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Absence of Discrete Spectrum in Highly Negative Ions*

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Abstract. Let H_N be the Hamiltonian for the Coulomb system consisting of N particles of like charge in the field of a fixed point charge Z. We show that if the particles are bosons, then H_N has no discrete spectrum when $N \geqq N_0 = cZ^2$ for some constant c. If the particles are fermions, then H_N is bounded below uniformly in N. These results can be extended to molecules and to other power law potentials.

I. Introduction

Let H_N be the Hamiltonian

$$H_N(W,Z) = -\sum_{j=1}^{N} \Delta_j - \sum_{j=1}^{N} Zr_j^{-1} + \sum_{j<k} Wr_{jk}^{-1}. \tag{1a}$$

When $W=1, H_N$ is the Hamiltonian of N charged particles in the field of an infinitely heavy nucleus of charge Z. If these particles are fermions and $Z \geqq N+1$, so that $H_N(1,Z)$ is the Hamiltonian for a negative ion, it is known [1–3, 18] that H_N has only finitely many bound states. However, very little is known about the precise number of bound states. When $N=2$, Hill [4, 5] has shown that $H_2(1,1)$ which is the Hamiltonian for H^-, has precisely one bound state in the sector of natural parity; Grosse and Pittner [6] have shown that H^- has precisely three degenerate bound states in the sector of unnatural parity. Hill's results can be extended to show that H^{--} has no bound states [7], but Hill's techniques are unlikely to be suitable for N much larger than 3 or 4. All other methods known for estimating the number of bound states of multi-particle systems are either very specialized or very weak [8–10].

In this paper we show that for a system of N charged *bosons*, $H_N(W,Z)$ has no discrete spectrum when N is sufficiently large. Then the only possible bound states are eigenvalues imbedded in the continuum. Because our method of proof uses smoothing functions which need not leave a given symmetry subspace invariant,

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we do not prove absence of bound states in each symmetry subspace, nor do we prove absence of discrete spectrum in the antisymmetric subspace corresponding to fermions. However, we believe that fermions also have no discrete spectrum for large N and discuss the extent to which our proof is valid for fermions in Sect. III. Furthermore, we can show that the Hamiltonian H_N is bounded below *uniformly* in N for fermions. Thus, at worst, the fermion binding energy can be made arbitrarily weak by making N sufficiently large.

For convenience we scale $H_N(W, Z)$ and consider instead

$$H_N(\omega) = -\sum_{j=1}^{N} \Delta_j - \sum_{j=1}^{N} r_j^{-1} + \sum_{j<k} \omega r_{jk}^{-1}, \tag{1b}$$

where $\omega = WZ^{-1}$. Let $\mathscr{D}(H_N)$ be a core for $H_N(\omega)$ with the following property: Whenever F is a bounded C^2 function and Ψ is in $\mathscr{D}(H_N)$, then $F\Psi$ is also in $\mathscr{D}(H_N)$. Note that $\mathscr{D}(H_N)$ is invariant under multiplication by smoothing functions, but the functions F need not have any properties which guarantee that a particular symmetry subspace of $\mathscr{D}(H_N)$ is also invariant. In particular, $F\Psi$ need not have the same permutational symmetry as Ψ. We now define

$$\varepsilon_N = \inf_{\Psi \text{ in } \mathscr{D}} \frac{\int \Psi H_N(\omega) \Psi dx}{\|\Psi\|^2}. \tag{2}$$

one can similarly define ε_N^+ and ε_N^- if the infimum is taken over Ψ in the symmetric and antisymmetric subspaces $\mathscr{D}^+$ and $\mathscr{D}^-$ respectively. We can now state our main result as:

Theorem 1. *For every fixed ω, there is an N_0 such that $N \geqq N_0$ implies $\varepsilon_N = \varepsilon_{N-1}$.*

We will prove Theorem 1 by showing that for sufficiently large N

$$\int \Psi_N H_N(\omega) \Psi_N dx > \varepsilon_{N-1} \|\Psi\|^2 \tag{3}$$

for all Ψ in $\mathscr{D}(H_N)$. This implies that $\varepsilon_N \geqq \varepsilon_{N-1}$. Since $\varepsilon_N \leqq \varepsilon_{N-1}$ always, we conclude that $\varepsilon_N = \varepsilon_{N-1}$. Furthermore, it follows from the Hunziker-van Winter-Zhislin (HVZ) theorem [11–14] that the essential spectrum of $H_N(\omega)$ begins at ε_{N-1}. Therefore $H_N(\omega)$ has discrete spectrum if and only if $\varepsilon_N < \varepsilon_{N-1}$, so that our theorem implies that $H_N(\omega)$ has no discrete spectrum for $N \geqq N_0$. Since (3) is a strict inequality, we can also conclude that ε_N is not an eigenvalue of $H_N(\omega)$ for sufficiently large N. Our method of proof will also show that $N_0 \leqq cZ^2$ for some constant c.

We emphasize again that our proof requires smoothing functions F which do not leave the symmetric and antisymmetric domains $\mathscr{D}^\pm$ invariant. Thus the above statements are valid only if we impose no permutational symmetry restrictions on Ψ. However, we can extend Theorem 1 and the discussion in the preceding paragraph to bosons as follows: Suppose $\varepsilon_N = \varepsilon_{N-1}$ and ε_{N-1} is not an eigenvalue of $H_{N-1}(\omega)$. Then the HVZ theorem implies that $\varepsilon_{N-1} = \varepsilon_{N-2}$. Therefore, there is an N' so that $\varepsilon_N = \varepsilon_{N-1} = \ldots = \varepsilon_{N'}$ and $\varepsilon_{N'}$ is an eigenvalue of $H_{N'}(\omega)$. It is well known [14] that the ground state of $H_{N'}(\omega)$ is unique and positive, which implies that the ground state is symmetric. Therefore $\varepsilon_{N'} = \varepsilon_{N'}^+$. Now $\varepsilon_N^+ \leqq \varepsilon_{N'}^+$, and $\varepsilon_N^+ \geqq \varepsilon_N = \varepsilon_{N'} = \varepsilon_{N'}^+$, so that $\varepsilon_N^+ = \varepsilon_N$ for all $N > N'$. Thus we conclude, as above, that for some constant c:

a) $\varepsilon_N^+ = \varepsilon_{N-1}^+ = \varepsilon_{N_0}^+$ for $N \geqq N_0$,
b) $H_N(\omega)$ has no discrete spectrum in the symmetric subspace $\mathscr{D}^+$ for $N \geqq N_0$,
c) ε_N^+ is not an eigenvalue of $H_N(\omega)$ for $N \geqq cZ^2$, and
d) $N_0 \leqq cZ^2$.

