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FINITENESS OF BOUND STATES OF GENERAL N-BODY OPERATORS

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

$$P_N = \sum_{j=1}^{N}(-\Delta_i - \frac{Z}{|x^i|}) + \sum_{1\le i<j\le N} \frac{1}{|x^i - x^j|}. \tag{1}$$

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 $x^i \in \mathbf{R}^3$ is the coordinate of the ith electron and Δ_i denotes the Laplacian in $\mathbf{R}^3$ 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. *(Zhislin (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 $Z \le N-1$.*

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

$$P = -\sum_{i=1}^{N}(2m_i)^{-1}\Delta_i + \sum_{i=1}^{N} v_{oi}(x^i) + \sum_{1\le i<j\le N} v_{ij}(x^i - x^j)\ , \tag{2}$$

where m_i is the mass of the ith electron. As in [2] we proceed from the foundation laid by Agmon[1] . Define

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

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

(3)
- (i) Each a^{ij} is a bounded, continuous, real-valued function on $\mathbf{R}^n$.
- (ii) The matrix $A(x) = [a^{ij}(x)]$ is symmetric and its smallest eigenvalue $\mu(x)$ is a positive continuous function on $\mathbf{R}^n$.
- (iii) $q \in L_1(\mathbf{R}^n)_{loc}$.
- (iv) $q_- = \max(-q,0) \in M_{loc}(\mathbf{R}^n)$, where $M(\mathbf{R}^n) = M_0(\mathbf{R}^n)$ is the Stummel class of functions.

The sesquilinear form which gives rise to H is

$$\rho[\varphi,\psi] = \int_{\mathbf{R}^n}\{< \nabla_A\varphi, \nabla_A\psi > + q\varphi\bar{\psi}\}\, dx \quad (\varphi,\psi \in C_0^\infty(\mathbf{R}^n)), \tag{4}$$

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

$$< \nabla_A\varphi, \nabla_A\psi > = \sum_{i,j=1}^{n} a^{ij}\nabla\varphi\nabla\bar{\psi}. \tag{5}$$

Define

$$\Lambda(H) = \inf\{\rho[\varphi] :\ \varphi \in C_0^\infty(\mathbf{R}^n), \|\varphi\| = 1\}. \tag{6}$$

If $\Lambda(H) > -\infty$, the sesquilinear form $\rho[\varphi,\psi]$ on $C_0^\infty(\mathbf{R}^n) \times C_0^\infty(\mathbf{R}^n)$ is proved to be a densely defined symmetric form which is bounded below and closable in $L_2(\mathbf{R}^n)$ - see Agmon[1] and [2] .

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Henceforth, let H denote the self-adjoint operator in $L_2(\mathbf{R}^n)$ associated with the form $\rho[\varphi,\psi]$. Then, the least point of the essential spectrum of H is given by

$$\Sigma(H) = \sup_{K:\text{compact}} \left[\inf\left\{\rho[\varphi] : \varphi \in C_0^\infty(\mathbf{R}^n - K), \|\varphi\| = 1\right\}\right]. \tag{7}$$

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

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

Let

$$\Sigma(\omega,\delta,R) = \inf\{\rho[\varphi] : \varphi \in C_0^\infty(\Gamma(\omega,\delta,R)), \|\varphi\| = 1\}$$

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

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

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

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

When H is a generalized N-body operator, Agmon shows that $K(\omega : H) \le 0$. 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

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

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

In the following, $suppJ_i$ denotes the support of J_i.

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

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

$$|\nabla J_1(x)|^2 + |\nabla J_2(x)|^2 \le (\epsilon J_1(x)^2 + C_\epsilon J_2(x)^2)|x|^{-2}$$

for all $x \in \mathbf{R}^n \setminus B(0;1)$.

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 ρ. This lemma gives the IMS localization formula[4] for H.

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

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

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 $\mathbf{R}^n$, 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,

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

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.

$\mathcal{H}(2)$: There exist $\epsilon_1, \epsilon_2 \in (0,1)$ and $C_{\epsilon_2} > 0$ such that

$$\int_{\mathbf{R}^n \setminus D} [|\nabla_A (J_1\phi)|^2 + (q - \frac{\epsilon_1}{|x|^2})|J_1\phi|^2] dx$$
$$\geq \Sigma(H) \int_{\mathbf{R}^n \setminus D} |J_1\phi|^2 dx - \epsilon_2 \int_D |\nabla_A \phi|^2 dx - C_{\epsilon_2} \int_D |\phi|^2 dx.$$

The "part" of the form described in $\mathcal{H}(2)$ is the "essential" part mentioned above that determines the finiteness or infiniteness of bound states. The term $-\epsilon_1/|x|^2$ 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 $\mathcal{H}(2)$ by the following two hypotheses:

$\mathcal{H}(2a)$: There exists $\epsilon_1 > 0$ and a function σ defined on ∂D such that

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

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

$\mathcal{H}(2b)$: 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 ϕ $C_0^\infty(\mathbf{R}^n)$.

Hypothesis $\mathcal{H}(2b)$ 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

$$\int_{\mathbf{R}^n} |\tilde{\nabla}_A w\phi|^2 dx := \int_D |\nabla_A \phi|^2 dx + \int_{\mathbf{R}^n \setminus D} |\nabla_A J_2 \phi|^2 dx,$$

for all $\phi \in C_0^\infty(\mathbf{R}^n)$. Note that $\nabla_A(w\phi)$ is not defined on ∂D.

$\mathcal{H}(3)$: Given ϵ_3 there exists $C_{\epsilon_3} > 0$ such that

$$\int_{\mathbf{R}^n} q|w\phi|^2 dx \le \epsilon_3 \int_{\mathbf{R}^n} |\tilde{\nabla}_A(w\phi)|^2 dx + C_{\epsilon_3} \int_{\mathbf{R}^n} |w\phi|^2 dx$$

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

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

$$H \ge J_1(x)\Sigma(H)J_1(x) + H_r$$

for some "remainder" operator H_r. The sesquilinear form for such an operator is defined for $C_0^\infty(D \cup supp J_2)$-functions. This form is much like ρ 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 orgin. Now, letting H be the Hamiltonian in $L^2(X) \cong L^2(\mathbf{R}^{3(N-1)})$, 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.

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