THE AGMON SPECTRAL FUNCTION
FOR MOLECULAR HAMILTONIANS
WITH SYMMETRY RESTRICTIONS

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Abstract. In this paper we introduce symmetry considerations into our earlier
work, which was concerned with geometric spectral properties of Schrödinger oper-
ators including the N-body operators of quantum mechanics. The point of emphasis
is a function introduced by Shmuel Agmon which we have named the Agmon spec-
tral function. We show that this function is symmetric for an N-body Schrödinger
operator restricted to a subspace of prescribed symmetry. We then show how it
can be used to obtain criteria for the finiteness and infiniteness of bound states of
polyatomic systems.

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School of Mathematics, Cardiff.
“Geometric spectral analysis” is a term which is used to described certain methods of quantum mechanics which have been developed over the past 30 years. These methods are used to study spectral properties of N-body Schrödinger operators using the geometry of phase space. (The term “localization techniques” has also been used in this regard.) The term “geometric methods” was first introduced by Simon (1977), but the methods go at least as far back as the fundamental work of Zhislin (1960). Sigal (1982), in particular, advanced and promoted their application. Our view here and in recent work builds mainly upon the work in chapters 2, 3, and 4 of Agmon (1982), but the work of many others as outlined in chapter 3 of Cycon et al (1987) is inherent here as well.

In his lecture notes Agmon (1982) defined a function $K(\omega)$ for $\omega$ on the unit sphere $S^{n-1}$ in $\mathbb{R}^n$ which is associated with a second order elliptic operator $P$ with domain in $L^2(\mathbb{R}^n)$. We refer to this function as the Agmon spectral function. Agmon showed that $K$ was lower semicontinuous on $S^{n-1}$ and that its minimum value on $S^{n-1}$ was the least point of the essential spectrum of $P$. This result recovered the classical result of Persson (1960) and the main part of the HVZ Theorem of quantum mechanics (named for Hunziker (1966), van Winter (1964), and Zhislin (1960)). For the case in which $P$ is an N-body Schrödinger operator, it gave an eloquent connection between the value of $K$ at any $\omega \in S^{n-1}$ and the least point of the spectrum of one of the different subsystems of $P$. Subsequently, the authors showed in (Evans and Lewis 1990) and (Evans, Lewis, Saitô 1991, 1992a) how an extension of these ideas could be used to characterize the finiteness and the infiniteness of eigenvalues below the least point of the essential spectrum of Schrödinger operators $P$ including N-body operators. However, neither Agmon’s work nor ours accounts for permutational symmetry required to accommodate the Pauli-exclusion principle. This is required before the results can be applied to Hamiltonians of real atomic and molecular systems. In this paper we develop the theory for the Agmon spectral function with permutational symmetry considerations for a certain polyatomic system. We refer freely to our past work in (Evans and Lewis 1990) and (Evans, Lewis, Saitô 1991, 1992a) in order to be as brief as possible. We do not look at the most general system which could be considered for the sake of clarity. However, the treatment below should make clear the needed changes to accommodate more complex systems. We also do not consider spin here, but its inclusion in the results below is not expected to cause any substantial change from what is given. For a relevant discussion we refer to Part IV of Lieb (1990).

We will consider a system of $N_1$ electrons of mass $M_1$ located at points $y^i \in \mathbb{R}^\nu$
and \( N_2 \) identical nuclei of mass \( M_2 \) at points \( z^i \in \mathbb{R}^\nu \). Denote the total mass by \( M := N_1 M_1 + N_2 M_2 \), set

\[
N = N_1 + N_2
\]

and let \( Y \) and \( Z \) be \( N_1 \) and \( N_2 \) copies of \( \mathbb{R}^\nu \) respectively. Set

\[
\tilde{X} := Y \times Z.
\]

The Hamiltonian of the system before the removal of the motion of the center of mass is of the form

\[
(1.1) \quad \tilde{P} := -\sum_{i=1}^{N} \frac{1}{2m_i} \Delta_i + q(x), \quad q(x) = \sum_{1 \leq i < j \leq N} v_{ij}(x^i - x^j)
\]

where we understand that \( x^i \) denotes the appropriate \( y^i \) or \( z^i \), \( m_i = M_1 \), \( i = 1, \ldots, N_1 \), and \( m_i = M_2 \), \( i = N_1 + 1, \ldots, N \). The Laplacian on the \( i \)-th copy of \( \mathbb{R}^\nu \) is given by \( \Delta_i \).

In order to consider symmetry among the electrons and nuclei we introduce \( G(n) \), the permutation group of degree \( n \), and define

\[
\alpha(y) = (y^{\alpha(1)}, \ldots, y^{\alpha(N_1)}), \quad y \in Y, \quad \alpha \in G(N_1),
\]

and, similarly, \( \beta(z) \) for \( z \in Z \) and \( \beta \in G(N_2) \). Let \( G := G(N_1) \times G(N_2) \) and define \( \sigma = (\alpha, \beta) \) for \( \alpha \in G(N_1) \) and \( \beta \in G(N_2) \). Henceforth, we will simply write \( \sigma = \alpha \beta \in G \) for which

\[
\sigma(x) = (\alpha(y), \beta(z)), \quad x = (y, z) \in \tilde{X}.
\]

The order of \( G(N_i), i = 1, 2, \) is denoted by \(|G_i|\) and \( |G| := |G_1||G_2| \). If \( \alpha \in G(N_i), i = 1, 2, \) then we define \( \epsilon(\alpha) = 1 \) if \( \alpha \) is an even permutation and \( \epsilon(\alpha) = -1 \) if \( \alpha \) is an odd permutation.

For any \( f \in L^2(\tilde{X}) \) we define

\[
(\sigma f)(x) := f(\sigma^{-1}x), \quad x \in \tilde{X}.
\]

A function \( f \) is said to be \textit{antisymmetric in} \( y \) and \( z \) if

\[
(\sigma f)(x) = \epsilon(\alpha)\epsilon(\beta)f(x), \quad x \in \tilde{X}, \quad \sigma \in G.
\]
In this case we define $\epsilon(\sigma) = \epsilon(\alpha)\epsilon(\beta)$. Similarly, $f$ is said to be antisymmetric in $y$ and symmetric in $z$ if

$$(\sigma f)(x) = \epsilon(\alpha)f(x), \quad x \in \tilde{X}, \quad \sigma \in G.$$ 

In this case we define $\epsilon(\sigma) = \epsilon(\alpha)$.

We denote by $S$ the set of functions which satisfy the symmetry imposed by the problem, i.e. antisymmetric in $Y$ and either antisymmetric or symmetric in $Z$. Define

$$f_S(x) := \frac{1}{|G|} \sum_{\sigma \in G} \epsilon(\sigma)(\sigma f)(x), \quad f \in L^2(\tilde{X}).$$

Then, $f_S \in S$ and since $x \mapsto \sigma(x)$ is a linear isometry on $\tilde{X}$ (endowed with the usual Euclidean norm) it follows that the map $R_S : f \mapsto f_S$ is a projection of $L^2(\tilde{X})$ onto the closed subspace $S \cap L^2(\tilde{X})$. We denote the latter subspace by $L^2_S(\tilde{X})$; it is clearly the closure in $L^2(\tilde{X})$ of

$$C^\infty_{S,0}(\tilde{X}) := S \cap C^\infty_0(\tilde{X}).$$

We shall assume throughout that

(i) $q \in L^1_{loc}(\tilde{X}),$

(ii) $(\sigma q)(x) = q(x)$ for all $\sigma \in G,$

(iii) $q_- := -\min(q(x),0) \in M_{loc}(\tilde{X}).$

(See (Agmon 1982) and (Evans, Lewis, Saitô (1991, 1992a)) for more details regarding the requirements of (1.2) and their relation to the representation of $q$ given in (1.1)).