Theorem 1 implies that $\varepsilon_N = \varepsilon_{N_0}$ for all $N \geqq N_0$, so that $\varepsilon_N^- \geqq \varepsilon_N \geqq \varepsilon_{N_0}$. Thus there is a constant A such that

$$\varepsilon_N^- \geqq -A, \tag{4}$$

i.e. the fermion ground state energy is bounded uniformly in N. This means that if Theorem 1 does not hold for fermions, then, at worst, $\varepsilon_{N-1}^- - \varepsilon_N^-$ can be made arbitrarily small.

Our results extend to more general Hamiltonians than (1). In particular, Theorem 1 holds for molecules and for Hamiltonians in which potentials of the form $1/r$ are replaced by $1/r^\gamma$ where $0<\gamma<2$. For simplicity we give a detailed proof of Theorem 1 in Sect. II only for the Hamiltonian given by (1). Generalizations are discussed in Sect. III.

We will use the following notation. Let $X = \{x = (x_1 \dots x_N)\}$ where $x_j = (\mathbf{r}_j, \alpha_j)$ denotes the space and (if necessary) spin coordinates, α_j, of the j^{th} particle. Integrals of the form $\int dx$ include both integration over $\mathbb{R}^{3N}$ and summation over spin; and $\int d\hat{x}_k$ means integration over coordinates of all particles except the k^{th}. As usual $r_k = |\mathbf{r}_k| = |x_k|$ and $r_{jk} = |\mathbf{r}_j - \mathbf{r}_k|$. We now fix $p \geqq 2$ and define

$$|r|_p = \left(\sum_{j=1}^N r_j^p \right)^{1/p},$$

$$|\hat{r}_k|_p = \left(\sum_{j \neq k} r_j^p \right)^{1/p} = (|r|_p^p - r_k^p)^{1/p},$$

$$\Omega_k(B) = \{x : |\hat{r}_k|_p < B r_k\},$$

and

$$\Gamma_k(B) = \Omega_k(B) - \bar{\Omega}_k\left(\frac{B}{2}\right) = \{x : 1 < r_k B |\hat{r}_k|_p^{-1} < 2\}.$$

In what follows, p is fixed and the dependence of $\Omega_k(B)$ and $\Gamma_k(B)$ on p is suppressed. The following properties of $\Omega_k(B)$ are extremely useful and easy to prove:

a) x in $\Omega_k(B) \Rightarrow r_{jk} < (B+1) r_k$
b) x in $\Omega_k(B) \Rightarrow r_k^{-1} < (B^p+1)^{1/p} |r|_p^{-1}$
c) $x \notin \Omega_k(B) \Rightarrow |\hat{r}_k|_p^{-1} \leqq (B^p+1)^{1/p} (B|r|_p)^{-1}$.

We can now sketch the main idea of our proof. In the cone $\Omega_N(B)$ one has by property (a) above

$$-r_N^{-1} + \sum_{j=2}^N \omega r_{jN}^{-1} \geqq -r_N^{-1} + \omega(N-1)(B+1)^{-1} r_N^{-1} = \lambda r_N^{-1}, \tag{5}$$

where $\lambda = \omega(N-1)(B+1)^{-1} - 1$ can be made positive by choosing ω or N

sufficiently large. It is then tempting to say

$$\int_{\Omega_N(B)} \Psi H_N \Psi dx \geqq \int_{\Omega_N(B)} \Psi H_{N-1} \Psi dx \geqq \varepsilon_{N-1} \int_{\Omega_N(B)} |\Psi|^2 dx.$$

However, the second inequality holds only when $\Psi = 0$ on $\partial\Omega_N(B)$ which is not true in general. Therefore, we will multiply Ψ by a smoothing function G so that $G\Psi = 0$ on $X\text{-}\Omega_N(B)$. This will, of course, introduce an error in the kinetic energy, but we will show that this can be bounded outside the region $\{|x|:|r|_p < R\}$ for sufficiently large R. We will further show that for $B \sim N^{1/p}$ the regions $\Omega_k(B)$ $(k = 1 \dots N)$ cover X. Thus, for sufficiently large N and R, the question of whether or not H_N has any discrete spectrum is determined entirely by $\int_{|r|_p < R} \Psi H_N \Psi dx$. We will show that $R \sim N^{3/p}$ and that this is sufficient to show that $\int_{|r|_p < R} \Psi H_N \Psi dx > 0$ for sufficiently large N.

The absence of discrete spectrum is therefore a consequence of the fact that the Coulomb repulsion $\sum_{j<k} \omega r_{jk}^{-1}$ dominates the attraction $-\sum_j r_j^{-1}$ when N is large. Screening occurs when particles are far from the nucleus. The Coulomb repulsion limits the number of particles which can be within a ball of fixed radius. Therefore, when N is large, the Coulomb repulsion forces particles away from the nucleus and into a region where screening gives an effective repulsive potential. This intuitive argument is independent of permutational symmetry and we expect our results to hold for both bosons and fermions. However we have only succeeded in proving that $\varepsilon_N^- \geqq \varepsilon_{N-1} \geqq -A$; we have not excluded the possibility that $\varepsilon_{N-1}^- > \varepsilon_N^- \geqq \varepsilon_{N-1}$. Further discussion of the fermion problem is given in Sect. III.

