R \}$ and $S^{n-1} := \{ x \in \mathbb{R}^n : \|x\| = 1 \}$. For $\omega \in S^{n-1}, \delta \in (0, \pi)$, and $R > 0$ define the truncated cone

$$\Gamma(\omega, \delta, R) = \{ x \in \mathbb{R}^n : < x, \omega > > |x| \cos \delta, |x| > R \}.$$ 

Let

$$\Sigma(\omega, \delta, R) = \inf \{ \rho[\varphi] : \varphi \in C^\infty_0(\Gamma(\omega, \delta, R)), \|\varphi\| = 1 \}$$

and

$$K(\omega : H) = \lim_{\delta \to 0} \lim_{R \to \infty} \Sigma(\omega, \delta, R).$$
Theorem 2. (Agmon[1], Lemma 2.7) $K(\cdot : H)$ is lower semicontinuous on $S^{n-1}$ and

$$\Sigma(H) = \min\{K(\omega : H) : \omega \in S^{n-1}\}.$$ 

Let

$$M := \{\omega \in S^{n-1} : K(\cdot : H) \text{ assumes its minimum at } \omega\}.$$ 

Note that $M$ is a closed subset of $S^{n-1}$ since $K(\omega : H)$ is lower semicontinuous on $S^{n-1}$. For $M$ we define the truncated conical region

$$\Gamma(M : R) := \{x \in \mathbb{R}^n : x = t\omega \text{ for } \omega \in M \text{ and } t > R\}.$$ 

Let $d_M(x) := \text{dist}(x : M)$. The first part of our main hypothesis is given by

$${\mathcal{H}}(1) : \text{Let } M \text{ be a proper subset of } S^{n-1} \text{ which is the finite union of closed sets } \{M_i\}_{i=1}^k. \text{ Suppose that each } d_{M_i} \text{ is } C^1 \text{ in a neighborhood of } M_i.$$ 

When $H$ is a generalized N-body operator, Agmon shows that $K(\omega : H) \leq 0$. In that special case, $M = S^{n-1}$ implies that $K(\omega : H) \equiv 0$. For 3-body operators this may result in a rather pathological case called the Efimov effect - see [4] and the references contained therein.

An important ingredient in our proof is the introduction of a certain partition of unity $\{J_0, J_1, J_2\}$ satisfying the properties given in Lemma 3 below. To this end we first define

$$M_{\delta} := \{\omega \in S^{n-1} : \text{dist}(\omega : M) < \delta\}.$$ 

We associate with $M_{\delta}$ the truncated conical region $\Gamma(M_{\delta} : R)$ defined as above.

In the following, $\text{supp} J_i$ denotes the support of $J_i$.

Lemma 3. There is a partition of unity $\{J_0, J_1, J_2\}$ satisfying

(i) $0 \leq J_i \leq 1$ for each $i$ and each $x \in \mathbb{R}^n$;
(ii) $\sum_{i=0}^2 J_i^2(x) \equiv 1$ for $x \in \mathbb{R}^n$;
(iii) each $J_i(x)$ is Lipschitz in $\mathbb{R}^n$;
(iv) $\text{supp } J_0 \subset B(0; 1)$;
(v) $\text{supp } J_1 \subset \Gamma(M_{\delta} : \frac{\delta}{2})$;
(vi) $\text{supp } J_2 \subset \mathbb{R}^n \setminus (\Gamma(M_{\delta}/2 : 0) \cup B(0; \frac{1}{2}))$;
(vii) $J_1$ and $J_2$ are homogeneous of degree zero in $\mathbb{R}^n \setminus B(0; 1)$; and
(viii) for any $\epsilon > 0$ there exists $C_\epsilon > 0$ such that

$$|\nabla J_1(x)|^2 + |\nabla J_2(x)|^2 \leq (\epsilon J_1(x))^2 + C_\epsilon J_2(x)^2 |x|^{-2}$$
for all \( x \in \mathbb{R}^n \setminus B(0; 1) \).