The self-adjoint realization, $\tilde{P}_S$, in $L^2_S(\tilde{X})$ of the formal operator $\tilde{P}$ is generated by the sesquilinear form

$$\tilde{\rho}[\phi, \psi] := \int_{\tilde{X}} \left\{ \sum_{i=1}^{N} \frac{1}{2m_i} < \nabla_i \phi, \nabla_i \psi > + q\phi \bar{\psi} \right\} dx, \quad \phi, \psi \in C^\infty_{S,0}(\tilde{X})$$

where $\nabla_i$ denotes the gradient on the $i$-th copy of $\mathbb{R}^\nu$ and $< \cdot, \cdot >$ is the Euclidean inner product in $C^\nu$. However, $\tilde{P}_S$ has no eigenvalues - see p. 79 of Agmon (1982). It is more appropriate to study the operator associated with the removal of the motion of the center of mass, i.e. we must restrict $\tilde{P}_S$ to the subspace

$$X := \{ x \in \tilde{X} : \sum_{i=1}^{N} m_i x^i = 0 \}.$$
We will do this by restricting \( \tilde{\rho} \) to the manifold \( X \). This new sesquilinear form will be denoted by \( \rho \); it is the form of the self-adjoint operator \( P_S = \tilde{P}_S|_X \) in \( L^2_X(X) \).

First, define the matrix \( G := \text{diag}(2m_1I_\nu, \ldots, 2m_NI_\nu) \) and the inner product

\[
(x, y)_{\tilde{X}} : = (Gx, y)_{\nu N} = \sum_{i=1}^N 2m_i < x^i, y^i > \quad x, y \in \tilde{X}.
\]

Then,

\[
\Delta_{\tilde{X}} : = \text{div}(G^{-1}\nabla) = \sum_{i=1}^N \frac{1}{2m_i} \Delta_i
\]

is the Laplace-Beltrami operator with respect to the inner product \((\cdot, \cdot)_{\tilde{X}}\). We wish to restrict \( \Delta_{\tilde{X}} \) to \( X \). If we let \( T : \tilde{X} \to \tilde{X} \) be any bijection on \( \tilde{X} \) (whose matrix representation with respect to the canonical basis on \( \tilde{X} \) we also denote by \( T \)) then for \( x, y \in \tilde{X} \)

\[
(x, y)_{\tilde{X}} = ((T^t)^{-1}GT^{-1}\hat{x}, \hat{y})_{\nu N} \quad \text{for } \hat{x} = Tx \text{ and } \hat{y} = Ty \text{ in } T\tilde{X},
\]

and

\[
(1.3) \quad \Delta_{\tilde{X}} = \text{div}(TG^{-1}T^t\nabla),
\]

where the equality of the operators above should be interpreted with respect to unitary equivalence, an interpretation which we will use freely without comment.

We can understand the restriction of \( \Delta_{\tilde{X}} \) to \( X \) by making certain choices of \( T \).

The classic cases are ones which produce Jacobi coordinates, atomic coordinates, or clustered coordinates.

To illustrate this let \( I_\nu \) be the identity matrix in \( \mathbb{R}^\nu \). Then, a nonsingular matrix \( T = (t_{ij}I_\nu) \), \( i, j = 1, \ldots, N \), is chosen such that \( Tx = (r^1, \ldots, r^{N-1}, R)^t \) for \( R := \sum_{i=1}^N m_i x^i/M \), the coordinate of the center of mass;

\[
(1.4) \quad T \begin{pmatrix}
  x^1 \\
  \vdots \\
  x^N
\end{pmatrix} = \begin{pmatrix}
  r^1_x \\
  \vdots \\
  r^{N-1}_x \\
  0
\end{pmatrix} ; \quad x \in X
\]

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and

\[
(1.4b) \quad T \begin{pmatrix} x^1 \\ \vdots \\ x^N \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \quad x \in X^\perp.
\]

(This implies that the last row of \( T \) is \( (\frac{m_1}{M}, \ldots, \frac{m_N}{M}) \) and that the sum of the elements of each of the first \( N-1 \) rows is zero.) The matrix appearing in (1.3) is now in block form

\[
(1.5) \quad TG^{-1}T^t = \text{diag}(G_X, \frac{1}{2M} I_\nu)
\]

where \( G_X \) is an \( (N-1)\nu \times (N-1)\nu \), positive definite, symmetric matrix. Similarly, this matrix is produced when the change of variable is made in the gradient term of \( \tilde{\rho} \). As a consequence,

\[
(x, y)_{\tilde{X}} := (Gx, y)_{\nu N} = (G_X^{-1}r_x, r_y)_{\nu(N-1)} + (2MR_x, R_y)_{\nu},
\]

and

\[
\sum_{i=1}^{N} \frac{1}{2m_i} \Delta_i = \text{div}(G^{-1}\nabla)
\]

\[
= \text{div}_r(G_X \nabla r) \otimes I_{L^2(TX^\perp)} + I_{L^2(TX)} \otimes \frac{1}{2M} \Delta R.
\]

In particular, this shows that \( \Delta_{\tilde{X}} \) restricted to \( X \) is

\[
\Delta_X = \text{div}_r(G_X \nabla r) \quad \text{for } x \in X \text{ and } Tx = \begin{pmatrix} r \\ 0 \end{pmatrix}
\]

which is the Laplace-Beltrami operator in \( X \) with respect to the inner product

\[
(1.6) \quad (x, y)_X := (G_X^{-1}r_x, r_y)_{\nu(N-1)}.
\]

We can now view \( \tilde{P}_S = -\Delta_{\tilde{X}} + q \) restricted to \( X \) as

\[
P_S := -\Delta_X + q|_X.
\]
We restrict $\tilde{\rho}$ in an analogous way. Define

$$C^\infty_{S,0}(X) := \{ \tilde{f}|_X : \tilde{f} \in C^\infty_{S,0}(\tilde{X}) \}$$

and for any subset $\Omega \subset X$

$$C^\infty_{S,0}(\Omega) := C^\infty_{S,0}(X) \cap C^\infty_{0}(\mathcal{G}(\Omega))$$

where

$$\mathcal{G}(\Omega) := \cup_{\sigma \in \mathcal{G}} \sigma(\Omega), \quad \mathcal{G}(x) := \mathcal{G}(\{x\}),$$

$$\sigma(\Omega) := \{ \sigma(x) : x \in \Omega \}.$$

Choose some matrix $T$ as defined above. (We will see that the spectrum of $P_S$ is independent of this choice.) For $1 \leq i < j \leq N$ and $\tilde{V}_{ij}(x) := v_{ij}(x_i - x_j)$, set

$$V_{ij}(r) := \tilde{V}_{ij}(x) \quad \text{for } x \in X \text{ and } x = T^{-1} \begin{pmatrix} r \\ 0 \end{pmatrix}. \tag{1.7}$$

We let $L^2(X) := L^2(TX; d_X r)$ where

$$d_X r := \sqrt{\det(G^{-1}_X)d r_1 \cdots d r_{N-1}} \tag{1.8}$$

is the measure induced by the inner product $(\cdot, \cdot)_X$ defined in (1.6). The closure of $C^\infty_{S,0}(X)$ in $L^2(X)$ is denoted by $L^2_S(X)$.

For all $\phi, \psi \in C^\infty_{S,0}(X)$ (with the variable change described in (1.7)) define

$$\rho[\phi, \psi] := \int_X \left( (\nabla_X \phi, \nabla_X \psi)_X + \sum_{1 \leq i < j \leq N} \tilde{V}_{ij}(x) \phi \psi \right) dx$$

$$= \int_{TX} \left( (G_X \nabla_r \phi, \nabla_r \psi)_{\nu(N-1)} + \sum_{1 \leq i < j \leq N} V_{ij}(r) \phi \psi \right) d_X r \tag{1.9}$$

with $\rho[\phi] := \rho[\phi, \phi]$. An immediate consequence of Proposition 1 of Evans and Lewis (1990) is
**Proposition 1.1.** Let (1.2) be satisfied and suppose that

\[(1.10) \quad \Sigma(P_S) := \sup_{K \text{ compact}} \left[ \inf \{ \rho[\phi] : \phi \in C_{S,0}^\infty(X \setminus K), \|\phi\|_{L^2(X)} = 1 \} \right] > -\infty. \]

Then, \( \rho \) is a symmetric form which is densely defined, bounded below, and closable in \( L^2_S(X) \).

We note that (1.10) is satisfied if we assume further to (1.2) that

(iv) \( q_- \in M(\tilde{X}) \) or, when \( \nu N \geq 3 \), \( q_- \in L^{\nu N}_{\nu N}(\tilde{X}) \).

