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Absence of Discrete Spectrum in Highly Negative Ions

II. Extension to Fermions

Mary Beth Ruskai

Department of Mathematics, University of Lowell, Lowell, MA 01854, USA

Abstract. We extend the results of [1] to fermions, i.e., we show that if H_N is the Hamiltonian for N electrons in the field of a fixed point charge Z, then there is a constant c such that H_N has no discrete spectrum for $N \geqq N_0 = cZ^{6/5}$.

In a recent paper [1], we showed that the N-particle Coulomb Hamiltonian

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

has no discrete spectrum for sufficiently large N if we make no permutational symmetry restrictions on the domain $\mathscr{D}(H_N)$. However, we were unable to extend these results to fermions and our extension to bosons was indirect. Sigal [2, 3] has recently proved this result for fermions. In this note, we show how to extend our proof to fermions. Despite Sigal's independent proof, we feel that the discussion which follows is valuable for several reasons. The modifications needed to extend our earlier proof to fermions are very minor. Furthermore, these changes lead to a simplification of the proof given in [1] and also allow us to give a direct proof in the boson case by restricting Ψ to the symmetric domain. In addition, our bound $N_0 \leqq cZ^{6/5}$ for the point at which additional electrons will not bind is better than Sigal's[1].

In what follows we use the notation, equation numbers, etc., of [1] unless otherwise stated. We can summarize the content of this note as: All results of [1] remain valid if $\mathscr{D}(H_N)$, ε_N are replaced by either $\mathscr{D}^+(H_N)$, ε_N^+ or by $\mathscr{D}^-(H_N)$, ε_N^-. Furthermore, in the case of fermions there are constants N_0 and c such that H_N has no discrete spectrum when $N \geqq N_0$ and $N_0 \leqq cZ^{6/5}$. The physical interpretation of this result is that a nucleus with infinite mass and charge Z cannot bind more than N_0 electrons[2].

1 Although Sigal does not explicitly give an estimate for N_0, the arguments in Sect. III.A and E of [1] can be used to show that his condition $\varrho \sim N^{2/3}$ implies $N_0 \sim Z^2$

2 We have not excluded the possibility of bound states corresponding to eigenvalues embedded in the continuous spectrum

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As we discussed in Sect. III.E, to extend the results of [1] to fermions one need only extend the proof of Lemma 5 to fermions. Lemma 5 did not preserve permutational symmetry because it used the asymmetric partition of unity

$$\sum_{k=1}^{N-1}\prod_{j=1}^{k-1}(1-G_j^2)G_k^2+\prod_{j=1}^{N-1}(1-G_j^2)=1\,.$$

Following Sigal [3], we define a symmetric partition of unity as follows. Let G_k be as before and define

$$F_k=G_k\Bigg/\left(\sum_{l=1}^{N}G_l^2\right)^{1/2},\qquad (k=1,\dots,N)\,.$$

Clearly $\sum_{k=1}^{N}F_k^2=1$. The argument following (23) can be modified to show that if $B=2N^{1/p}$, then the regions $\{\Omega_k(B/2):k=1,\dots,N\}$ cover $\mathbb{R}^{3N}$ so that $\sum_{l=1}^{N}G_l^2\geqq 1$. Therefore, the smoothing functions, F_k, are well-defined and satisfy $0\leqq F_k\leqq G_k\leqq 1$. Furthermore, $\operatorname{supp}F_k=\operatorname{supp}G_k$ so that both F_k and G_k vanish outside $\Omega_k(B)$.

