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Absence of an L^2-eigenfunction at the bottom of the spectrum of the Hamiltonian of the hydrogen negative ion in the triplet S-sector

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Abstract. It is shown that the Hamiltonian H of the hydrogenic anion has no bound state at the threshold in the triplet S-sector. This extends a result of Hill who showed that H has only an essential spectrum in the triplet sector.

We consider the Schrödinger operator describing the hydrogenic anion

$$H = -\tfrac{1}{2}\Delta_1 - \tfrac{1}{2}\Delta_2 - r_1^{-1} - r_2^{-1} + r_{12}^{-1} \tag{1}$$

on $L^2(\mathbb{R}^6, \mathrm{d}x_1\,\mathrm{d}x_2)$, $x_i \in \mathbb{R}^3$, $r_i = |x_i|$ $(i = 1, 2)$, $r_{12} = |x_1 - x_2|$. A few years ago Hill (1977) showed among other results that there is no bound state ψ in the triplet S-sector satisfying $(H - E)\psi = 0$ for $E < -\frac{1}{2}$. By bound state we mean L^2-solution and by triplet S-sector we denote the restriction of $L^2(\mathbb{R}^6)$ to the class of functions

$$\mathcal{M} = \{f \in L^2(\mathbb{R}^6, \mathrm{d}x_1\,\mathrm{d}x_2) | f(x_1, x_2) = -f(x_2, x_1), f = f(r_1, r_2, r_{12})\}. \tag{2}$$

Note that H has essential spectrum $[-\frac{1}{2}, \infty)$.

In this paper we extend the above result in the following way.

Theorem 1. Suppose $\psi \in \mathcal{M}$ and satisfies

$$(H + \tfrac{1}{2})\psi = 0 \tag{3}$$

on $\mathbb{R}^6$ with H given by (1). Then $\psi \equiv 0$.

Before giving the proof of the theorem some remarks might be appropriate:

(i) Stillinger (1966) conjectured this result on numerical grounds.

(ii) Theorem 1 should be compared to a result obtained by Hoffmann-Ostenhof *et al* (1983). In this paper the Hamiltonian $H(A) = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - r_1^{-1} - r_2^{-1} + Ar_{12}^{-1}$ on $L^2(\mathbb{R}^6, \mathrm{d}x_1\,\mathrm{d}x_2)$ has been considered with the smallest $A > 0$, so that $H(A)$ has only essential spectrum. It was proven that $H(A)$ has an L^2-solution at the bottom of its spectrum. Critical for this result was that $A > 1$ (because the hydrogen ion has a bound state). This fact was used to show that (loosely speaking) an electron far from the

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nucleus feels an effective potential by which binding could be deduced. However, in the present case no such mechanism will be available.

Proof of theorem 1. Suppose indirectly that $\psi \not\equiv 0$. Since ψ solves (3) it follows (see e.g. Simon 1982) that $\psi \in H^2(\mathbb{R}^6)$, the domain of the Hamiltonian H. (For a definition of the Sobolev space $H^2(\mathbb{R}^6)$ see e.g. Reed and Simon 1975.) Then due to Hill's result (1977) we have

$$-\tfrac{1}{2} = \inf_{f \in H^2 \cap \mathcal{M}} (f, Hf)/(f,f) = (\psi, H\psi)/(\psi, \psi). \tag{4}$$

However, it is obvious that $f(r_1, r_2, r_{12}) = 0$ for $r_1 = r_2$ for all $f \in \mathcal{M}$. This, together with (4), implies that ψ is the ground state of the Dirichlet problem (3) in the domain $|x_1| > |x_2|$ (resp. $|x_1| < |x_2|$). Such a ground state is non-degenerate and can be chosen to be non-negative (see e.g. Reed and Simon 1978). Further by Harnack's inequality (see Aizenman and Simon 1982) it is positive. Therefore we can choose $\psi > 0$ for $|x_1| > |x_2|$ and $\psi < 0$ for $|x_1| < |x_2|$.

Next we need the following lemma.

