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Geometric spectral properties of N-body Schrödinger operators. II

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Contents

Conditions for the finiteness and for the infiniteness of bound states of N-body Schrödinger operators are presented. These bound states correspond to eigenvalues below the essential spectrum of the operator. Previous work of the authors which extended geometric methods and localization techniques of Agmon are used to establish these conditions. An application to a diatomic system having N electrons and two nuclei is given.

1. Introduction

In Evans *et al.* (1991*a*) we extended geometric methods (or localization techniques) of Agmon (1982) to the study of the finiteness or infiniteness of the discrete spectra of Schrödinger-type operators with non-isotropic potentials. The methods have a long history of contributions coming largely from studies of N-body operators of quantum mechanics; see the extensive list of references in Cycon *et al.* (1987). The lecture notes of Agmon (1982) showed that much of this work fits well within the study of elliptic partial differential operators in a Hilbert space. However, this required that the potential be non-isotropic and not bounded below at ∞ contrary to much of the classical work in this area. It was in that spirit that the work in Evans *et al.* (1991*a*) was done.

Our purpose is to continue the work in Evans *et al.* (1991*a*) applying the results to Schrödinger operators of molecular-type. However, in this paper we do not restrict our operators to the symmetry subspaces required by the Pauli exclusion principle. This refinement will be pursued in later work. Our aim is to make the results as

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accessible as possible to researchers who are not necessarily specialist in this area. Many of the details appear in the Appendix.

In §2 the results in Evans *et al.* (1991*a*) are applied to N-body Schrödinger operators. It is shown that one of the hypotheses, $\mathscr{H}(1)$ in Evans *et al.* (1991*a*), required for non-isotropic Schrödinger operators always holds for N-body operators. This simplifies the basic theorem considerably. In §3 we show how the methods and results in Agmon (1982) and Evans *et al.* (1991*a*) complement the classical theory for N-body Schrödinger operators of molecular-type. In §4 criteria for the finiteness and for the infiniteness of bound states of N-body operators are given within the framework presented in §2 and §3. Here, we draw heavily upon ideas developed by Sigal (1982), who recognized the importance of geometric methods in the fundamental work of Zhislin (1960, 1969, 1971). We first look at the case in which the least point of the essential spectrum of the operator is equal to the infimum of the spectrum of subsystems which corresponds to an m-cluster decomposition in which m may be greater than 2. The typical assumption for criteria for the finiteness of bound states is that this happens only when $m = 2$. Making this assumption we present specific results which are easy to apply using the oscillation theory of ordinary differential equations. Finally, in §5 we give an application to a diatomic molecule with respect to the breakup of the system into two atomic subsystems. The nuclear motion is not restricted and the kinetic energy of both nuclei is included in the hamiltonian. Recent work of Ruskai (1989, 1990, 1991) concerned with the stability of such systems has been a significant source of information for us here. We compare these results with hers.

Agmon (1982) introduced the following generalized N-body Schrödinger operator:

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

Here, each a^{ij} is a real number and the matrix $A := (a^{ij})$ is assumed to be symmetric and positive definite. We will want to view $\Sigma_{i,j=1}^{n} a^{ij}\partial_i\partial_j$ as being the Laplace–Beltrami operator on $\boldsymbol{R}^n$ with the inner product defined by

$$(x, y) := \sum_{i,j=1}^{n} a_{ij}x_i y_j \quad \text{for} \quad A^{-1} := (a_{ij}).$$

The potential is assumed to be of the form

$$q(x) := \sum_{i=1}^{l} q_i(x).$$

For distinct non-zero projections Π_i, $i = 1, \dots, l$, on $\boldsymbol{R}^n$ each q_i is assumed to be a real-valued function on $\boldsymbol{R}^n$ satisfying

$$\left.\begin{array}{ll} \text{(i)} & q_i(x) = q_i(\Pi_i x), \\ \text{(ii)} & q_i(x) \to 0 \quad \text{as} \quad |\Pi_i x| \to \infty, \\ \text{(iii)} & \text{for} \quad Y_i = \text{Range}\,(\Pi_i), \quad q_i|_{Y_i} \in L^1_{\text{loc}}(Y_i), \\ \text{(iv)} & (q_i)_-|_{Y_i} \in M_{\text{loc}}(Y_i), \end{array}\right\} \tag{1.1}$$

where $|\cdot|$ denotes the norm in $\boldsymbol{R}^n$ (for any $n \geqslant 1$).

Here, $M(\boldsymbol{R}^n) = M_0(\boldsymbol{R}^n)$ is the Kato class of functions defined as follows: for $x, y \in \boldsymbol{R}^n$ define

$$g(x,y) = \begin{cases} |x-y|^{2-n} & \text{if} \quad n \geqslant 3, \\ |\ln|x-y|| & \text{if} \quad n = 2, \\ 1 & \text{if} \quad n = 1. \end{cases}$$

Then, $q \in M(\boldsymbol{R}^n)$, if, and only if $q \in L^1_{\text{loc}}(\boldsymbol{R}^n)$ and

$$\lim_{r \to 0} \int_{B(x;r)} g(x,y)\, |q(y)|\, \mathrm{d}y = 0$$

uniformly in x. If for every $x \in \boldsymbol{R}^n$ there is a neighbourhood U of x such that $\chi_U q \in M(\boldsymbol{R}^n)$, where χ_U is the characteristic function of U, then we will say that $q \in M_{\text{loc}}(\boldsymbol{R}^n)$. By $(q_i)_-|_{Y_i}$ we mean the restriction of $(q_i)_- := \max(-q, 0)$ to the subspace Y_i.

With these requirements we may regard P as being the operator associated with the closure of the form

$$\tau[\phi, \psi] := \int_{\boldsymbol{R}^n} ((A \nabla \phi(x), \nabla \psi(x))_{\boldsymbol{R}^n} + q(x)\, \phi(x)\, \overline{\psi(x)})\, \mathrm{d}x, \quad \phi, \psi \in C_0^\infty(\boldsymbol{R}^n).$$

The fact that τ is closable is discussed in Proposition 1 of Evans & Lewis (1990).

2. *N*-body Schrödinger operators

The classical N-body Schrödinger operator is given by

$$\tilde{H} := -\sum_{i=1}^{N} \frac{1}{2m_i} \Delta_i + \sum_{1 \leqslant i < j \leqslant N} \tilde{V}_{ij}, \quad x \in \times_{i=1}^{N} \boldsymbol{R}^\nu \approx \boldsymbol{R}^{\nu N},$$

where $\tilde{V}_{ij}(x) = v_{ij}(x^i - x^j)$ for $x = (x^1, \ldots, x^N)$ and $\times_{i=1}^{N} \boldsymbol{R}^\nu$ is the N-fold cartesian product of $\boldsymbol{R}^\nu$. The laplacian Δ_i is interpreted as the laplacian with respect to the variable $x^i \in \boldsymbol{R}^\nu$. Each x^i is considered to be the position of a particle of mass m_i.

The functions $v_{ij} : \boldsymbol{R}^\nu \to \boldsymbol{R}^\nu$ for $1 \leqslant i < j \leqslant N$ satisfy the following conditions:

$$\left.\begin{array}{ll} \text{(i)} & v_{ij} \in L^1_{\text{loc}}(\boldsymbol{R}^\nu), \\ \text{(ii)} & (v_{ij})_- \in M_{\text{loc}}(\boldsymbol{R}^\nu), \\ \text{(iii)} & \lim_{|y| \to \infty} v_{ij}(y) = 0. \end{array}\right\} \tag{2.1}$$

To see that $\tilde{H}$ is a special case of P, consider the projections

$$\Pi_{ij} : \times_{i=1}^{N} \boldsymbol{R}^\nu \to \times_{i=1}^{N} \boldsymbol{R}^\nu, \; 1 \leqslant i < j \leqslant N,$$

defined by

$$(\Pi_{ij}\, x)^k = \begin{cases} m_j/(m_i + m_j)\, (x^i - x^j) & \text{for} \quad k = i, \\ m_i/(m_i + m_j)\, (x^j - x^i) & \text{for} \quad k = j, \\ 0 & \text{when} \quad k \neq i \quad \text{and} \quad k \neq j. \end{cases}$$

Then each $\tilde{V}_{ij}(\Pi_{ij}\, x) = \tilde{V}_{ij}(x)$. Set

$$\tilde{V} := \sum_{1 \leqslant i < j \leqslant N} \tilde{V}_{ij}$$

corresponding to the potential q associated with P.

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Let $\tilde{X}$ be the set $\times_{i=1}^{N} \boldsymbol{R}^{\nu}$ with an inner product defined by

$$\langle x, y\rangle_{\tilde{X}} := \sum_{i=1}^{N} 2m_i(x^i, y^i)_{\nu}$$

where $(\cdot,\cdot)_{\nu}$ is the usual inner product in $\boldsymbol{R}^{\nu}$. Then, the Laplace–Beltrami operator associated with this new inner product is just

$$\Delta_{\tilde{X}} := \sum_{i=1}^{N} \frac{1}{2m_i}\Delta_i$$

and $\tilde{H} = -\Delta_{\tilde{X}} + \tilde{V}$. We denote the self-adjoint realization of $\tilde{H}$ in $L^2(\tilde{X})$ by $\tilde{H}$ also. (If $I_{\tilde{X}}$ is the natural identification of points in $\tilde{X}$ with points in $\boldsymbol{R}^{\nu N}$, recall that statements such as $\phi \in L^2(\tilde{X})$ or $\phi \in C_0^{\infty}(\tilde{X})$ should be interpreted as $\phi \circ I_{\tilde{X}}^{-1}$ being in either $L^2(\boldsymbol{R}^{\nu N})$ or $C_0^{\infty}(\boldsymbol{R}^{\nu N})$.)

It is common practice in quantum mechanics to study $\tilde{H}$ after the removal of the motion of the centre of mass of the system of particles. (The operator $\tilde{H}$ has no eigenvalues (see Agmon 1982).) This is done by restricting $\tilde{H}$ to a $\nu(N-1)$-dimensional subspace X of $\times_{i=1}^{N} \boldsymbol{R}^{\nu}$ in which the centre of mass is taken to be at the origin. Hence,

$$X := \left\{ x \in \times_{i=1}^{N} \boldsymbol{R}^{\nu} : \sum_{i=1}^{N} m_i x^i = 0 \right\}.$$

An inner product $\langle\cdot,\cdot\rangle_X$ on X is given by restricting $\langle\cdot,\cdot\rangle_{\tilde{X}}$ to X.

Denote the Laplace–Beltrami operator in X by Δ_X. Let

$$H := -\Delta_X + V(x), \quad \text{for} \quad V := \tilde{V}|_X$$

and $x \in X$. We may regard Δ_X as being the part of $\Delta_{\tilde{X}} = \Sigma_{i=1}^{N}(1/2m_i)\Delta_i$ acting on X. Let I_{ν} be the identity matrix in $\boldsymbol{R}^{\nu}$ and $G := \operatorname{diag}(2m_1 I_{\nu}, \ldots, 2m_N I_{\nu})$. There is a non-singular matrix $T_X = (t_{ij} I_{\nu})_{i,j=1,\ldots,N}$, such that

$$T_X \begin{bmatrix} x^1 \\ \vdots \\ \vdots \\ x^N \end{bmatrix} = \begin{bmatrix} y^1 \\ \vdots \\ y^{N-1} \\ 0 \end{bmatrix}, \quad x \in X$$

and

$$T_X \begin{bmatrix} x^1 \\ \vdots \\ \vdots \\ x^N \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ y^N \end{bmatrix}, \quad x \in X^{\perp}.$$

There is an $(N-1)\nu \times (N-1)\nu$ submatrix, G_X, of $T_X G^{-1} T_X^t$ such that

$$\Delta_X = \operatorname{div}_{\eta}(G_X \nabla_{\eta}) \quad \text{for} \quad \eta := \begin{bmatrix} y^1 \\ \vdots \\ y^{N-1} \\ 0 \end{bmatrix}.$$

We refer the reader to the Appendix for more details.

Agmon (1982) refers to H as the 'reduced N-body Schrödinger operator'. Let $V_{ij} := \tilde{V}_{ij}|_X$. Since each $\Pi_{ij}: X \to X$, then we still have that

$$V_{ij}(\Pi_{ij} x) = V_{ij}(x) = v_{ij}(x^i - x^j) \quad \text{for} \quad x = (x^1, \ldots, x^N) \in X$$

and $1 \leqslant i < j \leqslant N$. Therefore, we may also consider H as being an operator in the form given by P above. In particular, Lemma 4,8 of Agmon (1982) applies to the self-adjoint realization of H in $L^2(X)$ (which we continue to denote by H). This will be important for our later discussions.

In general, we take H to be the operator associated with the closure of the form

$$\rho[\phi, \psi] := \int_X \left((G_X \nabla_y \phi, \nabla_y \psi)_{\mathbf{R}^{\nu(N-1)}} + \sum_{1 \leqslant i < j \leqslant N} V_{ij}(y)\, \phi(y)\, \overline{\psi(y)} \right) \mathrm{d}_X y,$$

for $\phi, \psi \in C_0^\infty(X)$; we still denote the image of the subspace X under the transformation associated with T_X by X; and

$$\mathrm{d}_X y := \surd(\det(G_X^{-1}))\, \mathrm{d}y^1 \ldots \mathrm{d}y^{N-1}$$

is the measure induced by the inner product

$$\langle y, z \rangle_X = (G_X^{-1} y, z)_{\mathbf{R}^{\nu(N-1)}}, \quad y, z \in X.$$

Note that the inner product $\langle \cdot, \cdot \rangle_X$ is the restriction of $\langle \cdot, \cdot \rangle_{\tilde{X}}$ to X as shown in the Appendix. Henceforth, we write $\mathrm{d}y$ instead of $\mathrm{d}_X y$.

We denote the unit sphere in X by

$$S(X) := \{\omega \in X : |\omega|_X = 1\}$$

for $|\omega|_X := \surd\langle \omega, \omega \rangle_X$. For any set $U \subset S(X)$ we let

$$\operatorname{dist}(\omega : U) := \inf\{|\omega - u|_X : u \in U\}.$$

Here, $\|\cdot\|$ is the norm in $L^2(X)$.

