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A multiparticle Coulomb system with bound state at threshold

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Abstract. We consider the two-electron Hamiltonian $H=-\Delta_1-\Delta_2-r_1^{-1}-r_2^{-1}+Ar_{12}^{-1}$ at precisely that critical value of A where the ground state energy has just hit the continuum. For that A, it is proven that H has a square integrable eigenfunction at the bottom of the continuum.

1. Introduction

The class of Hamiltonians

$$H(A)=-\Delta_1-\Delta_2-r_1^{-1}-r_2^{-1}+Ar_{12}^{-1} \tag{1}$$

on $L^2(\mathbb{R}^6, \mathrm{d}x_1\,\mathrm{d}x_2)$, $x_1, x_2 \in \mathbb{R}^3$, $r_1=|x_1|$, $r_2=|x_2|$, $r_{12}=|x_1-x_2|$, enters naturally in the study of the $1/Z$ expansion for two-electron ions. Since the work of Stillinger (1966) there has been particular interest in the critical value of A (call it A_0) (see e.g. Stillinger and Stillinger 1974) as follows. For any $A>0$, H has continuous spectrum $[-\frac{1}{4}, \infty)$. At $A=0$, H has a ground state at energy $E(0)=-\frac{1}{2}$, and as A is increased, the ground state energy $E(A)$ increases until A_0, $E(A_0)=-\frac{1}{4}$. For simplicity, we have chosen here $-\Delta_1-\Delta_2$ for the kinetic energy, which poses no problem, since by scaling $2H$ is unitarily equivalent to the usual Hamiltonian $-\Delta_1/2-\Delta_2/2-1/r_1-1/r_2+A/r_{12}$. It can be proven (see e.g. Thirring 1979, Leinfelder and Simon 1982) that $A_0<\infty$, and since it is well known that the hydrogenic ion has a bound state, $A_0>1$. Numerically (Stillinger 1966), $A_0\sim 1.1$.

Our main goal in this paper is to prove that at $A=A_0$ there is a ground state, $\psi>0$, $\psi\in L^2(\mathbb{R}^6)$ with $H\psi=-\frac{1}{4}\psi$, i.e. there is a normalisable eigenfunction at threshold. Since short-range potentials in three dimensions do not produce normalisable ground states at thresholds (see e.g. Klaus and Simon 1980), this phenomenon is due to the long-range repulsion of r_{12}^{-1}. We mention that Klaus and Simon (1982) noted that for the three-dimensional model problem, $H=-\Delta+V+\alpha r^{-1}$ where V is spherically

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symmetric, negative, short range with $\inf \sigma(-\Delta+V)<0$, one has a threshold eigenvector at the critical coupling. For this reason, our result is to be expected.

In § 2, we prove that $H\psi=-\frac{1}{4}\psi$ has a bounded solution and in § 3 that the solution is L^2. In § 4 we discuss some further aspects. Critical to our considerations are various subharmonic comparison arguments as found e.g. in (Simon 1975, Hoffmann-Ostenhof 1980) and other results on properties of eigenfunctions as reviewed by Simon (1982).

One common theme of the analysis in §§ 2 and 3 will be to take a bounded solution ψ of $H(A)\psi=E(A)\psi$ for some A with $\psi(r_1, r_2, r_{12})=\psi(r_2, r_1, r_{12})$ and form

$$F(r_1)=\int \phi(r_2)\psi(x_1, x_2)\, \mathrm{d}x_2 \tag{2}$$

where ϕ is the ground state of $h=-\Delta_2-r_2^{-1}$. We will need:

Proposition 1.1. Let

$$G(r_1)=A\int \phi(r_2)r_{12}^{-1}\psi(x_1, x_2)\, \mathrm{d}x_2. \tag{3}$$

Then under the above assumptions F is a C^2 function away from $r_1=0$ obeying

$$(-\Delta_1-r_1^{-1}-E-\tfrac{1}{4})F=-G. \tag{4}$$

Proof. Since ψ is bounded by assumption and ϕ decays, both F and G are bounded. Indeed, since ψ is uniformly Lipschitz by estimates of Kato (1957), G is also Lipschitz. Thus, if we prove (4) in the distributional sense, standard elliptic estimates (see e.g. Gilbarg and Trudinger 1977, Simon 1982) imply that F is C^2 and (4) holds in the classical sense in $(0, \infty)$. In the distributional sense

$$[(-\Delta_1-r_1^{-1}-E-\tfrac{1}{4})F](r_1)=\int \phi(r_2)[(H-E)-(h+\tfrac{1}{4})-Ar_{12}]\psi(x_1, x_2)\, \mathrm{d}x_2=-G \tag{5}$$

if we integrate by parts.

