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Geometric Methods in the Quantum Many-Body Problem. Nonexistence of Very Negative Ions*

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Abstract. In this paper we develop the geometric methods in the spectral theory of many-body Schrödinger operators. We give different simplified proofs of many of the basic results of the theory. We prove that there are no very negative ions in Quantum Mechanics.

0. Introduction

In this paper we develop geometric methods for studying the spectral properties of the many-body Schrödinger operators. The adjective “geometric” refers to the basic role played by the analysis of the space configurations of a many-body system in question. To translate this geometry into the quantum-mechanical language, one uses partitions of unity on the state space, L^2 (configuration space). This approach commands a remarkable flexibility. As with trial functions in the variational principle, one can vary and optimize the partitions of unity depending on a problem at hand. This will be demonstrated in the present paper. Moreover, the method is naturally generalizable to operators on manifolds.

The basic property of the Schrödinger operators which permits such an analysis is their locality. Nevertheless, it is remarkable that basically local methods give detailed information about the spectra which are the global characteristics of operators.

The geometric methods in the many-body QM problem first appeared in the pioneering work of Zhislin [Z1]. In the West the geometric ideas come from the works of R. Haag and D. Ruelle on the scattering in the field theory and of Lax-Phillips on the acoustic scattering. The term “geometric methods” was dubbed by B. Simon [Sim1]. The importance of partitions of unity in the QM many-body problem was realized in the classical works of Enss [E] and Simon [Sim1] (see also Deift and Simon [DS]). (For more complete references and detailed comments see [RS3].)

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In this paper we discuss the following topics:

Section 2: Hunziker-van Winter-Zhislin (HVZ) theorem (warm up).

Section 3: Exponential fall-off of eigenfunctions.

Section 4: Number of bound states. Short-range systems and negative ions.

Section 5: Nonexistence of very negative ions.

In Sects. 2–4 we present simplified proofs of known results, while the result of Sect. 5 is new. Note that Ruskai [R] has earlier, and independently, obtained a similar but slightly weaker result (namely that the ground state energy of a negative ion is bounded from below by a constant¹). All the necessary definitions are given in Sect. 1 and some of the technical results are carried out into the appendices. Discussions of related results and extensions are presented under the title “Remarks” at the end of the paper. Finally we admit that in estimation we always favored short cuts whatever the price. Probably many of the estimates we use can be improved to give physically interesting results. An announcement of this paper appears in [S3].

1. Hamiltonians

The *configuration space* of an N -body system in \mathbb{R}^v with masses m_1, \dots, m_N in the *center-of-mass* frame is the hyperplane $X = \{x \in \mathbb{R}^{vN} | \sum m_i x_i = 0\}$. We equip X with the inner product [SS] $\langle x, y \rangle = 2 \sum m_i x_i y_i$. We assume $v \geq 2$.

The *potentials* $V_l: \mathbb{R}^v \rightarrow \mathbb{R}$ are supposed to be Laplacian-compact, i.e. compact as multiplication operators from the Sobolev space $H_2(\mathbb{R}^v)$ to $L^2(\mathbb{R}^v)$. By the same letter V_l we denote also the multiplication operator by $V_l(x^l)$ on $L^2(X)$. Here $x^l = x_i - x_j$ for $l = (ij)$.

The *Schrödinger operator* for an N -body system in question in the center-of-mass frame is

$$H = -\Delta + \sum V_l \quad \text{on} \quad L^2(X),$$

where Δ is the Laplacian on X .

The *partitions* $a = \{C_i\}$ of the set $\{1, \dots, N\}$ are collections of nonintersecting subsets C_i , called below the clusters, of which the union is entire $\{1, \dots, N\}$.

With each a we associate the intercluster interaction $I_a = \sum_{l \not\subseteq a} V_l$, truncated Hamiltonian $H_a = H - I_a$ and intercluster distance $|x|_a = \min_{l \not\subseteq a} |x^l|$. Here $l \not\subseteq a$ signifies that the indices of l belong to different clusters of a .

A *partition of unity* on $L^2(X)$ is a collection $\{X_i\}$ of (positive) C^2 -functions such that $\sum X_i^2 = 1$. (Note the difference with the standard definition.)

A *localization formula* (implicity [C, I, K, M, MS]). Let $\{X_i\}$ be a partition of unity on $L^2(X)$. Then

$$H = \sum X_i H X_i - \sum |\nabla X_i|^2. \tag{1.1}$$

Proof. In the identity $H = \sum X_i^2 H$ commute X_i one step to the right and use $\sum X_i \nabla X_i = 0$ and $\sum |\nabla X_i|^2 + \sum X_i \Delta X_i = 0$ to transform $\sum X_i [X_i, H]$. \square

The *local partition* $a(x)$ is defined by putting i and j into the same cluster of $a(x)$ iff $x_i = x_j$.

1 Ruskai proved also nonexistence of very negative ions with the electrons replaced by bosons

2. HVZ Theorem, Difficult Direction

The HVZ theorem states ([H, VW, Z1]) that $\sigma_{\text{ess}}(H) = \bigcup \sigma(H_a)$. The inclusion $\bigcup \sigma(H_a) \subset \sigma_{\text{ess}}(H)$, called normally the easy direction, is proven by an explicit construction of an approximate eigenfunction for each $\lambda \in \bigcup \sigma(H_a)$ and applying Weyl’s criterion [RSI]. We prove here the inclusion

$$\sigma_{\text{ess}}(H) \subset \bigcup \sigma(H_a), \tag{2.1}$$

called the difficult direction.

First, we introduce.

A Ruelle-Simon partition of unity $\{J_a\}$, *a runs* through all and only two-cluster partitions, is defined by $\text{supp } J_a = \{x \in X \mid |x|_a > d|x|\}$ for some number d depending only on N and such that the regions on the right hand side cover X . Such d exist by the Ruelle-Simon lemma ([Sim1]). This lemma and a standard construction (e.g. like the one used in the appendix) imply the existence of $\{J_a\}$.

In this paper we do not use directly the definition of $\{J_a\}$. Instead we use

The main property of $\{J_a\}$ ([Sim1, RS3]):

$|\nabla J_a|^n$ and $I_a J_a^n$, $n > 0$, are Δ -compact (in fact, they decay in X as $|x|^{-n}$ and the worst potential in I_a , respectively).

