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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 threshold in the triplet S-sector. This extends a result of R.N. Hill (1977) who showed that H has only essential spectrum in the triplet sector.

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We consider the Schrödinger operator describing the hydrogenic anion

$$H = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} \qquad (1)$$

on $L^2(\mathbb{R}^6, dx_1dx_2)$, $x_i \in \mathbb{R}^3$, $r_i = |x_i|$ $(i = 1,2)$, $r_{12} = |x_1 - x_2|$. A few years ago R.N. Hill (1977) has shown amoung other results that there is no bound state ψ in the triplet S-sector satisfying $(H - E)\psi = 0$ for $E < -1/2$. 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

$$M = \{f \in L^2(\mathbb{R}^6, dx_1dx_2) \mid f(x_1,x_2) = -f(x_2,x_1),\ f = f(r_1,r_2,r_{12})\} . \qquad (2)$$

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

In this note we extend the above result in the following way:

<u>Theorem 1</u>: Suppose $\psi \in M$, $\psi \not\equiv 0$ and satisfies

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

on $\mathbb{R}^6$ with H given by (1). Then $\psi \notin L^2(\mathbb{R}^6)$.

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

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

(ii) Theorem 1 should be compared to a result obtained by M. Hoffmann-Ostenhof et al. (1983): In this paper the Hamiltonian $H(A) = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{A}{r_{12}}$ on $L^2(\mathbb{R}^6, dx_1dx_2)$ 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 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 $\psi \in L^2(\mathbb{R}^6)$. 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

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

But obviously $f(r_1,r_2,r_{12}) = 0$ for $r_1 = r_2$ for all $f \in M$. 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 nondegenerate and can be chosen to be nonnegative (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 1: Let $g: \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ with $g = g(r_1,r_2,\theta)$, where $r_{12}^2 = r_1^2 + r_2^2 - 2r_1r_2\cos\theta$, $-\pi \le \theta \le \pi$ and define

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

Let

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

where $\psi \in C^2(\{(x_1,x_2) \in \mathbb{R}^3, 0 < r_2 < r_1\})$ and $\psi > 0$ for $r_2 < r_1$, then

$$[\frac{\Delta\psi}{\psi}] \ge \frac{\Delta f}{f} \quad \text{for} \quad r_2 < r_1 . \tag{7}$$

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

$$\Delta g = \sum_{i=1}^{2} \frac{1}{r_i^2} \{\frac{\partial}{\partial r_i}(r_i^2 \frac{\partial}{\partial r_i} g) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta} g)\} \tag{8}$$

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

$$\left[\frac{1}{r_{12}}\right] = \frac{1}{r_1} \quad \text{for} \quad r_2 < r_1 , \tag{10}$$

we obtain

$$\left(-\Delta_1 - \Delta_2 + 1 - \frac{2}{r_2}\right) f \geq 0 \quad \text{for} \quad r_2 < r_1 . \tag{11}$$

Now we consider

$$\left(-\Delta_2 - \frac{2}{r_2} + 1\right) \phi(r_2) = 0 \text{ with } \phi(r_2) = \frac{1}{\sqrt{\pi}} e^{-r_2} . \tag{12}$$

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

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

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 $\mathbb{R}^6$. Therefrom it follows easily that

$$\left| \left(\frac{\partial f}{\partial r_1} - \frac{\partial f}{\partial r_2}\right)\Big|_{r_2 = r_1} \right| \leq C \quad \text{for} \quad r_1 \geq R > 0 , \tag{15}$$

since

$$\frac{\partial f}{\partial r_2}\Big|_{r_2 = r_1} = \lim_{h \to 0} \frac{f(r_1, r_1 - h)}{-h} = -\exp\left[\ln \lim_{h \to 0} \frac{\psi(r_1, r_1 - h, \theta)}{h}\right] = \tag{16}$$

$$= - \exp \left[\ln\left(- \frac{\partial \psi(r_1, r_2, \theta)}{\partial r_2}\right)\Big|_{r_2 = r_1} \right]$$

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

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

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

Next we need

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

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

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

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

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 T. 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

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

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

$$v(r_1) \geq C(R)\, u_R(r_1) \quad \text{for} \quad r_1 > R \tag{22}$$

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

$$v(r_1) \geq \int_{|x_2|\leq R} \phi f \, dx_2 \geq \inf_{|x_2|\leq R} \phi \int_{|x_2|\leq R} \phi \, dx_2 \quad \text{for} \quad r_1 \geq R_1 > R . \tag{23}$$

Let $B = \{(x_1', x_2') \in \mathbb{R}^3 \times \mathbb{R}^3, |x_1' - x_1|^2 + |x_2'|^2 \leq R^2\}$ and let $\Omega = \{(x_1, x_2) \in \mathbb{R}^3 \times \mathbb{R}^3, r_2 < r_1\}$, then for $r_1 \geq R_1 > R$ 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 $C(R) > 0$

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

Combining (23) with (24) we arrive at

$$v(r_1) \geq C(R)\, \psi(x_1, x_2) \quad \text{for} \quad r_2 \leq R \leq r_1 \tag{25}$$

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

$$- \Delta_1 v + e^{-\beta r_1} v \geq 0 \quad \text{for} \quad r_1 \geq R \tag{26}$$

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

$$- w'' + e^{-\beta r} w \geq 0 , \quad - u'' + e^{-\beta r} u \leq 0 \quad \text{for} \quad r > r_m , m > 0 \tag{27}$$

for r_m sufficiently large. We are going to show now that $w \geq u_m$ for $r \geq r_m$:

Suppose indirectly that there is some $\bar{r}_m > r_m$ such that $(u_m - w)(\bar{r}_m) = 0$, $u_m \le w$ for $r_m < r < \bar{r}_m$ and $(u_m - w)'(\bar{r}_m) > 0$. Then $u_m - w$ is monotonously nondecreasing for $r_m \ge r_o$, 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))

$$[\psi] \ge f \quad \text{for} \quad r_2 \le r_1 \, . \tag{28}$$

By (28) and by Cauchy-Schwarz's inequality we conclude

$$\int_{|x_1| \ge R} \int_{|x_2| \le r_1} \psi^2 dx_1 dx_2 \ge (4\pi)^3 \int_R^\infty \Big(\int_0^{r_1} \phi[\psi] r_2^2 \, dr_2\Big)^2 r_1^2 \, dr_1 \ge \int_{|x_1| \ge R} v^2 dx_1 = \infty \, .$$

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

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