2. Existence of a bounded solution

In this section we will prove

Theorem 2.1. There exists a positive bounded function ψ, symmetric in x_1, x_2, which is a distributional solution of $H(A_0)\psi=-\frac{1}{4}\psi$.

We begin by noting that, by definition of A_0, we can find $E_n \uparrow -\frac{1}{4}$ and $\psi_n>0$, $\psi_n=\psi_n(r_1, r_2, r_{12})=\psi_n(r_2, r_1, r_{12})$ so that $H(A_n)\psi_n=E_n\psi_n$ with $A_n=A_0-1/n$. We will normalise ψ_n by requiring

$$\sup_{x\in\mathbb{R}^6} \psi_n(x)=1.$$

By the compactness of the unit ball in L^∞ in the weak-* topology (see e.g. Reed and Simon 1972, theorem IV.21), we can by passing to a subsequence find ψ in L^∞ so that

$$\int f(x)\psi_n(x)\, \mathrm{d}x \to \int f(x)\psi(x)\, \mathrm{d}x \qquad \text{for } n\to\infty \qquad \text{for all } f\in L^1(\mathbb{R}^6).$$

ψ is easily seen to be a distributional solution of $H(A_0)\psi = -\frac{1}{4}\psi$. The key fact is to show that ψ is not identically zero, i.e. that ψ_n does not run away to ∞. Once we show that ψ is not identically zero, it is somewhere non-negative, and then by Harnack's inequality (see e.g. Aizenman and Simon 1982) it is everywhere positive.

Lemma 2.2. Let $F_n(r_1) = \int \phi(r_2)\psi_n(x_1, x_2)\,\mathrm{d}x_2$ as in (2). Suppose that for some $R < \infty$ and $\varepsilon > 0$, $\sup_{r_1 \leqslant R} F_n(r_1) \geqslant \varepsilon$ for all large n; then ψ is not identically zero.

Proof. By Harnack's inequality there exists a constant C, so that for all n, $\psi_n(x_1, x_2) \geqslant C\psi_n(x_1', x_2)$ if $|x_1 - x_1'| \leqslant 1$. Thus, if $F_n(r_1') \geqslant \varepsilon$, we have that $F_n(r_1) \geqslant C\varepsilon$ if $|x_1' - x_1| \leqslant 1$; so if $\sup_{r_1 \leqslant R} F_n(r_1) \geqslant \varepsilon$, we have that

$$\int_{r_1 \leqslant R+1} F_n(r_1)\,\mathrm{d}r_1 \geqslant \tfrac{4}{3}\pi C\varepsilon.$$

Thus, since $\phi \in L^1$,

$$\int_{|x_1| \leqslant R+1} \phi(r_2)\psi(x_1, x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \geqslant \tfrac{4}{3}\pi\varepsilon C, \quad \text{so} \quad \psi \neq 0.$$

Lemma 2.3. For some $\varepsilon > 0$, $\sup_r F_n(r) \geqslant \varepsilon$ for all n.

Proof. Let K be the region where $r_1 > 8$, $r_2 > 8$. Then, on K, $-\Delta\psi_n = (E_n - A_n r_{12}^{-1} + r_1^{-1} + r_2^{-1})\psi_n \leqslant 0$ for n large. So ψ_n is subharmonic on K and thus, since $\psi_n \to 0$ at infinity (Simon 1982), we know that ψ_n takes its maximum value (which is 1) on the complement of K. Since ψ_n is symmetric in x_1, x_2 we can find $x_1^{(n)}$ and $x_2^{(n)}$ with $|x_2^{(n)}| \leqslant 8$, so that $\psi_n(x_1^{(n)}, x_2^{(n)}) = 1$. By Harnack's inequality, for some ε_0, $\psi_n(x_1^{(n)}, x_2) \geqslant \varepsilon_0$ if $r_2 \leqslant 1$. (Note that ε_0 does not depend on n.) Thus, with

$$\varepsilon = \varepsilon_0 \int_{|x_2| \leqslant 1} \phi(r_2)\,\mathrm{d}x_2$$

we see that $F_n(r_1^{(n)}) \geqslant \varepsilon$.