**Proof.** For the basic ideas of the proof we refer the reader to either [2] or Sigal[3].

As the next lemma illustrates, this partition of unity allows us to separate the essential “parts” of the form \( \rho \). This lemma gives the IMS localization formula[4] for \( H \).

**Lemma 4.** For any open set \( \Omega \subset \mathbb{R}^n \) and any \( \phi \in C_0^\infty (\mathbb{R}^n) \)

\[
\int_{\Omega} \left[ |\nabla_A \phi|^2 + q|\phi|^2 \right] \, dx = \sum_{i=0}^{2} \int_{\Omega} \left[ |\nabla_A (J_i \phi)|^2 + q|J_i \phi|^2 - |\nabla_A J_i|^2 |\phi|^2 \right] \, dx.
\]

**Proof.** An elementary calculation shows that

\[
|\nabla_A (J_i \phi)|^2 = J_i^2 |\nabla_A \phi|^2 + |\nabla_A J_i|^2 |\phi|^2 + \frac{1}{2} < \nabla_A J_i^2, \nabla_A \phi|^2 >
\]

on using the fact that the matrix \( A(x) \) is symmetric. Since \( \sum_{i=0}^{2} J_i^2 (x) \equiv 1 \), the identity follows.

Let \( D \) be a bounded open subset of \( \mathbb{R}^n \), which contains the unit ball \( B(0; 1) \), and for which

the embedding \( H^1(D) \hookrightarrow L^2(D) \) is compact.

This is the well-known Rellich property and is satisfied if \( D \) has a continuous boundary.

As a consequence of Lemma 4,

\[
\rho[\phi] = \int_{D} \left[ |\nabla_A \phi|^2 + q|\phi|^2 \right] \, dx
\]

\[
+ \sum_{i=1}^{2} \int_{\mathbb{R}^n \setminus D} \left[ |\nabla_A (J_i \phi)|^2 + q|J_i \phi|^2 - |\nabla_A J_i|^2 |\phi|^2 \right] \, dx.
\]

The finiteness of bound states of \( H \), or equivalently the finiteness of eigenvalues of \( H \) below \( \Sigma(H) \), depends upon the behavior of \( q \) in the truncated conical regions \( \Gamma(M_\delta : R) \) for \( R \) arbitrarily large. Roughly speaking, we need a certain degree of positivity of the “part” of the potential \( q \) which does not determine \( \Sigma(H) \). The next part of our basic hypothesis can be interpreted in such a manner.
The “part” of the form described in $H(2)$ is the “essential” part mentioned above that determines the finiteness or infiniteness of bound states. The term $-\frac{\epsilon_1}{|x|^2}$ arises from the error approximation associated with the partition of unity given in part (viii) of Lemma 3. At times it is helpful to replace $H(2)$ by the following two hypotheses:

$H(2a)$: There exists $\epsilon_1 > 0$ and a function $\sigma$ defined on $\partial D$ such that

$$\int_{\mathbb{R}^n \setminus D} [||\nabla_A (J_1 \phi)||^2 + (q - \frac{\epsilon_1}{|x|^2})|J_1 \phi|^2] dx \geq \Sigma(H) \int_{\mathbb{R}^n \setminus D} |J_1 \phi|^2 dx + \int_{\partial D} \sigma|J_1 \phi|^2 ds$$

for all $\phi \in C_0^\infty(\mathbb{R}^n)$.

$H(2b)$: For some $\epsilon_2 \in (0, 1)$ and $C_{\epsilon_2} > 0$

$$\int_{\partial D} \sigma|J_1 \phi|^2 dx \geq -\epsilon_2 \int_{D} |\nabla_A \phi|^2 dx - C_{\epsilon_2} \int_{D} |\phi|^2 dx$$

for all $\phi \in C_0^\infty(\mathbb{R}^n)$.