Results similar to Lemmas 2–6 have been obtained by Uchiyama [1] for $N = 2$ and $\omega > 1$, and by Zhislin [2] for $N - 1 > Z = 1/\omega$ using $p = 2$. However, Zhislin's R grows exponentially with N and his proofs are considerably more complicated.

II. Proof

All of the smoothing functions we need will be defined in terms of a fixed function $g : \mathbb{R}^+ \to \mathbb{R}$ such that

i) g has a continuous second derivative,
ii) $g(t) = 0$ if $t \leqq 1$,
iii) $g(t) = 1$ if $t \geqq 2$,
iv) $0 < g(t) < 1$ if $1 < t < 2$, and
v) $M = \sup_t |g'(t)|^2 (1 - g(t)^2)^{-1} < \infty$.

In order that (v) be satisfied it is sufficient that $g \sim \exp(-(2-t)^n)$ near $t = 2$.

We now give two Lemmas which will allow us to estimate the error in the kinetic energy which comes from our smoothing functions.

Lemma 2. *Fix B and k and let F be any positive function in $C^2(X)$ for which*

$\nabla_j F = 0$ *on* $X - \Gamma_k$ *for all* $j = 1 \dots N$. *Then*

$$\sum_{j=1}^{N} \int F^2 |\nabla_j \Psi|^2 dx = \sum_{j=1}^{N} \int |\nabla_j (F\Psi)|^2 dx + \sum_{j=1}^{N} \int |\Psi|^2 F \Delta_j F dx. \tag{6}$$

Proof. Let $\tilde{\nabla}_k = \bigoplus_{j \neq k} \nabla_j$. Then

$$\sum_{j \neq k} \int |\nabla_j F \Psi|^2 dx = \int |\Psi|^2 |\tilde{\nabla}_k F|^2 dx + \int F^2 |\tilde{\nabla}_k \Psi|^2 dx + 2 \int F \tilde{\nabla}_k F \cdot (|\Psi| \tilde{\nabla}_k |\Psi|) dx. \tag{7}$$

By Green's formula the last term on the right in (7) can be written as:

$$\tfrac{1}{2} \int dx \int_{r_k B/2 < |\hat{r}_k|_p < r_k B} (\tilde{\nabla} F^2) \cdot (\tilde{\nabla} |\Psi|^2) d\hat{x}_k = -\tfrac{1}{2} \int_{\Gamma_k(B)} |\Psi|^2 \tilde{\Delta}_k F^2 dx$$
$$= -\tfrac{1}{2} \int |\Psi|^2 \tilde{\Delta}_k F^2 dx = -\int |\Psi|^2 |\tilde{\nabla}_k F|^2 dx - \int |\Psi|^2 F \tilde{\Delta}_k F.$$

Substituting this in (7) gives

$$\int |\tilde{\nabla}_k (F\Psi)|^2 dx = \int F^2 |\tilde{\nabla}_k \Psi|^2 dx - \int |\Psi|^2 F \tilde{\Delta}_k F dx. \tag{8}$$

Similarly, one can show

$$\int |\nabla_k (F\Psi)|^2 dx = \int F^2 |\nabla_k \Psi|^2 dx - \int |\Psi|^2 F \Delta_k F dx. \tag{9}$$

Combining (8) and (9) gives (6).

We now introduce the smoothing functions $G_k(x_1 \dots x_N) = g(r_k B |\hat{r}_k|_p^{-1})$, where g is defined above.

Lemma 3. *Fix k and B. Then for all Ψ in $\mathcal{D}(H_N)$*

$$-\sum_{j=1}^{N} \int \Psi \Delta_j \Psi dx = \sum_{j=1}^{N} \int |\nabla_j (G_k \Psi)|^2 dx + \sum_{j=1}^{N} \int |\nabla_j (\sqrt{1 - G_k^2} \Psi)|^2 dx$$
$$- \sum_{j=1}^{N} \int |\Psi|^2 |\nabla_j G_k|^2 (1 - G_k^2)^{-1} dx. \tag{10}$$

Proof. Both G_k and $\sqrt{1 - G_k^2}$ satisfy the hypotheses of Lemma 2. Therefore

$$\sum_{j=1}^{N} - \int \Psi \Delta_j \Psi dx = \sum_{j=1}^{N} \int G_k^2 |\nabla_j \Psi|^2 dx + \sum_{j=1}^{N} \int (1 - G_k^2) |\nabla_j \Psi|^2 dx$$
$$= \sum_{j=1}^{N} \int |\nabla_j (G_k \Psi)|^2 dx + \sum_{j=1}^{N} \int |\nabla_j (\sqrt{1 - G_k^2} \Psi)|^2 dx$$
$$+ \sum_{j=1}^{N} \int |\Psi|^2 (G_k \Delta_j G_k + \sqrt{1 - G_k^2} \Delta_j \sqrt{1 - G_k^2}) dx.$$

The theorem then follows from the fact that for all j

$$G_k \Delta_j G_k + \sqrt{1 - G_k^2} \Delta_j \sqrt{1 - G_k^2} = -|\nabla_j G_k|^2 (1 - G_k^2)^{-1}. \tag{11}$$

We are now ready to estimate $E_N(\Psi) \equiv \int \Psi H_N \Psi dx$. We will let

$$H_{N-1}^k = -\sum_{j\neq k} \Delta_j - \sum_{j\neq k} r_j^{-1} + \sum_{\substack{i<j\\ i,j\neq k}} \omega r_{ij}^{-1}$$

$$= H_N - \left(-\Delta_k - r_k^{-1} + \sum_{j\neq k} \omega r_{jk}^{-1} \right) \tag{12}$$

and note that

$$\int \Psi H_{N-1}^k \Psi \, dx \geqq \varepsilon_{N-1} \|\Psi\|^2 \text{ for all } \Psi \text{ in } \mathscr{D}(H_N). \tag{13}$$