Definition 2.1. *For any set $U \subset S(X)$ and for positive numbers R and δ define*
(i) $\Lambda(H) := \inf\{\rho[\phi] : \phi \in C_0^\infty(X), \|\phi| = 1\}$;
(ii) $\Sigma(H) := \inf \sigma_e(H)$, *the least point of the essential spectrum of H*;
(iii) $U_\delta := \{\omega \in S(X) : \operatorname{dist}(\omega : U) < \delta\}$;
(iv) $\Gamma(U_\delta, R) := \{x \in X : x = t\omega$ *for* $\omega \in U_\delta$ *and* $t > R\}$;
(v) $K(U_\delta, R; H) := \inf\{\rho[\varphi] : \varphi \in C_0^\infty(\Gamma(U_\delta, R)), \|\varphi\| = 1\}$;
(vi) $K(U : H) := \lim_{\delta \downarrow 0} \lim_{R \to \infty} K(U_\delta, R; H)$; *and*
(vii) $\mathscr{M} := \{\omega \in S(X) : K(\omega : H) = \inf_{\omega \in S(X)} K(\omega : H)\}$, *where we write $K(\omega : H)$ instead of* $K(\{\omega\} : H)$.

The conditions which are required of $V(x)$ imply that $\Lambda(H) > -\infty$, which is needed to insure that ρ is bounded below (see Agmon 1982, p. 67). In Evans *et al.* (1991*a*) we have shown that for any $U \subset S(X)$

$$K(U : H) = K(\bar{U} : H) = \inf_{\omega \in \bar{U}} K(\omega : H). \tag{2.2}$$

Moreover, Agmon (1982) showed

Lemma 2.2. *The function $K(\omega) := K(\omega : H)$ of $\omega \in S(X)$ is lower semicontinuous and*

$$\min_{\omega \in S(X)} K(\omega) = \Sigma(H).$$

Therefore, we know that $K(\mathscr{M}:H) = \Sigma(H)$.

Next, we wish to apply our results in Evans *et al.* (1991*a*) to give criteria for the finiteness and for the infiniteness of $\sigma(H) \cap (-\infty, \Sigma(H)]$ where $\sigma(H)$ is the spectrum of H.

For $\delta > 0$ and $R > 0$ let χ_Δ be the characteristic function for

$$\Delta = \Delta(\delta, R) := \overline{\Gamma(\mathscr{M}_\delta, R)} \backslash \Gamma(\mathscr{M}_{\delta/2}, 2R),$$

where $\mathscr{M}$ is described in Definition 2.1. For δ, R, and each $\epsilon > 0$ we define the form

$$\rho_\epsilon[\phi] = \rho_\epsilon[\phi; \delta, R] := \rho[\phi] - \int_{B(R)^c} \frac{\epsilon}{|x|^2} \chi_\Delta |\phi|^2 \, dx, \quad \phi \in C_0^\infty(X).$$

Since ρ is closable in $L^2(X)$ and the perturbation above is ρ-bounded with ρ-bound 0, then ρ_ϵ is closable in $L^2(X)$. If

$$H_\epsilon := H - (\epsilon/|x|^2)\, \chi_\Delta$$

is the operator associated with the closure of ρ_ϵ then

$$\Sigma(H_\epsilon) = K(\mathscr{M}:H_\epsilon) = K(\mathscr{M}:H) = \Sigma(H).$$

Now, we state the main theorem of §2.

Theorem 2.3. *In order that $\sigma(H) \cap (-\infty, \Sigma(H)]$ be finite it is sufficient that there exist $\delta_0 > 0$, $\epsilon > 0$, and $R_0 > 0$ such that*

$$K(\mathscr{M}_{\delta_0}, R_0; H_\epsilon) = \Sigma(H).$$

A necessary condition for the finiteness of $\sigma(H) \cap (-\infty, \Sigma(H)]$ is that for some $\delta_0 > 0$ and some $R_0 > 0$

$$K(\mathscr{M}_{\delta_0}, R_0; H) = \Sigma(H).$$

Proof. A more general form of this theorem is given by Theorems 8 and 13 in Evans *et al.* (1991*a*). Hypothesis $\mathscr{H}(1)$ of Evans *et al.* (1991*a*) follows easily here by using (2.1)(ii) and (iii) to show that $V_- \in M(X)$. Then apply Lemma 0.3 of Agmon (1982). □

Recent results of Donig (1991) imply that when $P = -\Delta + q$ with $q_+ := \max(0, q) \in M_{\text{loc}}(\boldsymbol{R}^n)$ and $q_- \in M(\boldsymbol{R}^n)$, P has only a finite number of eigenvalues below the least point $\Sigma(P)$ of its essential spectrum if, and only if

$$K(S^{n-1}, R; P) = \Sigma(P)$$

for some $R > 0$. This settled an open question posed in Simon (1982).

As we see in the subsequent sections, applications to N-body operators require the local analysis of Theorem 2.3.

3. Schrödinger operators of molecular-type

By Lemma 4.8 of Agmon (1982),

$$K(\omega; H) = \Lambda(H_\omega),$$

where

$$H_\omega := -\Delta_X + \sum_{\omega_i = \omega_j} V_{ij}$$

for $\omega = (\omega^1, \ldots, \omega^N) \in S(X)$ and the sum being taken over all pairs ij for which $\omega_i = \omega_j$. As we show below, this statement includes the main part of the classical

HVZ Theorem of quantum mechanics (see Hunziker 1966; van Winter 1964; Zhislin 1960).

Here, H_ω is an operator associated with one of the classical cluster decompositions of particles. To illustrate that fact, first define

$$\begin{aligned} K_{ij} &:= \ker(\Pi_{ij}) \cap S(X) \\ &= \{\omega \in S(X) : \omega^i = \omega^j\}. \end{aligned}$$

For each $\omega \in S(X)$ define the equivalence relation R_ω on $\{1, \ldots, N\}$ by

$$iR_\omega j \Leftrightarrow i = j \quad \text{or} \quad \omega \in K_{ij}.$$

If $A_1(\omega), \ldots, A_m(\omega)$ are the equivalence classes of R_ω on $\{1, \ldots, N\}$, then $\boldsymbol{a}_\omega := \{A_1(\omega), \ldots, A_m(\omega)\}$ is an m-cluster decomposition of N particles. Conversely, if $\boldsymbol{a} := \{A_1, \ldots, A_m\}$ is a given m-cluster decomposition of N particles for $m \geqslant 2$, define

$$\left.\begin{aligned} U_{\boldsymbol{a}} &:= \bigcap_{(ij) \subset \boldsymbol{a}} K_{ij} \quad \text{for} \quad m < N, \\ U_{\boldsymbol{a}} &:= S(X) \setminus \bigcup_{(ij)} K_{ij} \quad \text{for} \quad m = N, \end{aligned}\right\} \tag{3.1}$$

where $(ij) \subset \boldsymbol{a} \Leftrightarrow i, j \in A_k \in \boldsymbol{a}$ for some k. Then

$$\boldsymbol{a} = \boldsymbol{a}_\omega \quad \text{for every} \quad \omega \in U_{\boldsymbol{a}} \setminus \bigcup_{(ij) \not\subset a} K_{ij}.$$

Consequently, for $m \geqslant 2$ there is a mapping from $S(X)$ onto the set of all m-cluster decompositions of N particles. An element $\boldsymbol{a}_\omega$ in the image of this mapping is called a 'local cluster' in Sigal (1982). In the following by a 'cluster decomposition' we shall mean an m-cluster decomposition with $m \geqslant 2$. We refer the reader to ch. 3 of Cycon *et al.* (1987) and Reed & Simon (1979) for a more extensive discussion of the ideas surrounding cluster decompositions.

Let $\boldsymbol{a} = \{A_1, A_2, \ldots, A_m\}$ be a cluster decomposition. It is customary to consider the $(m-1)\nu$-dimensional subspace

$$X_{\boldsymbol{a}} := \{x \in X : x^i = x^j \quad \text{for all} \quad (ij) \subset \boldsymbol{a}\},$$

see Sigal (1982) or Sigalov & Sigal (1970). To find the orthogonal complement of $X_{\boldsymbol{a}}$ in X choose $x \in X_{\boldsymbol{a}}, y \in X$ and observe that for k_i an arbitrary element of $A_i, i = 1, \ldots, m$,

$$\begin{aligned} \langle x, y \rangle_X &= \sum_{j=1}^{N} 2m_j (x^j, y^j)_{\boldsymbol{R}^\nu} \\ &= \sum_{i=1}^{m} \sum_{j \in A_i} 2m_j (x^{k_i}, y^j)_{\boldsymbol{R}^\nu} \\ &= \sum_{i=1}^{m} (x^{k_i}, \sum_{j \in A_i} 2m_j y^j)_{\boldsymbol{R}^\nu}. \end{aligned}$$

Hence, the orthogonal complement of $X_{\boldsymbol{a}}$ in X is

$$X^{\boldsymbol{a}} := \{x \in X : R_i^{\boldsymbol{a}}(x) = 0, i = 1, \ldots, m\}$$

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for

$$R_i^{\boldsymbol{a}}(x) := \frac{1}{M_i} \sum_{j \in A_i} m_j x^j, \quad M_i := \sum_{j \in A_i} m_j, \tag{3.2}$$

where $R_i^{\boldsymbol{a}}(x)$ is the centre of mass associated with the cluster $A_i \in \boldsymbol{a}$.

The next lemma illustrates the relation between the projections $\Pi_{ij}, 1 \leqslant i < j \leqslant N$, and the subspaces $X^{\boldsymbol{a}}$ and $X_{\boldsymbol{a}}$.

Lemma 3.1. *Let $\tilde{X}$ be the space $\times_{i=1}^N \boldsymbol{R}^\nu$ with the inner product*

$$\langle x, y \rangle_{\tilde{X}} := \sum_{i=1}^{N} 2m_i (x^i, y^i)_\nu.$$

Then for any given m-cluster decomposition $\boldsymbol{a} = \{A_1, \ldots, A_m\}$ of N particles

(i) $X^\perp = \{x \in \tilde{X} : x^1 = \cdots = x^N\}$,

(ii) $X_{\boldsymbol{a}} \oplus X^\perp = \{x \in \tilde{X} : x \in \ker(\Pi_{ij})$ *when* $(ij) \subset \boldsymbol{a}\}$, *and*

(iii) $X^{\boldsymbol{a}} = \operatorname{span}\{\bigcup_{(ij)\subset \boldsymbol{a}} \operatorname{Range}(\Pi_{ij})\}$.

For

$$X_{A_k}^{\boldsymbol{a}} := \operatorname{span}\left\{ \bigcup_{i,j \in A_k} \operatorname{Range}(\Pi_{ij}) \right\}, \quad k = 1, \ldots, m,$$

(iv) $X^{\boldsymbol{a}} = X_{A_1}^{\boldsymbol{a}} \oplus \cdots \oplus X_{A_m}^{\boldsymbol{a}}$ *and* $X_{A_k}^{\boldsymbol{a}} = \{x \in X : R_k^{\boldsymbol{a}}(x) = 0\}$.

By 'ker' and 'span' above we mean the kernel and linear span with $\operatorname{span}(\varnothing) := \{0\}$. Note that $X_{A_k}^{\boldsymbol{a}} = \{0\}$ when A_k is a singleton. The proof of Lemma 3.1 is given in the Appendix.

Given a cluster decomposition $\boldsymbol{a}$, the *intercluster interaction* is defined by

$$I_{\boldsymbol{a}} := \sum_{(ij) \not\subset \boldsymbol{a}} V_{ij}$$

and the *internal hamiltonian* is given by

$$H(\boldsymbol{a}) := H - I_{\boldsymbol{a}} = -\Delta_X + \sum_{(ij)\subset \boldsymbol{a}} V_{ij}.$$

We see that

$$H_\omega = H(\boldsymbol{a}_\omega) \quad \text{for all} \quad \omega \in S(X)$$

and for any m-cluster decomposition $\boldsymbol{a}$ with $m \geqslant 2$

$$H(\boldsymbol{a}) = H_\omega \quad \text{for all} \quad \omega \in U_{\boldsymbol{a}} \setminus \bigcup_{(ij)\not\subset \boldsymbol{a}} K_{ij}.$$

The self-adjoint realization of $H(\boldsymbol{a})$ in $L^2(X)$ will be denoted by $H(\boldsymbol{a})$ also.

Proposition 3.2. *Let $\boldsymbol{a}$ be an m-cluster decomposition of N particles. Then*

$$K(\omega : H) = K(\omega : H(a)) = \Lambda(H(\boldsymbol{a})) = \Sigma(H(\boldsymbol{a})), \quad \omega \in U_{\boldsymbol{a}} \setminus \bigcup_{(ij)\not\subset \boldsymbol{a}} K_{ij}.$$

Proof. The first equality follows from the fact implied by (2.1)(iii) that for $(ij) \not\subset \boldsymbol{a}$

$$V_{ij} \to 0 \quad \text{as} \quad |x| \to \infty \quad \text{in a cone} \quad \Gamma(\{\omega\}_\delta, 1)$$

for δ sufficiently small. If $\omega \in U_{\boldsymbol{a}}$, then $V_{ij}(x + t\omega) = V_{ij}(x)$ for all $(ij) \subset \boldsymbol{a}$ and $t > 0$, and it follows as in Lemma 4.6 of Agmon (1982) that $\Lambda(H(\boldsymbol{a})) = \Sigma(H(\boldsymbol{a})) = K(\omega : H(\boldsymbol{a}))$. If $m = N$, then $H(\boldsymbol{a}) = -\Delta_X$ and the statement still holds. □

The main part of the HVZ Theorem of quantum mechanics follows as a corollary of Proposition 3.2.

Corollary 3.3. (i) *$K(\omega:H)$ assumes only a finite number of values on $S(X)$.* (ii)

$$\begin{aligned}\Sigma(H) &= \inf\{K(\omega:H):\omega\in K_{ij} \text{ for some } (ij),\ 1\leqslant i<j\leqslant N\}\\ &= \inf\{K(U_a:H):\#\boldsymbol{a}\geqslant 2\}\\ &= \inf\{\Lambda(H(\boldsymbol{a})):\#\boldsymbol{a}\geqslant 2\}.\end{aligned}$$

Proof. Part (i) follows from Lemma 4.8 of Agmon (1982) which implies that $K(\omega:H) = \Lambda(H_\omega) = \Lambda(H(\boldsymbol{a}_\omega))$ for any $\omega \in S(X)$. There are only a finite number of the operators $H(\boldsymbol{a}_\omega)$.