The localization formula with $\{J_a\}$ reads

$$H = \Sigma(J_a H J_a - |\nabla J_a|^2).$$

Proof. Since $\Sigma(I_a J_a^2 - |\nabla J_a|^2)$ is Δ -compact, Weyl’s theorem [RS3] yields $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(\Sigma J_a H_a J_a)$. Furthermore, $\Sigma J_a H_a J_a \geq \min(\inf H_a)$. Hence $\sigma(\Sigma J_a H_a J_a) \subset \bigcup \sigma(H_a)$ (remember that the spectra of the H_a fill entire semiaxes since H_a are translationary invariant). Both relations give (2.1). \square

3. Exponential Fall-Off of Eigenfunctions

Theorem [DHSV]. *Let ψ be an eigenfunction of H corresponding to an isolated eigenvalue E . Then*

$$e^f \psi \in L^2(X) \quad \text{as long as} \quad \forall a, |\nabla f|^2 < \inf H_a - E \quad \text{in a vicinity of} \quad \{x \in X \mid a(x) = a\}.$$

Here we need another partition of unity.

A partition of unity $\{X_a\}$, *a runs* through all partitions, is defined with respect to the subspaces ([SS, DHSV, A]), $\{x \in X \mid a(x) = a\} \forall a$. X_a with two-cluster a live in a neighborhood of $\{x \in X \mid a(x) = a\}$ and so on.

Proof. By virtue of the Combes-Thomas argument (in the DHSV-form) (see [DHSV, CT, RS3] and Appendix 1) it suffices to show that

$$\text{Inf Re } \sigma_{\text{ess}}(H(i\lambda f)) > E \quad \text{for all} \quad 0 \leq \lambda \leq 1$$

as long as f is restricted as in the theorem. Here $H(f) = (-i\nabla - \nabla f)^2 + \Sigma V_f$. By the abstract inequality (see Appendix 2, cf. [A]),

$$\text{inf Re } \sigma_{\text{ess}}(A) \geq \text{inf } \sigma_{\text{ess}}(\text{Re } A), \quad \text{where} \quad \text{Re } A = \frac{1}{2}(A + A^*),$$

we find that $\inf \operatorname{Re} \sigma_{\text{ess}}(H(if)) \geq \inf \sigma_{\text{ess}}(H - |Vf|^2)$. Applying the proof of Sect. 2 with $\{J_a\}$ replaced by $\{X_a\}$ to $H - |Vf|^2$ we arrive at $\sigma_{\text{ess}}(H - |Vf|^2) \subset \bigcup \sigma(H_a - |Vf|^2 X_a^2)$. Together with the previous inequality this gives $\inf \operatorname{Re} \sigma_{\text{ess}}(H(if)) \geq \min_a \inf(H_a - |Vf|^2 X_a^2)$ which implies the desired inequality. \square

4. Finiteness of the Number of Bound States

Theorem 4.1. (Zhislin et al.) *The number of bound states of N -body short-range (more exactly $V^l \in L^p(\mathbb{R}^v)$, $p = v/2$) systems whose bottoms of continuous spectra are defined only by two-cluster breakups (i.e. $\inf H_a > \inf \sigma_{\text{ess}}(H)$ if a has more than two clusters) is finite.*

Theorem 4.2. [Yafaev (3 particles), Zhislin, Zhislin-Vugalter]. *Negative ions can have only a finite number of bound states.*

What makes the last theorem true is the QM Newton screening (by $N - 1$ electrons, in the ground state, of the nucleus of charge $Z \leq N - 1$ from the other electron). If the potentials are changed in such a way that the ground states of the $(N - 1)$ -electron system have different parities or do not have definite parities at all [which might happen if there is an additional (“accidental”) degeneracy], then the effective potential between this system and the other electron has a dipole leading term ($|x|^{-2}$ at infinity). This term when sufficiently large might lead to the infinite number of bound states for H .

Now we explain the main ideas of the proof of the theorems. First we transform H using the localization formula with the partition of unity $\{X_a\}$ defined in Sect. 3:

$$\begin{aligned} H &= \Sigma(X_a H X_a - |V X_a|^2) \\ &= \Sigma(X_a K_a X_a - |V X_a|^2), \end{aligned} \tag{4.1}$$

where $K_a = H_a + I_a \tilde{X}_a$ and $\tilde{X}_a = 1$ on $\operatorname{supp} X_a$. Here we have used that $\tilde{X}_a X_a = X_a$. This step is where the geometric methods enter changing radically the problem: $I_a \tilde{X}_a$ behaves as a multiparticle potential, namely, it vanishes in all directions, provided we choose $\operatorname{supp} \tilde{X}_a \subset \{x \in X \mid |x|_a > \tilde{d}|x|\}$.

Next we note that the operators K_a with a such that $\inf H_a > \Sigma$, where $\Sigma = \inf \sigma_{\text{ess}}(H)$, contribute only a finite number of eigenvalues $< \Sigma$. For the operators K_a with a such that $\inf H_a = \Sigma$ we use the Combes-Simon inequality $A \geq P A P - \delta^{-1} P A Q A P + Q(A - \delta)Q$, $\delta > 0$, to decouple the part along $P_a L^2(X)$ from the part along $Q_a L^2(X)$. Here $P_a =$ [projection on the eigenspace of H^a corresponding to $\inf H^a = \inf(H_a)$] $\otimes \mathbb{1}$ and $Q_a = \mathbb{1} - P_a$ with H^a the operator obtained from H_a after removal of the center-of-mass motion of the clusters in a . The resulting operators on $Q_a L^2(X)$ have $\inf(\text{essential spectrum}) > \Sigma$, so they contribute again only finite numbers of eigenvalues $< \Sigma$. The operators on $P_a L^2(X)$ are one-particle Schrödinger operators with the two-cluster effective potentials. Finally one takes care of the error term $\Sigma|V X_a|^2$ using the fact that it lives in the region of X where the system in question splits into three or more clusters. Collecting all the estimates above we observe that $H \geq \Sigma X_a F_a X_a$, where each F_a has only a finite number of eigenvalues $< \Sigma$. Hence so have $\Sigma X_a F_a X_a$ and, by the comparison theorem, H .

We deduce Theorems 4.1 and 4.2 from a general result given below. It is a slight generalization of the results of Zhislin and his collaborators [Z2, Z3, AZS, ZV].

Recall that H^a is the operator obtained from H_a after the removal of the center-of-mass motion of the clusters in a . The ground states, ψ^a , of the H^a are nondegenerate ([Zh4, RS3]). This is not, in general, true if one restricts H^a to functions of a certain symmetry type. However, we assume for the sake of notations that these ground states are nondegenerate too.