Lemma 1. Let $g: \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $g = g(r_1, r_2, \Theta)$, where $r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\Theta$, $-\pi \leq \Theta \leq \pi$ and define

$$[g](r_1, r_2) = \tfrac{1}{2} \int_{-1}^{+1} g \, \mathrm{d}\cos\Theta. \tag{5}$$

Let

$$f(r_1, r_2) = \exp[\ln \psi(r_1, r_2, \Theta)] \qquad \text{for } r_2 < r_1 \tag{6}$$

where $\psi \in C^2(\{(x_1, x_2) \in \mathbb{R}^6, 0 < r_2 < r_1\})$ and $\psi > 0$ for $r_2 < r_1$, then

$$[\Delta\psi/\psi] \geq \Delta f/f \qquad \text{for } r_2 < r_1. \tag{7}$$

Proof. This lemma is analogous to a result derived by Lieb (1981, lemma 7.17). Taking into account that for real valued $g \in C^2$

$$\Delta g = \sum_{i=1}^{2} \frac{1}{r_i^2}\left[\frac{\partial}{\partial r_1}\left(r_i^2 \frac{\partial}{\partial r_i} g\right) + \frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\left(\sin\Theta \frac{\partial}{\partial\Theta} g\right)\right] \tag{8}$$

and

$$(\nabla g)^2 = \sum_{i=1}^{2}\left[\left(\frac{\partial g}{\partial r_i}\right)^2 + \frac{1}{r_i^2}\left(\frac{\partial g}{\partial\Theta}\right)^2\right] \tag{9}$$

(see e.g. Hylleraas 1964) the proof runs in the same way as Lieb's proof.

Applying lemma 1 to equation (3) and noting that

$$[r_{12}^{-1}] = r_1^{-1} \qquad \text{for } r_2 < r_1, \tag{10}$$

we obtain

$$(-\Delta_1 - \Delta_2 + 1 - 2r_2^{-1})f \geq 0 \qquad \text{for } r_2 < r_1. \tag{11}$$

Now we consider

$$(-\Delta_2 - 2r_2^{-1} + 1)\phi(r_2) = 0 \qquad \text{with } \phi(r_2) = \pi^{-1/2}\,e^{-r_2}. \tag{12}$$

Multiplying inequality (11) from the left by ϕ and integrating over $|x_2| < r_1$, it is straightforward to calculate that

$$-\Delta_1 \int_{|x_2| \leq r_1} \phi f \, dx_2 + 4\pi r_1^2 \phi(r_1)(\partial f/\partial r_1 - \partial f/\partial r_2)|_{r_2 = r_1} \geq 0. \tag{13}$$

In the following we shall denote

$$v(r_1) = \int_{|x_2| \leq r_1} \phi f \, dx_2. \tag{14}$$

By a result of Kato (1957) $|\nabla \psi|$ is bounded in $\mathbb{R}^6$. It follows easily that

$$|(\partial f/\partial r_1 - \partial f/\partial r_2)|_{r_2 = r_1}| \leq C \qquad \text{for } r_1 \geq R > 0, \tag{15}$$

since

$$\partial f/\partial r_2|_{r_2=r_1} = \lim_{h\to 0}[f(r_1, r_1 - h)/-h] = -\exp\{\ln \lim_{h \to 0}[\psi(r_1, r_1 - h, \Theta)/h]\}$$

$$= -\exp\{\ln[-\partial\psi(r_1, r_2, \Theta)/\partial r_2]|_{r_2 = r_1}\} \tag{16}$$

and analogously for $\partial f/\partial r_1|_{r_2=r_1}$. Inserting (15) into (13) and taking into account (12) we arrive at

$$-\Delta_1 v + e^{-\alpha r_1} \geq 0 \qquad \text{for } r_1 \geq R \tag{17}$$

with some $0 < \alpha < 1$ and R large enough.

Next we need the following lemma.

Lemma 2. Let v be given according to (14), then for arbitrarily small $\delta > 0$ and sufficiently large R, there is some $C(R)$, such that

$$v(r_1) \geq C(R)\,e^{-\delta r_1} \qquad \text{for } r_1 \geq R. \tag{18}$$

Proof. First we note that for $0 \leq r_2 < R < \infty$ there is a $\phi_R(r_2) > 0$, $(\phi_R, \phi_R) = 1$ which solves the Dirichlet problem

$$(-\Delta_2 - 2r_2^{-1} + 1 - \delta_R)\phi_R = 0 \tag{19}$$

in the ball $B_R(0) = \{x_2 \in \mathbb{R}^3 | r_2 \leq R\}$, with some $\delta_R > 0$. Due to the variational principle $\delta_R \to 0$ for $R \to \infty$. Define

$$u_R(r_1) = \int \phi_R \psi \, dx_2 \tag{20}$$

with ψ given according to (3). Obviously $u_R > 0$ for $r_1 > R$. Since ψ obeys (3) and is by assumption in L^2 it follows from a result of Simon (1982) that $\psi \to 0$ for $r_1 \to \infty$ and therefore $u_R \to 0$ for $r_1 \to \infty$. Now we can use the same differential inequality techniques as derived by Hoffmann-Ostenhof (1979) to obtain $(-\Delta_1 + \delta)u_R \geq 0$ for all $\delta > \delta_R$, with $r > r_\delta$, r_δ sufficiently large, from which