If

$$\#(\boldsymbol{a}_\omega) = N \quad \text{then} \quad \omega \notin \bigcup_{1\leqslant i<j\leqslant N} K_{ij}$$

implying that $H(\boldsymbol{a}_\omega) = -\Delta_X$ and $\Lambda(H(\boldsymbol{a}_\omega)) = 0$. Such points ω form a dense subset of $S(X)$. Since $K(\omega:H)$ is lower semicontinuous (Lemma 2.2), it follows that $\max\{K(\omega, H):\omega\in S(X)\} = 0$. Therefore, $K(\omega:H)$ must assume its minimum at points in some K_{ij}. The remainder of the proof follows from Proposition 3.2 and the fact that

$$K(U_a:H) = \inf_{\omega\in U_a} K(\omega:H)$$

for any m-cluster $\boldsymbol{a}$. □

4. The finiteness and infiniteness of bound states

In the next two lemmas we discuss refinements T_a, associated with a cluster decomposition $\boldsymbol{a}$, of the matrix T_X mentioned in §2. These new matrices are used to change coordinates to *clustered coordinates*. An example of such coordinates is the *clustered Jacobi coordinates* discussed on p. 79 of Reed & Simon (1979). In the second lemma we give a specific matrix T_a to produce clustered coordinates differing from the clustered Jacobi coordinates. Many other variations on this theme are possible. Proofs are given in the Appendix.

Lemma 4.1. *Let $\boldsymbol{a} = \{A_1, \ldots, A_m\}$ be an m-cluster decomposition of N particles and set $M := \Sigma_{i=1}^N m_i$. Number the clusters in order that $\#(A_i) \geqslant \#(A_j)$ when $i<j$. Let m' be the number of clusters having more than one element. There is an $N\nu\times N\nu$ matrix T_a having the following properties:*

(*a*) *T_a is non-singular.*

(*b*) *For $G := \operatorname{diag}(2m_1 I_\nu, \ldots, 2m_N I_\nu)$ the matrix $G(\boldsymbol{a}) := T_a G^{-1} T_a^t$ has the form*

$$G(\boldsymbol{a}) = \begin{bmatrix} G_1^a & 0 & \cdots & & & 0\\ 0 & G_2^a & \cdots & & & 0\\ \vdots & \vdots & \ddots & & & \vdots\\ 0 & 0 & \cdots & G_{m'}^a & \cdots & 0\\ 0 & 0 & \cdots & & G_a & 0\\ 0 & 0 & \cdots & 0 & & (1/2M)\, I_\nu \end{bmatrix}.$$

Each G_i^a *is of dimension* $(n(i)-1)\nu \times (n(i)-1)\nu$ *for* $n(i) := \#(A_i)$, $i = 1, \ldots, m'$. *The submatrix* $G^a := \operatorname{diag}(G_1^a, \ldots, G_{m'}^a)$ *is of dimension* $(N-m)\nu \times (N-m)\nu$. *The submatrix* G_a *is of dimension* $(m-1)\nu \times (m-1)\nu$.

(*c*) *If* $x = (x^1, \ldots, x^N) \in X^a$ *then*

$$\begin{bmatrix} \eta^1 \\ \vdots \\ \eta^{N-m} \\ 0 \\ \vdots \\ 0 \end{bmatrix} = T_a x$$

for $\eta^l \in \mathbf{R}^\nu, l = 1, \ldots, N-m$. *Moreover, for* $x = (x^1, \ldots, x^N) \in X^a_{A_1}$

$$\begin{bmatrix} \eta(1) \\ 0 \\ \vdots \\ 0 \end{bmatrix} = T_a x \quad \textit{for} \quad \eta(1) := \begin{bmatrix} \eta^1 \\ \vdots \\ \eta^{n(1)-1} \end{bmatrix}.$$

In general, the result is analogous for $\eta(k)$, $k = 1, \ldots, m$, *and* x *in subspaces* $X^a_{A_k}$ *of* X^a.

(*d*) *If* $x = (x^1, \ldots, x^N) \in X_a$ *then*

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ \xi^1 \\ \vdots \\ \xi^{m-1} \\ 0 \end{bmatrix} = T_a x$$

for $\xi^i \in \mathbf{R}^\nu$, $i = 1, \ldots, m-1$.

(*e*) *If* $x = (x^1, \ldots, x^N) \in X^\perp$ *then*

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ R \end{bmatrix} = T_a x$$

for $R = x^1 = \cdots = x^N$.

Lemma 4.2. *For each m-cluster* $\boldsymbol{a}$ *there is a matrix* T_a *satisfying the properties of Lemma* 4.1 *as well as the following*:

(*a*) *In Lemma* 4.1*c each* $\eta^l = x^i - x^j$ *for some* $(ij) \subset \boldsymbol{a}$ *and* $l = 1, \ldots, N-m$. *For* $k = 1, \ldots, m$, *the components of* $\eta(k)$ *are equal to* $x^i - x^j$ *for some* $i, j \in A_k$.

(*b*) *In Lemma* 4.1*d each*

$$\xi^l = (M_l/M)\,(R_l^a(x) - R_m^a(x)), \quad l = 1, \ldots, m-1,$$

for $M := \Sigma_{i=1}^N m_i$ *and* R_l^a, M_l *given by* (3.2).

(c) *The* $(m-1)\nu \times (m-1)\nu$ *matrix*

$$G_a = \frac{1}{2M_m M^2}\begin{bmatrix} M_1(M_1+M_m)I_\nu & M_1M_2I_\nu & \cdots & M_1M_{m-1}I_\nu \\ M_2M_1I_\nu & M_2(M_2+M_m)I_\nu & \cdots & M_2M_{m-1}I_\nu \\ \vdots & \vdots & \ddots & \vdots \\ M_{m-1}M_1I_\nu & M_{m-1}M_2I_\nu & \cdots & M_{m-1}(M_{m-1}+M_m)I_\nu \end{bmatrix}.$$

In these new coordinates the Laplace–Beltrami operator in $\tilde{X}$ is given by

$$\Delta_{\tilde{X}} = \operatorname{div}_{T_a x}(G(\boldsymbol{a})\nabla_{T_a x}).$$

For each m-cluster decomposition $\boldsymbol{a}$ let Δ_{X^a} and Δ_{X_a} be the Laplace–Beltrami operators on the subspaces X^a and X_a respectively. Then Lemma 4.1 implies that

$$\Delta_{X^a} = \operatorname{div}_\eta (G^a\nabla_\eta), \quad \eta := (\eta^1, \dots, \eta^{N-m}, 0, \dots, 0) \in T_a X^a \tag{4.1}$$

and

$$\Delta_{X_a} = \operatorname{div}_\xi (G_a\nabla_\xi), \quad \xi := (0, \dots, 0, \xi^1, \dots, \xi^{m-1}, 0) \in T_a X_a. \tag{4.2}$$

Moreover, Δ_X splits into a tensor product

$$\Delta_{X^a} \otimes I + I \otimes \Delta_{X_a}$$

on $L^2(X^a) \otimes L^2(X_a) \approx L^2(X)$, where I is the identity operator on either X_a or X^a in accordance to its position. Define

$$H^a := -\Delta_{X^a} \otimes I + \Sigma_{(ij)\subset a} V_{ij} \tag{4.3}$$

and

$$H_a := I \otimes (-\Delta_{X_a}) + I_a, \tag{4.4}$$

where I_a is the intercluster interaction for the cluster $\boldsymbol{a}$.

We may view H_a and H^a as being (unitarily equivalent to) the operators associated with the closures in $L^2(T_a X)$ of the forms

$$\rho_a[\phi, \psi] := \int_{T_a X^a}\int_{T_a X_a} [(G_a\nabla_\xi\phi, \nabla_\xi\psi) + I_a(\eta, \xi)\,\phi\bar{\psi}]\,\mathrm{d}_{X_a}\xi\,\mathrm{d}_{X^a}\eta, \quad \phi, \psi \in C_0^\infty(T_a X)$$

and

$$\rho^a[\phi, \psi] := \int_{T_a X_a}\int_{T_a X^a}\left[(G^a\nabla_\eta\phi, \nabla_\eta\psi) + \sum_{(ij)\subset a} V_{ij}(\eta)\,\phi\bar{\psi}\right]\mathrm{d}_{X^a}\eta\,\mathrm{d}_{X_a}\xi, \quad \phi, \psi \in C_0^\infty(T_a X)$$

respectively, where $\mathrm{d}_{X^a}\eta := \sqrt{(G^a)^{-1}}\,\Pi_{ij}\,\mathrm{d}\eta^i_j$ and $\mathrm{d}_{X_a}\xi := \sqrt{(G_a)^{-1}}\,\Pi_{ij}\,\mathrm{d}\xi^i_j$; see the discussion of 'The restriction of $\Delta_{\tilde{X}}$ to X' in the Appendix for more details. Henceforth, we simply write $\mathrm{d}\eta$ and $\mathrm{d}\xi$ for $\mathrm{d}_{X^a}\eta$ and $\mathrm{d}_{X_a}\xi$ respectively. Then, $\rho = \rho_a + \rho^a$ and $H = H_a + H^a$. (We make no notational distinction between unitarily equivalent operators.)

Lemma 4.3. *Let* $\boldsymbol{a}$ *be an m-cluster decomposition. Let* $H(\boldsymbol{a})$ *be the internal hamiltonian. For* H^a *defined by* (4.3)

$$\Lambda(H(\mathbf{a})) = \Lambda(H^a), \tag{4.5}$$

if $m < N$ *and* $\Lambda(H(\boldsymbol{a})) = 0$ *if* $m = N$.

Since the proof of Lemma 4.3 follows in the same manner as Lemma 4.10 of Agmon (1982), we do not repeat it here.

Now, we are prepared to state one of our main theorems.

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Theorem 4.4. *Let $\mathscr{M}$, given in Definition 2.1, be the disjoint union of sets U_a, $\boldsymbol{a}\in\mathscr{A}$, for some set $\mathscr{A}$ of cluster decompositions. Given δ and R set*

$$\Delta_a := \Gamma(\overline{(U_a)_\delta}, R)\backslash\Gamma((U_a)_{\delta/2}, 2R).$$

If there exists positive numbers δ, ϵ and R such that

$$([H_a-(\epsilon/|x|^2)\,\chi_{\Delta_a}]\,\phi,\phi)_{L^2(X)} \geqslant 0 \tag{4.6}$$

for all $\phi\in C_0^\infty(\Gamma((U_a)_\delta, R))$ and each $\boldsymbol{a}\in\mathscr{A}$, then $\sigma(H)\cap(-\infty,\Sigma(H)]$ is finite.

Proof. We may assume that δ has been chosen sufficiently small in order that the $(U_a)_\delta$, $\boldsymbol{a}\in\mathscr{A}$, are disjoint. If $\|\phi\|_{L^2(X)}=1$, then for each $\boldsymbol{a}\in\mathscr{A}$

$$\begin{aligned}([H-(\epsilon/|x|^2)\,\chi_{\Delta_a}]\,\phi,\phi)_{L^2(X)} &\geqslant (H^a\phi,\phi)_{L^2(X)}\\ &\geqslant \Lambda(H^a)\\ &= \Sigma(H)\end{aligned}$$

by (4.5), (4.6), and Proposition 3.2. Therefore,

$$K(\mathscr{M}_\delta, R; H_\epsilon) \geqslant \Sigma(H).$$

It follows from the Definition 2.1, Lemma 2.2, and (2.2) that

$$K(\mathscr{M}_\delta, R; H_\epsilon) \leqslant \Sigma(H).$$

Hence, the condition required in Theorem 2.3 is met. □

Note that Theorem 4.4 does not require that the cluster decompositions $\boldsymbol{a}\in\mathscr{A}$ be 2-cluster decompositions, contrary to the typical assumption for finiteness of bound states. However, if $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are distinct 2-cluster decompositions then U_{a1} and U_{a2} are disjoint, meeting the requirement of the theorem. We look at a consequence of this fact below.

Inequality (4.6) requires that for given δ and ϵ the operator determined by

$$H_a-(\epsilon/|x|^2)\,\chi_{\Delta_a} \quad \text{on} \quad C_0^\infty(\Gamma((U_a)_\delta, 1))$$

has finite negative spectrum.

The conical region $\Gamma((U_a)_\delta, 1)$ compares with the support of the localizing function j_a used in the *Deift–Agmon–Sigal partition* of unity given in Definition 3.19 of (Cycon *et al.* 1987). There $\{|x|>1\}\cap\operatorname{supp} j_a$ is contained in the set

$$\{x\in X: |x^i-x^j|_\nu \geqslant C|x| \quad \text{whenever} \quad (ij)\not\subset \boldsymbol{a}\}$$

for a suitable constant C, and it is not hard to see that this is also the case for $\Gamma((U_a)_\delta, 1)$ for all δ small enough.

When $\mathscr{M}$ is not the disjoint union of sets U_a, an analogue of Theorem 4.4 can be proved, but we do not pursue that here. In reference to the results in §2 the reader may notice that the condition (4.6) is equivalent to the requirement that

$$K((U_a)_\delta, R; (H_a-(\epsilon/|x|^2)\,\chi_{\Delta_a})) \geqslant 0.$$

To show that H has an infinite number of bound states, according to Theorem 2.3 it will suffice that we can find a function $\phi\in C_0^\infty(\Gamma(\mathscr{M}_\delta, R))$ such that

$$(H\phi,\phi)_{L^2(X)} < \Sigma(H)\,\|\phi\|^2_{L^2(X)}$$

for every $\delta>0$ and every $R>0$. Roughly speaking, this will require that the inequality (4.6) with $\epsilon=0$ be reversed for some sequence $\{\phi_n\}$.

Earlier results of this type have used techniques developed in the fundamental

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paper of Kato (1951) (see also Reed & Simon 1978, p. 89; Titchmarsh 1958). Here, we use recent results in Agmon (1982) concerning the decay of eigenfunctions and a consequence regarding the decay of the gradient of eigenfunctions. The proposition and its corollary are stated for the general operator P introduced in §2, but it applies to H and H^a as well. The next proposition is a corollary of Theorem 4.9 of Agmon (1982). It is a modification of Proposition 4.2 in Evans *et al.* (1991*b*).

Proposition 4.5. *Assume* (1.1) (i)–(iv). *Let ψ be an eigenfunction of P with eigenvalue $\mu < \Sigma(P) := \inf \sigma_e(P)$ and let $\lambda_1(A^{-1})$ be the minimum eigenvalue of the matrix $A^{-1} = (a_{ij})$.*

(i) *For* $c_0 := \frac{1}{2}\sqrt{[(\Sigma(P)-\mu)\,\lambda_1(A^{-1})]}$

$$\int_{R^n} |\psi(x)|^2\, e^{2c_0|x|}\, dx < \infty. \tag{4.7}$$

(ii) *If* (1.1) (i)–(iii) *hold and*

$$q_i|_{Y_i} \in M_{\text{loc}}(Y_i), \quad i = 1, \ldots, l, \tag{4.8}$$

then

$$\int_{R^n} |\nabla\psi(x)|^2\, e^{c_0|x|}\, dx < \infty. \tag{4.9}$$

Recall that τ is the form associated with the operator P in $L^2(\boldsymbol{R}^n)$.