For then, it follows that given \( \epsilon > 0 \) there exists \( C_\epsilon > 0 \) such that

\[
\int_{\tilde{X}} q_- |\phi|^2 \, dx \leq \epsilon \int_{\tilde{X}} |\nabla \phi|^2 \, dx + C_\epsilon \int_{\tilde{X}} |\phi|^2 \, dx, \quad \phi \in C_{S,0}^\infty(\tilde{X}).
\]

Hence, with \( 2\delta = \min \{ \frac{1}{2m_i} : i = 1, \ldots, N \} \), there exists \( C_\delta > 0 \) such that

\[
\tilde{\rho}[\phi] + C_\delta \|\phi\|^2 \geq \delta \int_{\tilde{X}} |\nabla \phi|^2 \, dx + \int_{\tilde{X}} q_+ |\phi|^2 \, dx + \|\phi\|^2_{L^2(\tilde{X})}, \quad \phi \in C_{S,0}^\infty(\tilde{X}),
\]

and, in particular, this implies (1.10). Condition (iv) includes the case in which each \( v_{ij} \) is a Coulomb potential and short-range potentials as well - see p. 67 of Agmon (1982) and (Evans, Lewis, Saitô (1992a)).

Now, \( P_S \) is the self-adjoint operator associated with the closure of the form \( \rho \) in \( L^2_S(X) \). It is important to note that while there are many choices for \( T \) which could be made, the associated operators \( P_S \) defined as above would be unitarily equivalent. Hence, we don’t distinguish between them. It may also be helpful to view the maps \( x \mapsto r_x, x \in X \), as coordinate maps given by each \( T \) from the manifold \( X \) to \( \mathbb{R}^{\nu(N-1)} \). For other discussions in this regard see Agmon (1982), Chavel (1984), Cycon *et al* (1987), and the appendix in (Evans, Lewis, Saitô (1992a)).

Denoting the spectrum and essential spectrum of \( P_S \) by \( \sigma(P_S) \) and \( \sigma_e(P_S) \) respectively, it follows as in Theorem 3.2 of Agmon (1982) that

\[
\inf \sigma(P_S) = \Lambda(P_S) := \inf \{ \rho[\phi] : \phi \in C_{S,0}^\infty(X), \|\phi\|_{L^2(X)} = 1 \}
\]

and \( \inf \sigma_e(P_S) = \Sigma(P_S) \) when the hypothesis of Proposition 1.1 holds.
§2 THE AGMON SPECTRAL FUNCTION IN $X$ WITH SYMMETRY

Let $S(\tilde{X}) := \{\omega \in \tilde{X} : |\omega|_{\tilde{X}} = 1\}$, $S(X) = S(\tilde{X}) \cap X = \{\omega \in X : |\omega|_X = 1\}$ be the unit spheres in $\tilde{X}$ and $X$ respectively where $| \cdot |_{\tilde{X}}$ and $| \cdot |_X$ are the norms induced by the inner products in $\tilde{X}$ and $X$ respectively.

**Definition 2.1.** Let $\text{dist}$ be the metric defined by $| \cdot |_X$ in $X$.

(i) For $\delta > 0$ and $U \subset S(X)$,

$$U_\delta := \{\omega \in S(X) : \text{dist}(\omega, U) < \delta\}, \quad \omega_\delta := \{\omega\}_\delta$$

and

(ii) $\Gamma(U; R) := \{x = \omega t : \omega \in U, t > R\}$.

Next, we compile several basic facts about the action of $G$ on subsets of $X$.

**Lemma 2.2.** For $U \subset S(X)$, $\sigma \in G$, and $\delta > 0$,

(i) $\sigma(U_\delta) = [\sigma(U)]_\delta$;

(ii) $G(U_\delta) = [G(U)]_\delta$;

(iii) $\sigma(\Gamma(U_\delta; R)) = \Gamma([\sigma(U)]_\delta; R)$;

(iv) if $\omega \in S(X)$ and

\begin{equation}
0 < \delta < \frac{1}{2} \min\{|\sigma(\omega) - \omega|_X : \sigma \in G, \sigma(\omega) \neq \omega\},
\end{equation}

then $[\sigma(\omega)]_\delta \cap [\tau(\omega)]_\tau = \emptyset$ for all $\sigma, \tau \in G$ such that $\sigma(\omega) \neq \tau(\omega)$;

(v) for each $\sigma \in G$, $\sigma(X) = X$, $\sigma(S(X)) = S(X)$, $f \in L^2_S(X)$ if, and only if $\sigma f \in L^2_S(X)$, and $\sigma(x) = x$ for all $x \in X^\perp$;

(vi) if $\phi \in C_{S,0}^\infty(\Omega)$ for some $\Omega \subset X$, then $\sigma \phi \in C_{S,0}^\infty(\sigma(\Omega))$ for all $\sigma \in G$ and $(\sigma \phi)(x) = \epsilon(\sigma)\phi(x)$ for all $x \in \sigma(\Omega)$.

**Proof.** Assertions (i)-(iv) are straightforward consequences of the fact that $x \mapsto \sigma(x)$ is a linear isometry on $X$. For instance, to prove (iv) we suppose there exist $\sigma, \tau \in G$ with $\sigma(\omega) \neq \tau(\omega)$ and $[\sigma(\omega)]_\delta \cap [\tau(\omega)]_\tau \neq \emptyset$. Then, there exists $\omega_0 \in [\sigma(\omega)]_\delta \cap [\tau(\omega)]_\tau$, i.e.

$$|\omega_0 - \sigma(\omega)|_X < \delta \quad \text{and} \quad |\omega_0 - \tau(\omega)|_X < \delta.$$
Hence, $\sigma^{-1}\tau(\omega) \neq \omega$, but
\[
|\omega - \sigma^{-1}\tau(\omega)|_X = |\sigma(\omega) - \tau(\omega)|_X < 2\delta,
\]
contrary to the choice of $\delta$.

Since
\[
\sum_{i=1}^N m_i x^i = \sum_{i=1}^N m_i x^{\sigma(i)} \quad \text{for all } x \in \tilde{X} \text{ and all } \sigma \in G
\]
then $\sigma(X) = X$, and $\sigma(S(X)) = S(X)$ for all $\sigma \in G$ since each $\sigma$ is an isometry.

It then follows that $f \in L_0^2(S(X))$ if, and only if $\sigma f \in L_0^2(S(X))$ for all $\sigma \in G$. To complete the proof of (v) note that $\sigma^\perp$ is spanned by elements $x = (x^1, \ldots, x^N)$ where $x^i = \alpha$, $i = 1, \ldots, N$, for any $\alpha \in \mathbb{R}^\nu$. Therefore, any $x \in \sigma^\perp$ can be written as a linear combination of such elements implying that $\sigma(x) = x$.

To show (vi) let $\phi \in C_0^\infty(S(\tilde{X}))$, then
\[
\phi = \tilde{\phi}|_{\chi} \in C_0^\infty(G(\Omega)) \quad \text{for some } \tilde{\phi} \in C_0^\infty(\tilde{X}).
\]
Since $\tilde{\phi} \in S$, then for $\sigma \in G$ and $x \in \sigma(\Omega)$
\[
(\sigma \phi)(x) = \phi(\sigma^{-1} x) = \tilde{\phi}(\sigma^{-1} x) = (\sigma \tilde{\phi})(x) = \epsilon(\sigma) \tilde{\phi}(x) = \epsilon(\sigma) \phi(x).
\]
Therefore, $\sigma \phi \in C_0^\infty(\sigma(\Omega))$. □

**Definition 2.3.** For $\omega \in S(X)$, $G_\omega := \{\sigma \in G : \sigma(\omega) = \omega\}$.

Then, $G_\omega$ is a subgroup of $G$ and we have a coset decomposition
\[
G = \bigcup_{j=1}^p \sigma_j [G_\omega]
\]
for each $\omega \in S(X)$ where $\sigma_1$ is the identity of $G$ and $\sigma_j \sigma_k^{-1} \notin G_\omega$ for $j \neq k$. If $\delta$ satisfies (2.1) we have the disjoint union
\[
G(\Gamma(\omega_\delta; R)) = \bigcup_{j=1}^p \Gamma(\sigma_j(\omega)_\delta; R).
\]
Hereafter, we will assume that $\delta$ satisfies (2.1).