The next lemma will be needed again in the next section. We remark that it only uses $\sup_{x \in \mathbb{R}^6} \psi_n(x) \leqslant 1$.

Lemma 2.4. For any $\delta > 0$, there is a function $H_\delta(r_1)$ obeying

$$H_\delta(r_1) \leqslant C\,\mathrm{e}^{-Dr_1} \tag{6}$$

for some $C, D > 0$ so that for all $r_1 \geqslant 1$

$$G_n(r_1) \geqslant (A_0 - \tfrac{1}{4})(1-\delta)r_1^{-1}F_n(r_1) - H_\delta(r_1) \tag{7}$$

with $G_n = (\Delta_1 + r_1^{-1} + E_n - \frac{1}{4})F_n$. (Note. We emphasise that C, D are independent of n.)

Proof. Let $b = \delta(1-\delta)^{-1}$. Then, since $r_{12} \leqslant r_1 + r_2$,

$$G_n(r_1) \geqslant A_n \int_{|x_2| \leqslant br_1} (r_1 + r_2)^{-1}\phi\psi_n\,\mathrm{d}x_2 \geqslant A_n(1+b)^{-1}r_1^{-1} \int_{|x_2| \leqslant br_1} \phi\psi_n\,\mathrm{d}x_2$$
$$\geqslant A_n(1-\delta)r_1^{-1}F_n(r_1) - H_\delta(r_1)$$

where

$$H_\delta(r_1) = A_0 r_1^{-1} \int_{|x_2| \geq b r_1} \phi(r_2)\, dx_2$$

which is easily seen to obey (6) since ϕ decreases exponentially.

Proof of theorem 2.1. Due to lemmas 2.2 and 2.3 it suffices to show that for some $R > 0$, $\sup_r F_n(r) = \sup_{r \leq R} F_n(r)$ for $n \geq N$, N large. Choose r_n such that $F_n(r_n) = \sup_r F_n(r)$ and pick δ and N so that $(A_0 - 1/N)(1-\delta) \geq 1 + \delta$, which is possible since $A_0 > 1$. Suppose r_n becomes arbitrarily large for $n \to \infty$; then by proposition 1.1 and lemma 2.4

$$(\Delta F_n)(r_n) \geq G_n(r_n) - (1/r_n) F_n(r_n) \geq \delta F_n(r_n)/r_n - C\, e^{-Dr_n}$$

with C, D given in (6). This together with lemma 2.3 implies

$$(\Delta F_n)(r_n) \geq r_n^{-1}(\varepsilon\delta - C r_n\, e^{-Dr_n}) > 0.$$

But this is impossible if F_n is maximised at r_n and thus $r_n \leq R$. Lemma 2.2 is therefore applicable and theorem 2.1 follows.

3. Existence of an L^2 solution

In this section we will prove

Theorem 3.1. The solution $\psi(x_1, x_2)$ of theorem 2.1 obeys

$$|\psi(x_1, x_2)| \leq C_m (1 + r_1^2 + r_2^2)^{-m} \tag{8}$$

for any $m > 0$ and in particular, $\psi \in L^2$.

We want first to reduce the theorem to the study of the function F of (2).

Lemma 3.2. If

$$F(r_1) \leq \tilde{C}_m (1 + r_1^2)^{-m} \tag{9}$$

then (8) follows.

Proof. Since ϕ is bounded away from zero on $r_2 < 17$, we see that if (9) holds and $r_2 < 16$, then

$$\int_{|x'-x| \leq 1} \psi(x')\, d^6x' \leq C_m^{(1)} (1 + r_1^2 + r_2^2)^{-m}$$

and so by subsolution estimates (Simon 1982), if $r_2 < 16$ (or by symmetry if $r_1 < 16$), then (8) holds. In the region where $r_1 > 16$ and $r_2 > 16$ we have that

$$\Delta\psi \geq \tfrac{1}{8}\psi.$$

On the other hand, if $\psi_- = (r_1^2 + r_2^2 + 1)^{-m}$ and $\psi_+ = (r_1^2 + r_2^2 + 1)^m$, then (with $r = (r_1^2 + r_2^2)^{1/2}$)