Corollary 4.6. *Assume* (1.1) (i)–(iii) *and* (4.8). *Let P, ψ, μ, and c_0 be given as in Proposition 4.5 with $\|\psi\|_{L^2(\boldsymbol{R}^n)} = 1$. Then there is a sequence $\{\phi_k\} \subset C_0^\infty(\boldsymbol{R}^n)$ having the following properties for each positive integer k:*

$$\left.\begin{array}{ll} \text{(i)} & \|\phi_k\|_{L^2(\boldsymbol{R}^n)} = 1; \\ \text{(ii)} & \operatorname{supp}(\phi_k) \subset \{x \in \boldsymbol{R}^n : |x| \leqslant 2k\}; \\ \text{(iii)} & \tau[\phi_k, \phi_k] \leqslant \mu + \dfrac{C}{k\, e^{c_0 k}} \displaystyle\int_{|x|>k} e^{c_0|X|}(|\psi|^2 + |\nabla\psi|^2)\, dx, \end{array}\right\} \tag{4.10}$$

for some constant $C > 0$ independent of k.

The proofs of Proposition 4.5 and Corollary 4.6 can be found in the Appendix. The next theorem is an application of these two results. Although it is quite technical, it does sketch a general method of proving the infiniteness of bound states for H. Below we use it to obtain specific criteria in the special case in which U_a for a 2-cluster decomposition $\boldsymbol{a}$ is an isolated subset of the minimizing set $\mathscr{M}$.

Theorem 4.7. *Assume that*

$$v_{ij} \in M_{\text{loc}}(\boldsymbol{R}^\nu), \quad 1 \leqslant i < j \leqslant N, \tag{4.11}$$

and for some m-cluster decomposition $\boldsymbol{a}$ assume that

$$\left.\begin{array}{l} U_a \subset \mathscr{M} \quad \textit{and} \\ A(H^a) = \Sigma(H) \quad \textit{is an isolated eigenvalue of } H^a. \end{array}\right\} \tag{4.12}$$

Let $\{\phi_k^a\} \subset C_0^\infty(\boldsymbol{R}^{(N-m)\nu})$ *be a sequence given by Corollary* 4.6 *associated with* $\Lambda(H^a)$. *For each* $k \geqslant 1$ *define*

$$V_k(\xi) := \int_{\boldsymbol{R}^{(N-m)\nu}} I_a(\eta, \xi)\, |\phi_k^a(\eta)|^2 \, \mathrm{d}\eta.$$

If for some $\epsilon > 0$ *there is a sequence* $\{\psi_k(\xi)\} \subset C_0^\infty(\boldsymbol{R}^{(m-1)\nu})$ *with*

$$\left.\begin{array}{ll} \text{(i)} & \operatorname{supp}(\psi_k) \subset \boldsymbol{R}^{(m-1)\nu} \backslash B(0; k^q) \text{ for some fixed } q > 1, \\ \text{(ii)} & \|\psi_k\|_{L^2(\boldsymbol{R}^{(m-1)\nu})} = 1, \quad \text{and} \\ \text{(iii)} & \displaystyle\int_{\boldsymbol{R}^{(m-1)\nu}} [(G_a \nabla_\xi \psi_k, \nabla_\xi \psi_k) + V_k(\xi)\, |\psi_k|^2]\, \mathrm{d}\xi + \frac{\epsilon}{k\, \mathrm{e}^{c_0 k}} < 0, \end{array}\right\} \tag{4.13}$$

then H *has an infinite number of bound states.*

Proof. By Corollary 4.6 we may assume that the sequence $\{\phi_k^a\} \subset C_0^\infty(\boldsymbol{R}^{(N-m)\nu})$ has the following properties:

$$\left.\begin{array}{ll} \text{(i)} & \|\phi_k^a\|_{L^2(\boldsymbol{R}^{(N-m)\nu})} = 1; \\ \text{(ii)} & \operatorname{supp}(\phi_k^a) \subset \{x \in \boldsymbol{R}^{(N-m)\nu} : |x| \leqslant 2k\}; \quad \text{and} \\ \text{(iii)} & \displaystyle\int_{\boldsymbol{R}^{(N-m)\nu}} \left[(G^a \nabla_\eta \phi_k^a, \nabla_\eta \phi_k^a) + \sum_{(ij) \subset a} V_{ij}(\eta)\, |\phi_k^a|^2\right] \mathrm{d}\eta \leqslant \Sigma(H) + \frac{\epsilon}{k\, \mathrm{e}^{c_0 k}} \end{array}\right\} \tag{4.14}$$

for any $\epsilon > 0$ and all k sufficiently large. Define

$$\Phi_k(\eta, \xi) := \phi_k^a(\eta)\, \psi_k(\xi), \quad \text{for} \quad (\eta, \xi, 0)^t \in T_a X \quad \text{and} \quad k \geqslant 1.$$

Then each $\Phi_k \in C_0^\infty(T_a X)$. Also, note that

$$\operatorname{supp} \Phi_k \subset \{(\eta, \xi, 0)^t \in T_a X : |\eta|_{\boldsymbol{R}^{(N-m)\nu}} \leqslant 2k \quad \text{and} \quad |\xi|_{\boldsymbol{R}^{(m-1)\nu}} \geqslant k^q\}.$$

Next, we show that for positive constants $C_0 > 0, c_1$, and $\delta_k := C_0/k^{q-1}, k \geqslant 1$,

$$T_a^{-1}(\operatorname{supp} \Phi_k) \subset \Gamma((U_a)_{\delta_k}, c_1 k^q).$$

Let $x \in T_a^{-1}(\operatorname{supp} \Phi_k)$. Then, $T_a x = (\eta, \xi, 0)^t \in \operatorname{supp} \Phi_k$ and, according to Lemma 4.1, there exist $x_a \in X_a$ and $x^a \in X^a$ such that

$$T_a x^a = \begin{pmatrix} \eta \\ 0 \\ 0 \end{pmatrix}, \quad T_a x_a = \begin{pmatrix} 0 \\ \xi \\ 0 \end{pmatrix}, \quad \text{and} \quad T_a x = \begin{pmatrix} \eta \\ \xi \\ 0 \end{pmatrix}$$

with $x = x^a \oplus x_a \in X$. Then there are positive constants c_1 and c_2 such that (i) $|x^a| \leqslant c_2 k$ and (ii) $|x_a| \geqslant c_1 k^q$. Set $C_0 = 2c_2/c_1$. Since $|x_a|_X^{-1} x_a \in U_a$, then

$$\begin{aligned} \operatorname{dist}(x/|x|_X : U_a) &\leqslant |x/|x|_X - x_a/|x_a|_X|_X \\ &\leqslant (1/|x|_X |x_a|_X)\, \| x_a|_X x^a + (|x_a|_X - |x|_X)\, x_a|_X \\ &\leqslant (1/|x|_X)\, (|x^a|_X + (|x|_X - |x_a|_X)) \\ &\leqslant 2\, |x^a|_X / |x|_X \\ &\leqslant C_0/k^{q-1} \\ &= \delta_k, \end{aligned}$$

which is what we wanted to show.

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Hence, for all k sufficiently large

$$\begin{aligned}\rho[\Phi_k] &= \rho^a[\Phi_k]+\rho_a[\Phi_k]\\ &= \int_{R^{(N-m)\nu}}\Big[(G^a\nabla_\eta\phi^a_k,\nabla_\eta\phi^a_k)+\sum_{(ij)\subset a}V_{ij}(\eta)\,|\phi^a_k|^2\Big]\,d\eta\\ &\quad+\int_{R^{(m-1)\nu}}[(G_a\nabla_\xi\psi_k,\nabla_\xi\psi_k)+V_k(\xi)\,|\psi_k|^2]\,d\xi\\ &< \Sigma(H).\end{aligned}$$

Therefore, H has an infinite number of bound states. □

We conjecture that $V_k(\xi)$ in Theorem 4.7 can be replaced by

$$V_a(\xi) := \int_{R^{(N-m)\nu}} I_a(\eta,\xi)\,|\psi_a(\eta)|^2\,d\eta$$

for ψ_a being the ground state of H^a. In that case the problem would be reduced essentially to showing that

$$-\Delta_{X_a}+V_a(\xi)$$

has an infinite negative spectrum.

(a) *Bounds for H_a when a is a 2-cluster decomposition*

A common assumption for criteria for the finiteness of bound states of H is that $U_a\subset\mathscr{M}$ only for 2-cluster decompositions $\boldsymbol{a}$ (cf. Sigal 1982). In the absence of this condition it can be shown that some 3-body operators have an infinite number of bound states even if the v_{ij} have compact support. This phenomenon is known as the 'Efimov effect' (see Efimov 1970, 1971) and Cycon *et al.* (1987).

When $\boldsymbol{a}$ is a 2-cluster decomposition, we will be able to use Lemma 4.8 below to approximate I_a as follows:

$$V^-_a(|\xi|;\delta)\leqslant I_a(\eta,\xi)\leqslant V^+_a(|\xi|;\delta),\quad T^{-1}_a(\eta,\xi,0)^t\in\Gamma((U_a)_\delta,1) \tag{4.15}$$

for δ sufficiently small and functions V^-_a and V^+_a given below. Using these approximations to the intercluster interaction we identify operators, which are lower and upper bounds for H_a,

$$H^-_a := -\Delta_{X_a}+V^-_a \quad\text{and}\quad H^+_a := -\Delta_{X_a}+V^+_a \tag{4.16}$$

with domains in $L^2(X_a)$.

A basic hypothesis, which holds for N-body operators, is as follows:

Hypothesis $\mathscr{H}$. *For a given cluster decomposition* $\boldsymbol{a}$ *and each* $(ij)\not\subset\boldsymbol{a}$, *assume that there is a function* v'_{ij}: $(0,\infty)\to\boldsymbol{R}$ *such that*

(i) $V_{ij}(x)=v_{ij}(x^i-x^j)=v'_{ij}(|x^i-x^j|_{R^\nu})$;

(ii) *each* v'_{ij} *is of one sign on* $(0,\infty)$;

(iii) $|v'_{ij}|$ *is non-increasing on* $(0,\infty)$.

Lemma 4.8. *Assume that* $\mathscr{H}$ *holds for a 2-cluster decomposition* $\boldsymbol{a}:=\{A_1,A_2\}$. *Let*

$$M:=\sum_{i=1}^N m_i \quad\text{and}\quad M_j:=\sum_{l\in A_j} m_l.$$

Then for all δ sufficiently small there is a constant $C > 0$ depending only upon $m_1, \dots, m_N$ such that (4.15) *holds with*

$$\left.\begin{aligned} V_a^-(|\xi|;\delta) &:= \sum_{\{(ij)\notin a:\, v'_{ij}\leqslant 0\}} v'_{ij}\left(\left(\frac{M}{M_1}-C\delta\right)|\xi|\right)+\sum_{\{(ij)\notin a:\, v'_{ij}\geqslant 0\}} v'_{ij}\left(\left(\frac{M}{M_1}+C\delta\right)|\xi|\right), \\ V_a^+(|\xi|;\delta) &:= V_a^-(|\xi|;-\delta). \end{aligned}\right\} \quad (4.17)$$

If $\boldsymbol{a} = \{A_1, A_2\}$, it follows from Lemma 4.2*b* that $|\xi|$ is a constant multiple of the distance between the centres of mass of the clusters of particles corresponding to A_1 and A_2. Note that

$$\delta_1 \geqslant \delta_0 > 0 \Rightarrow \begin{cases} V_a^-(|\xi|;\delta_1) \leqslant V_a^-(|\xi|;\delta_0), \\ V_a^+(|\xi|;\delta_1) \geqslant V_a^+(|\xi|;\delta_0), \end{cases}$$

for each $\xi \in \boldsymbol{R}^\nu$. The proof of Lemma 4.8 depends upon the following lemma. The proofs are given in the Appendix.

Lemma 4.9. *For an m-cluster* $\boldsymbol{a}$ *let* T_a *be given by Lemma* 4.1 *and let* $\eta := (\eta^1, \dots, \eta^{N-m})^t$ *and* $\xi := (\xi^1, \dots, \xi^{m-1})^t$ *as given in parts* (*c*) *and* (*d*) *of Lemma* 4.1. *If*

$$\begin{pmatrix}\eta\\ \xi\\ 0\end{pmatrix} \in \{T_a x : x \in \Gamma((U_a)_\delta, 1)\}$$

and δ is sufficiently small, then

$$|\eta|_{\boldsymbol{R}^{(N-m)\nu}} < 2\delta|\xi|_{\boldsymbol{R}^{(m-1)\nu}}.$$

For each 2-cluster decomposition $\boldsymbol{a}$ define H_a^+ and H_a^- according to (4.16) associated with the closure of the forms

$$\rho_a^\pm[\phi,\psi] := \int_{\boldsymbol{R}^\nu} [(G_a \nabla_\xi \phi, \nabla_\xi \psi) + V_a^\pm \phi\bar{\psi}]\,\mathrm{d}\xi, \quad \phi, \psi \in C_0^\infty(\boldsymbol{R}^\nu),$$

in $L^2(\boldsymbol{R}^\nu)$. According to Lemma 4.2*c* the matrix $G_a = (M_1/2M_2M)I_\nu$. It follows from (2.1)(iii) that $V_a^\pm \to 0$ as $|\xi| \to \infty$. Using this fact it can be shown that $\Sigma(H_a^-) = \Sigma(H_a^+) = 0$.

The next corollary to Theorem 4.4 shows that in the case of N-body operators (4.6) is satisfied for $\boldsymbol{a}$ being a 2-cluster decomposition if an associated operator in $L^2(\boldsymbol{R}^\nu)$ has finite negative spectrum (see Donig 1991). This is the classical problem of the existence of positive solutions studied in the oscillation theory of partial differential equations.

Recall that $B(R)$ denotes the ball centred at the origin and with radius R.

Corollary 4.10. *Assume that*

$$\mathscr{M} \subset \bigcup_{\#(a)=2} U_a.$$

If $\mathscr{H}$ *holds for each* $\boldsymbol{a}$ *for which* $U_a \subset \mathscr{M}$, δ *is sufficiently small in order that* (4.15) *holds, and for some* $R > 0$

$$\left(\left[H_a^- - \frac{\epsilon}{|\xi|^2}\right]\phi(\xi), \phi(\xi)\right)_{L^2(\boldsymbol{R}^\nu)} \geqslant 0, \quad \phi \in C_0^\infty(\boldsymbol{R}^\nu \setminus B(R)), \quad (4.18)$$

then H has no more than a finite number of bound states.