Lemma 4. *Fix $p \geqq 2$ and $B \geqq 2$. Then for all Ψ in $\mathscr{D}(H_N)$*

$$E_N(\Psi) \geqq \varepsilon_{N-1} \|G_k \Psi\|^2 + E_N(\sqrt{1-G_k^2}\Psi) - 2^{1+2/p} M B^2 \cdot \int |\Psi|^2 |r|_p^{-2} dx + \lambda \int |G_k \Psi|^2 |r|_p^{-1} dx, \tag{14}$$

where $\lambda = \omega(N-1)(B+1)^{-1} - 1$. (15)

Proof. It follows from Lemma 3 that

$$E_N(\Psi) = E_N(G_k\Psi) + E_N(\sqrt{1-G_k^2}\Psi) - \sum_{j=1}^{N} \int |\Psi|^2 |\nabla_j G_k|^2 (1-G_k^2)^{-1} dx. \tag{16}$$

Now, using (12), one sees easily that

$$E_N(G_k\Psi) \geqq \int (G_k\Psi) H_{N-1}^k (G_k\Psi) dx + \int |G_k|^2 |\Psi|^2 \left(-r_k^{-1} + \sum_{j\neq k} \omega r_{jk}^{-1} \right) dx. \tag{17}$$

Since $G_k\Psi = 0$ for x in $X - \Omega_k(B)$, the last term on the right in (17) becomes

$$\int_{\Omega_k(B)} |G_k|^2 |\Psi|^2 \left(-r_k^{-1} + \sum_{j\neq k} \omega r_{jk}^{-1} \right) dx > \int \lambda |G_k\Psi|^2 r_k^{-1} dx \geqq \lambda \int |G_k\Psi|^2 |r|_p^{-1} dx,$$

where we proceed first as in (5) and then use the fact that $r_k < |r|_p$. If we combine this with (13) applied to $G_k\Psi$, (17) becomes

$$E_N(G_k\Psi) \geqq \varepsilon_{N-1} \|G_k\Psi\|^2 + \lambda \int |G_k\Psi|^2 |r|_p^{-1} dx. \tag{18}$$

We now need to estimate $\sum_{j=1}^{N} \int |\Psi|^2 |\nabla_j G_k|^2 (1-G_k^2)^{-1} dx$. We first note that $\nabla_j G_k \neq 0 \Rightarrow 1 < r_k B |\hat{r}_k|_p^{-1} < 2$. Then for $j \neq k$

$$|\nabla_j G_k|^2 = \left| \frac{\partial}{\partial r_j} g(r_k B |\hat{r}_k|_p^{-1}) \right|^2 = |\hat{r}_k|_p^{-2} (r_k B |\hat{r}_k|_p^{-1})^2 (r_j |\hat{r}_k|_p^{-1})^{2p-2} \cdot |g'(r_k B |\hat{r}_k|_p^{-1})|^2$$

so that for all $p \geqq 2$

$$\sum_{j\neq k} |\nabla_j G_k|^2 (1-G_k^2)^{-1} \leqq 4M |\hat{r}_k|_p^{-2} |\hat{r}_k|_p^{-p} \sum_{j\neq k} r_j^p (r_j/|\hat{r}_k|_p)^{p-2} \leqq 4M |\hat{r}_k|_p^{-2}.$$

Similarly,

$$|\nabla_k G_k|^2 (1-G_k^2)^{-1} \leqq M B^2 |\hat{r}_k|_p^{-2}.$$

Combining these estimates and applying property (c) of $\Omega_k(B/2)$, one finds that for all $B \geqq 2$

$$\sum_{j=1}^{N} |\nabla_j G_k|^2(1-G_k^2)^{-1} \leqq M(B^2+4)|\hat{r}_k|_p^{-2} \leqq M(1+4B^{-2})(B^p+2^p)^{2/p}|r|_p^{-2}$$
$$\leqq 2^{1+2/p}MB^2|r|_p^{-2}. \tag{19}$$

Substituting (18) and (19) in (16) gives (14).

We will prove our main theorem by repeated application of Lemma 4. To sketch the idea we consider $N=3$. Applying Lemma 4 twice one gets

$$E_3(\Psi) \geqq \varepsilon_2(\|G_1\Psi\|^2 + \|G_2\sqrt{1-G_1^2}\Psi\|^2) + E_3(\sqrt{1-G_1^2}\sqrt{1-G_2^2}\Psi)$$
$$-8MB^2\int|\Psi|^2|r|_p^{-2}dx + \lambda\int[|G_1\Psi|^2 + G_2(1-G_1^2)|\Psi|^2]|r|_p^{-1}dx.$$

As we will see below, for suitable choices of B,

$$E_3(\sqrt{1-G_1^2}\sqrt{1-G_2^2}\Psi) \geqq \varepsilon_2\|\sqrt{1-G_1^2}\sqrt{1-G_2^2}\Psi\|^2$$
$$+\lambda\int(1-G_1^2)(1-G_2^2)|\Psi|^2|r|_p^{-1}dx,$$

so that

$$E_3(\Psi) \geqq \varepsilon_2\|\Psi\|^2 + \int|\Psi|^2(\lambda|r|_p - 8MB^2)|r|_p^{-2}dx. \tag{20}$$

We need to generalize this to arbitrary N and to find conditions under which the last term can be made positive. Since $\lambda|r|_p - 8MB^2 > 0$ only for large $|r|_p$ we will also need to smooth around $\{x : |r|_p \leqq R\}$ for a suitable choice of R.

Lemma 5. *Fix $p \geqq 2$ and let $B = 2^{1+1/p}(N-1)^{1/p}$. Then for all Ψ in $\mathscr{D}$,*

$$E_N(\Psi) \geqq \varepsilon_{N-1}\|\Psi\|^2 + \int|\Psi|^2(\lambda|r|_p - 2^{1+2/p}M(N-1)B^2)|r|_p^{-2}dx, \tag{21}$$

where $\lambda = \omega(N-1)(B+1)^{-1} - 1$.