**Lemma 2.4.** For $\delta$ satisfying (2.1) and $\sigma_j$, $j = 1, \ldots, p$, given in (2.2)
\[
\phi(x) = \sum_{j=1}^p \epsilon(\sigma_j)(\sigma_j \phi)(x), \quad x \in G(\Gamma(\omega_\delta; R))
\]
for all $\phi \in C_0^\infty(\Gamma(\omega_\delta; R))$ with each $\sigma_j \phi \in C_0^\infty(\Gamma(\sigma_j(\omega)_\delta; R))$, $j = 1, \ldots, p$.

**Proof.** This follows from Lemma 2.2(vi) and (2.3). □
Definition 2.5. Let $\rho$ be given by (1.9). For all $\omega \in S(X)$ define
\[ K_S(\omega; R) := \inf \{ \rho[\phi] : \phi \in C_{\infty}^\infty(\Gamma(\omega_\delta; R)) \text{ and } \|\phi\|_{L^2(\nu)} = 1 \} \]
and
\[ K_S(\omega) := \lim_{\delta \to 0} \lim_{R \to \infty} K_S(\omega_\delta; R) = \sup_{\delta>0,R<\infty} K_S(\omega; R) \]

The function $K_S(\omega)$, $\omega \in S(X)$, is the Agmon spectral function with symmetry restrictions.

Proposition 2.6. The Agmon spectral function $K_S(\omega)$ is symmetric on $S(X)$, i.e.
\[ K_S(\sigma(\omega)) = K_S(\omega), \quad \text{for all } \omega \in S(X) \text{ and all } \sigma \in G. \]

Proof. First, we need to show that for any $\sigma \in G$
\begin{equation}
\tilde{\rho}[\tilde{\phi}] = \tilde{\rho}[\sigma \tilde{\phi}], \quad \tilde{\phi} \in C_{\infty}^\infty(\tilde{X}).
\end{equation}
Here, it is helpful to write each permutation as the product of two-cycles. Then represent each two-cycle by an elementary matrix $E_{ij}$ where $E_{ij}$ is formed by interchanging the $i$-th and the $j$-th rows of the identity matrix. Then, a matrix representation for $\sigma$ is given by
\[ E_\sigma := \Pi E_{ij}, \quad \sigma \in G, \]
where the product is taken over all $E_{ij}$ representing the two-cycles forming $\sigma$. Note that each $E_{ij}$ associated with some $\sigma \in G$ is symmetric, commutes with $G^{-1} = \text{diag}(\frac{1}{2m_1}I_{\nu}, \ldots, \frac{1}{2m_N}I_{\nu})$, and $E_{ij}^{-1} = E_{ij}$. This implies that each $E_\sigma$ is orthogonal, i.e. $E_\sigma^t = E_\sigma^{-1}$, and that $E_\sigma$ commutes with $G^{-1}$. Therefore, we have the representation
\[ \sigma^{-1}x = E_\sigma^{-1}x = E_\sigma^t x, \quad x \in \tilde{X}. \]
For a given $\sigma \in G$ let $z = \sigma^{-1}x$. Then, for any $\tilde{\phi} \in C_{\infty}^\infty(\tilde{X})$
\[ \tilde{\rho}[\sigma \tilde{\phi}] = \int_{\tilde{X}} \left[ < G^{-1} \nabla_x \sigma \tilde{\phi}, \nabla_x \sigma \tilde{\phi} > + q(x)|\sigma \tilde{\phi}(x)|^2 \right] dx 
\]
\[ = \int_{\tilde{X}} \left[ < G^{-1} \nabla_x \tilde{\phi}(\sigma^{-1}x), \nabla_x \tilde{\phi}(\sigma^{-1}x) > + q(x)|\tilde{\phi}(\sigma^{-1}x)|^2 \right] dx 
\]
\[ = \int_{\tilde{X}} \left[ < E_\sigma^{-1} G^{-1}(E_\sigma^{-1})^t \nabla_z \tilde{\phi}(z), \nabla_z \tilde{\phi}(z) > + q(\sigma z)|\tilde{\phi}(z)|^2 \right] dz 
\]
\[ = \int_{\tilde{X}} \left[ < G^{-1} \nabla_z \tilde{\phi}(z), \nabla_z \tilde{\phi}(z) > + q(z)|\tilde{\phi}(z)|^2 \right] dz 
\]
\[ = \tilde{\rho}[\tilde{\phi}] \]
since \( q \) is symmetric.

Next, we claim that for \( \Omega \subset X \) and each \( \sigma \in \mathcal{G} \)
\begin{equation}
(2.5) \quad \rho[\phi] = \rho[\sigma \phi] \quad \text{for all } \phi \in C^\infty_{S,0}(\Omega).
\end{equation}

Choose \( \psi \in C^\infty_0(X^\perp) \) and \( \phi \in C^\infty_{S,0}(\Omega) \). Extend these functions into all of \( \tilde{X} \) by
\[
\phi(\tilde{x}) := \phi(x) \quad \text{and} \quad \psi(\tilde{x}) := \psi(x^\perp) \quad \text{for } \tilde{x} = x + x^\perp
\]
with \( x \in X \) and \( x^\perp \in X^\perp \). Extend each \( \sigma \phi, \sigma \in \mathcal{G} \), in the same manner. Define
\[
\tilde{\phi}(\tilde{x}) := \phi(\tilde{x}) \psi(\tilde{x}), \quad \tilde{x} \in \tilde{X}.
\]
Then,
\[
\sigma \tilde{\phi} = (\sigma \phi)(\sigma \psi) = (\sigma \phi)\psi = \epsilon(\sigma)\phi \psi, \quad \sigma \in \mathcal{G}
\]
by Lemma 2.2(v) showing that \( \tilde{\sigma} \in C^\infty_{S,0}(\tilde{X}) \).

Let \( T\tilde{x} = (r, R)^t := y \) as described in (1.4a) and (1.4b), and set \( V(r) := \sum_{1 \leq i < j \leq N} V_{ij}(r) \) as used in (1.9). It follows from (1.1) and the characterization of \( x^\perp \in X^\perp \) given in the proof of Lemma 2.2(v) that
\[
q(\tilde{x}) = q(x + x^\perp) = q(x) = q(T^{-1}(r, 0)^t) = V(r), \quad \tilde{x} \in \tilde{X}.
\]
Now, using the fact that \( \nabla_x = T^t \nabla_y \) and (1.5) we have that
\[
\tilde{\rho}[\sigma \tilde{\phi}] = \int_{T \tilde{X}^\perp} \int_{T X^\perp} \left\{ (T G^{-1} T^t \nabla_y \sigma \tilde{\phi}, \nabla_y \sigma \tilde{\phi})_{R^\nu N} + V(r) |\sigma \tilde{\phi}|^2 \right\} d_x r d_{X^\perp} R
\]
\[
= \int_{T \tilde{X}^\perp} |\psi|^2 d_{X^\perp} R \int_{T X^\perp} \left\{ (G_X \nabla_r \sigma \phi, \nabla_r \sigma \phi)_{R^\nu (N-1)} + V(r) |\sigma \phi(r)|^2 \right\} d_x r
\]
\[
+ \frac{1}{2M} |\sigma \phi|^2 L_2(X^\perp) \int_{T \tilde{X}^\perp} |\nabla_R \psi|^2 d_{X^\perp} R
\]
\[
= \rho[\sigma \phi]|\psi|^2 L_2(X^\perp) + \frac{1}{2M} |\sigma \phi|^2 L_2(X^\perp) \| \nabla_R \psi \|_{L_2(T \tilde{X}^\perp)}^2
\]
where \( d_x r \) is defined in (1.8) and \( d_{X^\perp} R = \sqrt{2MdR} \) for \( R \) given by (1.4b). A similar calculation shows that
\[
\tilde{\rho}[\tilde{\phi}] = \rho[\phi]|\psi|^2 L_2(X^\perp) + \frac{1}{2M} \| \phi \|_{L_2(X)}^2 \| \nabla_R \psi \|_{L_2(T \tilde{X}^\perp)}^2.
\]
Since \( |\sigma \phi|^2 L_2(X^\perp) = |\phi|^2 L_2(X^\perp) \) and \( \tilde{\rho}[\sigma \tilde{\phi}] = \tilde{\rho}[\tilde{\phi}] \) by (2.4), then (2.5) follows.