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Proof. Since only 2-cluster decompositions are being considered, then $\mathscr{M}$ must be the disjoint union of sets U_a as required by Theorem 4.4. If δ is sufficiently small and $\phi \in C_0^\infty(\Gamma((U_a)_\delta, R)$ for $U_a \subset \mathscr{M}$ then the left-hand side of inequality (4.6) is equal to

$$\rho_a[\phi] - \int_X \frac{\epsilon}{|x|^2}|\phi|^2\,\mathrm{d}x \geqslant \int_{T_a X^a}\int_{T_a X_a}\left[\left(G_a \nabla_\xi \phi, \nabla_\xi \phi\right) + \left(V_a^-(|\xi|;\delta) - \frac{\epsilon}{|\xi|^2}\right)|\phi|^2\right]\mathrm{d}\xi\,\mathrm{d}\eta \geqslant 0$$

according to (4.18). □

For δ sufficiently small (4.18) obviously holds if

$$V_a^-(|\xi|;\delta) - \epsilon/|\xi|^2 \geqslant 0$$

for all R sufficiently large and all ϵ sufficiently small. This is the way one can show that an atom with N electrons and an infinitely heavy nucleus of charge $Z < N-1$ has at most a finite number of bound states. Another more general criterion is given by the next corollary. Below Ω_ν denotes the volume of the unit ball in $\boldsymbol{R}^\nu$.

Corollary 4.11. *Assume that*

$$\mathscr{M} \subset \bigcup_{\#(a)=2} U_a,$$

$\mathscr{H}$ holds for each $\boldsymbol{a}$ for which $U_a \subset \mathscr{M}$, and δ is sufficiently small in order that (4.15) *holds. If for each of these 2-cluster decompositions $\boldsymbol{a} = \{A_1, A_2\}$*

$$\lim_{R\to\infty}\sup_{l\geqslant R} l^{2-\nu}\int_{1\leqslant|x|<l}(V_a^-(|x|;\delta))_-\,\mathrm{d}x < \frac{(\nu-2)\,M_1}{8M_2 M},$$

then H has no more than a finite number of bound states.

Corollary 4.11 is a modification of Example 5 of Evans & Lewis (1990). It is an adaptation of a classical one-dimensional result of Hille (1948). In contrast, we give a corollary to Theorem 4.7.

Corollary 4.12. *Assume* (4.11) *and that* (4.12) *holds for some 2-cluster decomposition $\boldsymbol{a}$. Suppose that $V_a^+(|\xi|;\delta) \leqslant 0$ for some δ and all $|\xi|$ sufficiently large. If*

$$\lim_{R\to\infty}\sup_{l\geqslant R} l^{2-\nu-\beta}\int_{2l\leqslant|\xi|\leqslant 3l}|\xi|^\beta\, V_a^+(|\xi|;\delta)\,\mathrm{d}\xi < -\frac{\Omega_\nu M_1(8+|\beta|)^2}{8M_2 M(2-\nu-\beta)},$$

for some $\beta \in (-\nu, 2-\nu)$, then H has an infinite number of bound states.

The proof of Corollary 4.12 depends upon the next lemma.

Lemma 4.13. *Let p_0 be a positive constant and let $p_1 \in L^1_{\mathrm{loc}}[1,\infty)$ with $p_1(t) \leqslant 0$ for all t sufficiently large. For $n \geqslant 3$ define*

$$Ly := -(p_0 t^{n-1} y')' + t^{n-1} p_1(t)\, y, \quad y \in C^2(0,\infty),$$

where $' = \mathrm{d}/\mathrm{d}t$. Assume that for some $\alpha < 1$

$$\lim_{R\to\infty}\sup_{l>R} l^{1-\alpha}\int_{2l}^{3l} t^\alpha p_1(t)\,\mathrm{d}t < -\frac{p_0(8+|\alpha+1-n|)^2}{4(1-\alpha)}. \tag{4.19}$$

Then for any constant $q \geqslant 1$ *there is a sequence* $\{\phi_k\} \subset C_0^\infty(0,\infty)$ *and* $\epsilon > 0$ *such that*

$$\left.\begin{aligned} \operatorname{supp}(\phi_k) &\subset [k^q, \infty), \\ (L\phi_k, \phi_k)_{L^2(0,\infty)} &< -\epsilon k^{q(\alpha-1)}. \end{aligned}\right\} \tag{4.20}$$

Proof. Choose $\beta(t) \in C^\infty(-\infty,\infty)$ for which

$$\beta(t) = \begin{cases} 0, & t \leqslant 0, \\ 1, & t \geqslant 1, \end{cases}$$

$\beta(t) \in [0,1]$, and $\beta'(t) \in [0,2]$ for all t. For each $k \geqslant 1$ define

$$\phi_k(t) := t^{(\alpha+1-n)/2} \begin{cases} \beta((t-k^q)/k^q), & t \in [k^q, 2k^q), \\ 1, & t \in [2k^q, 3k^q), \\ \beta((6k^q - t)/3k^q), & t \in [3k^q, 6k^q), \\ 0, & t \notin [k^q, 6k_q]. \end{cases}$$

Note that

$$|\phi_k'(t)| \leqslant \tfrac{1}{2}(|\alpha+1-n|+8)\, t^{(\alpha-1-n)/2}$$

for all t. Therefore,

$$\int_{k^q}^\infty p_0\, t^{n-1}\, |\phi_k'(t)|^2\, \mathrm{d}t \leqslant \frac{p_0(8+|\alpha+1-n|)^2}{4(1-\alpha)} k^{q(\alpha-1)}. \tag{4.21}$$

Since $p_1(t) \leqslant 0$ for t large, then by (4.19) with $l := k^q$ and (4.21), there exists $\epsilon > 0$ such that

$$\begin{aligned} (L\phi_k, \phi_k)_{L^2(0,\infty)} &\leqslant \int_{2k^q}^{3k^q} t^\alpha\, p_1(t)\, \mathrm{d}t + \frac{p_0(8+|\alpha+1-n|)^2}{4(1-\alpha)} k^{q(\alpha-1)} \\ &< -\epsilon k^{q(\alpha-1)} \end{aligned}$$

for k large enough. The conclusion now follows. □

A consequence of Lemma 4.13 is the fact that all solutions of $Ly = 0$ have unbounded zeros on $[1,\infty)$, i.e. all solutions are *oscillatory* at ∞.

Proof of Corollary 4.12. In Theorem 4.7 considered for this case ($m = 2$) we have that

$$V_k(\xi) \leqslant V_{\boldsymbol{a}}^+(|\xi|;\delta), \quad k \geqslant 1.$$

Set $\alpha := \beta + \nu - 1$ and

$$p_1(t) := V_{\boldsymbol{a}}^+(t;\delta).$$

Then (4.19) holds. Recall that $G_{\boldsymbol{a}} = (M_1/2M_2M)/I_\nu$ for $\boldsymbol{a} = \{A_1, A_2\}$. Set $p_0 := M_1/2M_2M$ and $n = \nu$. Now, the hypothesis of Lemma 4.13 holds. To complete the proof we need only use (4.20) to construct the sequence required by (4.13), i.e. set

$$\psi_k(\xi) := \phi_k(|\xi|), \quad k \geqslant 1.$$

Now,

$$\begin{aligned} \int_{\boldsymbol{R}^\nu} [(G_{\boldsymbol{a}} \nabla_\xi \psi_k, \nabla_\xi \psi_k) + V_k(\xi)\, |\psi_k|^2]\, \mathrm{d}\xi &\leqslant \Omega_\nu \int_0^\infty [p_0\, r^{\nu-1} |\phi_{k(r)}'|^2 + r^{\nu-1} p_1(r) |\phi_k(r)|^2]\, \mathrm{d}r \\ &< -\epsilon \Omega_\nu\, k^{q(\beta+\nu-2)} \end{aligned}$$

and, for $\beta\in(-\nu, 2-\nu)$ and some constant $C>0$ independent of k,

$$\|\psi_k\|^2_{L^2(\mathbf{R}^\nu)} \leqslant C^{-1}\Omega_\nu k^{q(\beta+\nu)}.$$

Hence

$$\left(H_a^+\frac{\psi_k}{\|\psi_k\|},\frac{\psi_k}{\|\psi_k\|}\right)+\frac{\epsilon}{kc^{c_0k}} < -\epsilon\left(\frac{C}{k^{2q}}-\frac{1}{k\epsilon^{c_0k}}\right)$$
$$< 0$$

for k large. □

We conclude this section with another corollary to Theorem 4.4, which is concerned with N-body short-range systems. The proof of this result was first given by Yafaev (1972*a*, 1976). The reader may note that Corollary 4.11 also applies to N-body short-range systems.

Corollary 4.14. *Suppose that*

$$\mathscr{M} \subset \bigcup_{\#(a)=2} U_a.$$

If $\mathscr{A}$ *is the set of all 2-cluster decompositions for which* $U_a \subset \mathscr{M}$, *suppose that*

$$(v_{ij})_- \in L^{\nu/2}(\mathbf{R}^\nu), \quad (ij) \not\subset \mathbf{a}\in\mathscr{A}.$$

Then H *has no more than a finite number of bound states.*

Proof. We need to show that (4.6) holds (after the change of variable $(\eta,\xi,0) = T_a x$). It follows from Lemma 4.9 that $|\xi|_{X_a} \geqslant cR$ for some constant c when $(\eta,\xi,0) = T_a \mathbf{x}$ and $x\in\Gamma((U_a)_\delta, R)$. If $(ij)\not\subset \mathbf{a}\in\mathscr{A}$, then by Hölder's inequality and the Sobolev Imbedding Theorem

$$\int_{T_aX}(v_{ij}(\eta,\xi))_-|\phi|^2\,d\xi\,d\eta \leqslant \int_{T_aX^a}\left[\left(\int_{|\xi|\geqslant cR}|(v_{ij})_-|^{\nu/2}\,d\xi\right)^{2/\nu}\left(\int_{|\xi|\geqslant cR}|\phi|^{2\nu/(\nu-2)}\,d\xi\right)^{(\nu-2)/\nu}\right]d\eta$$
$$\leqslant C\int_{T_aX^a}\left[\left(\int_{|\xi|\geqslant cR}|(v_{ij})_-|^{\nu/2}\,d\xi\right)^{2/\nu}\int_{|\xi|\geqslant cR}|\nabla_\xi\phi|^2\,d\xi\right]d\eta$$

for some constant C and all $\phi\in C_0^\infty(T_a(\Gamma((U_a)_\delta,R))$. Hence, we may choose R large enough in order that

$$\int_{T_aX}(v_{ij}(\eta,\xi))_-\,|\phi|^2\,d\xi\,d\eta \leqslant \epsilon\int_{T_aX}(G_a\nabla_\xi\phi,\nabla_\xi\phi)\,d\xi\,d\eta, \quad \phi\in C_0^\infty(T_a(\Gamma((U_a)_\delta,R)).$$

By Hardy's inequality we also have that

$$\epsilon\int_{T_aX}(G_a\nabla_\xi\phi,\nabla_\xi\phi)\,d\xi\,d\eta \geqslant \frac{(\nu-2)^2M_1}{8M_2M}\int_{T_aX}\frac{\epsilon}{|\eta|^2+|\xi|^2}|\phi|^2\,d\xi\,d\eta, \quad \phi\in C_0^\infty(T_aX).$$

Inequality (4.6) now follows for all ϵ sufficiently small. □

5. An application to diatomic systems

In this section we assume that our system is a diatomic molecule consisting of N electrons and two nuclei. The results can easily be extended to the polyatomic case with assumptions similar to those which we make here. For the sake of simplicity, we do not restrict our operator to the symmetry subspace required by the Pauli exclusion principle as should be the case for a complete consideration of a diatomic molecule.

The electrons have mass m and coordinates x^i, $i = 1, \ldots, N$. The two nuclei have coordinates R_1, R_2, masses M_{R_1}, M_{R_2}, and charges Z_1, Z_2, respectively. Therefore, letting $x = (R_1, R_2, x^1, \ldots, x^N)^t \in \tilde{X}$ the hamiltonian before the removal of the centre of mass is given by

$$\tilde{H} := -\sum_{i=1}^{2} \frac{1}{2M_{R_i}} \Delta_{R_i} - \sum_{i=1}^{N} \frac{1}{2m} \Delta_{x^i} - \sum_{i=1}^{N} \left(\frac{Z_1}{|x^i - R_1|} + \frac{Z_2}{|x^i - R_2|} \right) + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x^i - x^j|} + \frac{Z_1 Z_2}{|R_1 - R_2|}. \tag{5.1}$$

As discussed in §2 the motion of centre of mass can be removed by changing variables using a matrix T_X and then restricting $\tilde{H}$ to X to obtain H.

Recent work of Ruskai (1989, 1990, 1991) and Solovej (1990) study the stability of such systems. However, the work of Solovej studies diatomic systems in the Born–Oppenheimer approximation and does not compare directly with the results here. The work of Ruskai does not require this restriction. Earlier fundamental work of Lieb (1984*a*, *b*) considers this problem for atoms and molecules in which the nuclei are assumed to be fixed.

We are interested in finding criteria concerning the relation between N and Z_1, Z_2, which insure either the finiteness or the infiniteness of bound states of H particularly with respect to the breakup of the system into two atomic subsystems. Consequently, we assume that the least point of the essential spectrum $\Sigma(H)$ is determined only by 2-cluster decompositions which separate the nuclei, i.e.

$$\mathscr{M} = \bigcup_{j=1}^{p} U_{\boldsymbol{a}_j} \quad \text{where} \quad \boldsymbol{a}_j = \{A_1^j, A_2^j\}. \tag{5.2}$$

For $i = 1, 2$, the ith nucleus is assumed to be in the cluster $A_i^j, j = 1, \ldots, p$. (We continue to write $l \in A_i^j$ meaning that the electron in position x^l corresponds to the cluster A_i^j.) As a consequence of the HVZ Theorem (Hunziker 1966; van Winter 1964; Zhislin 1960), (5.2) implies that the least point of the spectrum of each $H^{\boldsymbol{a}_j}$ is an isolated eigenvalue.