Theorem 4.3. (Essentially Zhislin et al.) *Assume that $\inf\sigma_{\text{ess}}(H)$ is defined only by two-cluster breakups (i.e. $\inf H_a > \inf\sigma_{\text{ess}}(H)$ for all three-cluster decompositions a) and assume that for any two-cluster partition a with $\inf H^a = \inf\sigma_{\text{ess}}(H)$ the one-body hamiltonian $-\Delta + W_a$ (on $L^2(\mathbb{R}^v)$), where*

$$W_a \equiv \langle \psi^a, I_a \psi^a \rangle - \delta^{-1} (\langle \psi^a, I_a^2 \psi^a \rangle - \langle \psi^a, I_a \psi^a \rangle^2), \quad \delta > 0, \tag{4.2}$$

has only a finite number of bound states. Then the discrete spectrum of H is finite. The analogous result holds also on the subspaces of functions of definite symmetry types.

Proof. Denote by $\#(a)$ the number of clusters in a partition a . Set, as usual, $\langle x \rangle = (1 + |x|^2)^{1/2}$. Let \tilde{W}_a is obtained from W_a by the substitution $I_a \rightarrow I_a \tilde{X}_a$.

Lemma 4.4. *For any $\delta > 0$ and $\varepsilon > 0$ the following inequality holds*

$$H \geq \sum_{\#(a)=2} X_a B_a X_a + \sum_{\#(a) \geq 3} X_a (H_a + I_a \tilde{X}_a + C_\varepsilon \langle x \rangle^{-2}) X_a, \tag{4.3}$$

where $B_a = C_a \oplus D_a$ on $P_a L^2(X) \oplus Q_a L^2(x)$ with

$$C_a = -\Delta + \tilde{W}_a - \varepsilon \langle x \rangle^{-2} - \Sigma \quad \text{on} \quad L^2(\mathbb{R}^v) \tag{4.4}$$

and

$$D_a = Q_a (H_a - \delta + I_a \tilde{X}_a - \varepsilon \langle x \rangle^{-2}) Q_a.$$

Proof. We apply the Combes-Simon decoupling inequality [Sim1]

$$K_a \geq P_a K_a P_a - \delta^{-1} P_a K_a Q_a K_a P_a + Q_a (K_a - \delta) Q_a, \tag{4.5}$$

obtained by applying the Schwartz inequality to $P_a K_a Q_a + Q_a K_a P_a$ [see Remark (a) to this section], to each K_a with $\#(a) = 2$ on the right hand side of (4.1).

Next, we estimate the localization error as

$$\Sigma |\mathcal{V}X_a|^2 \leq \left(\varepsilon \sum_{\#(a)=2} X_a^2 + C_\varepsilon \sum_{\#(a) \geq 3} X_a^2 \right) \langle x \rangle^{-2}, \tag{4.6}$$

for any $\varepsilon > 0$. To understand this estimate it is useful to note that

$$\text{supp} \Sigma |\mathcal{V}X_a|^2 \subset \bigcup_{\#(b) \geq 3} \text{supp} X_b.$$

To prove (4.6) we observe that since $\Sigma |\mathcal{V}X_a|^2 = 0$ on the set $\left\{ x \in X \mid \sum_{\#(a)=2} X_a^2(x) = 1 \right\}$, there is a δ -neighborhood of this set and a number $0 < \varepsilon_2 \leq \frac{1}{2}$ such that $\sum_{\#(a)=2} X_a^2 \geq 1 - \varepsilon_2$ and $\Sigma |\mathcal{V}X_a|^2 \leq \varepsilon_1$ on this neighborhood and $1 - \sum_{\#(a)=2} X_a^2 \geq \varepsilon_2$ outside of it. This implies (4.6) with $\varepsilon = \varepsilon_1 (1 - \varepsilon_2)^{-1}$ and $C_\varepsilon = \varepsilon_2^{-1} \text{sup}(\Sigma |\mathcal{V}X_a|^2)$.

Inserting (4.5) and (4.6) into (4.1) and recalling (4.2) we arrive at (4.3). \square

Now we pick \tilde{X}_a so that

$$|x|_a \geq \text{const}|x| \quad \text{on} \quad \text{supp} \tilde{X}_a.$$

Lemma 4.5. *Let $\Sigma_1 = \min_a \inf H_a Q_a$. Fix positive $\delta < \Sigma_1 - \Sigma$. Then the operators B_a have only finite numbers of eigenvalues $< \Sigma$.*

Proof. Each C_a has a finite number of negative eigenvalues because of the restriction on W_a . Operators D_a have finite numbers of eigenvalues $\leq \Sigma$ because $\inf \sigma_{\text{ess}}(D_a) = \Sigma_1 + \delta > \Sigma$. Since $B_a = C_a \oplus D_a$, the statement follows. \square

Lemma 4.6. *The operators $H_b + I_b \tilde{X}_b - C_\varepsilon \langle x \rangle^{-2}$ with $\#(b) \geq 3$ have finite numbers of eigenvalues $\leq \Sigma$.*

Proof. Since $I_b \tilde{X}_b - C_\varepsilon \langle x \rangle^{-2}$ is H_b -compact, the essential spectra of the operators under consideration equal $\sigma_{\text{ess}}(H_b)$. Since by the condition of Theorem 4.3, $\inf H_b > \Sigma$ for all b with $\#(b) \geq 3$, those operators have only finite numbers of eigenvalues $\leq \Sigma$. \square

Lemma 4.7. *Let each operator F_a be self-adjoint with negative spectrum finite. Then $\Sigma X_a F_a X_a$ has a finite number of negative eigenvalues.*

Proof. Let π_a be the projection operator on the eigenspace of F_a corresponding to the spectrum in $(-\infty, 0)$. Then

$$\Sigma X_a F_a X_a \geq \Sigma F_a \pi_a.$$

Since each π_a is finite dimensional, $\Sigma F_a \pi_a$ has a finite number of negative eigenvalues. Thus by the comparison theorem [RS3], $\Sigma X_a F_a X_a$ has only a finite negative spectrum. \square

Lemmas 4.4–4.7 imply via the comparison theorem the first statement of Theorem 4.3 (no symmetry). The proof with an allowance for symmetry is obtained by adding a few extra indices to the proof above (cf. Appendix 4). \square

Now we deduce Theorems 4.1 and 4.2 from Theorem 4.3.

