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On the Existence of the Discrete Eigenvalue of the Schrödinger Operator for the Negative Hydrogen Ion*

By

Jun UCHIYAMA**

In this note, we shall consider the Schrödinger operator of the form

$$H=-\Delta_1-\Delta_2-\frac{Z_1}{r_1}-\frac{Z_2}{r_2}+\frac{Z_3}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}, \tag{1}$$

where $\Delta_i=\sum_{\nu=0}^{2}\frac{\partial^2}{\partial x_{3i-\nu}^2}$, $r_i=|\boldsymbol{r}_i|=(\sum_{\nu=0}^{2}x_{3i-\nu}^2)^{1/2}$ $(i=1,2)$, $|\boldsymbol{r}_1-\boldsymbol{r}_2|=(\sum_{\nu=1}^{3}(x_\nu-x_{3+\nu})^2)^{1/2}$, and $Z_1\geq Z_2>0$, $Z_3>0$ are constants. Let $C_0^\infty(R^6)$ be the space of all C^∞ functions with compact support, and $\mathcal{D}_{L^2}^n(R^6)$ be the completion of $C_0^\infty(R^6)$ with the norm $\|f\|_{\mathcal{D}_{L^2}^n(R^6)}=\left(\sum_{|\alpha|\leq n}\int_{R^6}|D^\alpha f|^2dx\right)^{1/2}$, where $D^\alpha f=\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1}\cdots\partial x_6^{\alpha_6}}f$ and $|\alpha|=\alpha_1+\cdots+\alpha_6$. If the domain of H is $\mathcal{D}_{L^2}^2(R^6)$, H is a lower semi-bounded selfadjoint operator in $L^2(R^6)$ and the essential spectrum $\sigma_e(H)$ of H consists of $[-Z_1^2/4, \infty)$ (see Žislin [4], or the introduction of the author [1]).

In case $Z_2=Z_3$, it is interesting whether H has a discrete eigenvalue in $(-\infty, -Z_1^2/4)$ or not. In fact the Schrödinger operator for the negative hydrogen ion has the form (1) with $Z_1=Z_2=Z_3$. In other cases, there are some results as for the existence of discrete eigenvalues in $(-\infty, -Z_1^2/4)$ (see the author [1], [2] and [3]). Especially if Z_1 and Z_2 are smaller enough than Z_3, H has no discrete eigenvalues in $(-\infty, -Z_1^2/4)$ (see the author [2]). Here we shall show that the operator of the form (1) with Z_1 and Z_2, which are close to Z_3, has

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** Mathematical Institute, Kyoto University of Industrial Arts and Textile Fibres.

at least one discrete eigenvalue in $(-\infty, -Z_1^2/4)$. Namely we have

Theorem. *There exists some constant $\delta > 0$ depending only on Z_3 such that for any Z_1 and Z_2 satisfying $Z_3+\delta \geq Z_1 \geq Z_2 \geq Z_3-\delta$, the Schrödinger operator H of the form* (1) *has at least one discrete eigenvalue in $(-\infty, -Z_1^2/4)$.*

Proof. Let for any $\psi \in \mathcal{D}_{L^2}^1(R^6)$

$$(2)\qquad L[\psi;\, Z_1, Z_2, Z_3] \equiv \int_{R^6} \Big\{ |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_1}{r_1}|\psi|^2 - \frac{Z_2}{r_2}|\psi|^2 + \frac{Z_3}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}|\psi|^2 + \frac{Z_1^2}{4}|\psi|^2 \Big\} dx$$

$$= \int_{\Omega_1} + \int_{\Omega_2} \equiv L_1[\psi;\, Z_1, Z_2, Z_3] + L_2[\psi;\, Z_1, Z_2, Z_3],$$

where $|\nabla_i \psi|^2 = \sum_{\nu=0}^{2} \left| \frac{\partial \psi}{\partial x_{3i-\nu}} \right|^2$ $(i=1, 2)$, $\Omega_1 = \{x = (\boldsymbol{r}_1, \boldsymbol{r}_2) = (x_1, \cdots, x_6) \in R^6;\ r_1 \geq r_2\}$ and $\Omega_2 = \{x \in R^6;\ r_2 \geq r_1\}$. If and only if $L[\psi;\, Z_1, Z_2, Z_3] < 0$ for some $\psi \in \mathcal{D}_{L^2}^1(R^6)$, the Schrödinger operator H of the form (1) has at least one discrete eigenvalue in $(-\infty, -Z_1^2/4)$ (see Theorem 1 in Žislin [4]). Then we shall look for some suitable function to satisfy $\psi(x) = \psi(r_1, r_2) \in \mathcal{D}_{L^2}^1(R^6)$ and $L[\psi;\, Z_1, Z_2, Z_3] < 0$. In case $\psi(x) = \psi(r_1, r_2)$ depends only on r_1 and r_2, we have

$$(3)\qquad \int_{\Omega_1} \frac{|\psi|^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} dx = 2\pi \int_{R^3} d\boldsymbol{r}_1 \int_0^{r_1} |\psi|^2 r_2^2 dr_2 \int_0^{\pi} \frac{\sin\theta\, d\theta}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta)^{1/2}}$$

$$= 2\pi \int_{R^3} d\boldsymbol{r}_1 \int_0^{r_1} |\psi|^2 r_2^2 \Big(\frac{1}{r_1 r_2} (r_1 + r_2 - |r_1 - r_2|) \Big) dr_2 = \int_{\Omega_1} \frac{|\psi|^2}{r_1} dx,$$

and similarly

$$(4)\qquad \int_{\Omega_2} \frac{|\psi|^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} dx = \int_{\Omega_2} \frac{|\psi|^2}{r_2} dx.$$