For each \( \phi \in C^\infty_{S,0}(\Gamma(\omega_\delta, R)) \) with \( \| \phi \|_{L_2(X)} = 1 \) and any \( \sigma \in \mathcal{G} \), we have \( \sigma \phi \in C^\infty_{S,0}(\Gamma([\sigma \omega_\delta, R]) \) by Lemma 2.2(vi) with \( |\sigma \phi|^2 L_2(X) = 1 \) and \( \rho[\sigma \phi] = \rho[\phi] \) by (2.5). This implies that
\[
K([\sigma \omega_\delta; R]) \leq K(\omega_\delta; R), \quad \text{for all } \sigma \in \mathcal{G}.
\]
A similar argument gives the reverse inequality and the Proposition follows. \( \square \)
The next lemma is proved by Agmon (1982) (Lemma 2.7, p.38) for \( K \) without symmetry considerations. The same proof applies to \( K_S \).

**Lemma 2.7.** The Agmon spectral function \( K_S \) is lower semi-continuous on \( S(X) \).

An immediate consequence of Proposition 2.6 and Lemma 2.7 is

**Corollary 2.8.** Let \( M \) denote the subset of \( S(X) \) on which \( K_S \) attains its minimum value. Then, \( M \) is a closed subspace of \( S(X) \) which is \( \mathcal{G} \)-invariant, i.e. \( \sigma M = M \) for all \( \sigma \in \mathcal{G} \).

### §3 Properties of the Bound States of Polyatomic Systems

Here, we look at criteria for the finiteness and for the infiniteness of bound states of \( P_S \) analogous to our earlier work, (Evans and Lewis 1990) and (Evans, Lewis, Saitô (1991, 1992a)), in which symmetry restrictions were not included. An important new ingredient will be a partition of unity in which the functions are symmetric. Therefore, the product of these functions with an element of \( S \) will be in \( S \).

**Lemma 3.1.** Let \( U \) be a closed, proper subset of \( S(X) \) which is \( \mathcal{G} \)-invariant, i.e. \( \sigma U = U \) for all \( \sigma \in \mathcal{G} \), and let \( \delta, R > 0 \). Then, there exist symmetric functions \( \alpha, \beta \in C^\infty(X) \) satisfying

(i) \( \alpha(x), \beta(x) \in [0, 1] \) and \( \alpha(x)^2 + \beta(x)^2 \equiv 1 \) for all \( x \in X \);

(ii) \( \text{supp}(\alpha) \subset \Gamma(U_\delta; R/2) \), with \( \alpha \equiv 1 \) in \( \Gamma(U_{\frac{3}{4}}; R) \);

(iii) \( \text{supp}(\beta) \subset X \setminus \Gamma(U_{\frac{3}{4}}; R) \);

(iv) \( \alpha \) and \( \beta \) are homogeneous of degree 0 in \( X \setminus B(R) \); and

(v) given \( \epsilon > 0 \) there exists \( C_\epsilon > 0 \) such that

\[
|\nabla_X \alpha(x)|_X^2 + |\nabla_X \beta(x)|_X^2 \leq (\epsilon \alpha(x)^2 + C_\epsilon \beta(x)^2) \chi_\Delta/|x|_X^2, \quad x \in X,
\]

where \( \chi_\Delta \) is the characteristic function with \( \Delta := \Gamma(U_\delta; R/2) \setminus \Gamma(U_\frac{3}{4}; R) \) being its support.

**Proof.** Choose nonnegative \( f, g \in C^\infty[0, \infty) \) satisfying

\[
g(t) = \begin{cases} 
0, & \text{for } t \in [0, \frac{1}{2}) \\
1, & \text{for } t > \frac{3}{4}
\end{cases}
\]

and

\[
f(t) = \begin{cases} 
1, & \text{for } t \in [0, \frac{3}{4}) \\
0, & \text{for } t > 1.
\end{cases}
\]
Choose nonnegative $h_1, h_2 \in C^\infty(S(\mathcal{X}))$ satisfying
\[
h_1(\omega) = \begin{cases} 
1, & \text{for } \omega \in U_{\text{44}}^3 \\
0, & \text{for } \omega \in S(\mathcal{X}) \setminus U_\delta 
\end{cases}
\]
and
\[
h_2(\omega) = \begin{cases} 
0, & \text{for } \omega \in U_\delta^4 \\
1, & \text{for } \omega \in S(\mathcal{X}) \setminus U_\delta^4.
\end{cases}
\]

Henceforth, we shall drop the subscript “$\mathcal{X}$” and write $| \cdot |$ for $| \cdot |_{\mathcal{X}}$ and $\nabla$ for $\nabla_{\mathcal{X}}$. Define
\[
\theta_1(x) := h_1 \left( \frac{x}{|x|} \right) g \left( \frac{|x|}{R} \right); \\
\theta_2(x) := h_2 \left( \frac{x}{|x|} \right) g \left( \frac{|x|}{R} \right); \text{ and }
\theta_3(x) := f \left( \frac{|x|}{R} \right).
\]

Next, let
\[
J_i(x) := \frac{1}{|\mathcal{G}|} \sum_{\sigma \in \mathcal{G}} \sigma \theta_i(x), \quad i = 1, 2, 3.
\]

Then, each $J_i$ is symmetric as well as the function
\[
J_0(x) := \sqrt{J_2(x)^2 + J_3(x)^2}.
\]

Note that $J_0(x)^2 + J_1(x)^2 \geq 1$ for all $x$. Now, define
\[
\alpha(x) := \frac{J_1(x)}{\sqrt{J_0(x)^2 + J_1(x)^2}} \quad \text{and} \quad \beta(x) := \frac{J_0(x)}{\sqrt{J_0(x)^2 + J_1(x)^2}}.
\]

It is not hard to see that properties (i)-(iii) are satisfied since each $\sigma \in \mathcal{G}$ is an isometry and $U$ is $\mathcal{G}$-invariant. Part (iv) follows since both $\alpha$ and $\beta$ are functions of $\frac{x}{|x|}$ only in $\mathcal{X} \setminus B(R)$.

To see (v) first note that $|\nabla \alpha|^2 + |\nabla \beta|^2$ is supported inside $\Delta$. In view of (iv) it suffices to prove (v) in $\mathcal{X} \setminus B(R)$ on the surface of the ball $B(R)$. This follows in the same manner as given in Appendix 2 of (Evans and Lewis 1990) which
followed the proof of (4.6) of Sigal (1982). In $A_R := B(R) \setminus B(R/2)$ we prove (v) in a similar way. Define
\[
C(\eta) := \{ x \in A_R : \alpha(x)^2 > 1 - \eta \}
\]
for $\eta < \frac{1}{2}$. By uniform continuity there exists $\eta = \eta(\epsilon) > 0$ such that
\[
|x|^2 \left( |\nabla \alpha(x)|^2 + |\nabla \beta(x)|^2 \right) < \frac{\epsilon}{2} < \epsilon \alpha(x)^2, \quad x \in C(\eta).
\]
Let
\[
C'_{\epsilon} := \frac{1}{\eta} \max_{x \in A_R} |x|^2 \left( |\nabla \alpha(x)|^2 + |\nabla \beta(x)|^2 \right).
\]
Then,
\[
|x|^2 \left( |\nabla \alpha(x)|^2 + |\nabla \beta(x)|^2 \right) \leq \eta C'_{\epsilon} \leq C'_{\epsilon} \beta(x)^2, \quad x \in A_R \setminus C(\eta).
\]
The last two inequalities imply (v) inside $A_R$. Combining this with the inequality in $X \setminus B(R)$ gives (v) in all of $X$. □

It follows from the IMS-Localization Formula, named for Ismagilov (1961), Morgan (1979), and Morgan and Simon (1980) (see Lemma 6 of (Evans and Lewis 1990)), that for all $\phi \in C^\infty_{S,0}(X)$
\[
\rho[\phi] = \rho[\alpha \phi] + \rho[\beta \phi] - \int_X \left( |\nabla \alpha|^2 + |\nabla \beta|^2 \right) |\phi|^2 dx.
\]
In light of Lemma 3.1(v) we have
\[
(3.1) \quad \rho[\phi] \geq \rho[\alpha \phi] - \epsilon \int_X \frac{\chi_\Delta}{|x|^2} |\alpha \phi|^2 dx + \rho[\beta \phi] - C'_{\epsilon} \int_X \frac{\chi_\Delta}{|x|^2} |\beta \phi|^2 dx
\]
for all $\phi \in C^\infty_{S,0}(X)$.

