ON THE SPECTRUM OF THE SCHRÖDINGER OPERATOR

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Abstract

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MATHEMATICS

G. M. ZHISLIN

ON THE SPECTRUM OF THE SCHRÖDINGER OPERATOR

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§ 1. In the present note the form of the spectrum of the operator*

$$H = -\sum_{i=1}^{n} a_i \Delta_i - 2a_0 \sum_{\substack{i,j=1 \\ i<j}}^{n} \left(\frac{\partial^2}{\partial x_i \partial x_j} + \frac{\partial^2}{\partial y_i \partial y_j} + \frac{\partial^2}{\partial z_i \partial z_j} \right) - \sum_{i=1}^{n} b_i \frac{1}{r_i} + \sum_{\substack{i,j=1 \\ i<j}}^{n} c_{ij} \frac{1}{r_{ij}}, \tag{1}$$

where $a_i = a_0 + a'_i$, a'_i, b_i, c_{ij} $(i, j = 1, 2, \dots, n)$ are arbitrary positive numbers; a_0 is any nonnegative number.

In the case $a_0 = 0$, i.e. without taking into account the motion of the nucleus, the author proved$^{(1)}$ the existence of a sequence of eigenvalues of the operator $\widetilde{H}$** when the conditions

$$b_i > \sum_{\substack{j=1 \\ j\neq i}}^{n} c_{ij}, \qquad i = 1, 2, \dots, n \tag{2}$$

are satisfied (where $c_{ij} = c_{ji}$ for $j < i$), to which atoms with any number of electrons and positive ions correspond.

In the present note this result is generalized to the case $a_0 > 0$. In addition, the existence of the limiting spectrum*** of the operator $\widetilde{H}$ is established. We use the notation and definitions introduced in $^{(1)}$.

§ 2. **Theorem.** *There exists a number $\mu_1 < 0$ such that the entire limiting spectrum of the operator $\widetilde{H}$ consists of all numbers λ, $\lambda \geq \mu_1$. Moreover, if conditions (2) are satisfied, then all points of the spectrum lying to the left of μ_1 form an increasing sequence of eigenvalues $\lambda^{(p)}$, accumulating at μ_1, whose eigenfunctions ψ_p are differentiable any number of times and satisfy the equation $H\psi_p = \lambda^{(p)}\psi_p$ at every point of the space R_{3n} that lies on none of the manifolds $r_i = 0$ $(i = 1, 2, \dots, n)$, $r_{ij} = 0$ $(i, j = 1, 2, \dots, n;\ i \neq j)$.*

In what follows it is sufficient to consider only real functions. Let ψ and φ be arbitrary real functions respectively from

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* The Schrödinger operator for atoms and ions is reduced to the form (1) with $a_0 > 0$ if the motion of their nuclei is taken into account.

** $\widetilde{H}$ is the self-adjoint extension of H, obtained in the same way as in $^{(1)}$.

*** For the definition of the limiting spectrum see $^{(2)}$, p. 391.

$W_2^1(R_{3n})$ and $W_2^1(R_{3n-3,i})$. Introduce the following notation:

$$\begin{aligned} L[\psi] = \sum_{j=1}^{n} a_j \int_{R_{3n}} |\operatorname{grad}_j \psi|^2 \, d\Omega + 2a_0 \int_{R_{3n}} \sum_{\substack{l,j=1 \\ l<j}}^{n} (\operatorname{grad}_l \psi, \operatorname{grad}_j \psi) \, d\Omega \\ - \sum_{j=1}^{n} b_j \int_{R_{3n}} \frac{|\psi|^2}{r_j} \, d\Omega + \sum_{\substack{l,j=1 \\ l<j}}^{n} c_{lj} \int_{R_{3n}} \frac{|\psi|^2}{r_{lj}} \, d\Omega, \end{aligned} \tag{3}$$

where

$$(\operatorname{grad}_l \psi, \operatorname{grad}_j \psi) = \frac{\partial\psi}{\partial x_l}\frac{\partial\psi}{\partial x_j} + \frac{\partial\psi}{\partial y_l}\frac{\partial\psi}{\partial y_j} + \frac{\partial\psi}{\partial z_l}\frac{\partial\psi}{\partial z_j};$$

$$\begin{aligned} L^i[\varphi] = \sum_{\substack{j=1 \\ j\neq i}}^{n} a_j \int_{R_{3n-3,i}} |\operatorname{grad}_j \varphi|^2 \, d\Omega + 2a_0 \int_{R_{3n-3,i}} \sum_{\substack{l,j=1 \\ \neq i}}^{n} (\operatorname{grad}_l \varphi, \operatorname{grad}_j \varphi) \, d\Omega \\ - \sum_{\substack{j=1 \\ j\neq i}}^{n} b_j \int_{R_{3n-3,i}} \frac{|\varphi|^2}{r_j} \, d\Omega + \sum_{\substack{l,j=1 \\ l\neq i,\ l<j,\ j\neq i}}^{n} c_{lj} \int_{R_{3n-3,i}} \frac{|\varphi|^2}{r_{lj}} \, d\Omega; \end{aligned} \tag{4}$$

$$\lambda_{3n-3,i} = \inf_{\varphi\in W_2^1(R_{2n-2,i}),\ \|\varphi\|=1} L^i[\varphi], \qquad n > 1, \qquad \lambda_{0,1} = 0.$$