Proof. Let $\Psi_1 = \Psi$, $\Psi_{k+1} = \sqrt{1-G_k^2}\Psi_k (k = 1 \dots N-1)$. Then by repeated application of Lemma 4

$$E_N(\Psi) \geqq \varepsilon_{N-1}\sum_{k=1}^{N}\|G_k\Psi_k\|^2 + E_N(\Psi_N) - 2^{1+2/p}M(N-1)B^2\int|\Psi|^2|r|_p^{-2}dx$$
$$+\lambda\sum_{k=1}^{N-1}\int|G_k\Psi_k|^2|r|_p^{-1}dx. \tag{22}$$

Now $\Psi_{k+1} \neq 0 \Rightarrow G_k \neq 1 \Rightarrow r_k B|\hat{r}_k|_p^{-1} < 2$, and $\Psi_N \neq 0 \Rightarrow \Psi_k \neq 0$ for all $k \leqq N$. Thus, whenever $\Psi_N \neq 0$ we have

$$r_k^p B^p \leqq 2^p \sum_{j \neq k} r_j^p \quad (k = 1 \dots N-1). \tag{23}$$

Adding these $N-1$ inequalities gives

$$|\hat{r}_N|_p^p (B/2)^p \leqq (N-2)|\hat{r}_N|_p^p + (N-1)r_N^p,$$

so that

$$r_N^p \geqq [(B/2)^p - (N-2)](N-1)^{-1}|\hat{r}_N|_p^p.$$

Now choose $B = 2(2(N-1))^{1/p}$. Then $N \geqq 2$ implies $B > 2$ so that

$$r_N \geqq (N(N-1)^{-1})^{1/p}|\hat{r}_N|_p > |\hat{r}_N|_p > B^{-1}|\hat{r}_N|_p.$$

Thus $\left(-r_N^{-1}+\sum_{j=1}^{N-1}\omega r_{jN}^{-1}\right)>\lambda r_N^{-1}$ whenever $\Psi_N\neq 0$. Then, using (12) and (13) as in the proof of Lemma 4, one finds

$$E_N(\Psi_N)\geqq \varepsilon_{N-1}\|\Psi_N\|^2+\lambda\int|\Psi_N|^2|r|_p^{-1}dx. \tag{24}$$

Substituting (24) in (22) and using

$$\sum_{j=1}^{N-1}|G_k\Psi_k|^2+|\Psi_N|^2=|\Psi|^2,$$

one finds

$$E_N(\Psi)\geqq \varepsilon_{N-1}\|\Psi\|^2+\lambda\int|\Psi|^2|r|_p^{-1}dx-2^{1+2/p}M(N-1)B^2\int|\Psi|^2|r|_p^{-2}dx.$$

Remark. Let $R_1=2^{1+2/p}M(N-1)B^2\lambda^{-1}$. If $\Psi=0$ whenever $|r|_p<R_1$, then Lemma 5 implies that $E_N(\Psi)\geqq\varepsilon_{N-1}\|\Psi\|^2$. Since $B<B+1\leqq 3B/2$

$$\omega 2^{-1-1/p}(N-1)^{1-1/p}>\lambda\geqq\omega 3^{-1}2^{-1/p}(N-1)^{1-1/p}-1, \tag{25}$$

so that when N is large $\lambda>(\omega/5)(N-1)^{1-1/p}$ and $R_1<40\cdot 2^{4/p}M(N-1)^{3/p}\omega^{-1}$.

Lemma 6. *For every fixed ω there are constants N_ω and c_ω such that for every $N\geqq N_\omega$ and for every Ψ in $\mathscr{D}(H_N)$ there is a Ψ_0 in $\mathscr{D}(H_N)$ such that*

a) $\Psi_0=0$ *whenever* $r\geqq 2R$ *where* $(2/5)c_\omega(N-1)^{3/p}<R\leqq c_\omega(N-1)^{3/p}$, and

b) $E_N(\Psi)\geqq\varepsilon_{N-1}(\|\Psi\|^2-\|\Psi_0\|^2)+\int\Psi_0H_N(\omega/2)\Psi_0\,dx.$ (26)

Proof. Let $G_0(x)=g(|r|_pR^{-1})$ and $\tilde\nabla=\bigoplus_{j=1}^{N}\nabla_j$. Then proceeding as in the proofs of Lemmas 2 and 3 one can show that

$$\int G_0^2|\tilde\nabla\Psi|^2dx=\int|\tilde\nabla G_0\Psi|^2dx+\int|\Psi|^2G_0\tilde\Delta G_0\,dx$$

and similarly for $\sqrt{1-G_0^2}$. Thus

$$-\sum_{j=1}^{N}\int\Psi\Delta_j\Psi\,dx=\sum_{j=1}^{N}\int|\nabla_j(G_0\Psi)|^2dx+\sum_{j=1}^{N}\int|\nabla_j\sqrt{1-G_0^2}\,\Psi|^2dx$$
$$-\sum_{j=1}^{N}\int_{R<|r|_p<2R}|\nabla_jG_0|^2(1-G^2)^{-1}|\Psi|^2dx. \tag{27}$$

Since $|\nabla_jG_0|=R^{-1}r_j^{p-1}|r|_p^{-(p-1)}|g'(|r|_pR^{-1})|$,

$$\sum_{j=1}^{N}|\nabla_jG_0|^2(1-G^2)^{-1}\leqq R^{-2}M|r|_p^{-p}\sum_{j=1}^{N}r_j^p=R^{-2}M.$$