Theorem 5.1. *Let $\tilde{H}$ be given by* (5.1) *and let H be the resulting operator after the removal of the motion of the centre of mass. Assume* (5.2) *and let $n_i^j := (\#(A_i^j) - 1)$, i.e. the number of electrons associated with the ith nucleus in cluster $A_i^j, j = 1, \ldots, p$ and $i = 1, 2$. If*

$$(Z_1 - n_1^j)(Z_2 - n_2^j) > 0, \quad \text{for} \quad j = 1, \ldots, p, \tag{5.3}$$

then H has no more than a finite number of bound states. Conversely, if H has no more than a finite number of bound states, then

$$(Z_1 - n_1^j)(Z_2 - n_2^j) \geqslant 0 \quad \text{for} \quad j = 1, \ldots, p. \tag{5.4}$$

Proof. The proof follows as a corollary of Corollaries 4.11 and 4.12. Hypothesis $\mathscr{H}$ holds for this system. For each 2-cluster decomposition $\boldsymbol{a}_j, j = 1, \ldots, p$, in (5.2) the matrix $T_{\boldsymbol{a}_j}$ given in Lemmas 4.1 and 4.2 maps $x \mapsto (\eta(1), \eta(2), \xi, 0)^t, x \in \tilde{X}$, where the components of $\eta(i)$, $i = 1, 2$, are $R_i - x^l$ for some $l \in A_i^j$ according to the proof of Lemmas 4.1 and 4.2 given in the Appendix. Here,

$$\xi = (M_1/M)\,(R_1^{a_j}(x) - R_2^{a_j}(x)), \quad \text{for} \quad M_1 = M_{R_1} + n_1^j m \quad \text{and} \quad M = mN + \sum_{i=1}^{2} M_{R_i},$$

where each $R_i^{a_j}(x)$ is the centre of mass of the cluster A_i^j defined in (3.2).

Let $\boldsymbol{a} = \boldsymbol{a}_j$ for some $j = 1, \ldots, p$ which will be suppressed for our subsequent discussion. By Lemma 4.8 for all positive δ sufficiently small we can bound the intercluster interaction as given in (4.15) with

$$\begin{aligned} V_{\boldsymbol{a}}^-(|\xi|) &= V_{\boldsymbol{a}}^-(|\xi|\,;\delta) \\ &= \frac{Z_1 Z_2}{(M/M_1 + C\delta)|\xi|} + \sum_{l \in A_1, k \in A_2} \frac{1}{(M/M_1 + C\delta)|\xi|} \\ &\quad - \sum_{l \in A_2} \frac{Z_1}{(M/M_1 - C\delta)|\xi|} - \sum_{l \in A_1} \frac{Z_2}{(M/M_1 - C\delta)|\xi|} \\ &= \frac{1}{(M/M_1 - C\delta)|\xi|}\left((Z_1 Z_2 + n_1 n_2)\frac{M - CM_1\delta}{M + CM_1\delta} - (n_2 Z_1 + n_1 Z_2)\right) \end{aligned}$$

and $V_{\boldsymbol{a}}^+(|\xi|) = V_{\boldsymbol{a}}^-(|\xi|\,; -\delta)$ where C is a positive constant depending only upon M_{R_1}, M_{R_2}, and m. If (5.3) holds then $V_{\boldsymbol{a}}^-(|\xi|) \geqslant 0$ for all δ sufficiently small. Since this can be done for each 2-cluster $\boldsymbol{a}^j, j = 1, \ldots, p$, then Corollary 4.11 implies that H has no more than a finite number of bound states.

If (5.4) does not hold for some j, then

$$V_{\boldsymbol{a}^j}^+(|\xi|) \leqslant -\epsilon/|\xi|$$

for all δ sufficiently small and some $\epsilon = \epsilon(\delta)$. By choosing $\beta \in [1-\nu, 2-\nu)$ in Corollary 4.12, we can now conclude that H has an infinite number of bound states. □

Vugal'ter & Zhislin (1977) (Theorems 2.5 and 2.6) have shown that the number of bound states of H is finite if one of the 2-clusters A_i^j has a neutral subsystem, i.e. inequality (5.3) is an equality (see also Yafaev 1976; Vugal'ter & Zhislin 1984).

The proof that (5.4) is a necessary condition for finiteness of the bound states of H in the case of 2-cluster breakups also follows from Theorem 1 of Simon (1970). The finiteness criterion of Theorem 5.1 can be shown to follow from Theorem 3.23 in Cycon *et al.* (1987) with a little more work than is required here. (The relationship given by(4.15) is quite helpful in applying Theorem 3.23 in (Cycon *et al.* 1987).)

For homonuclear diatomic systems with $Z = Z_1 = Z_2$ we have by Theorem 5.1 that

$$Z > N \Rightarrow \sigma(H) \cap (-\infty, \Sigma(H)] \quad \text{is finite}$$

provided that (5.2) holds, i.e. provided that the least point of the spectrum of every 2-cluster subsystem is an isolated eigenvalue. Ruskai (1989) has shown that for N sufficiently large

$$Z > 2N \Rightarrow \sigma(H) \cap (-\infty, \Sigma(H)] = \varnothing.$$

It is interesting to compare this with the case of an atomic system $P(Z\!:\!N)$ with N electrons and a nucleus of charge Z. Results of Yafaev (1972*b*, 1976) and Zhislin (1960, 1969, 1971) show that for 2-cluster breakups

$$Z \leqslant N-1 \Leftrightarrow \sigma(P(Z\!:\!N)) \cap (-\infty, \Sigma(P(Z\!:\!N))] \quad \text{is finite}$$

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while Lieb (1984*a*, *b*) has shown that

$$Z < \tfrac{1}{2}(N-1) \Rightarrow \sigma(P(Z:N)) \cap (-\infty, \Sigma(P(Z:N))] = \varnothing.$$

Hence, the results are also related by a factor of 2.

To treat the case in which $Z_2 < N < Z_1$ for asymmetric diatomic molecules Ruskai (1991) has shown that for every fixed pair of values Z_2 and N, there exists a constant $Z_1^c > 0$ for which

$$Z_1 > Z_1^c \Rightarrow \sigma(H) \cap (-\infty, \Sigma(H)] = \varnothing.$$

A key ingredient in the proof is the fact that when Z_1 is sufficiently large

$$U_{\boldsymbol{a}_0} \subset \mathscr{M} \quad \text{for} \quad \boldsymbol{a}_0 = \{A_1, A_2\}$$

when $\#(A_1) = N+1$ and $\#(A_2) = 1$, i.e. all electrons are associated with the nucleus of greater charge implying that $n_1 = N$ and $n_2 = 0$. Note that (5.3) is satisfied in this case. In contrast (5.4) in Theorem 5.1 indicates that if (5.2) holds and $\boldsymbol{a}_0 = \boldsymbol{a}_j$ for some $j \in \{1, \dots, p\}$ then

$$0 < Z_2 \leqslant Z_1 < N \Rightarrow \sigma(H) \cap (-\infty, \Sigma(H)] \quad \text{is infinite.}$$

Also, if it were the case that for some $j \in \{1, \dots, p\}$ given by (5.2)

$$0 < Z_2 < n_2^j \leqslant n_1^j < Z_1, \quad \text{then} \quad \sigma(H) \cap (-\infty, \Sigma(H)] \quad \text{is infinite.}$$

However, it appears that (5.4) should be taken more as an indication of the types of 2-cluster decompositions which constitute (5.2) than as a statement about the infiniteness of bound states of H.

Appendix

(*a*) *The restriction of* $\Delta_{\tilde{X}}$ *to* X

If

$$X := \left\{ x \in \tilde{X} : \sum_{i=1}^{N} m_i x^i = 0 \right\},$$

then

$$X^{\perp} = \{ x \in \tilde{X} : x^1 = x^2 = \dots = x^N \},$$

a ν-dimensional subspace of $\tilde{X}$. To understand the restriction of $\Delta_{\tilde{X}}$ to X it helps to change coordinates. We want a real non-singular matrix $T = (t_{ij} I_\nu)$, $i, j = 1, \dots, N$, such that

$$T \begin{bmatrix} x^1 \\ \vdots \\ \vdots \\ x^N \end{bmatrix} = \begin{bmatrix} y^1 \\ \vdots \\ y^{N-1} \\ 0 \end{bmatrix}, \quad x \in X$$

and

$$T \begin{bmatrix} x^1 \\ \vdots \\ \vdots \\ x^N \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ y^N \end{bmatrix}, \quad x \in X^{\perp}.$$

This requires the sum of the elements in the first $N-1$ rows to be 0, i.e. $\Sigma_{j=1}^N t_{ij} = 0$, $i = 1, \dots, N-1$. For the last row choose $t_{Nj} = m_j / M$, $j = 1, \dots, N$.

Now, look at the transformation of $\Delta_{\tilde{X}}$ under T. For $G := \mathrm{diag}(2m_1 I_\nu, \ldots, 2m_N I_\nu)$ and $\phi, \psi \in C_0^\infty(\tilde{X})$

$$\int_{\tilde{X}} -\Delta_{\tilde{X}} \phi \bar{\psi} \, \mathrm{d}_{\tilde{X}} x = \int_{\tilde{X}} (G^{-1} \nabla_x \phi, \nabla_x \psi)_{\mathbf{R}^{\nu N}} \, \mathrm{d}_{\tilde{X}} x$$
$$= \int_{\tilde{X}} (T G^{-1} T^t \nabla_y \phi, \nabla_y \psi)_{\mathbf{R}^{\nu N}} \, \mathrm{d}_{\tilde{X}} y,$$

where $\mathrm{d}_{\tilde{X}} x := \det(G^{\frac{1}{2}}) \, \mathrm{d}x^1 \ldots \mathrm{d}x^N$, $\mathrm{d}_{\tilde{X}} y := \det(G^{\frac{1}{2}}) \det(T^{-1}) \, \mathrm{d}y^1 \ldots \mathrm{d}y^N$. Note the form of

$$T G^{-1} T^t = \begin{pmatrix} G_X & 0 \\ 0 & (1/2M) I_\nu \end{pmatrix},$$

where G_X is an $(N-1)\nu \times (N-1)\nu$ non-singular, positive definite matrix. Clearly,

$$(\det T)^2 \det(G^{-1}) = (2M)^{-\nu} \det(G_X),$$

whence

$$(\det(G^{\frac{1}{2}}) \det(T^{-1}))^2 = (2M)^\nu \det(G_X^{-1})$$

indicating that

$$\mathrm{d}_{\tilde{X}} y = \sqrt{\det(G_X^{-1})} \, \mathrm{d}y^1 \ldots \mathrm{d}y^{N-1} (2M)^{\nu/2} \, \mathrm{d}y^N$$
$$= \mathrm{d}_X \eta \, \mathrm{d}_{X^\perp} R$$

for

$$(\eta, 0) := (y^1, \ldots, y^{N-1}, 0) \in X;$$
$$(0, R) := (0, \ldots, 0, y^N) \in X^\perp;$$
$$\mathrm{d}_X \eta := \sqrt{\det(G_X^{-1})} \, \mathrm{d}y^1 \ldots \mathrm{d}y^{N-1};$$

and

$$\mathrm{d}_{X^\perp} R := (2M)^{\frac{1}{2}} \mathrm{d}y^N.$$

For $\phi, \psi \in C_0^\infty(\tilde{X})$

$$\int_{\tilde{X}} -\Delta_{\tilde{X}} \phi \bar{\psi} \, \mathrm{d}_{\tilde{X}} x = \int_{\tilde{X}} (G^{-1} \nabla_x \phi, \nabla_x \psi)_{\mathbf{R}^{\nu N}} \, \mathrm{d}_{\tilde{X}} x$$
$$= \int_{\tilde{X}} (T G^{-1} T^t \nabla_y \phi, \nabla_y \psi)_{\mathbf{R}^{\nu N}} \, \mathrm{d}_{\tilde{X}} y$$
$$= \int_{X^\perp} \int_X (G_X \nabla_\eta \phi, \nabla_\eta \psi)_{\mathbf{R}^{\nu(N-1)}} \, \mathrm{d}_X \eta \, d_{X^\perp} R$$
$$+ \frac{1}{2M} \int_{X^\perp} \int_X (\nabla_R \phi, \nabla_R \psi)_{\mathbf{R}^\nu} \, \mathrm{d}_X \eta \, \mathrm{d}_{X^\perp}$$
$$= \int_{X^\perp} \int_X -\mathrm{div}_\nu (G_X \nabla_\eta \phi) \bar{\psi} \, \mathrm{d}_X \eta \, \mathrm{d}_{X^\perp} R$$
$$+ \int_X \int_{X^\perp} -\frac{1}{2M} \Delta_R \phi \bar{\phi} \, \mathrm{d}_{X^\perp} R \, \mathrm{d}_X \eta$$

indicating that

$$\Delta_X = \mathrm{div}_\nu (G_X \nabla_\eta)$$

and that $\Delta_{\tilde{X}}$ splits into a tensor product:

$$\Delta_{\tilde{X}} = \Delta_X \otimes I_{L^2(\boldsymbol{R}^\nu)} + I_{L^2(\boldsymbol{R}^{\nu(N-1)})} \otimes (1/2M)\,\Delta_R.$$

If $\eta_x + R_x = Tx$ and $\eta_y + R_y = Ty$ for $x, y \in \tilde{X}$, $\eta_x, \eta_y \in X$, and $R_x, R_y \in X^\perp$, then it is not hard to show that

$$\langle x, y\rangle_{\tilde{X}} = (G_X^{-1}\eta_x, \eta_y)_{\boldsymbol{R}^{\nu(n-1)}} + 2M(R_x, R_y)_{\boldsymbol{R}^\nu}.$$

Consequently, for $x, y \in X$

$$\langle x, y\rangle_X = (G_X^{-1}\eta_x, \eta_y)_{\boldsymbol{R}^{\nu(N-1)}}.$$

To illustrate the transformation above in one set of coordinates, we recall the classical Jacobi transformation $J : x \mapsto \tilde{\xi}, x \in \times_{i=1}^N \boldsymbol{R}^\nu$, defined by

$$\xi^j := x^{j+1} - \frac{1}{M_j}\sum_{i=1}^{j} m_i x^i, \quad j = 1, \dots, N-1,$$

with

$$\xi^N = \frac{1}{M_n}\sum_{i=1}^{N} m_i x^i$$

and $M_j = \Sigma_{i=1}^j m_i, j = 1, \dots, N$ (see Reed & Simon 1979). Then, $\xi^N \equiv 0$ in X and

$$\Delta_X = \sum_{i=1}^{N-1} \frac{1}{2\mu_i}\Delta_{\xi^i} \quad \text{for} \quad \mu_i^{-1} := m_{i+1}^{-1} + M_i^{-1}.$$

Proof of Lemma 3.1. Parts (i) and (ii) follow directly from the definitions of X, $X^\perp$, X_a, and the Π_{ij}s.