Lemma. If, for a completely spreading sequence $\{u_m\}$ from $W_2^1(R_{3n})$,

$$\|u_m\| = 1, \qquad \|u_m\|_{W_2^1(R_{3n})} < M, \qquad m = 1, 2, \dots,$$

then

$$\lim L[u_m] \geq \min_{1\leq i\leq n} \{\lambda_{3n-3,i}\}.$$

§ 3. Let α_k $(k = 0, 1, \dots, l-1)$ be l arbitrary distinct natural numbers, $1 \leq \alpha_k$, $l \leq n$;

$$H^{\alpha_0\alpha_1\cdots\alpha_{l-1}} = -\sum_{i=1}^{n}{}' a_i\Delta_i -$$

$$-2a_0\sum_{\substack{i,j=1\\ i<j}}^{n}{}'\left(\frac{\partial^2}{\partial x_i\partial x_j}+\frac{\partial^2}{\partial y_i\partial y_j}+\frac{\partial^2}{\partial z_i\partial z_j}\right)-\sum_{i=1}^{n}{}'\frac{b_i}{r_i}+\sum_{\substack{i,j=1\\ i<j}}^{n}{}' c_{ij}\frac{1}{r_{ij}}\ast; \qquad (5)$$

$R^{\alpha_0\cdots\alpha_{l-1}}$ is the $3(n-l)$-dimensional Euclidean space of the variables x_i, y_i, z_i, $i \neq \alpha_k$, $k = 0, 1, \ldots, l-1$; $R^{(\alpha_0\cdots\alpha_{l-1})}$ is the $3l$-dimensional Euclidean space of the variables x_i, y_i, z_i, $i = \alpha_k$, $k = 0, 1, \ldots, l-1$. Define the spaces $\mathcal{L}_2(R^{\alpha_0\cdots\alpha_{l-1}})$, $W_2^1(R^{\alpha_0\cdots\alpha_{l-1}})$ by analogy with $\mathcal{L}_2(R_{3n})$, $W_2^1(R_{3n})$.

* Here and below, a prime on a sum means that the terms with $i, j = \alpha_k$, $k = 0, 1, \ldots, l{-}1$, are absent.

Let ψ be an arbitrary function from $W_2^1(R^{\alpha_0\cdots\alpha_{l-1}})$,

$$\begin{aligned}L^{\alpha_0\cdots\alpha_{l-1}}[\psi] = &\sum_{i=1}^{n}{}' a_i\int_{R^{\alpha_0\cdots\alpha_{l-1}}}|\operatorname{grad}_i\psi|^2\,d\Omega\\ &+2a_0\sum_{\substack{i,j=1\\ i<j}}^{n}{}'\int_{R^{\alpha_0\cdots\alpha_{l-1}}}(\operatorname{grad}_i\psi,\operatorname{grad}_j\psi)\,d\Omega-\sum_{i=1}^{n}{}' b_i\int_{R^{\alpha_0\cdots\alpha_{l-1}}}\frac{|\psi|^2}{r_i}\,d\Omega\\ &+\sum_{\substack{i,j=1\\ i<j}}^{t}{}' c_{ij}\int_{R^{\alpha_0\cdots\alpha_{l-1}}}\frac{|\psi|^2}{r_{ij}}\,d\Omega;\end{aligned} \qquad (6)$$

$$Q^{\alpha_0\cdots\alpha_{l-1}} = \left\{\psi,\ \psi\in W_2^1(R^{\alpha_0\cdots\alpha_{l-1}}),\ \|\psi\|_{\mathcal{L}_2(R^{\alpha_0\cdots\alpha_{l-1}})}=1\right\};$$

$$\lambda_{\alpha_0\cdots\alpha_{l-1}} = \inf_{\psi\in Q^{\alpha_0\cdots\alpha_{l-1}}} L^{\alpha_0\cdots\alpha_{l-1}}[\psi]; \qquad \mu_l = \min\{\lambda_{\alpha_0\cdots\alpha_{l-1}}\};$$

$$l = 1, 2, \ldots, n-1; \qquad \mu_n = 0.$$

We shall prove that μ_1 is the number whose existence is asserted in the theorem.