The partition of unity constructed in Lemma 3.1 and (3.1) play a vital role in the proof of the next proposition which itself is an important step in the proof of Theorem 3.7.

**Definition 3.2.** Let $U \subseteq S(X)$ be $G$-invariant and define
\[
\ell_R(U) := \inf\{ \rho[\phi] : \phi \in C^\infty_S(\Gamma(U; R), \|\phi\|_{L^2(X)} = 1 \}
\]
and
\[
\ell(U) := \lim_{R \to \infty} \ell_R(U).
\]
Proposition 3.3. Assume that (1.2) holds and let $U$ be an open $G$-invariant subset of $S(X)$. Then,
\[
\min_{\omega \in U} K_S(\omega) \leq \ell(U) \leq \inf_{\omega \in U} K_S(\omega).
\]

Proof. (i) $\ell(U) \geq \min_{\omega \in U} K_S(\omega)$:
Let $\delta$ be given and for $\omega \in U$ set
\[
\eta(\delta, \omega) := \frac{1}{3} \min \left\{ \delta, \min \{ |\sigma(\omega) - \omega| : \sigma \in G, \sigma(\omega) \neq \omega \} \right\}.
\]
Since $\{\omega_{\eta(\delta, \omega)} : \omega \in \overline{U}\}$ is an open covering of the compact set $\overline{U}$, there exists a finite number of distinct points $\omega_1, \omega_2, \ldots, \omega_M \in U$ such that
\[
\overline{U} \subset \bigcup_{j=1}^{M} [\omega_j]_{\eta(\delta, \omega_j)}.
\]
For each $R > 0$ there exists $\phi_R \in C_{S,0}^\infty(\Gamma(U; R))$ with $\|\phi_R\|_{L^2(X)} = 1$ and
\[
(3.2) \quad \ell_R(U) + \frac{1}{R} \geq \rho[\phi_R].
\]
Since
\[
\sum_{j=1}^{M} \int_{\Gamma([\omega_j]_{\eta(\delta, \omega_j)}; R)} |\phi_R|^2 dx \geq \|\phi_R\|^2_{L^2(X)} = 1,
\]
we conclude that, for each $R > 0$, there exists $j_0 = j_0(R) \in \{1, \ldots, M\}$ such that
\[
(3.3) \quad \int_{\Gamma([\omega_0]_{\eta_0}; R)} |\phi_R|^2 dx \geq \frac{1}{M}
\]
where $\omega_0 = \omega_{j_0}$ and $\eta_0 = \eta(\delta, \omega_0)$.

We now invoke Lemma 3.1 with $U = G(\omega_0)$ and $\delta, R$ replaced by $2\eta_0$ and $1$ respectively. Note that
\[
\Gamma([G(\omega_0)]_{2\eta_0}; R) = G(\Gamma([\omega_0]_{2\eta_0}; R))
\]
as indicated in Lemma 2.2, and that
\[
0 < 2\eta_0 < \min \{ |\sigma(\omega) - \omega| : \sigma \in G, \sigma(\omega) \neq \omega \}
\]
\[
0 < 2\eta_0 < \delta.
\]
Let \( G = \bigcup_{j=1}^{p} \sigma_j [G_{\omega_0}] \) be a coset decomposition of \( G \) as in (2.2) with \( p = p(\omega_0) \). By Lemma 3.1, \( \alpha \phi_R, \beta \phi_R \in C_{S,0}^{\infty}(\Gamma(U;R)) \), and
\[
\text{supp}(\alpha \phi_R) \subset G(\Gamma([\omega_0]2\eta_0;1/2)) \cap \Gamma(U;R) \\
\text{supp}(\beta \phi_R) \subset \{X \setminus G(\Gamma([\omega_0]_{\eta_0};1))\} \cap \Gamma(U;R).
\]
By Lemma 2.2
\[
G(\Gamma([\omega_0]2\eta_0;1/2)) = \bigcup_{j=1}^{p} \sigma_j (\Gamma([\omega_0]2\eta_0;1/2))
\]
which is a disjoint union. Also, \( \alpha \equiv 1 \) on \( \Gamma([\omega_0]2\eta_0;1) \) and hence, for \( R \geq 1 \), (3.3) yields
\[
\|\alpha \phi_R\|^2 \geq \frac{1}{M}.
\]
From (3.1)
\[
\rho[\phi_R] \geq \rho[\alpha \phi_R] + \rho[\beta \phi_R] - C(\delta,\omega_0)R^{-2}
\]
where \( C(\delta,\omega_0) \) is a positive constant depending on \( \delta \) and \( \omega_0 \) only. For each \( R, \omega_0(R) \in \{\omega_1, \ldots, \omega_M\} \). Hence, there exists an increasing sequence \( R_n \to \infty \) such that \( \omega_0(R_n) = \omega_j := \hat{\omega} \) for some fixed \( j \in \{1, \ldots, M\} \). Set \( \hat{\eta} := \eta(\delta,\hat{\omega}) \) and \( \phi_n = \phi_{R_n} \) to obtain
\[
\rho[\phi_n] \geq \rho[\alpha \phi_n] + \rho[\beta \phi_n] - C(\delta)R_n^{-2}.
\]
Let \( \alpha_1 \) be the restriction of \( \alpha \) to \( \Gamma([\hat{\omega}]2\hat{\eta};R_n/2) \). Since \( \rho[\alpha \phi_n] = p \cdot \rho[\alpha_1 \phi_n] \) by (2.5) and \( \|\alpha \phi_n\| = p\|\alpha_1 \phi_n\| \), then
\[
\frac{\rho[\alpha \phi_n]}{\|\alpha \phi_n\|^2} = \frac{\rho[\alpha_1 \phi_n]}{\|\alpha_1 \phi_n\|^2} \geq K_S([\hat{\omega}]2\hat{\eta};R_n).
\]
Similarly, since \( \beta \phi_n \) is compactly supported in \( \Gamma(U;R_n) \) we have for each positive integer \( n \)
\[
\rho[\beta \phi_n] \geq \ell_{R_n}(U)\|\beta \phi_n\|^2
\]
Thus, from (3.2), (3.5), (3.6), and (3.7)
\[
\ell_{R_n}(U) + \frac{1}{R_n} \geq K_S([\hat{\omega}]2\hat{\eta};R_n)\|\alpha \phi_n\|^2 + \ell_{R_n}(U)\|\beta \phi_n\|^2 - C(\delta)R_n^{-2}
\]
whence
$$\ell_{R_n}(U)\|\alpha\phi_n\|^{2} \geq K_{S}([\hat{\omega}]_{2\hat{\eta}}; R_n)\|\alpha\phi_n\|^{2} - \frac{1}{R_n} - C(\delta)R_n^{-2}. $$

Using (3.4), we obtain
$$\ell(U) \geq \ell_{R_n}(U)$$
$$\geq K_{S}([\hat{\omega}]_{2\hat{\eta}}; R_n) - \frac{M}{R_n} - MC(\delta)R_n^{-2}$$
$$\geq K_{S}([\hat{\omega}]_{\delta}; R_n) - \frac{M}{R_n} - MC(\delta)R_n^{-2}.$$

Now, let $n \to \infty$ and then $\delta \to 0$ to obtain
$$\ell(U) \geq K_{S}(\hat{\omega}) \geq \min_{\omega \in U} K_{S}(\omega)$$
which proves (i).