Proof of Theorem 4.1. Writing $\langle \psi^a, I_a \psi^a \rangle$ and $\langle \psi^a, I_a^2 \psi^a \rangle$ as sums of the convolutions of V_l and V_l^2 , respectively, $l \leq a$, with one-particle densities (see e.g. the proof of Theorem 4.2 below) and using the Young (or generalized Young) inequality [RS2] and the fact that $\psi^a \in L^q$ for any q , we find that $\langle \psi^a, I_a \psi^a \rangle \in L^p \cap L^q$ and $\langle \psi^a, I_a^2 \psi^a \rangle \in L^{p/2} \cap L^r$ with p the same as in the statement and $\infty \geq q > p$ and $\infty \geq r \geq p/2$. Hence, since $p = v/2$ and $\langle \psi^a, I_a \psi^a \rangle^2$ is positive, W_a has only a finite number of bound states [RS3]. \square

Before proceeding to the proof of Theorem 4.2, we recall the Hamiltonian of an ion with N electrons and a nucleus of charge Z (the masses are not restricted)

$$H(N) = -\Delta - \sum_{i=1}^N \frac{Z}{|x_{i0}|} + \sum_{i \neq j}^N \frac{1}{|x_{ij}|}. \tag{4.7}$$

Here the nucleus is labeled by 0, the electron charge is taken to be 1 and X is, of course, the vN -dimensional hyperplane in $\mathbb{R}^{v(N+1)}$. The fact that the electrons are fermions is reflected in the restriction of $H(N)$ to functions of the permutation-symmetry types corresponding to one- and two-column Young tables.

Next we note that in accordance with the HVZ theorem (Sect. 2 and Appendix 4) the bottom of the continuous spectrum of $H(N)$ (also if restricted to certain symmetry type functions) is defined only by two-cluster breakups of the form

$$a_s = \{(0 \dots \hat{s} \dots N)(s)\}, \quad s = 1, \dots, N,$$

i.e. by the one-electron ionizations. Here we *assume* that $H(N-1)$ has isolated eigenvalues. We *conjecture* that this always holds in the case when $H(N)$ has isolated eigenvalues (presently, it is known only for $N = Z + 1$).

Finally, we mention that [RS3] the ground state, ψ_N , of $H(N)$ is unique and therefore rotationaly invariant in the sense

$$\psi_N(gx) = \psi_N(x) \quad \text{with} \quad gx = (gx_1 \dots gx_N) \quad \text{and} \quad g \in O(3). \quad (4.8)$$

This is not, however, known for different permutation-symmetry types. If (4.8) fails to hold we use the fact that the ground states of the same symmetry type have the same parities [see Remark (b) to this section].

Proof of Theorem 4.2. To estimate W_{a_s} we note that the intercluster interaction for a_s is

$$I_{a_s} = \sum_{i \neq 0, s} \frac{1}{|x_{is}|} - \frac{Z}{|x_{0s}|} \quad (4.9)$$

and use standard screening estimates given in the two lemmas below. There we use the notations $y = x_s$, $I(y) = I_{a_s}$ and ψ for the ground state of H^{a_s} of a definite permutation symmetry type. We assume ψ is rotationaly invariant [in the sence of (4.8)]. If the latter fails to hold then we proceed as prescribed in Remark (b).

Lemma 4.9. (QM Newton screening theorem.) *We have (here $x = (x_1 \dots x_{N-1})$ and $dx = \prod_1^{N-1} dx_i$)*

$$\langle \psi, I(y)\psi \rangle \geq [N - 1 - Z - (N - 1) \int_{|x_1| \geq |y|} |\psi|^2 dx] |y|^{-1}. \quad (4.10)$$

Proof. First we compute in a standard way ($M =$ mass of the nucleus/mass of the electron)

$$\langle \psi, I(y)\psi \rangle = (N - 1) \int \frac{|\psi(x)|^2}{|x_1 - y|} dx - Z \int \frac{|\psi(x)|^2 dx}{|M^{-1} \sum x_j - y|}. \quad (4.11)$$

Since ψ is rotationaly invariant [in the sence of (4.8)] the one-particle densities entering (4.11) are spherically symmetric. Hence by the Newton electrostatic theorem

$$\int \frac{|\psi(x)|^2}{|x_1 - y|} dx = |y|^{-1} \int_{|x_1| \leq |y|} |\psi(x)| dx$$

and similarly for the second integral on the right hand side of (4.11). Together with (4.11) this gives (4.10). \square

Lemma 4.10. (Simon.) *The following estimate holds*

$$\langle \psi, I(y)^2 \psi \rangle - \langle \psi, I(y)\psi \rangle^2 \leq \text{const}(1 + |y|)^{-4}.$$

Proof. Using the elementary inequality

$$||a - y|^{-1} - |y|^{-1} - (a \cdot y)|y|^{-3}| \leq 3|a|^2|y|^{-2}|a - y|^{-1},$$

we obtain

$$\left| I(y) - (N - 1 - Z)|y|^{-1} + \left(\sum_{i \neq 0, s} x_i - Zx_0 \right) \cdot y|y|^{-3} \right| \leq 3|y|^{-2} \sum_{i \neq s} |x_i| |x_i - y|^{-1}.$$

Consider $\langle \psi, I(y)\psi \rangle$. Since $|\psi|^2$ is even, the integral, produced by the term $\left(\sum_{i \neq 0, s} x_i - Zx_0 \right) \cdot y|y|^{-3}$, is zero. Using that $|\psi|^2$ falls off at infinity we estimate

$$|\langle \psi, I(y)\psi \rangle - (N - 1 - Z)|y|^{-1}| \leq C(1 + |y|)^{-3} \tag{*}$$

(the dipole moment is zero for an even density). Similarly, we obtain

$$|\langle \psi, I(y)^2\psi \rangle - (N - 1 - Z)^2|y|^{-2}| \leq C(1 + |y|)^{-4}.$$

These two inequalities imply the desired estimate.

These two lemmas and the fact that the bound states are exponentially bounded [see Remark (c) to Sect. 3] imply the inequality ($a = a_s$)

$$W_a(y) \geq (N - 1 - Z)|y|^{-1} - \text{const}(1 + |y|)^{-4}.$$

So for $Z \leq N - 1$, the negative part of W_a is short-range (the Newton screening theorem in QM). Hence W_a have only finite number of bound states. This by virtue of Theorem 4.3 completes the proof. \square

5. Nonexistence of Very Negative Ions

Theorem. *There is no very negative ions in QM.*

To give a mathematical formulation of the theorem we consider an N -electron ion with a nucleus of charge Z . For the sake of notational convenience we assume the nuclear mass to be infinite. In the units in which the electron charge and mass are 1 and $\frac{1}{2}$ respectively, the Schrödinger operator of such an ion is

$$H_N = \sum_{i=1}^N \left(-\Delta_i - \frac{Z}{|x_i|} \right) + \sum_{i < j} \frac{1}{|x_i - x_j|} \quad \text{on } L^2(\mathbb{R}^{vN}).$$

Here Δ_i stands for the Laplacian in $x_i \in \mathbb{R}^v$.