Let $\Psi_0=\sqrt{1-G_0^2}\,\Psi$ and $\Psi_1=G_0\Psi$. Then $\Psi_0\neq0\Rightarrow|r|_p<2R$ and $\Psi_1\neq0\Rightarrow|r|_p>R$. Using (27) and then applying Lemma 5 to Ψ_1 one finds

$$E_N(\Psi)\geqq E_N(\Psi_1)+E_N(\Psi_0)-MR^{-2}\int_{R<|r|_p<2R}|\Psi|^2dx$$
$$\geqq\varepsilon_{N-1}\|\Psi_1\|^2+\lambda\int|\Psi_1|^2|r|_p^{-1}dx-2^{1+2/p}M(N-1)B^2\int|\Psi_1|^2|r|_p^{-2}dx$$
$$+\int\Psi_0H_N(\omega)\Psi_0\,dx-MR^{-2}\int_{R<|r|_p<2R}|\Psi|^2dx$$

$$\geqq \varepsilon_{N-1}\|\Psi_1\|^2 + \int |\Psi_1|^2 |r|_p^{-2}[|r|_p\lambda/2 - 2^{1+2/p}M(N-1)B^2]dx$$
$$+ \int \Psi_0 H_N(\omega/2)\Psi_0 dx$$
$$+ \int_{R<|r|_p<2R} \left[(\lambda/2)|r|_p^{-1}|\Psi_1|^2 + \tfrac{1}{2}\sum_{i<k} \omega r_{jk}^{-1}|\Psi_0|^2 - MR^{-2}|\Psi|^2\right]dx. \quad (28)$$

Choose

$$R = 2^{2+2/p}M(N-1)B^2\lambda^{-1} \text{ with } B = 2^{1+1/p}(N-1)^{1/p}. \quad (29)$$

Since $\Psi_1 = 0$ when $|r|_p < R$, (29) implies

$$\int |\Psi_1|^2 |r|_p^{-2}(|r|_p\lambda/2 - 2^{1+2/p}M(N-1)B^2)dx > 0. \quad (30)$$

Now use (25) to choose N_ω so that $N \geqq N_\omega$ implies

$$\lambda > \left(\frac{\omega}{5}\right)(N-1)^{1-1/p} > 0.$$

Then $\omega N(N-1)/4 > \lambda$ for all $N \geqq N_\omega$, so that the last term on the right in (28) is bounded below by

$$\int_{R<|r|_p<2R} [(\lambda/2)(2R)^{-1}|\Psi_1|^2 + 4^{-1}\omega N(N-1)(4R)^{-1}|\Psi_0|^2 - MR^{-2}|\Psi|^2]dx$$
$$\geqq \int_{R<|r|_p<2R} [\lambda(4R)^{-1}(|\Psi_1|^2 + |\Psi_0|^2) - MR^{-2}|\Psi|^2]dx$$
$$= \int_{R<|r|_p<2R} |\Psi|^2 R^{-1}(\lambda/4 - MR^{-1})dx$$
$$= \int_{R<|r|_p<2R} |\Psi|^2 \lambda 4^{-1}R^{-1}[1 - (2^{2+4/p}(N-1)^{1+2/p})^{-1}]dx > 0. \quad (31)$$

Thus $N \geqq N_\omega$ implies

$$E_N(\Psi) \geqq \varepsilon_{N-1}\|\Psi_1\|^2 + \int \Psi_0 H_N(\omega/2)\Psi_0 dx.$$

Since $|\Psi|^2 = |\Psi_1|^2 + |\Psi_0|^2$, this gives (26). To complete the proof we note that (25), and (29) imply that for $N \geqq N_\omega$

$$\omega^{-1}2^{5+5/p}M(N-1)^{3/p} < R \leqq \omega^{-1}2^{4+4/p}\cdot 5(N-1)^{3/p}. \quad (32)$$

This gives (a) if $c_\omega = 80\cdot 2^{4/p}M\omega^{-1}$.

Proof of Theorem 1. By Lemma 6, if suffices to show that

$$\int_{|r|_p<2R} \Psi_0 H_N(\omega/2)\Psi_0 dx \geqq \varepsilon_{N-1}\|\Psi_0\|^2,$$

where $H_N(\omega/2) = H_N^0 + \frac{1}{2}\sum_{j<k} \omega r_{jk}^{-1}, H_N^0 = -\sum_{j=1}^{N}(\Delta_j + r_j^{-1})$, and R is given by (29). It is well-known that $H_0 \geqq -N/4$ and, as before, $|r|_p < 2R \Rightarrow r_{jk} < 4R$. Therefore,

$$\int_{|r|_p<2R} \Psi_0 H_N(\omega/2)\Psi_0 dx \geqq \left[-\frac{N}{4} + \omega N(N-1)(16R)^{-1}\right]\|\Psi_0\|^2$$
$$\geqq \left(\frac{N}{16}\right)[-4 + \omega c_\omega^{-1}(N-1)^{1-3/p}]\|\Psi_0\|^2, \quad (33)$$

where the last inequality follows from (32) for $N \geqq N_\omega$. When $p > 3$, (33) can be made arbitrarily large by choosing N sufficiently large. Let $p = 4$ and choose $N_0 \geqq N_\omega$ so that $(N_0/16)[\omega c_\omega^{-1}(N-1)^{1/4} - 4] > \varepsilon_{N-1}$. Then by Lemma 6

$$E_N(\Psi) > \varepsilon_{N-1}(\|\Psi\|^2 - \|\Psi_0\|^2) + \varepsilon_{N-1}\|\Psi\|_0^2 = \varepsilon_{N-1}\|\Psi\|^2.$$