(ii) $\ell(U) \leq \min_{\omega \in U} K_{S}(\omega)$:

Let $\omega \in U$ and $\epsilon > 0$. Then, there exists $R_\epsilon$ such that

$$\ell(U) \leq \ell_{R}(U) + \epsilon, \quad R \geq R_\epsilon.$$ 

Let $\delta_0 = \delta_0(\omega) > 0$ be such that $\omega_{\delta_0} \in U$. Since $\Gamma(\omega_{\delta}; R) \subset \Gamma(U; R)$ for $0 < \delta < \delta_0$, it follows that
$$\ell_{R}(U) \leq K_{S}(\omega_{\delta}; R) \quad \text{for} \ 0 < \delta < \delta_0,$$
which, on using (3.8), gives
$$\ell(U) \leq K_{S}(\omega_{\delta}; R) + \epsilon \quad \text{for} \ 0 < \delta < \delta_0 \ \text{and} \ R \geq R_\epsilon.$$

This implies (ii) which completes the proof. □

The next theorem establishes the connection between $\inf \sigma_e(P_S)$ and $K_{S}$ which is analogous to a result of Agmon (1982). It recovers the main part of the celebrated HVZ-Theorem of quantum mechanics.

**Theorem 3.4.** Let the hypothesis of Proposition 1.1 hold. Then,
$$\inf \sigma_e(P_S) = \Sigma(P_S) = \min_{\omega \in \mathcal{S}(X)} K_{S}(\omega).$$
Proof. The fact that the first equality holds follows as the proof of Theorem 3.2 of Agmon (1982) as indicated in §1. Clearly, $\Sigma(P_S) = \ell(S(X))$. Therefore, by Proposition 3.3

$$\min_{S(X)} K_S(\omega) \leq \Sigma(P_S) \leq \inf_{S(X)} K_S(\omega) = \min_{S(X)} K_S(\omega). \quad \square$$

Next, we consider a natural extension of $K_S(\omega)$, $\omega \in S(X)$, to subsets $U$ of $S(X)$ which was introduced in (Evans et al (1991)). The proposition which follows establishes its relevance to Proposition 3.3 and a proof is given which is simpler than our earlier version.

Definition 3.5. For $U \subset S(X)$ define

$$K_S(U_\delta; R) := \inf \{ \rho[\phi] : \phi \in C_0^\infty(\Gamma(U_\delta; R), \|\phi\|_{L^2(X)} = 1\}$$

and

$$K_S(U) := \lim_{\delta \to 0, R \to \infty} K_S(U_\delta; R) = \sup_{0 < \delta, R < \infty} K_S(U_\delta; R).$$

Proposition 3.6. Let the hypothesis of Proposition 1.1 hold and let $U$ be a $G$-invariant subset of $S(X)$. Then,

$$K_S(U) = \min_{\omega \in U} K_S(\omega).$$

Proof. First, consider the case in which $U$ is closed. Since $\ell(R(U_\delta)) = K_S(U_\delta; R)$, then it follows from Proposition 3.3 that

$$\lim_{R \to \infty} K_S(U_\delta; R) = \ell(U_\delta) \geq \min_{\omega \in U_\delta} K_S(\omega).$$

Therefore, for each positive integer $n$ there exists $\omega_n \in U_\frac{1}{n}$ such that

$$\lim_{R \to \infty} K_S(U_\frac{1}{n}; R) \geq K_S(\omega_n).$$

We infer from this that there exists a subsequence $\{\omega_{n_k}\}$ of $\{\omega_n\}$ such that $\omega_{n_k} \to \omega_0 \in \overline{U} = U$ as $k \to \infty$ and

$$K_S(U) = \lim_{k \to \infty} \lim_{R \to \infty} K_S(U_{\frac{1}{n_k}}; R) \geq \lim_{k \to \infty} \inf_{m \geq k} K_S(\omega_{n_m}) \geq K_S(\omega_0) \geq \min_{\omega \in U} K_S(\omega)$$

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since $K_S$ is lower semi-continuous by Lemma 2.7. Conversely, $K_S(U_\delta; R) \leq K_S(\omega_\delta; R)$ for any $\omega \in U$ for each pair $\delta, R$ of positive numbers. Consequently, $K_S(U) \leq K_S(\omega)$, for every $\omega \in U$, and

$$K_S(U) \leq \inf_{\omega \in U} K_S(\omega) = \min_{\omega \in U} K_S(\omega)$$

since $U$ is closed. This completes the proof for the case in which $U$ is closed.

If $U$ is not closed, we still have that $\overline{U}_\delta = U_\delta$ and hence, $K_S(U) = K_S(\overline{U})$. Therefore, if we apply the above results to $K_S(\overline{U})$ we can conclude that $K_S(U) = K_S(\overline{U}) = \min_{\omega \in \overline{U}} K_S(\omega)$ which is what we wanted to show. □

We are now prepared to prove our main theorem. Here, we write $K_S(U : P_S)$ and $K_S(U; R : P_S)$, instead of $K_S(U)$ and $K_S(U; R)$, to emphasize the dependence on the operator $P_S$ discussed in §1. Let $M \subset S(X)$ be the minimizing set for $K_S$ defined in Corollary 2.8. Given positive numbers $\epsilon, \delta, R$ define the characteristic function

$$\chi(M) := \chi_{\Delta(M)} \quad \text{for} \quad \Delta(M) := \Gamma(M_\delta ; R/2) \setminus \Gamma(M_{\frac{\delta}{2}} ; R)$$

and

$$P_S(\epsilon) := P_S - \frac{\epsilon}{|x|^2} \chi(M)$$

where we understand $P_S(\epsilon)$ to be the operator realized from a sesquilinear form associated in the appropriate manner with $\rho$ defined in (1.9). As in Lemma 12 of (Evans et al (1991))

$$\Sigma(P_S(\epsilon)) = K_S(M : P_S(\epsilon)) = K_S(M : P_S) = \Sigma(P_S).$$

**Theorem 3.7.** Let the hypothesis of Proposition 1.1 hold, and let $M$ as defined in Corollary 2.8 be a proper subset of $S(X)$.

(i) If $\sigma(P_S) \cap (-\infty, \Sigma(P_S))$ is finite, then for some positive $\delta_0, R_0$

$$K_S(M_\delta ; R : P_S) = K_S(M : P_S) = \Sigma(P_S)$$

for all $\delta \leq \delta_0$ and $R \geq R_0$.

(ii) If there exist positive $\epsilon, \delta_0, R_0$ such that

$$K_S(M_\delta ; R : P_S(\epsilon)) = \Sigma(P_S)$$

for all $\delta \leq \delta_0$ and $R \geq R_0$, then $\sigma(P_S) \cap (-\infty, \Sigma(P_S))$ is finite.
Proof. The proof of (i) is essentially the same as that given in Theorem 8 of (Evans et al. (1991)) and we do not repeat it here.

To show (ii) let \( \{\alpha, \beta\} \) be the partition of unity constructed in Lemma 3.1 with \( \delta \leq \delta_0/2 \), \( R \geq 2R_0 \) and \( U = \mathcal{M} \) which is closed and \( G \)-invariant. From (3.1) we have for all \( \phi \in \mathcal{C}^\infty_S(X) \)

\[
(3.9) \quad \rho[\phi] \geq K_S(\mathcal{M}_{\delta_0}; R_0 : P_S(\epsilon)) \|\phi\|^2 + \rho_\beta[\phi]
\]

where

\[
(3.10) \quad \rho_\beta[\phi] = \rho[\beta\phi] - C_\epsilon \int_X \frac{\chi(M)}{|x|^2}|\beta\phi|^2 dx.
\]

The map \( \phi \mapsto \beta^{-1}\phi \) is a linear isometry of \( L^2_S(X) \) onto the weighted space \( L^2_S(X; \beta^2 dx) \). Since \( q - C_\epsilon \chi(M)|x|^{-2} \) satisfies the necessary properties, as \( q \) does, it follows that \( \rho_\beta \) is closable in \( L^2_S(X; \beta^2 dx) \), cf. Proposition 9 of (Evans and Lewis 1990). Let \( P_\beta \) denote the associated self-adjoint operator in \( L^2_S(X; \beta^2 dx) \). Note that by Lemma 2.2 \( \mathcal{M}_{\frac{3}{2}} \) is \( G \)-invariant since \( \mathcal{M} \) is, and consequently, \( S(X) \setminus \mathcal{M}_{\frac{3}{2}} \) is an open \( G \)-invariant set. Since \( \text{supp}(\beta) \subset \Gamma(\mathcal{M}_{\frac{3}{2}}; R) \), we have from Theorem 3.4 and Proposition 3.3 that, with \( B(k) \) the ball in \( X \) with center the origin and radius \( k \),

\[
\inf \sigma_e(P_\beta) = \Sigma(P_\beta) \\
\geq \lim_{k \to \infty} \inf \{\rho_\beta[\phi] : \phi \in \mathcal{C}^\infty_S(X \setminus B(k)), \|\beta\phi\|_{L^2(X)} = 1\} \\
\geq \lim_{k \to \infty} \left\{ \ell_k(S(X) \setminus \mathcal{M}_{\frac{3}{2}}) - C_\epsilon k^{-2} \right\} \\
= \ell(S(X) \setminus \mathcal{M}_{\frac{3}{2}}) \\
\geq \min_{\omega \notin \mathcal{M}_{\frac{3}{2}}} K_S(\omega) \\
> \Sigma(P_S).
\]