Ignoring the symmetry, the theorem asserts that

$$H_N \geq \inf \sigma_{\text{ess}}(H_N) = \inf H_{N-1} \quad \text{for sufficiently large } N.$$

[The second equality follows from the HVZ theorem (Sect. 2).] The symmetry can be taken into account in a routine simple way (see Appendix 4).

In this section we use a new partition of unity $\{K_s\}_0^N$ tailored for the problem. Let $x = (x_1, \dots, x_N)$ and $|x|_p = N^{-1/p}(\sum |x_i|^p)^{1/p}$. We define K_s by

$$\text{supp } K_s \subset \{x \in \mathbb{R}^{vN} \mid |x|_p \leq \gamma |x_s| \text{ and } |x_s| > N^{-1/p} \varrho\}, \tag{5.1}$$

where $\gamma > 1$ is a given number, e.g. $\gamma = 2$, for $s = 1, \dots, N$ and

$$K_0 \in C_0^\infty(\mathbb{R}^{vN}) \quad \text{and} \quad \text{supp } K_0 \subset \{x \in \mathbb{R}^{vN} \mid |x_i| < N^{-1/p} \gamma \varrho\}, \tag{5.2}$$

$K_s, s = 1, \dots, N$, is invariant under the action of the group $S_{N-1}^{(s)}$ and K_0 , under the action of S_N . (5.3)

Here S_N and $S_{N-1}^{(s)}$ are the groups of permutations of the indices $\{1, \dots, N\}$ and $\{1, \dots, N\} \setminus \{s\}$, respectively.

The localization formula with $\{K_s\}$ is

$$H_N = \sum_{s=0}^N K_s H_N K_s - \sum_{s=0}^N |\nabla K_s|^2. \tag{5.4}$$

Proof. In each cone K_s , $s=1, \dots, N$, we estimate (from below) the electrostatic interaction of the s^{th} electron with the rest of the ion, using that

$\sum_{i:i \neq s} |x_{is}|^{-1} \geq (N/\gamma + 1 - \frac{1}{2})|x_s|^{-1}$ on $\text{supp } K_s$ (this inequality is derived by evaluating the minimum of $\sum_1^N (1+a_i)^{-1}$ under the restrictions $a_i \geq 0$ and $\sum_1^N a_i^p \leq \gamma^p N$; here $a_i = |x_i|/|x_s|$) and that $H_{N-1}^{(s)} \geq \Sigma_N$, where $H_{N-1}^{(s)}$ is the Hamiltonian of the ion without the s^{th} electron:

$$K_s H_N K_s \geq (\Sigma_N + (N/\gamma + 1 - \frac{1}{2} - Z)|x_s|^{-1}) K_s, \quad \text{where } \Sigma_N = \inf H_{N-1}. \tag{5.5}$$

This estimate expresses a simple fact that this electron sees the nucleus shielded by the other electrons whose electrostatic repulsion prevails for sufficiently large N (the classical Newton screening). In K_0 we estimate (again from below) the electrostatic repulsion between electrons using the fact that they cannot get more than $2\gamma\varrho$ apart in K_0 and then we estimate the ground state energy of N independent electrons by the classical Fermi method filling first $N/2$ levels (counting the multiplicities) of the corresponding Dirichlet one-particle Hamiltonian with two electrons each (the Pauli principle!):

$$K_0 H_N K_0 \geq L_N K_0^2, \quad \text{where } L_N = N(N-1)/4\gamma\varrho + \text{Fermi term.}$$

The Fermi term is twice the sum of the first $N/2$ eigenvalues (counting the multiplicities) of the one-particle Hamiltonian $-\Delta - Z/|x|$ on $L^2(B_{\gamma\varrho})$, where $B_\varrho = \{x \in \mathbb{R}^3 \mid |x| \leq \varrho\}$, with the Dirichlet boundary conditions. A good estimate of this term is tedious but its asymptotic behavior as $N \rightarrow \infty$ is easy to derive (using e.g. the hydrogen levels till the cutoff energy and a box model for the positive eigenvalues): it tends to $+\infty$ as $N \rightarrow \infty$.

Finally we estimate the localization error $-\Sigma |\nabla K_s|^2$ using an explicit construction of $\{K_s\}$ (see Appendix 3), (we set $p=N^2$ and absorb the factors $N^{1/p}$ into the constants which otherwise are p -independent):

$$\Sigma |\nabla K_s(x)|^2 \leq CN^{2/3} (|x|_p + \varrho)^{-2}.$$

Putting together these inequalities and localization formula (5.4), we get

$$H_N \geq (L_N - CN^{1/2}\varrho^{-2}) K_0^2 + \Sigma_N (1 - K_0^2) + W, \tag{5.6}$$

where

$$W = \sum_1^N (N/\gamma + 1 - \frac{1}{2} - Z - CN^{1/2}\varrho^{-1}) |x_s|^{-1} K_s^2.$$

For N sufficiently large and $\varrho \geq 1$ we have that

$$N \geq \alpha Z \quad \text{for some } \alpha > 2 \quad \text{implies } W \geq 0.$$

Furthermore, since $L_N = O(N^2 \varrho^{-1})$ and Σ_N does not grow as $N \rightarrow \infty$ we can choose N so that $L_N \geq \Sigma_N + C\varrho^{-2}N^{2/3}$. Together with the former inequality this implies $H_N \geq \Sigma_N$. \square

Appendix 1: Combes-Thomas Argument

Combes-Thomas Argument (in the DHSV form) [CT, DHSV]. *Let ψ be an eigenfunction of H with an eigenvalue E , f a measurable function with the measurable weak derivative. Then*

$$e^f \psi \in L^2(X) \text{ iff } E \notin \sigma_{\text{ess}}(H(i\lambda f)) \quad \forall 0 \leq \lambda \leq 1.$$

Here, recall, $H(f) = (-i\nabla - \nabla f)^2 + V$ with $V = \Sigma V_1$.