Let R_i^a be given by (3.2). To show (iii), first note that each $\Pi_{ij} : \tilde{X} \to X$. Moreover, if $i, j \in A_k$ for some k, then R_k^a (Range $(\Pi_{ij})) = \{0\}$ by the definition of Π_{ij}. In fact, R_l^a (Range $(\Pi_{ij})) = \{0\}$ when $l \neq k$ since the A_ks are disjoint and all components of $x \in$ Range (Π_{ij}) are zero except for the ith and jth components. Since the R_k^as are linear operators, then

$$\operatorname{span}\left\{\bigcup_{(ij)\subset a} \operatorname{Range}(\Pi_{ij})\right\} \subset X^a.$$

The definitions of the Π_{ij}s and the disjointness of the A_ks give the fact that

$$X_{A_1}^a \oplus \dots \oplus X_{A_m}^a = \operatorname{span}\left\{\bigcup_{(ij)\subset a} \operatorname{Range}(\Pi_{ij})\right\}.$$

Viewing X^a as the set of solutions to a system of m equations in N unknowns, it is clear that the dimension of X^a is $(N-m)\nu$. The definition of the Π_{ij}s shows that the dimension of $X_{A_k}^a$ is $(\#(A_k)-1)\nu$ for $k = 1, \dots, m$. Hence,

$$\dim(X_{A_1}^a \oplus \dots \oplus X_{A_m}^a) = \sum_{k=1}^{m} (\#(A_k)-1)\nu = (N-m)\nu$$

finishing the proof of (iii) and (iv). □

Proof of Lemmas 4.1 *and* 4.2. We prove these lemmas by constructing such a matrix. It will be obvious from our construction that the matrix which we give is not unique.

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Example: clustered coordinates. Given an m-cluster $\boldsymbol{a} = \{A_1, \ldots, A_m\}$, it is convenient to enumerate the A_ks defining $\boldsymbol{a}$ in order that $\#(A_1) \geqslant \#(A_2) \geqslant \ldots \geqslant \#(A_m)$. Furthermore, let the elements of each $A_k \in \boldsymbol{a}$ be arranged in ascending order, say

$$A_k = \{a_1^k, \ldots, a_{n(k)}^k\} \quad \text{with} \quad a_1^k < \ldots < a_{n(k)}^k, \quad \text{and} \quad n(k) := \#(A_k). \tag{A 1}$$

Define the first $N-m$ rows of a $\nu N \times \nu N$ block matrix $\tilde{T}_{\boldsymbol{a}}$ consisting of $\nu \times \nu$ blocks as follows.

Row 1 of $\tilde{T}_{\boldsymbol{a}}$ has I_ν in the position a_1^1; $-I_\nu$ in position a_2^1; and zeros elsewhere.

Row 2 of $\tilde{T}_{\boldsymbol{a}}$ has I_ν in the position a_1^1; $-I_\nu$ in position a_3^1; and zeros elsewhere...

Row $n(1)-1$ of $\tilde{T}_{\boldsymbol{a}}$ has I_ν in the position a_1^1; $-I_\nu$ in the position $a_{n(1)}^1$; and zeros elsewhere.

Row $n(1)$ of $\tilde{T}_{\boldsymbol{a}}$ has I_ν in the position a_1^2; $-I_\nu$ in position a_2^2; and zeros elsewhere...

This process is continued until the elements of A_2 are exhausted...

This process is continued for each A_k with $\#(A_k) \geqslant 2$.

In this manner we construct the first $(N-m)\nu$ linearly independent rows of $\tilde{T}_{\boldsymbol{a}}$ corresponding to all $A_k \in \boldsymbol{a}$ with two or more elements. The last m rows of $\tilde{T}_{\boldsymbol{a}}$ consist of $\nu \times \nu$ blocks given as follows.

Row $N-m+1$ has $(m_k/M_1) I_\nu$ in position $k = a_i^1 \in A_1, i = 1, \ldots, n(1)$ and zeros elsewhere.

Row N has $(m_k/M_m) I_\nu$ in position $k = a_i^m \in A_m, i = 1, \ldots, n(m)$ and zeros elsewhere.

Recall that $M_i := \Sigma_{j \in A_i} m_j$. When multiplied by $x \in \tilde{X}$, these rows will give the location of the centres of mass of the different clusters. However, the centre of mass of the entire system has not been separated, which is a requirement for the matrix $T_{\boldsymbol{a}}$.

Notice that the last m rows of $\tilde{T}_{\boldsymbol{a}}$ are mutually orthogonal. Analogous to part (*b*), we have that

$$\tilde{T}_{\boldsymbol{a}} G^{-1} \tilde{T}_{\boldsymbol{a}}^t = \begin{bmatrix} G_1^{\boldsymbol{a}} & 0 & \cdots & & 0 \\ 0 & G_2^{\boldsymbol{a}} & \cdots & & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & \cdots & G_m^{\boldsymbol{a}} \cdots & 0 \\ 0 & 0 & \cdots & G_{\boldsymbol{a}}^1 & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & & G_{\boldsymbol{a}}^m \end{bmatrix}$$

partly because the last m rows of $\tilde{T}_{\boldsymbol{a}} G^{-\frac{1}{2}}$ are orthogonal to its first $N-m$ rows. If we perform elementary row operations on these last m rows, say $E\tilde{T}_{\boldsymbol{a}} G^{-\frac{1}{2}}$ for some elementary matrix E, each of the last m rows of the resulting matrix $E\tilde{T}_{\boldsymbol{a}} G^{-\frac{1}{2}}$ will still be a linear combination of the original m rows maintaining this orthogonality property.

Define elementary matrices $E_i, i = 1, 2, 3, 4$, as follows:

$$E_1 := \begin{bmatrix} I_{(N-m)\nu} & 0 & \cdots & 0 & 0 \\ 0 & (M_1/M) I_\nu & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & & (M_{m-1}/M) I_\nu & \vdots \\ 0 & 0 & \cdots & \cdots & I_\nu \end{bmatrix},$$

$$E_2 := \begin{bmatrix} I_{(N-m)\nu} & 0 & \cdots & 0 & 0 \\ 0 & I_\nu & \cdots & 0 & -\beta_1(M_m/M)\,I_\nu \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & & I_\nu & -\beta_{m-1}(M_m/M)\,I_\nu \\ 0 & 0 & \cdots & \cdots & I_\nu \end{bmatrix},$$

where the $\beta_i, i = 1, \ldots, m-1$ are to be determined below,

$$E_3 := \begin{bmatrix} I_{(N-M)\nu} & 0 & \cdots & 0 & & 0 \\ 0 & I_\nu & \cdots & 0 & & 0 \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ \vdots & \vdots & & I_\nu & & 0 \\ 0 & 0 & \cdots & \cdots & (M_m/M) & (1+\Sigma_{i=1}^{m-1}\beta_i)I_\nu \end{bmatrix},$$

and

$$E_4 := \begin{bmatrix} I_{(N-m)\nu} & 0 & \cdots & 0 & 0 \\ 0 & I_\nu & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & & I_\nu & 0 \\ 0 & I_\nu & \cdots & \cdots & I_\nu \end{bmatrix}.$$

Let $E := E_4 E_3 E_2 E_1$. Finally, we define

$$T_a := E\tilde{T}_a.$$

Notice that for any choice of the β_is

$$\mathrm{Row}_N(T_a) = ((m_1/M)\,I_\nu, \ldots, (m_N/M)\,I_\nu)$$

corresponding to the location of the centre of mass of the entire system. For $j = 1, \ldots, m-1$, $\mathrm{Row}_{N-m+j}(T_a)$ has $(m_k/M)\,I_\nu$ in column $k = a_i^j \in A_j$, $i = 1, \ldots, n(j)$; $-\beta_j(m_k/M)\,I_\nu$ in column $k = a_i^m \in A_m$, $i = 1, \ldots, n(m)$; and zeros elsewhere. By defining

$$\beta_j := M_j/M_m, \quad j = 1, \ldots, m-1.$$

the first $m-1$ elements of the last row of $T_a G^{-1} T_a^t$ are given by

$$(\mathrm{Row}_{N-m+j}(T_a)\,G^{-\frac{1}{2}}) \cdot (Row_N(T_a)\,G^{-\frac{1}{2}}) = \sum_{k\in A_j}\left(\frac{m_k}{\surd(2m_k)M}\right)^2 - \beta_j \sum_{k\in A_m}\left(\frac{m_k}{\surd(2m_k)M}\right)^2 = 0,$$

$j = 1, \ldots, m-1$, which is required by part (b). Then, for $i, j = 1, \ldots, m-1$,

$$(G_a)_{ij} = (\mathrm{Row}_{N-m+i}(T_a)\,G^{-\frac{1}{2}}) \cdot (\mathrm{Row}_{N-m+j}(T_a)\,G^{-\frac{1}{2}}) = \begin{cases} (1/2M^2)\,M_i(M_i+M_m)/M_m, & \text{for} \quad i = j, \\ (1/2M^2)\,M_i M_j/M_m, & \text{for} \quad i \neq j. \end{cases}$$

Therefore, the matrix

$$G_a = \frac{1}{2M_m M^2}\begin{bmatrix} M_1(M_1+M_m)\,I_\nu & M_1 M_2 I_\nu & \cdots & M_1 M_{m-1} I_\nu \\ M_2 M_1 I_\nu & M_2(M_2+M_m)\,I_\nu & \cdots & M_2 M_{m-1} I_\nu \\ \vdots & \vdots & \ddots & \vdots \\ M_{m-1} M_1 I_\nu & M_{m-1} M_2 I_\nu & \cdots & M_{m-1}(M_{m-1}+M_m)\,I_\nu \end{bmatrix}.$$

Finally, we have for any $x = (x^1, \ldots, x^N) \in \tilde{X}$

$$T_a x = \begin{bmatrix} x^{a_1^1} - x^{a_2^1} \\ \vdots \\ x^{a_1^1} - x^{a_{n(1)}^1} \\ \vdots \\ \vdots \\ x^{a_1^{m'}} - x^{a_2^{m'}} \\ \\ \vdots \\ x^{a_1^{m'}} - x^{a_{n(m')}^{m'}} \\ (M_1/M)\,(R_1^a(x) - R_m^a(x)) \\ \vdots \\ (M_{m-1}/M)\,(R_{m-1}^a(x) - R_m^a(x)) \\ (1/M)\,\sum_{i=1}^N m_i x^i \end{bmatrix}.$$

The conclusions of Lemmas 4.1 and 4.2 follow from the construction above and from Lemma 3.1. □

Proof of Proposition 4.5. Part (i) follows directly from Theorem 4.9 of Agmon (1982) by setting $\epsilon = \frac{1}{2}$ and noting that $\rho(x) \geqslant 2c_0 |x|$.

From (1.1)(ii) and (4.8) we can conclude that $q \in M(\boldsymbol{R}^n)$. Therefore by Lemma 0.3 of Agmon (1982), for every $\epsilon > 0$ there is a positive constant C_ϵ such that

$$\int_{\boldsymbol{R}^n} |q||\phi|^2 \,\mathrm{d}x \leqslant \epsilon \int_{\boldsymbol{R}^n} |\nabla\phi|^2 \,\mathrm{d}x + C_\epsilon \int_{\boldsymbol{R}^n} |\phi|^2 \,\mathrm{d}x \tag{A 2}$$

for all $\phi \in C_0^\infty(\boldsymbol{R}^n)$. Recall that the sesquilinear form τ giving rise to P is the closure, $\tilde{\tau}$, of

$$\tau[\phi, \psi] := \int_{\boldsymbol{R}^n} [(A\nabla\phi, \psi) + q\phi\bar{\psi}] \,\mathrm{d}x$$

on $C_0^\infty(\boldsymbol{R}^n) \times C_0^\infty(\boldsymbol{R}^n)$. Since $C_0^\infty(\boldsymbol{R}^n)$ is dense in the domain $\mathscr{D}(\tilde{\tau})$ of $\tilde{\tau}$ we can conclude from (A 2) that $\psi \in H^1(\boldsymbol{R}^n)$ and $|q|^{\frac{1}{2}}\psi \in L^2(\boldsymbol{R}^n)$; in fact (A 2) insures that the τ-norm is equivalent to the $H^1(\boldsymbol{R}^n)$-norm on $C_0^\infty(\boldsymbol{R}^n)$ and hence, $\mathscr{D}(\tilde{\tau}) = H^1(\boldsymbol{R}^n)$. Moreover, there is a sequence $\{\phi_m\} \subset C_0^\infty(\boldsymbol{R}^n)$ such that

$$\left.\begin{aligned} \phi_m &\to_{\tilde{\tau}} \psi, \\ \phi_m &\longrightarrow \psi, \quad \text{in} \quad H^1(\boldsymbol{R}^n), \\ |q|^{\frac{1}{2}}\phi_m &\longrightarrow |q|^{\frac{1}{2}}\psi, \quad \text{in} \quad L^2(\boldsymbol{R}^n), \end{aligned}\right\} \tag{A 3}$$

as $m \to \infty$. (The first condition in (A 3) requires $\tilde{\tau}$-convergence defined on p. 313 of Kato (1984).) Set

$$\eta = \eta(x) = \mathrm{e}^{c_0|x|}.$$

From (i) we have $\eta\psi \in L^2(\boldsymbol{R}^n)$.

