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

By

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

\[ H = -\Delta_1 - \Delta_2 - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} + \frac{Z_3}{|r_1 - r_2|}, \]

where \( \Delta_i = \sum_{\nu=0}^3 \frac{\partial^2}{\partial x_{3,\nu}^2}, \) \( r_i = |r_i| = (\sum_{\nu=0}^3 x_{3,\nu}^2)^{1/2} \) \( (i = 1, 2), \) \( |r_1 - r_2| = (\sum_{\nu=1}^3 (x_\nu - x_\nu^*)^2)^{1/2}, \) and \( Z_i \geq Z_2 > 0, \) \( Z_3 > 0 \) are constants. Let \( C^\infty_c(\mathbb{R}^3) \) be the space of all \( C^\infty \) functions with compact support, and \( \mathcal{D}_c(\mathbb{R}^3) \) be the completion of \( C^\infty_c(\mathbb{R}^3) \) with the norm \( ||f||_{\mathcal{D}_c(\mathbb{R}^3)} = \left( \int_{\mathbb{R}^3} |D^a f|^2 \, dx \right)^{1/2}, \)

where \( D^a f = \sum_{|\alpha| = |a|} \frac{\partial^{|a|}}{\partial x_{1}^{a_1} \cdots \partial x_{3}^{a_3}} f \)

and \( |\alpha| = a_1 + \cdots + a_3. \) If the domain of \( H \) is \( \mathcal{D}_c(\mathbb{R}^3), \) \( H \) is a lower semi-bounded self-adjoint operator in \( L^2(\mathbb{R}^3) \) and the essential spectrum \( \sigma_*(H) \) of \( H \) consists of \( [ -Z_3^2/4, \infty ] \) (see Zislin [4], or the introduction of the author [1]).

In case \( Z_2 = Z_3, \) it is interesting whether \( H \) has a discrete eigenvalue in \( ( -\infty, -Z_3^2/4 ) \) 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 \( ( -\infty, -Z_3^2/4 ) \) (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 \( ( -\infty, -Z_3^2/4 ) \) (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

* This research was partly supported by the Sakkokai Foundation.
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at least one discrete eigenvalue in \((-\infty, -Z_i^2/4)\). Namely we have

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

**Proof.** Let for any \(\psi \in D_1^3(R^n)\)

\[
L[\psi; Z_1, Z_2, Z_3] = \int_{R^n} \left( |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_1}{r_1} |\psi|^2 - \frac{Z_2}{r_2} |\psi|^2 + \frac{Z_3^2}{4} |\psi|^2 \right) dx
\]

where \( |\nabla_i \psi|^2 = \sum_{j=0}^{n-1} \left| \frac{\partial \psi}{\partial x_{3j+i}} \right|^2 \) (i = 1, 2), \( \Omega_1 = \{x = (r_1, r_2) = (x_1, \ldots, x_n) \in R^n; \ r_1 \geq r_2 \}\) and \( \Omega_2 = \{x \in R^n; r_2 \geq r_1 \}\). If and only if \(L[\psi; Z_1, Z_2, Z_3] < 0\) for some \(\psi \in D_1^3(R^n)\), the Schrödinger operator \(H\) of the form (1) has at least one discrete eigenvalue in \((-\infty, -Z_i^2/4)\) (see Theorem 1 in Žislin [4]). Then we shall look for some suitable function to satisfy \(\psi(x) = \psi(r_1, r_2) \in D_1^3(R^n)\) 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

\[
L_1[\psi; Z_1, Z_2, Z_3] = \int_{\Omega_1} \left( |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_1}{r_1} |\psi|^2 - \frac{Z_2}{r_2} |\psi|^2 + \frac{Z_3^2}{4} |\psi|^2 \right) dx
\]

and similarly

\[
L_2[\psi; Z_1, Z_2, Z_3] = \int_{\Omega_2} \left( |\nabla_1 \psi|^2 + |\nabla_2 \psi|^2 - \frac{Z_1}{r_1} |\psi|^2 - \frac{Z_2}{r_2} |\psi|^2 + \frac{Z_3^2}{4} |\psi|^2 \right) dx.
\]
Moreover if $\psi(r_1, r_2) = \psi(r_2, r_1)$, we have $L_2[\psi; Z_2, Z_3, Z_3] = L_2[\psi; Z_3, Z_3, Z_3]$. Taking into consideration the fact that $e^{-(x^2+y^2)}$ is an eigenfunction of the operator $-\Delta - (Z/r)$ in $L^2(R^3)$ belonging to the least eigenvalue $-Z^2/4$, we put

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

Then we have $f(x) = f(r_1, r_2) = f(r_2, r_1) \in D_{1/2}(R^3)$ and

$$L_1[f; Z_3, Z_3, Z_3] = \frac{(4\pi)^2}{Z^3_3} \left\{ \frac{\varepsilon^2}{4} \int_0^\infty e^{-r_1^2} r_1^3 dr_1 \int_0^{r_1} e^{-r_2^2} r_2^3 dr_2 + \frac{1}{4} \int_0^\infty e^{-r_1^2} r_1^3 dr_1 \int_0^{r_1} e^{-r_2^2} r_2^3 dr_2 \right\}$$

$$+ \frac{1}{2} \int_0^\infty e^{-r_1^2} r_1^3 dr_1 \int_0^{r_1} e^{-r_2^2} r_2^3 dr_2$$

$$= \frac{(4\pi)^2}{Z^3_3} \left\{ \frac{\varepsilon^2}{4} \int_0^\infty e^{-r_1^2} r_1^3 (2 - 2e^{-r_1^2} - 2r_1 e^{-r_1^2} - r_1^2 e^{-r_1^2}) dr_1 \right\}$$

$$- \frac{1}{2} \int_0^\infty e^{-r_1^2} r_1^3 dr_1$$

$$= \frac{(4\pi)^2}{Z^3_3} \frac{(2\varepsilon - 1)(5\varepsilon - 1)}{(1+\varepsilon)^5}.$$

Then if we choose $\varepsilon$ 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

$$L[f; Z_3, Z_3, Z_3] = 0.$$

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

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

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

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

$$L[f; Z_1, Z_2, Z_3] < 0.$$

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

[2] ————, Corrections to the above article, Publ. RIMS Kyoto Univ., this issue.

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 \(-\infty, -\frac{Z_1^2}{4}\) for the case \(Z_1=\cdots=1\).