Sketch of the proof. Introduce the one parameter group of gauge transformations:

$$U(\lambda) : u \rightarrow e^{i\lambda f} u.$$

The gauge-transformed Hamiltonian is given by

$$H(\lambda f) = U(\lambda) H U(\lambda)^{-1}.$$

We compute $H(f) = (-i\nabla - \nabla f)^2 + V$. Hence the family $H(\lambda f)$ has an analytic continuation to $\lambda \in \mathbb{C}$. Applying the O'Connor projection lemma and the first Balslev-Combes theorem [RS3] one concludes that ψ is $U(\lambda)$ -analytic as long as E stays away from $\sigma_{\text{ess}}(H(\lambda f))$. So $e^f \psi \in L^2(X)$ if $E \notin \sigma_{\text{ess}}(H(i\lambda f))$ for all $0 \leq \lambda \leq 1$. \square

Appendix 2: An Inequality

Proposition. *Let A be a densely defined closed operator on a Hilbert space such that $\text{Re } A = \frac{1}{2}(A + A^*)$ and $\text{Im } A = \frac{1}{2i}(A - A^*)$ are defined and self-adjoint and $\text{Im } A$ is $(\text{Re } A)$ -bounded. Then*

$$\inf \text{Re } \sigma_{\text{ess}}(A) \geq \inf \sigma_{\text{ess}}(\text{Re } A). \tag{*}$$

The same inequality is also true for the full spectra.

Proof. Note first that $\text{Re } A$ and $\text{Im } A$ are self-adjoint by the assumptions. For any $\varepsilon > 0$ there is an n -dimensional eigen-projection P^n , $n < \infty$, for $\text{Re } A$ so that $T \equiv (\text{Re } A)(\mathbb{1} - P^n) \geq \inf \sigma_{\text{ess}}(\text{Re } A) - \varepsilon$. The real spectrum of $A - (\text{Re } A)P^n$ lies in $[\inf \sigma_{\text{ess}}(\text{Re } A) - \varepsilon, \infty)$ as follows from the invertibility of

$$T + i \text{Im } A - \lambda = (T - \lambda)^{1/2} [\mathbb{1} + i(T - \lambda)^{-1/2} (\text{Im } A)(T - \lambda)^{-1/2}] (T - \lambda)^{1/2} \tag{**}$$

for any $\lambda < \inf \sigma_{\text{ess}}(\text{Re } A) - \varepsilon$. Since $\sigma_{\text{ess}}(A) \subset \sigma(A - (\text{Re } A)P^n)$ by Weyl-type theorem of [S4, Theorem AI, 1], (*) follows. The second part of the proposition follows from the invertibility of (**) with $T = \text{Re } A$. \square

Appendix 3: Construction of $\{K_s\}$

Let $\Omega_s = \{x \in \mathbb{R}^{vN} \mid |x|_p \leq |x_s|, |x_s| \geq \varrho\}$ for $s = 1, \dots, N$ and $\Omega_0 = \{x \in \mathbb{R}^{vN} \mid |x|_p \leq \varrho\}$. Then $\bigcup_0^N \Omega_s = \mathbb{R}^{vN}$. Let $\{F_s\}_0^N$ be a collection of real C^∞ -functions such that $F_s = 1$

on Ω_s . We define $K_s = F_s(\Sigma F_i^2)^{-1/2}$. So $\Sigma K_i^2 = 1$. Note that $\Sigma F_i^2 \geq 1$ since $F_s = 1$ on $\Omega_s \forall s$ and $\bigcup \Omega_s = \mathbb{R}^N$.

Now we construct F_s . Let $\chi \in C^\infty$ and $\chi(t) = 1$ if $t \leq 1$ and $= 0$ if $t > 1 + \alpha$ for some fixed $\alpha > 0$. Then $F_s(x) = (1 - \chi(|x_s|N^{1/p}/\varrho))\chi(|x|_p/|x_s|)$ if $|x_s| > 0$ and $= 0$ if $|x_s| = 0$ for $s = 1, \dots, N$ and $F_0(x) = \chi(|x|_p N^{1/p}/\varrho)$. With this definition K_s obeys (5.1)–(5.3). We show now that it obeys (5.5) as well.

First we prepare the ground for the estimation of $\sum |VK_s|^2$. We compute

$$\nabla K_s = \nabla F_s (\sum F_j^2)^{-1/2} - F_s (\sum F_j \nabla F_j) (\sum F_j^2)^{3/2}.$$

So as vectors on \mathbb{R}^{N+1} and $\mathbb{R}^{v(N+1)N}$

$$\begin{aligned} \|\nabla K\|^2 &= \|\nabla F\|^2 \|F\|^{-2} - |\langle F, \nabla F \rangle|^2 \|F\|^{-4} \\ &\leq \|\nabla F\|^2 \|F\|^{-2}. \end{aligned} \tag{A.1}$$

Finally, we note the following simple inequalities [cf. (4.6)]

$$\chi'^2 \leq C_1(\varepsilon^{-1}\chi^2 + \varepsilon) \quad \text{and} \quad \chi'^2 \leq C_1(\delta^{-1}(1-\chi)^2 + \delta), \tag{A.2}$$

where C_1 is a constant depending only on α . This can be derived using e.g. the explicit construction

$$\chi(t) = 2\left(\frac{t-1}{\alpha}\right)^3 - 3\left(\frac{t-1}{\alpha}\right)^2 + 1 \quad \text{for} \quad 1 \leq t \leq 1 + \alpha.$$

Now we proceed directly to an estimation of $\|\nabla F\|$. First we compute explicitly

$$\begin{aligned} |\nabla F_s|^2 &= [\varrho^{-1}\psi_s + \partial/\partial|x_s|(|x|_p|x_s|^{-1})g_s]^2 \\ &\quad + |x_s|^{-2}N^{-2/p}\left(\sum_{i \neq s} |x_i|^{2(p-1)}\right)\left(\sum_j |x_j|^p\right)^{-\frac{2(p-1)}{p}}g_s^2, \end{aligned}$$

where we have introduced the notation $\psi_s \equiv -\chi'(|x_s|/\varrho)\chi(|x|_p/|x_s|)$ and $g_s = (1 - \chi(|x_s|/\varrho))\chi'(|x|_p/|x_s|)$. Since $|x_p| \leq (1 + \alpha)|x_s|$ on $\text{supp } g_s$ and $|x_s|^{p-1} \leq (\sum |x_j|^p)^{\frac{p-1}{p}}$ we have $|\partial/\partial|x_s|(|x|_p|x_s|^{-1})| \leq (1 + \alpha + N^{-1/p})|x_s|^{-1}$. Furthermore, using the inequalities $(a+b)^2 \leq 2a^2 + 2b^2$ and $\sum |x_j|^{2(p-1)} \leq (\sum |x_j|^p)^{\frac{2(p-1)}{p}}$ we find

$$|\nabla F_s|^2 \leq 2\varrho^{-2}\psi_s^2 + |x_s|^{-2}(2(1 + \alpha + N^{-1/p})^2 + N^{-2/p})g_s^2.$$