For each positive integer k choose $\alpha_k \in C_0^\infty(\boldsymbol{R}^n)$ with

$$\alpha_k(x) := \begin{cases} 1 & \text{for} \quad |x| \leqslant k, \\ 0 & \text{for} \quad |x| \geqslant 2k, \end{cases}$$

and

$$|\alpha_k(x)|, |\nabla \alpha_k(x)| \leqslant 1 \quad x \in \boldsymbol{R}^n. \tag{A 4}$$

Consequently, for $\{\phi_m\} \subset C_0^\infty(\boldsymbol{R}^n)$ given in (A 3)

$$\tau[\phi_m, \alpha_k^2 \eta \phi_m] = \int_{\boldsymbol{R}^n} (A\nabla\phi_m, \nabla \alpha_k^2 \eta \phi_m)\,\mathrm{d}x + \int_{\boldsymbol{R}^n} q(x)\,\alpha_k^2\,\eta\,|\phi_m|^2\,\mathrm{d}x$$
$$:= I_1 + I_2. \tag{A 5}$$

Let $\lambda_1(A) :=$ minimum eigenvalue of A and $\lambda_n(A) :=$ maximum eigenvalue of A. Let $B(k) := \{x \in \boldsymbol{R}^n : |x| < k\}$. Now,

$$I_1 = \int_{\boldsymbol{R}^n} [\alpha_k^2\,\eta(A\nabla\phi_m, \nabla\phi_m) + 2\alpha_k\,\eta\overline{\phi_m}(A\nabla\phi_m, \nabla\alpha_k) + \alpha_k^2\,\overline{\phi_m}(A\nabla\phi_m, \nabla\eta)]\,\mathrm{d}x$$

from which we obtain the inequality

$$I_1 \geqslant \lambda_1(A) \int_{\boldsymbol{R}^n} \alpha_k^2\,\eta\,|\nabla\phi_m|^2\,\mathrm{d}x - c_1 \left\{ \int_{B(2k)} |\nabla\phi_m|^2\,\mathrm{d}x + \int_{B(2k)} \eta^2\,|\phi_m|^2\,\mathrm{d}x \right\} \tag{A 6}$$

for some constant $c_1 > 0$ depending on $\lambda_n(A)$ and c_0. By (A 2) for any $\epsilon > 0$ there exists a constant $c(\epsilon) > 0$ such that

$$|I_2| \leqslant \epsilon \int_{\boldsymbol{R}^n} |\nabla(\alpha_k\,\eta^{\frac{1}{2}}\phi_m)|^2\,\mathrm{d}x + c(\epsilon) \int_{B(2k)} \eta\,|\phi_m|^2\,\mathrm{d}x.$$

Therefore, we have for any $\epsilon > 0$

$$I_2 \geqslant -\epsilon \int_{\boldsymbol{R}^n} \alpha_k^2\,\eta\,|\nabla\phi_m|^2\,\mathrm{d}x - c'(\epsilon) \int_{B(2k)} \eta^2\,|\phi_m|^2\,\mathrm{d}x. \tag{A 7}$$

Here the constant $c'(\epsilon) > 0$ depends only on ϵ and c_0.

It follows from (A 5), (A 6), and (A 7) that for any $\epsilon > 0$ there are positive constants $C = C(\epsilon, c_0, \lambda_n(A))$ and $c_1 = c_1(\lambda_n(A), c_0)$ such that

$$\tau[\phi_m, \alpha_k^2\,\eta\phi_m] \geqslant (\lambda_1(A) - \epsilon) \int_{\boldsymbol{R}^n} \alpha_k^2\,\eta\,|\nabla\phi_m|^2\,\mathrm{d}x - c_1 \int_{B(2k)} |\nabla\phi_m|^2\,\mathrm{d}x - C \int_{B(2k)} \eta^2\,|\phi_m|^2\,\mathrm{d}x. \tag{A 8}$$

Letting $m \to \infty$ in (A 8) it follows from (A 3) and Theorem VI-1.17 of Kato (1984) that

$$(\lambda_1(A) - \epsilon) \int_{\boldsymbol{R}^n} \alpha_k^2\,\eta\,|\nabla\psi|^2\,\mathrm{d}x \leqslant \mu(\psi, \alpha_k^2\,\eta\psi)_{L^2(\boldsymbol{R}^n)} + c_1 \int_{B(2k)} |\nabla\psi|^2\,\mathrm{d}x + C \int_{B(2k)} \eta^2\,|\psi|^2\,\mathrm{d}x$$

for any k. Therefore for ϵ sufficiently small

$$(\lambda_1(A) - \epsilon) \int_{B(k)} \eta\,|\nabla\psi|^2\,\mathrm{d}x \quad \leqslant c_1 \int_{B(2k)} |\nabla\psi|^2\,\mathrm{d}x + (C + |\mu|) \int_{B(2k)} \eta^2\,|\psi|^2\,\mathrm{d}x.$$

The proof of (ii) follows by letting $k \to \infty$ and using part (i). □

Proof of Corollary 4.6. Let $\beta = \beta(r) \in C^{\infty}[0, \infty)$ satisfy

$$\beta(r) = \begin{cases} 1 & \text{for} \quad r \in [0, 1], \\ 0 & \text{for} \quad r \geqslant \tfrac{3}{2}, \end{cases}$$

and $\beta(r) \in [0, 1]$ for all r. Define

$$\alpha_k(x) := \beta(|x|/k), \quad x \in \boldsymbol{R}^n,$$

for positive integers $k \geqslant 1$. Choose an integer K_0 large enough to insure that

$$c_k := \|\alpha_k \psi\| \geqslant \tfrac{1}{2} \quad \text{for all} \quad k \geqslant K_0.$$

Therefore, for all $k \geqslant K_0$ the sequence

$$\psi_k := \alpha_k \psi / \|\alpha_k \psi\|_{L^2(\boldsymbol{R}_n)}$$

is well defined and has the following properties:

$$\left.\begin{aligned} \|\psi_k\|_{L^2(\boldsymbol{R}^n)} &= 1, \\ \psi_k \in H^1(\boldsymbol{R}^n), &\quad \text{and} \\ \operatorname{supp}(\psi_k) \subset \{x \in \boldsymbol{R}^n &: |x| \leqslant \tfrac{3}{2}k\}. \end{aligned}\right\} \tag{A 9}$$

Recall that for real numbers a^{ij} the matrix $A = (a^{ij})$ is symmetric and positive definite. We have that

$$A^{\frac{1}{2}} \nabla \psi_k(x) = c_k^{-1} A^{\frac{1}{2}} (\alpha_k(x) \nabla \psi(x) + \psi(x) k^{-1} \beta'(|x|/k)\, x/|x|), \quad k \geqslant K_0,$$

implying that there is a constant C' independent of k such that

$$(A \nabla \psi_k, \nabla \psi_k)_{L^2(\boldsymbol{R}^n)} \leqslant c_k^{-2} (A \alpha_k \nabla \psi, \alpha_k \nabla \psi)_{L^2(\boldsymbol{R}^n)} + \frac{C'}{k} \int_{k \leqslant |x| \leqslant 3k/2} (|\psi(x)|^2 + |\nabla \psi(x)|^2)\, dx \tag{A 10}$$

since $B'(r)$ vanishes for $r \notin (1, \frac{3}{2})$. Therefore,

$$\tilde{\tau}[\psi_k] \leqslant \frac{1}{c_k^2} \int_{\boldsymbol{R}^n} [(A \nabla \psi, \alpha_k^2 \nabla \psi) + q(x)\, \psi \overline{\alpha_k^2 \psi}]\, dx + \frac{C'}{k} \int_{k \leqslant |x| \leqslant 3k/2} (|\psi(x)|^2 + |\nabla \psi(x)|^2)\, dx. \tag{A 11}$$

Since

$$\alpha_k^2 \nabla \psi = \nabla(\alpha_k^2 \psi) - \psi \nabla(\alpha_k^2),$$

then for $|A| = \max\{(A\xi, \xi) : |\xi| = 1\}$

$$\begin{aligned} c_k^{-2}(A \nabla \psi, \alpha_k^2 \nabla \psi)_{L^2(\boldsymbol{R}^n)} &\leqslant (A \nabla \psi, \nabla(\alpha_k^2/c_k^2)\, \psi)_{L^2(\boldsymbol{R}^n)} \\ &\quad + |A| \frac{2}{k} \int_{k \leqslant |x| \leqslant 3k/2} B'(|x|/k)\, |\nabla \psi\, \|\psi|\, dx \\ &\leqslant (A \nabla \psi, \nabla(\alpha_k^2/c_k^2)\, \psi)_{L^2(\boldsymbol{R}^n)} \\ &\quad + \frac{C'}{k} \int_{k \leqslant |x| \leqslant 3k/2} (|\psi(x)|^2 + |\nabla \psi(x)|^2)\, dx, \end{aligned}$$

where we may assume that C' is the same as given in (A 10). Substituting this inequality into (A 11) we obtain

$$\begin{aligned}\tilde{\tau}[\psi_k] &\leqslant \tilde{\tau}[\psi, (\alpha_k^2/c_k^2)\,\psi] + \frac{2C'}{k}\int_{k\leqslant|x|\leqslant 3k/2} (|\psi(x)|^2 + |\nabla\psi(x)|^2)\,\mathrm{d}x \\ &\leqslant \mu(\psi, (\alpha_k^2/c_k^2)\,\psi)_{L^2(\boldsymbol{R}^n)} + \frac{2C'}{k\mathrm{e}^{c_0 k}}\int_{k\leqslant|x|\leqslant 3k/2} \mathrm{e}^{c_0|x|}(|\psi(x)|^2 + |\nabla\psi(x)|^2)\,\mathrm{d}x \\ &\leqslant \mu + \frac{2C'}{k\mathrm{e}^{c_0 k}}\int_{|x|\geqslant k} \mathrm{e}^{c_0|x|}(|\psi(x)|^2 + |\nabla\psi(x)|^2)\,\mathrm{d}x.\end{aligned}$$

To conclude the proof we use the fact that $C_0^\infty(\boldsymbol{R}^n)$ is dense in the domain $\mathscr{D}(\tilde{\tau})$. This implies that for each ψ_k there is a sequence $\{\theta_l^k\}_{l=1}^\infty \subset C_0^\infty(\boldsymbol{R}^n)$ converging to ψ_k in $L^2(\boldsymbol{R}^n)$ for which $\tau[\theta_l^k] \to \tilde{\tau}[\psi_k]$ as $l\to\infty$. Since $\|\psi_k\|_{L^2(\boldsymbol{R}^n)} = 1$, then $\|\theta_l^k\|_{L^2(\boldsymbol{R}^n)} \to 1$ as $l\to\infty$. Since $\operatorname{supp}(\psi_k) \subset \{x\in\boldsymbol{R}^n : |x| \leqslant \frac{3}{2}k\}$, then we may choose the θ_l^ks with support in $\{x\in\boldsymbol{R}^n : |x| \leqslant 2k\}$. If we normalize the θ_l^ks in $L^2(\boldsymbol{R}^n)$, then

$$|\tau[\theta_l^k/\|\theta_l^k\|] - \tilde{\tau}[\psi_k]| \leqslant |\tau[\theta_l^k] - \tilde{\tau}[\psi_k]| + |\tau[\theta_l^k]|\,|1/\|\theta_l^k\|^2 - 1| \to 0 \quad \text{as} \quad l\to\infty.$$

Now for each $k \geqslant K_0$ choose $\phi_k := \theta_{l_0}^k/\|\theta_{l_0}^k\|$ for l_0 chosen sufficiently large in order that

$$|\tilde{\tau}[\psi_k] - \tau[\phi_k]| \leqslant \frac{C'}{k\,\mathrm{e}^{c_0 k}}\int_{|x|\geqslant k} \mathrm{e}^{c_0|x|}(|\psi(x)|^2 + |\nabla\psi(x)|^2)\,\mathrm{d}x.$$

Hence, the sequence $\{\phi_k\}$ satisfies the requirements of the conclusion with $C := 3C'$. □

Proof of Lemma 4.8. We first need a lemma. Let $A_{k(i)}$ be the cluster containing i. The inner products $(\cdot,\cdot)$ in the next lemma are euclidean inner products of appropriate dimension.

Lemma A 1. *If* $(ij) \not\subset \boldsymbol{a} = \{A_1, \ldots, A_m\}$, *then for* $i\in A_{k(i)}$ *and* $j\in A_{k(j)}$

$$\begin{aligned}x^i - x^j &= R^{\boldsymbol{a}}_{k(i)}(x) - R^{\boldsymbol{a}}_{k(j)}(x) + (c(k(i)), \eta(k(i))) + (c(k(j)), \eta(k(j))) \\ &= (M/M_{k(i)})\,\xi^{k(i)} - (M/M_{k(j)})\,\xi^{k(j)} + (c(k(i)), \eta(k(i))) + (c(k(j)), \eta(k(j)))\end{aligned}$$

for $\xi^m := 0$, $\eta(k)$ *defined in Lemma* 4.1c, *and* $(n(k)-1)\nu$*-dimensional vectors* $c(k)$, $n(k) := \#(A_k)$, *which depend only on* $m_1, \ldots, m_N$.

Proof. Using the notation scheme in (A 1) (in the proofs of Lemmas 4.1 and 4.2) the corollary follows from the fact that

$$x^{a_1^k} = R^{\boldsymbol{a}}_k(x) + \frac{1}{M_k}\sum_{l\in A_k\backslash\{a_1^k\}} m_l(x^{a_1^k} - x^l).$$ □

Since $\boldsymbol{a}$ is a 2-cluster decomposition in this lemma, then by Lemma 4.1, $\xi = \xi_1 \in \boldsymbol{R}^\nu$. Then for $(ij) \not\subset \boldsymbol{A}$ there is some constant C depending only upon $m_1, \ldots, m_N$ such that

$$|\,|x^i - x^j| - (M/M_1)\,|\xi|\,|_{\boldsymbol{R}^\nu} \leqslant C\delta\,|\xi|$$

by Lemma A 1 and Lemma 4.9. The proof of Lemma 4.8 now follows from $\mathscr{H}$. □

Proof of Lemma 4.9. We may assume that $m < N$. Otherwise, $X_a = X$. We choose some $x\in\Gamma((U_a)_\delta, 1)$ and set $y := T_a x$ with $y = (\eta, \xi)^t$ and the zero suppressed throughout the proof. Then there is some $\omega \in U_a$ such that

$$|x/|x|_X - \omega|_X < \delta.$$

Set $x' := |x|_X \, \omega$, $y' := T_a x'$, and

$$y' = \begin{pmatrix} \eta' \\ \xi' \end{pmatrix}.$$

Therefore, $|T_a^{-1}(y-y')|_X < \delta |x|_X$ from which we can conclude that

$$\begin{aligned} |y-y'|_X &= |T_a T_a^{-1}(y-y')|_X \\ &\leqslant \|T_a\| \, |T_a^{-1}(y-y')|_X \\ &\leqslant \delta \, \|T_a\| \, |x|_X. \end{aligned} \tag{A 12}$$

By Lemma 3.1 (ii), $x' \in X_a$ and by Lemma 4.1 *d*, $\eta' = 0$. Therefore, by (A 12),

$$\delta^2 \, \|T_a\|^2 \, |x|_X^2 \geqslant \left| \begin{pmatrix} \eta \\ 0 \end{pmatrix} \oplus \left(\begin{pmatrix} 0 \\ \xi \end{pmatrix} - \begin{pmatrix} 0 \\ \xi' \end{pmatrix} \right) \right|_X^2 \geqslant |\eta|_X^2.$$

Since $|x|_X^2 \leqslant \|T_a^{-1}\|^2 (|\eta|_X^2 + |\xi|_X^2)$ and $\|T_a^{-1}\| = \|T_a\|^{-1}$, then

$$\delta^2 (|\eta|_X^2 + |\xi|_X^2) \geqslant |\eta|_X^2.$$

Hence,

$$|\eta|_X \leqslant \delta(1-\delta^2)^{-\frac{1}{2}} |\xi|_X < 2\delta \, |\xi|_X$$

for δ sufficiently small. □

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