$$\Delta\psi_- = (r^2+1)^{-1}\psi_-[4m(m+1)r^2(r+1)^{-1} - 12m],$$

$$\Delta\psi_+ = (r^2+1)^{-1}\psi_+[4m(m-1)r^2(r+1)^{-1} + 12m].$$

Thus, in the region $r_1 \geqslant 16$, $r_2 \geqslant 16$, $r \geqslant R_0$,

$$\Delta(c\psi_- + \varepsilon\psi_+) \leqslant \tfrac{1}{8}(c\psi_- + \varepsilon\psi_+)$$

for all $c, \varepsilon > 0$ and with suitable R_0 (depending on m). Let R_1 be given with $R_1 > R_0$. By the foregoing considerations there is some $c > 0$ such that $\psi \leqslant c\psi_-$ for $r_1 = 16$ or $r_2 = 16$ or $r = R_0$. Further, since ψ is bounded $\psi \leqslant \varepsilon\psi_+$ for $r = R_1$ with $\varepsilon \geqslant \sup \psi/(R_1^2+1)^m$. Hence $\psi \leqslant c\psi_- + \varepsilon\psi_+$ on the boundary of the region $\Omega = \{(x_1, x_2) \in \mathbb{R}^6 | r_1 \geqslant 16, r_2 \geqslant 16, R_0 \leqslant r \leqslant R_1\}$. Using a standard comparison argument for differential inequalities (see e.g. Simon 1975), we get $\psi \leqslant c\psi_- + \varepsilon\psi_+$ in Ω. As can be seen from above, c is independent of R_1 and $\varepsilon \to 0$ as $R_1 \to \infty$. Hence we recover (8) for $r \geqslant R_0$. If $r < R_0$, (8) is trivial.

To prove theorem 3.1 we shall further need the following lemmas.

Lemma 3.3. Let $v(r) \geqslant 0$ obey

$$-v'' + m(m+1)r^{-2}v \leqslant 0$$

on $[R, \infty)$, $R > 0$. Then either v grows at least as fast as r^{m+1} at infinity or decreases at least as fast as r^{-m}.

Proof. If $v'v^{-1} \leqslant -mr^{-1}$ on $[R, \infty)$, then obviously for some $C > 0$, $v \leqslant Cr^{-m}$, so it suffices to show that if $v'(r_0) > -mr_0^{-1}v(r_0)$ for some $r_0 > R$, then v grows at least like r^{m+1}. The functions

$$u(c, r) = r^{m+1} + cr^{-m}$$

with $c \in [-r_0^{2m+1}, \infty)$ are positive on $[r_0, \infty)$ and obey $-u'' + m(m+1)r^{-2}u = 0$. As c runs through that interval, $u'(r_0)/u(r_0)$ runs from $+\infty$ to $-mr_0^{-1}$, so we can find such a u with $u'(r_0)/u(r_0) \leqslant v'(r_0)/v(r_0)$ and thus a multiple of u (call it $\tilde{u}$) with $v'(r_0) > \tilde{u}'(r_0)$ and $\tilde{u}(r_0) = v(r_0)$. We claim that $v(r) > \tilde{u}(r)$ for all $r > r_0$, proving the desired result. For if r_1 is the smallest $r > r_0$ where $v(r) = \tilde{u}(r)$, then

$$0 \geqslant \int_{r_0}^{r_1} [\tilde{u}(-v'' + m(m+1)r^{-2}v) - v(-\tilde{u}'' + m(m+1)r^{-2}\tilde{u})]\, \mathrm{d}r$$

$$= {}_{r_0}^{r_1}|(v\tilde{u}' - \tilde{u}v') = v(r_1)(\tilde{u}'(r_1) - v'(r_1)) + v(r_0)(-\tilde{u}'(r_0) + v'(r_0)) > 0$$

which is a contradiction.

Lemma 3.4. Let $g(r) = Cr\,\mathrm{e}^{-Dr}$ and let $v(r) \geqslant 0$ obey

$$-v'' + m(m+1)r^{-2}v \leqslant g(r)$$

on $[R_m, \infty)$, $R_m > 0$. Then either v grows at least as fast as r^{m+1} at infinity or decays at least as fast as r^{-m}.