$$u_R(r_1) \geq C(R)\,e^{-\delta r} \qquad \text{for } r_1 > R \tag{21}$$

follows for some $C(R)>0$. Finally we shall show that

$$v(r_1)\geqslant C(R)u_R(r_1) \qquad \text{for } r_1>R \tag{22}$$

for some $C(R)>0$ which together with (21) verifies (18). Evidently

$$v(r_1)\geqslant \int_{|x_2|\leqslant R} \phi f\,\mathrm{d}x_2 \geqslant \inf_{|x_2|\leqslant R} \psi \int_{|x_2|\leqslant R} \phi\,\mathrm{d}x_2 \qquad \text{for } r_1\geqslant R_1>R. \tag{23}$$

Let $B=\{(x_1', x_2')\in\mathbb{R}^3\times\mathbb{R}^3,\ |x_1'-x_1|^2+|x_2'|^2\leqslant R^2\}$ and let $\Omega=\{(x_1,x_2)\in\mathbb{R}^3\times\mathbb{R}^3,\ r_2<r_1\}$, then for $r_1\geqslant R_1>R$ we have $B\subset\Omega$. Since $\psi>0$ in Ω and obeys (3) we obtain by Harnack's inequality (Aizenman and Simon 1982) for some $C(R)>0$

$$\begin{aligned}\inf_{|x_2|\leqslant R} \psi(x_1, x_2')&\geqslant \inf_B \psi \geqslant C(R)\sup_B \psi\\ &\geqslant C(R)\sup_{|x_2|\leqslant R}\psi(x_1,x_2')\geqslant C(R)\psi(x_1,x_2) \qquad \text{for } r_2\leqslant R<R_1<r_1.\end{aligned} \tag{24}$$

Combining (23) with (24) we arrive at

$$v(r_1)\geqslant C(R)\psi(x_1,x_2) \qquad \text{for } r_2\leqslant R\leqslant r_1 \tag{25}$$

with some $C(R)>0$. Multiplying (25) by ϕ_R and integrating over x_2 (22) results.

Applying lemma 2 to inequality (17) we arrive at

$$-\Delta_1 v+\mathrm{e}^{-\beta r_1}v\geqslant 0 \qquad \text{for } r_1\geqslant R \tag{26}$$

with some $0<\beta<1$. Let $w=rv$ and $u_m=r^{-m}c_m$, $m>0$ with $(w-u_m)(r_m)>0$ for some $r_m>0$ with suitable $c_m>0$. Then

$$-w''+\mathrm{e}^{-\beta r}w\leqslant 0 \qquad -u''+\mathrm{e}^{-\beta r}u\leqslant 0 \qquad \text{for } r>r_m,\ m>0 \tag{27}$$

for r_m sufficiently large. We are going to show now that $w\geqslant u_m$ for $r\geqslant r_m$. Suppose indirectly that there is some $\bar r_m>r_m$ such that $(u_m-w)(\bar r_m)=0$, $u_m\leqslant w$ for $r_m<r<\bar r_m$ and $(u_m-w)'(\bar r_m)>0$. Then u_m-w is monotonously non-decreasing for $r_m\geqslant r_0$, since due to (27) it cannot have a maximum there. But $u_m\to 0$ for $r\to\infty$ and $w>0$, therefore $w\to 0$ for $r\to\infty$. Hence $u_m-w\to 0$ for $r\to\infty$ which is a contradiction.

Thus we have shown that $v\notin L^2(\mathbb{R}^3)$.

By Jensen's inequality (see e.g. Hayman and Kennedy 1976)

$$[\psi]\geqslant f \qquad \text{for } r_2\leqslant r_1. \tag{28}$$

By (28) and by the Cauchy–Schwarz inequality we conclude

$$\int_{|x_1|\geqslant R}\int_{|x_2|\leqslant r_1}\psi^2\,\mathrm{d}x_1\,\mathrm{d}x_2\geqslant(4\pi)^3\int_R^\infty\left(\int_0^{r_1}\phi[\psi]r_2^2\,\mathrm{d}r_2\right)^2 r_1^2\,\mathrm{d}r_1\geqslant\int_{|x_1|\geqslant R} v^2\,\mathrm{d}x_1=\infty.$$

Hence $\psi\notin L^2(\mathbb{R}^6)$, which contradicts our assumption.

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