Hence, \( P_\beta \) has only a finite number of eigenvalues (counting multiplicities) in \( (-\infty, \Sigma(P_S)) \). Let \( E_1 := \{\psi_1, \ldots, \psi_m\} \) be the corresponding eigenfunctions and set \( E_2 := \{\beta^2\psi_1, \ldots, \beta^2\psi_m\} \). It follows from (3.9) that \( D(\tilde{\rho}) \subset D(\tilde{\rho}_\beta) \) where \( \tilde{\rho} \) and \( \tilde{\rho}_\beta \) denote the closures of the forms \( \rho \) and \( \rho_\beta \) respectively and that (3.9) continues to hold for \( \phi \in D(\tilde{\rho}) \). Consequently, if \( \phi \in D(\tilde{\rho}_\beta) \) is orthogonal to \( E_2 \) in \( L^2_S(X) \), then \( \phi \in D(\tilde{\rho}_\beta) \) and is orthogonal to \( E_1 \) in \( L^2_S(X; \beta^2 dx) \). In this case

\[
\tilde{\rho}[\phi] \geq K_S(\mathcal{M}_{\delta_0}; R_0 : P_S(\epsilon)) \|\alpha\phi\|^2 + \Sigma(P_S) \|\beta\phi\|^2 \\
= \Sigma(P_S) \|\phi\|^2
\]
by the hypothesis. Therefore, \( P_S \) can have no more than \( m \) eigenfunctions in \((−∞, \Sigma(P_S))\), and the proof is complete. \( \square \)

As an application of Theorem 3.7, we present an example which is analagous to Theorem 5.1 of (Evans, Lewis, Saitô (1992a)) and we refer the reader to that paper for details. These results also follow from earlier work of Simon (1970), Zhislin (1960, 1969, 1971), Vugal’ter and Zhislin (1977), and Sigal (1982) - see Chapter 3 of Cycon et al (1987). We also wish to refer the reader to more recent, related work of Vugal’ter and Zhislin (1984, 1986, 1991) and of Ahia (1992).

**Example 3.8.** Let \( \tilde{P} \) be given by (1.1) where we denote the charge of each nucleus by \( Z \). Then,

\[
\tilde{P} := -\sum_{i=1}^{N_1} \frac{1}{2M_1} \Delta_i - \sum_{k=1}^{N_2} \frac{1}{2M_2} \Delta_k - \sum_{i=1}^{N_1} \sum_{k=1}^{N_2} \frac{Z}{|y^i - z^k|} + \sum_{1 \leq i < j \leq N_1} \frac{1}{|y^i - y^j|} + \sum_{1 \leq k < \ell \leq N_2} \frac{Z^2}{|z^k - z^\ell|}.
\]

As in §1, we assume that the nuclei are either fermions or bosons. The Hamiltonian of the system after the removal of the motion of the center of mass is given by \( P_S \). We assume that the minimizing set \( M \) is determined only by 2-cluster decompositions

\[ a_j = \{A^j_1, A^j_2\}, \quad j = 1, \ldots, q. \]

The clusters \( A^j_1, A^j_2, j = 1, \ldots, q \), may or may not have electrons or nuclei. Because of the symmetry restrictions, the minimizing set \( M \) is \( G \)-invariant (Corollary 2.8) showing no distinction among electrons and among nuclei. For each of these 2-cluster decompositions \( a_j, j = 1, \ldots, q \), let \( N(A^j_1) \) and \( N(A^j_2) \) be the number of electrons in clusters \( A^j_1 \) and \( A^j_2 \) respectively. Let \( Z(A^j_1) = N(A^j_1) \cdot Z \) and \( Z(A^j_2) = N(A^j_2) \cdot Z \) - the total charge of the nuclei in the respective clusters. Then,

\[
(3.11) \quad \left(Z(A^j_1) - N(A^j_1)\right) \left(Z(A^j_2) - N(A^j_2)\right) > 0, \quad j = 1, \ldots, q,
\]

is a sufficient condition in order that the number of bound states of \( P_S \) be finite and

\[
(3.12) \quad \left(Z(A^j_1) - N(A^j_1)\right) \left(Z(A^j_2) - N(A^j_2)\right) \geq 0, \quad j = 1, \ldots, q,
\]

is a necessary condition.
Proof. The proof follows as a corollary of Theorem 3.7 and of Corollaries 4.11 and 4.12 in (Evans, Lewis, Saitô (1992a)). We refer to the discussion there for the definition of many of the terms used below. Let $a = \{A_1, A_2\}$ be one of the cluster decompositions mentioned above where we suppress the superscript. The intercluster interaction is given by

$$I_a(y, z) = \sum_{y^i \in A_1} \sum_{z^k \in A_2} \frac{Z}{|y^i - z^k|} - \sum_{y^i \in A_2} \sum_{z^k \in A_1} \frac{Z}{|y^i - z^k|} + \sum_{y^i \in A_1, y^j \in A_2} \frac{1}{|y^i - y^j|} + \sum_{z^k \in A_1, z^\ell \in A_2} \frac{Z^2}{|z^k - z^\ell|}.$$ 

Lemma 4.8 of (Evans, Lewis, Saitô (1992a)) shows that for all $\delta$ sufficiently small

$$V_a^- (|\xi|; \delta) \leq I_a(\eta, \xi) \leq V_a^+(|\xi|; \delta), \quad (\eta, \xi) \in T_a(\Gamma(U_a; 1))$$

where $V_a^+(|\xi|; \delta) = V_a^- (|\xi|; -\delta)$. Here,

$$V_a^- (|\xi|; \delta) = -\frac{N(A_1)Z(A_2) + N(A_2)Z(A_1)}{|M - C\delta||\xi|} + \frac{N(A_1)N(A_2) + Z(A_1)Z(A_2)}{|M + C\delta||\xi|}.$$

Here, $M$ is the total mass of all electrons and nuclei in the system and $\hat{M}_1$ is the total mass for the cluster $A_1$. If (3.11) holds, then $V_a^- (|\xi|; \delta) \geq 0$ for all $\delta$ sufficiently small. The fact that there are no more than a finite number of bound states follows from Corollary 4.11 of (Evans, Lewis, Saitô (1992a)). If (3.12) does not hold for some $a = a_j$, then $V_a^+(|\xi|; \delta) \leq -\frac{\epsilon(\delta)}{|\xi|}$ for all $\delta$ sufficiently small. In that case Corollary 4.12 of (Evans, Lewis, Saitô (1992a)) would imply that there must be an infinite number of bound states. $\square$

We note that this example includes the case of an atom whose nucleus is not assumed to be infinitely heavy. In this case, familiar criteria for the finiteness of bound states and for the infiniteness of bound states is recovered.

The assumption that $\mathcal{M}$ is determined only by 2-cluster decompositions is typical for results of this type. For an atom whose electrons are treated as bosons it is known that $\mathcal{M}$ is determined only by 2-cluster decompositions when $Z > N - 2$, see Theorem 3.26 of Cycon et al (1987) and (Evans, Lewis, Saitô (1992b)), and in certain cases for which $Z < N - 1$, see Bach (1991). However, the actual structure of $\mathcal{M}$ is not very well understood in general.

Ahia, F. 1992 Finiteness of the discrete spectrum of \((N \geq 3)\) \(N\)-body Schrödinger operators, which have some determinate subsystems that are virtual at the bottom of the continuum. \textit{J. Math. Phys.} \textbf{33} (1), 189-202.