Proof. Define for $r \geqslant R_m$

$$\eta(r) = \frac{1}{2m+1}\left(r^{m+1}\int_r^\infty x^{-m}g(x)\,\mathrm{d}x + r^{-m}\int_{R_m}^r x^{m+1}g(x)\,\mathrm{d}x\right).$$

Then $-\eta'' + m(m+1)r^{-2}\eta = g$ and since $\int_{R_m}^\infty x^{m+1}g(x)\,\mathrm{d}x < \infty$, $\eta(r) \leqslant \mathrm{d}r^{-m}$ for some $0 < d < \infty$. Let $\tilde{v} = v + \mathrm{d}r^{-m} - \eta$; then $\tilde{v} \geqslant 0$ and obeys $-\tilde{v}'' + m(m+1)\tilde{v} \leqslant 0$ on $[R_m, \infty)$.

But by the foregoing lemma $\tilde{v}$ grows at least like r^{m+1} or decays at least as fast as r^{-m}, and according to the definition of $\tilde{v}$, v has the same properties.

Proof of theorem 3.1. Due to lemma 3.2 it suffices to verify inequality (9) by proposition 1.1 and lemma 2.4 we know that for $r>1$

$$\Delta F - \delta r^{-1} F \geqslant -C\,\mathrm{e}^{-Dr}$$

and so, for $r \geqslant R_m$, where $R_m > m(m+1)/\delta$,

$$\Delta F - m(m+1) r^{-2} F \geqslant -C\,\mathrm{e}^{-Dr}.$$

The fact that F is spherically symmetric and bounded (since ψ is bounded) together with lemma 3.4 implies that F decays at least as fast as r^{-m}, finishing the proof of the theorem.

4. Remarks

(1) As explained in (Simon 1977), the fact that the ground state is L^2 at A_0 immediately implies that for $A \leqslant A_0$, $E(A) \leqslant E(A_0) + d(A - A_0)$ with $d>0$ so that $E(A)$ cannot turn into an antibound state at A_0. We agree with Reinhardt's analysis (Reinhardt 1977) that it probably turns into a resonance pair.

(2) Following the 'Schrödinger inequality' methods (Hoffmann-Ostenhof and Hoffmann-Ostenhof 1977, Ahlrichs *et al* 1981), it can be shown that at A_0, the one-particle density ρ obeys

$$\sqrt{\rho(r)} \underset{\geqslant}{\leqslant} C_\pm(\delta)(r+1)^{-\frac{3}{4}\pm\delta} \exp\{-[4(A_0-1)r]^{\frac{1}{2}}\}.$$

(3) The Coulomb nature of the potential was unimportant. What was critical was that at the critical coupling the electron about to be unbound sees a potential which is repulsive at infinity with a slower decay than r^{-2}.

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References

Alriches R, Hoffmann-Ostenhof M, Hoffmann-Ostenhof T and Morgan J 1981 *Phys. Rev.* A **23** 2106
Aizenman M and Simon B 1982 *Commun. Pure Appl. Math.* **35** 209
Gilbarg D and Trudinger N S 1977 *Elliptic Partial Differential Equations of Second Order* (Berlin: Springer)
Hoffmann-Ostenhof M and Hoffmann-Ostenhof T 1977 *Phys. Rev.* A **16** 1782
Hoffmann-Ostenhof T 1980 *J. Phys. A: Math. Gen.* **13** 417
Kato T 1957 *Commun. Pure Appl. Math.* **10** 151
Klaus M and Simon B 1980 *Ann. Phys.* **130** 251
—— 1982, in preparation
Leinfelder H and Simon B 1982 *Recent Results on Schrödinger Operators* (Paris: Dunod) in preparation

Reed M and Simon B 1972 *Methods of Modern Mathematical Physics I, Functional Analysis* (New York: Academic)
Reinhardt W 1977 *Phys. Rev.* A **15** 832
Simon B 1975 *Trans. Am. Math. Soc.* **208** 317
—— 1977 *J. Funct. Anal.* **25** 338
—— 1982 *Bull. Am. Math. Soc.* **7** 447
Stillinger F H 1966 *J. Chem. Phys.* **45** 3623
Stillinger F H and Stillinger D K 1974 *Phys. Rev.* A **10** 1109
Thirring W 1979 *Lehrbuch der Mathematischen Physik* III (Wien: Springer)