To estimate the error in the kinetic energy introduced by these smoothing functions, we again follow Sigal [3] and instead of Lemma 3 use the formula:

$$|\nabla_i\Psi|^2=\sum_{k=1}^{N}|\nabla_i(F_k\Psi)|^2-|\Psi|^2\sum_{k=1}^{N}|\nabla_iF_k|^2\,. \tag{38}$$

This can be proven by modifying (7), summing over all F_k, and noting that $\sum_{k=1}^{N}F_k\nabla_iF_k=0$. It will be useful to bound the last term in (38) by using

$$\begin{aligned}\sum_{k=1}^{N}|\nabla_iF_k|^2&=\left(\sum_{k=1}^{N}|\nabla_iG_k|^2\right)\left(\sum_{k=1}^{N}G_k^2\right)^{-1}-\left(\sum_{k=1}^{N}G_k\nabla_iG_k\right)^2\left(\sum_{k=1}^{N}G_k^2\right)^{-2}\\&\leqq\sum_{k=1}^{N}|\nabla_iG_k|^2\,.\end{aligned}\tag{39}$$

Finally we note that the estimates obtained from (39) will involve $M_1=\sup_t|g'(t)|$ rather than the M used[3] in [1]. We can now replace Lemmas 4 and 5 by the following slightly modified version of Lemma 5 which we call

Lemma 4 1/2. *Fix $p\geqq 2$ and let $B=2N^{1/p}$. Then for all Ψ in $\mathscr{D}$,*

$$E_N(\Psi)\geqq\varepsilon_{N-1}\|\Psi\|^2+\int|\Psi|^2[\lambda|r|_p-2^{1+2/p}NM_1^2B^2]|r|_p^{-2}dx\,, \tag{40}$$

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

3 Condition (v) in the definition of $g(t)$ can now be eliminated provided a suitable modification is also made in the smoothing by G_0 in the proof of Lemma 6

Proof. Proceeding as in the proof of Lemma 4 and using (38) and (39), we find

$$\begin{aligned} E_N(\Psi) &= \sum_{k=1}^{N} E_N(F_k\Psi) - \sum_{i=1}^{N}\sum_{k=1}^{N} \int |\Psi|^2 |\nabla_i F_k|^2 dx \\ &\geqq \sum_{k=1}^{N} \varepsilon_{N-1} \|F_k\Psi\|^2 + \lambda \sum_{k=1}^{N} \int |F_k\Psi|^2 r_k^{-1} dx \\ &\quad - \sum_{i=1}^{N}\sum_{k=1}^{N} \int |\Psi|^2 |\nabla_i G_k|^2 dx \\ &\geqq \varepsilon_{N-1} \|\Psi\|^2 + \lambda \int |\Psi|^2 |r|_p^{-1} dx \\ &\quad - \sum_{k=1}^{N}\sum_{i=1}^{N} \int |\Psi|^2 |\nabla_i G_k|^2 dx . \end{aligned} \tag{41}$$

To estimate the last term on the right in (41) we use a slight modification of (19),

$$\sum_{k=1}^{N} |\nabla_i G_k|^2 \leqq 2(2^{1/p} M_1 B)^2 |r|_p^{-2} .$$

Substituting this in (41) and summing over k merely introduces a factor of N so that we conclude

$$E_n(\Psi) \geqq \varepsilon_{N-1} \|\Psi\|^2 + \lambda \int |\Psi|^2 |r|_p^{-1} dx - 2N(2^{1/p} M_1 B)^2 \int |\Psi|^2 |r|_p^{-2} dx ,$$

which is the desired result.

With the understanding that Lemmas 4 and 5 are to be replaced by the above Lemma 4 1/2, we now claim that all results in [1] remain valid if $\mathscr{D}$, ε_N are replaced by $\mathscr{D}^+$, ε_N^+ or $\mathscr{D}^-$, ε_N^-. In fact, it is easy to see, as we discussed in Sect. III.E, that all steps in the proofs of Lemma 4 1/2 and [1] remain valid if Ψ is restricted to either the symmetric or antisymmetric domain and ε_N is replaced by ε_N^+ or ε_N^-. The only change in the proofs of Lemma 6 and the main theorem come from slightly changing the definition of R from (29) to

$$R = 4N(M_1 B 2^{1/p})^2 \lambda^{-1}$$

with $B = 2N^{1/p}$. Since this change does affect the dependence of R on N, i.e. $R \sim N^{3/p}$, the arguments given in [1] remain valid.

The proof that $N_0 \leqq cZ^{6/5}$ in the fermion case, was already given at the end of Sect. III.E.

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