Finally, since

$$\begin{aligned} |x|_p &\leq (1 + \alpha)|x_s| \leq (1 + \alpha)^2\varrho \quad \text{on} \quad \text{supp } \psi_s, \\ \varrho &\leq |x_s| \quad \text{and} \quad |x|_p \leq (1 + \alpha)|x_s| \quad \text{on} \quad \text{supp } g_s \end{aligned} \tag{A.3}$$

and, by virtue of (A.2),

$$\psi_s^2 \leq C_1(\delta + \delta^{-1}F_s^2) \quad \text{and} \quad g_s^2 \leq C_1(\varepsilon + \varepsilon^{-1}F_s^2)$$

we get taking $\delta = \varepsilon < 1$

$$|\nabla F_s|^2 \leq 24(1 + \alpha)^4 C_1(\varepsilon + \varepsilon^{-2}F_s^2)(\varrho + |x|_p)^{-2}N^{1/p}.$$

Summing up these inequalities we find

$$\|\nabla F\|^2 \leq C_2(\varepsilon N + \varepsilon^{-2}\|F\|^2)(\varrho + |x|_p)^{-2}N^{1/p},$$

where $C_2 = 24(1 + \alpha)^4 C_1$, obviously N -independent. Picking here $\varepsilon = N^{-1/3}$ and recalling (A.1) we arrive at

$$\sum_1^N |(VK_s)(x)|^2 \leq CN^{1/2 + 1/p} (|x|_p + \varrho)^{-2}$$

with a p - and N -independent constant C . \square

Appendix 4: The Symmetry Groups

Let G and $G(a)$ be symmetry groups (or subgroups) of H and H_a , respectively, and let σ and α label the types of their irreducible representations. We always choose $G(a)$ to be a subgroup of G . The examples of $G(G(a))$ are trivial group, S , $S \times O(3)$ [trivial group, $\bigotimes_{C_i \in a} S(C_i)$, $(\bigotimes_{C_i \in a} S(C_i)) \otimes O(3)$]. Here S and $S(C)$ are the groups of permutations of the identical particles in the whole system and in the cluster C , respectively. The trivial group, $\{id\}$, is considered when we do not want to take the symmetry into account. Let $\alpha < \sigma$ express the fact that the irreducible representation α of $G(a)$ is present in the decomposition of the restriction of the irreducible representation σ of G to the subgroup $G(a)$. Finally, we denote by H^σ and H_a^α the restrictions of H and H_a to the invariant subspaces on which the representations of G and $G(a)$ are multiple to irreducible of the types σ and α , respectively. The projections on the invariant subspaces above will be denoted by P^σ and P_a^α . Then $H^\sigma = HP^\sigma = P^\sigma H$ and similarly $H_a^\alpha = H_a P_a^\alpha = P_a^\alpha H_a$.

To obtain the HVZ-theorem with the symmetry we note first that the J_a can be constructed to commute with the symmetry groups $G(a)$.

Since $\sum_{\alpha < \sigma} P_a^\alpha P^\sigma = P^\sigma$ by the definition of the restriction $\alpha < \sigma$, the proof above applied to H^σ yields that $\sigma_{\text{ess}}(H^\sigma) \subset \bigcup_{a, \alpha < \sigma} \sigma(H_a^\alpha)$. Together with the easy direction of which proof in the case of symmetry remains the same, this gives $\sigma_{\text{ess}}(H^\sigma) = \bigcup_{a, \alpha < \sigma} \sigma(H_a^\alpha)$, which is the HVZ theorem with symmetry.

Now we point out the allowances which have to be made in the proof of the theorem of Sect. 5 in order to take into account the symmetry consistently. Recall that S_N and $S_{N-1}^{(s)}$ denote the groups of the permutations of $(1 \dots N)$ and $(1 \dots \hat{s} \dots N)$, respectively. Let P^σ and P_s^α be the projections on the subspaces on which the representations of S_N and $S_N^{(s)}$ are multiple to irreducible of the types σ and α , respectively. Finally, let $\Sigma_N^\sigma = \inf \sigma_{\text{ess}}(H_N^\sigma)$. Then the obvious inequality $K_s H_{N-1}^{(s)} K_s \geq \inf H_{N-1} K_s^2$ used to obtain (5.6) should be replaced by $P^\sigma K_s H_{N-1}^{(s)} K_s P^\sigma \geq \Sigma_N^\sigma P^\sigma K_s^2 P^\sigma$, which follows readily if we use:

(α) $\sum_{\alpha < \sigma} P_s^\alpha P^\sigma = P^\sigma$,

(β) invariance of K_s with respect to permutation $S_{N-1}^{(s)}$ (so K_s commutes with P_s^α), and

(γ) $\Sigma_N^\sigma = \min_{\alpha < \sigma} \inf H_{N-1}^\alpha$ by the HVZ-theorem with the symmetry.

The second and last remark is about inequality (5.6): It should be placed between the $P^{\sigma'}$'s.

Remarks

Section 2. Our proof of the HVZ theorem is related to that of Enss [E]. It is shorter than the latter since it uses the Weyl theorem while Enss' proof is based on the Weyl criterion (which is more powerful) and proves the Weyl theorem in its course. Besides, Enss' proof is more intuitive.

Section 3. (a) For almost all x , $a(x) = \{(1) \dots (N)\}$, so $|Vf|^2 < -E$, which gives the fastest possible decay.

(b) As was noticed by Agmon (see [CS]) the DHSV exponential bounds are equivalent to the Agmon optimal bounds.

(c) [DHSV] has shown that the DHSV L^2 -exponential bound implies the DHSV L^p -exponential bound [i.e. $e^f \psi \in L^p(X)$].

(d) The references and comments on other works on the exponential fall off of bound states can be found in [DHSV, H-O²AM, and RS3] (we note only that the first general exponential bounds were obtained by O'Connor [OC]).

(e) The subspaces $\{x \in X | a(x) = a\}$ can be also written as ([SS])

$$\{x \in X | x_i = x_j \text{ iff } i \text{ and } j \text{ belong to the same cluster of } a\}.$$

Section 4. (a) The Combes-Simon inequality can be given the following abstract form:

Lemma. *Let A and P be self-adjoint operators with $R(P) \subset D(A)$ and $R(A) \subset D(P)$. Denote $Q = \mathbb{1} - P$. Then*

$$A \geq PAP - PAQW^{-1}QAP + Q(A - W)Q \tag{*}$$

for any invertible, positive operator W for which the right hand side is defined.