Therefore by (3) and (4) we have for any $\psi(x) = \psi(r_1, r_2) \in \mathcal{D}_{L^2}^1(R^6)$

$$(5)\qquad L_1[\psi;\, Z_3, Z_3, Z_3] = \int_{\Omega_1} \Big\{ |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_3}{r_2}|\psi|^2 + \frac{Z_3^2}{4}|\psi|^2 \Big\} dx,$$

$$L_2[\psi;\, Z_3, Z_3, Z_3] = \int_{\Omega_2} \Big\{ |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_3}{r_1}|\psi|^2 + \frac{Z_3^2}{4}|\psi|^2 \Big\} dx.$$

Moreover if $\psi(r_1, r_2)=\psi(r_2, r_1)$, we have $L_1[\psi; Z_3, Z_3, Z_3]=L_2[\psi; Z_3, Z_3, Z_3,]$. Taking into consideration the fact that $e^{-(Z/2)r}$ is an eigenfunction of the operator $-\Delta-(Z/r)$ in $L^2(R^3)$ belonging to the least eigenvalue $-Z^2/4$, we put

$$(6)\qquad f(x)=\begin{cases} e^{-(\varepsilon Z_3/2)r_1}e^{-(Z_3/2)r_2} & \text{for } r_1\geq r_2 \\ e^{-(Z_3/2)r_1}e^{-(\varepsilon Z_3/2)r_2} & \text{for } r_2\geq r_1 . \end{cases} \quad (\varepsilon>0)$$

Then we have $f(x)=f(r_1, r_2)=f(r_2, r_1)\in\mathcal{D}^1_{L^2}(R^6)$ and

$$(7)\qquad L_1[f; Z_3, Z_3, Z_3]=\frac{(4\pi)^2}{Z_3^4}\left\{\frac{\varepsilon^2}{4}\int_0^\infty e^{-\varepsilon r_1}r_1^2dr_1\int_0^{r_1}e^{-r_2}r_2^2dr_2\right.$$

$$+\frac{1}{4}\int_0^\infty e^{-\varepsilon r_1}r_1^2dr_1\int_0^{r_1}e^{-r_2}r_2^2dr_2-\int_0^\infty e^{-\varepsilon r_1}r_1^2dr_1\int_0^{r_1}e^{-r_2}r_2dr_2$$

$$\left.+\frac{1}{4}\int_0^\infty e^{-\varepsilon r_1}r_1^2dr_1\int_0^{r_1}e^{-r_2}r_2^2dr_2\right\}$$

$$=\frac{(4\pi)^2}{Z_3^4}\left\{\frac{\varepsilon^2}{4}\int_0^\infty e^{-\varepsilon r_1}r_1^2(2-2e^{-r_1}-2r_1e^{-r_1}-r_1^2e^{-r_1})dr_1\right.$$

$$\left.-\frac{1}{2}\int_0^\infty e^{-(1+\varepsilon)r_1}r_1^4dr_1\right\}$$

$$=\frac{(4\pi)^2}{Z_3^4}\frac{(2\varepsilon-1)(5\varepsilon-1)}{(1+\varepsilon)^5}.$$

Then if we choose ε to satisfy $1/5<\varepsilon<1/2$, we have $L_1[f; Z_3, Z_3, Z_3]=L_2[f; Z_3, Z_3, Z_3]<0$, and then

$$(8)\qquad L[f; Z_3, Z_3, Z_3]<0.$$

Now fix $\varepsilon>0$ to satisfy $1/5<\varepsilon<1/2$ and f defined by (6). By (8) and

$$(9)\qquad L[f; Z_1, Z_2, Z_3]=L[f; Z_3, Z_3, Z_3]+(Z_3-Z_1)\int_{R^6}\frac{|f|^2}{r_1}dx$$

$$+(Z_3-Z_2)\int_{R^6}\frac{|f|^2}{r_2}dx+\frac{Z_1^2-Z_3^2}{4}\int_{R^6}|f|^2dx,$$

there exists some $\delta>0$ such that for any Z_1 and Z_2 satisfying $Z_3+\delta\geq Z_1\geq Z_2\geq Z_3-\delta$ we have

$$(10)\qquad L[f; Z_1, Z_2, Z_3]<0.$$

By (10) we have the assertion of the theorem.

References

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Note added in proof (July 1, 1970): After this work was finished, we found the review article by A. G. Sigalov, "The mathematical problem in the theory of atomic spectra", Russian Math. Survey **22**, No. 2 (1967), 1–18, in which he said that P. Gombás ["Theorie und Lösungsmethoden des Mehrteichenproblems der Wellenmechanik" Birkhäuser, Basel, 1950, p. 170] had also given a trial function to ensure the existence of a discrete eigenvalue in $\left(-\infty, -\frac{Z_1^2}{4}\right)$ for the case $Z_1 = \cdots = 1$.