III. Remarks and Generalization

A. Dependence of N_0 on Z

We consider the case $W = 1$ so that $\omega = Z^{-1}$. By the remark following Lemma 5, it follows that the N_ω of Lemma 6 grows no worse than $Z^{p/p-1}$. In fact (25) implies $(N_\omega - 1) \leqq [15/(5 \cdot 2^{-1/p} - 3)]^{p/p-1}\, Z^{p/p-1}$. Since p can be chosen arbitrarily large, we find $N_\omega < 8Z + 1$. Thus, we conclude that for large Z the dependence of N_0 on Z is determined by (33). Since ε_{N-1} is not known exactly, we will find N_0 large enough to satisfy $-1 + \omega(4c_\omega)^{-1}(N-1)^{1-3/p} \geqq 0$. Thus

$$(N_0 - 1)^{(p-3)/p} = 4c_\omega \omega^{-1} = 5 \cdot 2^6 2^{4/p} M Z^2.$$

when $p = 4$, this gives $N_0 \leqq 5^4 2^{28} M^4 Z^8$. However, since p can be made arbitrarily large, we obtain the better estimate

$$N_0 - 1 \leqq 320 M Z^2. \tag{34}$$

B. Molecules

Our results remain true if we replace $-Zr_k^{-1}$ in $H_N(W, Z)$ by $-\sum_{\ell=1}^{L} Z_\ell |\mathbf{r}_k - \mathbf{R}_\ell|^{-1}$ where $\mathbf{R}_\ell$ are fixed. Choose $\tilde{R}$ so that $(B^p + 1)^{-1/p}\tilde{R}/2 = \max\{R_1 \ldots R_L\}$. Then if $|r|_p \geqq \tilde{R}$ and x in $\Omega_k(B)$, $R_\ell \leqq (B^p + 1)^{-1/p}|r|_p/2 < r_k/2$, and

$$\begin{aligned} -\sum_{\ell=1}^{L} Z_\ell |\mathbf{r}_k - \mathbf{R}_\ell|^{-1} + W \sum_{j \neq k} r_{jk}^{-1} &\geqq -2\sum_{\ell=1}^{L} Z_\ell r_k^{-1} + W(N-1)(B+1)^{-1} r_k^{-1} \\ &= Z\lambda r_k^{-1}, \end{aligned}$$

where $Z = 2\sum_{\ell=1}^{L} Z_\ell$ and $\lambda = WZ^{-1}(N-1)(B+1)^{-1} - 1$ as before. Since $\tilde{R} \sim B \sim (N-1)^{1/p}$ and $R \sim B^3 \sim (N-1)^{3/p}$ in Lemma 6, $R > \tilde{R}$ for sufficiently large N. Let Ψ_1 be as in Lemma 6. Then $\Psi_1 = 0$ for $r < \tilde{R} < R$ and Lemmas 4 and 5 remain valid when applied to Ψ_1. Thus Lemma 6 holds with $\omega = W\left(2\sum_{\ell=1} Z_\ell\right)^{-1}$ and a possibly larger N_ω.

C. Other Power Law Potentials

Our methods can easily be generalized to show that the Hamiltonian

$$H_N^\gamma(\omega) = -\sum_{j=1}^{N} \Delta_j - \sum_{j=1}^{N} r_j^{-\gamma} + \omega \sum_{j<k} r_{jk}^\gamma$$

also satisfies Theorem 1, when $0 < \gamma < 2$.

Since x in $\Omega_k(B)$ implies that $-r_k^{-\gamma}+\omega\sum_{j\neq k} r_{jk}^{-\gamma}\geqq\lambda_\gamma r_k^{-\gamma}$, where $\lambda_\gamma=\omega(N-1)(B+1)^{-\gamma}-1$, Lemmas 4 and 5 remain valid if $\lambda\int|G_k\Psi|^2|r|_p^{-1}dx$ is replaced by $\lambda_\gamma\int|G_k\Psi|^2|r|_p^{-\gamma}dx$. Then in the proof of Lemma 6, (30) becomes $\int|\Psi_1|^2|r|_p^{-2}(|r|_p^{2-\gamma}\lambda_\gamma-2^{2+2/p}M(N-1)B^2)dx>0$ if $R^{2-\gamma}=2^{2+2/p}M(N-1)B^2\lambda_\gamma^{-1}=c_1(N-1)^{(2+\gamma)/p}$ for some constant c_1. The last integral in (28) can again be made positive as in (31) since

$$(\lambda_\gamma/4)R^{-\gamma}-MR^{-2}=(\lambda_\gamma/4)R^{-\gamma}[1-(2^{2+4/p}(N-1)^{1+2/p})^{-1}]>0.$$

Thus Lemma 6 holds with $R\leqq c_2(N-1)^{1/s}$ where $s=p(2-\gamma)/(2+\gamma)$ for some constant c_2. We complete the proof as before using

$$\begin{aligned}\int_{|r|_p<2R}\Psi_0H_N(\omega/2)\Psi_0dx &\geqq\left(-\frac{N}{4}+\omega N(N-1)16^{-1}R^{-\gamma}\right)\|\Psi_0\|^2\\ &=\frac{N}{4}(-1+c_3(N-1)^{1-\gamma/s})\|\Psi_0\|^2,\end{aligned}\tag{35}$$

for some positive constant c_3. For each fixed $\gamma<2$, we can choose p so that $s>\gamma$ and (35) can be made arbitrarily large.

D. Increasing the Interaction

If N is fixed, $H_N(W,Z)$ has no bound states if the nuclear charge Z is sufficiently small or the interaction parameter W is sufficiently large. To be precise, for each fixed N there is an ω_0 such that $\omega=WZ^{-1}>\omega_0$ implies that $H_N(\omega)$ has no discrete spectrum.

When $N=2$ this result was first proven by Uchiyama [15]. Since the fermion ground state is always a singlet when $N=2, \varepsilon_2^+=\varepsilon_2^-=\varepsilon_2$ so that both bosons and fermions have the same critical ω_0. Using a perturbation expansion in ω, Stillinger [16] has estimated $\omega_0\simeq 1.0975$. Ruskai [17] has used Hill's techniques [4, 5] to obtain the less accurate, but rigorous bound $\omega_0<1.343$.