Let ν be an arbitrary point of the limiting spectrum of $\widetilde{H}$. We shall show that $\nu \geq \mu_1$. Let E_λ be the spectral function of the operator $\widetilde{H}$; let $\sigma_{\nu,\varepsilon}$ be the subspace onto which the operator $E_{\nu+\varepsilon}-E_{\nu-\varepsilon}$ projects functions from $\mathcal{L}_2(R_{3n})$. For an arbitrary sequence $\{\varepsilon_k\}$, $\varepsilon_k > 0$, $\varepsilon_k \underset{k\to\infty}{\longrightarrow} 0$, one can indicate an orthonormal sequence of functions $\{\psi_{\varepsilon_k}\}$ such that $\psi_{\varepsilon_k} \in \sigma_{\nu,\varepsilon_k}$ ((2), pp. 391–392). Obviously, $\psi_{\varepsilon_k} \in D_{\widetilde{H}} \subset W_2^1(R_{3n})$ and

$$\lim_{k\to\infty} L[\psi_{\varepsilon_k}] = \lim_{k\to\infty} (\widetilde{H}\psi_{\varepsilon_k}, \psi_{\varepsilon_k}) = \nu. \tag{7}$$

It follows that $\|\operatorname{grad}\psi_{\varepsilon_k}\| < M$, $k = 1, 2, \ldots$. By virtue of the lemma and (4),

$$\lim_{k\to\infty} L[\psi_{\varepsilon_k}] \geq \mu_1. \tag{8}$$

From (7) and (8) the required inequality $\nu \geq \mu_1$ follows.

In order to prove that every fixed number ν, $\nu \geq \mu_1$, is a point of the limiting spectrum of the operator $\widetilde{H}$, it is enough ((2), pp. 392–393) to indicate a sequence of functions $\{F_m\}$ such that

$$\begin{aligned}
&\text{a)}\quad F_m \in D_{\widetilde{H}};\\
&\text{b)}\quad \|F_m\| = 1;\\
&\text{c)}\quad F_m \xrightarrow{\text{weakly}} 0 \text{ in } \mathcal{L}_2(R_{3n});\\
&\text{d)}\quad \|\widetilde{H}F_m - \nu F_m\| \underset{m\to\infty}{\longrightarrow} 0.
\end{aligned} \tag{9}$$

We shall construct the sequence $\{F_m\}$ for the operator $\widetilde{H}$ of the form (1) with $a_0 = 0$.

It can be shown that $\mu_n > \mu_{n-1} \geq \cdots \geq \mu_1$. Let μ_s be the smallest of the numbers μ_k $(1 \leq k \leq n-1)$ for which

$$\mu_k < \mu_{k+1} \tag{10}$$

holds, and $\mu_s = \lambda_{i_0\cdots i_{s-1}}$, where $i_0, i_1, \ldots, i_{s-1}$ are some fixed numbers. It follows from (10) that $\lambda_{i_0\cdots i_{s-1}} < \lambda_{i_0\cdots i_{s-1}i_s}$ for any i_s $(1 \leq i_s \leq n$, $i_s \neq i_\alpha$, $\alpha = 0, 1, \ldots, s-1)$. Hence, using the lemma of the present note and general—

applying Lemma 2 from (1), we obtain that $\lambda_{i_0\cdots i_{s-1}}$ is the least eigenvalue of the operator $\widetilde{H}^{i_0\cdots i_{s-1}}*$; let $\theta(x_i, y_i, z_i)$, $i = 1, 2, \ldots, n$, $i \neq i_\alpha$, $\alpha = 0, 1, \ldots, s-1$, be the corresponding eigenfunction. Consider the operator

$$H_3 = -a_{i_0}\Delta_{i_0} - b_{i_0}\frac{1}{r_{i_0}}.$$

It has limiting spectrum filling the whole ray $[0, +\infty)$ (5). Therefore (4) implies that for each number ν, $\nu \geqslant \mu_1$, there exists a completely spreading sequence of functions f_m, for which:

a) $f_m \in C_2(R^{(i_0)}) **$;

$$\text{b) } \|f_m\|_{\mathcal{L}_2(R^{(i_0)})} = 1;$$

$$\text{c) } \|H_3 f_m - (\nu - \mu_1) f_m\|_{\mathcal{L}_2(R^{(i_0)})} \xrightarrow[m\to\infty]{} 0.$$

Let $g(x_p, y_p, z_p)$, $p = i_1, i_2, \dots, i_{s-1}$, be an arbitrary finite twice continuously differentiable function in $R^{(i_1,\dots,i_{s-1})}$, $\|g\|_{\mathcal{L}_2(R^{(i_1,\dots,i_{s-1})})} = 1$,

$$g_m(x_p, y_p, z_p) = m^{-3/2(s-1)} g(m^{-1}x_p, m^{-1}y_p, m^{-1}z_p), \quad m = 1, 2, \dots$$

Put $F_m = \theta f_m g_m$, $m = 1, 2, \dots$. Using the properties of θ, $\{f_m\}$, and $\{g_m\}$, one can show that the functions F_m satisfy the relations (9). The first part of the theorem is proved.

The proof of the second part of the theorem is carried out, using the lemma, in the same way as the proof of the main theorem in (1).

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Gorky State University
named after N. I. Lobachevsky

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CITED LITERATURE

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* $\widetilde{H}^{i_0 \cdots i_{s-1}}$ is a self-adjoint extension of the operator $H^{i_0 \cdots i_{s-1}}$.

** $C_2(R^{(i_0)})$ is the space of twice continuously differentiable functions in $R^{(i_0)}$ belonging to $\mathcal{L}_2(R^{(i_0)})$ together with all their derivatives up to order 2 inclusive.

Note: Figure translations are in progress. See original paper for figures.

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