Proof. The equality

$$A = PAP + QAQ + PAQ + QAP$$

and inequality

$$|\langle QAP\varphi, \varphi \rangle| \leq \frac{1}{2} (\|U^{-1}QAP\varphi\|^2 + \|U^*Q\varphi\|^2),$$

where U is any invertible operator, resulting from the Schwartz inequality, imply (*) with $W = UU^*$. \square

(b) $H(N)$ has a finite number of eigenvalues on a subspace of any irreducible S_N - or $S_N \times O(3)$ -symmetry type or if the symmetry group is dropped altogether. Here S_N is the group of permutations of N indices (electrons). If the ground states of $H(N-1)$ of a certain S_{N-1} -symmetry type are not rotationary invariant [in the sence of (4.8)] as it is the case with the ground states of the $S_{N-1} \times O(3)$ -symmetry types with nonzero total momenta, estimate (4.10) is not, in general, valid (the negative part of $\langle \psi, I(y)\psi \rangle$ does not fall off exponentially for $Z \leq N-1$). However, since the ground states have same parity [the parity transformation is contained in $O(3)$], negative part of $\langle \psi, I(y)\psi \rangle \leq \text{const}(1 + |y|)^{-3}$ for $Z \leq N-1$ as follows from inequality (*) of the proof of Lemma 4.10 (the dipole moment is zero for even densities). Note that if the potentials are changed in such a way that the ground states have different parities or do not have definite parities at all (which might happen if there is an additional ("accidental") degeneracy (see [LL]), then the

effective potential $\langle \psi, I(y)\psi \rangle$ has a dipole leading term ($|x|^{-2}$ at infinity) which when sufficiently large might lead to the infinite number of bound states for $H(N)$.

(c) Note again that $\Sigma|\nabla X_a|^2$ falls off at infinity as $|x|^{-2}$, i.e. it behaves as a long-range N -body potential. This does not lead to the infinite number of bound states of H in our case since $\Sigma|\nabla X_a|^2$ lives in the region of X where the system splits into more than two clusters and therefore has the lowest threshold $> \Sigma = \inf \sigma_{\text{ess}}(H)$. If we remove the restriction on Σ , e.g. allow for three-cluster thresholds to be at Σ , then $\Sigma|\nabla X_a|^2$ is supported also in the region with the lowest threshold Σ . This, in our opinion (also, B. Simon, private communication) might account for the Effimov effect, the appearance of the infinite number of bound states in some short-range systems.

(d) One might try to use inequality (4.3) together with the comparison theorem [RS3] in order to obtain effective estimates of the number of bound states of H along the lines of works [B1, B2, BF1, BF2, H1] (see also [G, WS, W]). Note that such estimates were given using different generalizations of the Birman-Schwinger principle by Yafaev [Y2], Klaus and Simon [KS], and Sigal [S2].

(e) The restriction on Σ , that it is defined only by two-cluster breakups, is a technical one. The essentially most general conditions under which the finiteness of $\sigma_a(H)$ is still true were given in [S1]. To obtain this result by the method presented here one might try to counter $-\Sigma|\nabla X_a|^2$ with $\varepsilon(-\Delta)$ borrowed from $-\Delta$.

(f) Theorem 4.2 can be obviously generalized to include molecular ions.

(g) In the case $Z = N - 1$ the proof of Lemma 4.10 is especially simple. Indeed, by virtue of

$$||a - y|^{-1} - |y|^{-1}| \leq |a||y|^{-2}(1 + |a||a - y|^{-1})$$

we get

$$\begin{aligned} |I(y)| &\leq \sum_{i \neq 0, s} ||x_i - y|^{-1} - |x_0 - y|^{-1}| \\ &\leq |y|^{-2} \sum_{i \neq s} |x_i|(1 + |x_i||x_i - y|^{-1}), \end{aligned}$$

which, along with the fact that $|\psi|^2$ is bounded and fast decreasing, implies that $\langle \psi, I(y)^2 \psi \rangle \leq C(1 + |y|)^{-4}$.

Section 5. (a) Different generalizations (not discussed here) of the theorem of this section are possible. Among them we list the extensions of this theorem to molecules and to non-Coulomb potentials (cf. [R]).

(b) The idea of using $|x|_p$ with $p < \infty$ comes from Ruskai [R]. (Originally the author used the K_s -partition with $p = \infty$.)

(c) This section has many common points with Ruskai [R] and Zhislin [Z1, Z2].

Appendix 3. (a) We used the same function χ in different, independent constructions. The reason for this is our laziness.

(b) We believe that the estimate (A.4) can be improved considerably:

Our conjecture is that $\sum_{s=0}^N |(\nabla K_s)(x)|^2 \leq C(1 + \Sigma \varphi_s(x))(|x|_p + \varrho)^{-2}$, where $\varphi_s = (\|\psi_s\|/\|\psi_s\|_\infty)^2$, is true. Note that (A.3) implies that $\text{supp } \varphi_s \subset \{x \in \mathbb{R}^{3N} \mid |x_j| < \gamma^2 \varrho \forall i\}$. The factor $N^{1/2}$ should, in our opinion, disappear due to a compensation in $\|\nabla F\|^2 - |\langle F, \nabla F \rangle|^2 / \|F\|^2$.

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Note added in proof. The technique above is effective within the framework of Agmon's method of proving the exponential bounds. More specifically, the localization formula $H = \Sigma(X_a H X_a - |\nabla X_a|^2)$ implies $H \geq \omega + I$, where $\omega = \Sigma(\inf H_a) X_a^2$ and $I = \Sigma(I_a X_a^2 - |\nabla X_a|^2)$. Since I is H -compact, $\chi_R I (H + 1)^{-1} \rightarrow 0$ as $R \rightarrow \infty$ for bounded C^2 functions χ_R with $\text{supp } \chi_R \subset \{|x| > R\}$. So for any $\varepsilon > 0$ there is R s.t. $\chi_R H \chi_R \geq [\omega - \varepsilon(H + a)] \chi_R^2$, where $a = \inf H + 1$. The latter inequality plays an important role in Agmon's method [together with the elementary inequality $\langle (H - E - |\nabla f|^2) e^f \chi_R \psi, e^f \chi_R \psi \rangle \leq M \|e^f \chi_R \psi\|^2$, where $M = \|e^f \Delta \chi\| \|\psi\| + 2 \|e^f \nabla \chi\| \|\nabla \psi\|$, valid for any bounded C^2 function f and an eigenfunction ψ of H with the eigenvalue E , it implies validity the DHSV bound (see Sect. 3)].