We now sketch the proof that $H_N(\omega)$ has no discrete spectrum for sufficiently large ω. As before, the proof for bosons follows from the proof for particles without any permutational symmetry restrictions. Lemmas 2–5 do not depend on the value of ω. Lemma 6 holds for arbitrary N if ω_1 is chosen so that $\lambda>(\omega/5)(N-1)^{1-1/p}$ whenever $\omega>\omega_1$ as in (25). To complete the proof, we write (33) as

$$\int_{|r|_p<2R}\Psi_0H_N(\omega/2)\Psi_0dx\geqq(N/4)[-1+\omega^2c_N]\|\Psi_0\|^2\tag{36}$$

for some constant c_N. Since (36) can be made arbitrarily large by choosing ω sufficiently large, the argument following (33) can be used to show $E_N(\Psi)\geqq\varepsilon_{N-1}\|\Psi\|^2$ for ω sufficiently large.

E. Fermions

We now indicate which portions of our proof in Sect. II remain valid for fermions, i.e. if we restrict Ψ to $\mathscr{D}^-$ and replace ε_N by ε_N^-. Lemmas 2 and 3 obviously do not depend on permutational symmetry. Before discussing Lemmas 4–6, we note that G_k is symmetric with respect to the interchange $i \leftrightarrow j$ provided $i \neq k$ and $j \neq k$, but not with respect to $i \leftrightarrow k$. Therefore $G_k \Psi$ is antisymmetric in the coordinates of the $N-1$ particles $(1, \ldots, k-1, k+1, \ldots, N)$, so that

$$\int (G_k \Psi) H_{N-1}^k G_k \Psi \, dx \geqq \varepsilon_{N-1}^- \| G_k \Psi \|^2.$$

This is sufficient to extend the proof of Lemma 4 to fermions.

The proof of Lemma 5 does not, unfortunately, hold for fermions. The problem is that $\Psi_k = \prod_{j=1}^{k-1} \sqrt{1 - G_j^2}\, \Psi$ and $G_k \Psi_k$ will not be antisymmetric in general so that Lemma 4 cannot be applied to Ψ_k. The functions $G_k \Psi_k$ are antisymmetric within the clusters $(1, \ldots, k-1)$ and $(k+1, \ldots, N)$ but not with respect to interchanges between clusters. Therefore (13) becomes $\int G_k \Psi_k H_{N-1}^k G_k \Psi_k \geqq \varepsilon_{N-1}^k \| G_k \Psi_k \|^2$ where ε_{N-1}^k is defined by taking the infimum in (2) over the subspace $\mathscr{D}^k(H_{N-1})$ consisting of functions antisymmetric within the clusters $(1, \ldots, k-1)$ and $(k+1, \ldots, N)$. It would suffice to show $\varepsilon_{N-1}^k \geqq \varepsilon_{N-1}^-$, but we know of no reason to expect this to hold in general. We note, however, that $\mathscr{D}^k$ is an invariant subspace of H_{N-1} containing $\mathscr{D}^-$. Choose N' so that $\varepsilon_{N'}^k$ is an eigenvalue of $H_{N'}$ and $\varepsilon_{N'+1}^k = \varepsilon_{N'}^k$. If $N' > 3$ and this ground state happens to be unique, it must be antisymmetric since there are no totally symmetric functions in $\mathscr{D}^k$. Then by the same argument used to show that $\varepsilon_N^+ = \varepsilon_N$, we could conclude $\varepsilon_{N-1}^- = \varepsilon_{N-1}^k$. Unlike the symmetric case, however, we know of no physical or mathematical reason which would justify the assumption that H_N has a unique ground state on $\mathscr{D}^k(H_N)$. Therefore, we cannot conclude that $\varepsilon_N^k = \varepsilon_N^-$, except by occasional accident.

Lemma 6 and the proof of Theorem 1 are invalid for fermions only because they depend on Lemma 5. In fact, our entire analysis extends to fermions except for the application of (13) to $G_k \Psi_k$. If a suitable extention of Lemma 5 could be found, Lemma 6 would also hold. The completion of Theorem 1 can even be modified, if necessary, to accommodate a different dependence of R on N. Since ε_N^- is bounded uniformly in N, we can use (4) to replace (33) by

$$\begin{aligned} \int \Psi_0 H_N(\omega/2) \Psi_0 &\geqq \int \Psi_0 H_N(\omega/4) \Psi_0 \, dx + (\omega/4) \sum_{j<k} \int_{|r|_p \leqq 2R} \Psi_0 r_{jk}^{-1} \Psi_0 \, dx \\ &\geqq (-A + \omega N(N-1)/(32R)) \| \Psi_0 \|^2, \end{aligned} \tag{37}$$

which can be made arbitrarily large by making N large, provided that R grows more slowly than N^2. In the boson case (33) needed R growing more slowly than N, which was satisfied by choosing $p > 3$ since Lemma 5 implied $R \sim (N-1)^{3/p}$. Because the boson result implies uniform boundedness of ε_N^-, (37) can tolerate $R \sim N^t$ for some $t < 2$. Thus a weaker version of Lemma 5 would suffice in the fermion case.

If the fermion proof could be completed with $R \sim N^{k/p}$ for some fixed k and arbitrarily large p, then one could similarly improve the bound on N_0. We first use the well-known fact that the eigenfunctions of H are Slater determinants of the hydrogenic eigenfunctions, $\phi_n^k (k = 1, \ldots, qn^2)$, of $-\Delta + r^{-1}$ which have eigenvalues $\lambda_n^k = -1/4n^2 (k = 1, \ldots, qn^2)$ where q is the number of spin states. Then there is an n_0 such that

$$N \geqq \sum_{n=1}^{n_0-1} qn^2 \geqq c_1 n_0^3$$

and the ground state energy of H^0 is $\geqq -\sum_{n=1}^{n_0} qn^2/4n^2 \geqq -(qc_1^{1/3}/4)N^{1/3}$. Then (33) could be replaced by

$$\int_{|r|_p<2R} \Psi_0 H_N(\omega/2)\Psi_0 dx \geqq [-\alpha N^{1/3} + \beta Z^{-2} N(N-1)^{1-k/p}] \|\Psi_0\|^2$$

for some constants α and β. Then we could conclude, as in Sect. A above, that $N_0 \leqq BZ^{6/5}$ for some constant B.

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