Hypothesis $H(2b)$ holds if $\sigma_- \in L^\gamma(\partial D)$ for $\gamma = n - 1$ when $n > 2$ and $\gamma \in (1, \infty]$ when $n = 2$.

The final part of our hypothesis assures us that the remainder of the form is under control. First, it is helpful to define the weight

$$w(x) := \begin{cases} 1 & \text{for } x \in D \\ J_2(x) & \text{for } x \notin D. \end{cases}$$

Now, we introduce the notation

$$\int_{\mathbb{R}^n} |\nabla_A w\phi|^2 dx := \int_{D} |\nabla_A \phi|^2 dx + \int_{\mathbb{R}^n \setminus D} |\nabla_A J_2 \phi|^2 dx,$$

for all $\phi \in C_0^\infty(\mathbb{R}^n)$. Note that $\nabla_A (w\phi)$ is not defined on $\partial D$. 
\( \mathcal{H}(3) \): Given \( \epsilon_3 \) there exists \( C_{\epsilon_3} > 0 \) such that
\[
\int_{\mathbb{R}^n} q|w\phi|^2 \, dx \leq \epsilon_3 \int_{\mathbb{R}^n} |\nabla_A (w\phi)|^2 \, dx + C_{\epsilon_3} \int_{\mathbb{R}^n} |w\phi|^2 \, dx
\]
for all \( \phi \in C_0^\infty (\mathbb{R}^n) \).

This last part of the hypothesis is satisfied by the N-body potentials briefly mentioned above.

Now, we state our main theorem. Due to space limitations, we cannot give a full proof here. We will give a sketch of the main ideas of the proof.

**Theorem 5.** If (3)(i)-(iv) and \( \mathcal{H}(1), \mathcal{H}(2), \& \mathcal{H}(3) \) hold, then \( H \) has only a finite number of bound states.

**Proof (Sketch).** If we interpret \( \mathcal{H}(2) \) in terms of operators, then we might expect that
\[
H \geq J_1(x)\Sigma(H)J_1(x) + H_r
\]
for some “remainder” operator \( H_r \). The sesquilinear form for such an operator is defined for \( C_0^\infty (D \cup \text{supp}J_2) \)-functions. This form is much like \( \rho \) with some additional error terms. Part \( \mathcal{H}(3) \) of the hypothesis is a key ingredient in the proof of the fact that this form is closeable. Now, \( H_r \) arises as the operator associated with this form. A result like Theorem 2 applies to \( H_r \). Part \( \mathcal{H}(3) \) of the hypothesis assures that \( \Sigma(H_r) > \Sigma(H) \). It follows that \( H_r \) can have only a finite number of eigenvalues below \( \Sigma(H) \). Finally, we show that the number of eigenvalues of \( H \) below \( \Sigma(H) \) can be no more than the number of eigenvalues of \( H_r \) below \( \Sigma(H) \), which completes the proof.

A version of Theorem 5 with a more restrictive hypothesis was used in [2] to establish results for atomic-type operators (2). There it was assumed that \( K(\cdot : P) \) assumes its minimum at no more than a finite number of points. That assumption excluded the consideration of molecules and an atom with a nucleus which was not assumed to be infinitely heavy. In these latter cases it is common to first remove the motion of the center of mass via a Jacobi coordinate change restricting the operator to “configuration space” \( X \) - see [4]. In \( X \) we can think of the motion of the center of mass as being held fixed at the origin. Now, letting \( H \) be the Hamiltonian in \( L^2(X) \cong L^2(\mathbb{R}^{3(N-1)}) \), then \( K(\cdot : H) \) assumes its minimum on curves in \( S^{3N-4} \) or on their intersections. These curves correspond to \( x = (x^1, x^2, \ldots, x^{N-1}) \in S^{3N-4} \) where \( x^i = x^j \) for distinct \( i \) and \( j \). Theorem 5 now allows us to consider these other cases.
References


