Reports of the Academy of Sciences of the USSR

MATHEMATICS

1962

SovietRxiv

Abstract

Full Text

Reports of the Academy of Sciences of the USSR
1962. Volume 142, No. 3

MATHEMATICS

L. A. SAKHNOVICH

ON THE DISCRETE SPECTRUM OF THE RADIAL SCHRÖDINGER EQUATION

(Presented by Academician A. N. Kolmogorov on 28 VIII 1961)

1. Consider the Schrödinger equation

$$-\frac{d^2u}{dx^2} + \left[\frac{\mu(\mu-1)}{x^2} - 2q(x)\right]u - \lambda u = 0, \tag{1}$$

$$u(0) = 0, \qquad 0 \leq x < \infty, \qquad \mu > 1.$$

Many problems of physics lead to equations of this kind. In particular, for $q(x) = A/x$ $(A > 0)$ one obtains the equation for the radial part of the wave function of the hydrogen atom ([1]).

We shall be interested in the behavior of the smallest eigenvalue $\varphi(\mu)$ of equation (1), as well as in the behavior of the corresponding eigenfunction $u(x, \mu)$.

In doing so we shall assume that $q(x)$ is a function continuous for $x > 0$ and, moreover,

$$q(x) = \begin{cases} \dfrac{\beta}{x} + O(1), & 0 \leq x \leq x_0, \\ \dfrac{A_1}{x} + \dfrac{A_2}{x^2} + O\left(\dfrac{1}{x^3}\right), & x \geq x_0, \end{cases} \tag{2}$$

where $A_1 > 0$.

As is known ([2]), the continuous spectrum of the problem under consideration fills the positive half-axis. On the negative half-axis only a discrete spectrum is possible, bounded from below.

If, for a given μ, there exist negative eigenvalues of equation (1), then the function $\varphi(\mu)$ is defined and the inequality ([3])

$$\varphi(\mu) \leq \int_0^\infty \left\{ y'(x)^2 + \left[\frac{\mu(\mu-1)}{x^2} - 2q(x) \right] y^2(x) \right\} dx, \tag{3}$$

holds, where y is an absolutely continuous function satisfying the conditions

$$\int_0^\infty y^2(x)\, dx = 1, \qquad y(0) = 0.$$

Equality in (3) holds only for the eigenfunction $u(x, \mu)$ corresponding to the eigenvalue $\varphi(\mu)$.

We shall set $\varphi(\mu) = 0$ if, for the corresponding μ, problem (1) has no negative eigenvalues.

Then

$$\varphi(\mu) = \inf \int_0^\infty \left\{ y'(x)^2 + \left[\frac{\mu(\mu-1)}{x^2} - 2q(x) \right] y^2(x) \right\} dx,$$

where the absolutely continuous function y satisfies the conditions:

$$\int_0^\infty y^2(x)\, dx = 1, \qquad y(0) = 0.$$

We shall call the function $\varphi(\mu)$ the **minimum function** of problem (1), and the corresponding eigenfunction the **minimizing eigenfunction**.

If $q(x) = A/x$ $(A > 0)$, then, as is known,

$$\varphi(\mu) = -\frac{A^2}{\mu^2}, \qquad u(x, \mu) = x^\mu e^{-\frac{A}{\mu} x}.$$

Theorem 1. *The minimum function $\varphi(\mu)$ has the form*

$$\varphi(\mu) = -\frac{A_1^2}{\mu^2} - \frac{4A_2A_1^2}{\mu^4} + O\left(\frac{1}{\mu^6}\right), \qquad \mu > 1.$$

From this theorem and from the monotone increase of the minimum function it follows that

$$\varphi(\mu) < 0,$$

i.e., $\varphi(\mu)$ is a point of the discrete spectrum, and there always corresponds to it a minimizing eigenfunction $u(x, \mu)$ (by $\bar{u}(x, \mu)$ we shall denote the normalized minimizing eigenfunction: $\|\bar{u}\| = 1$).

Thus, the existence of a discrete spectrum for problem (1) depends only on the behavior of $q(x)$ at infinity ($A_1 > 0$).

Theorem 2. *The minimizing eigenfunction* $u(x,\mu)$ *has the form:*

$$u(x,\mu) = x^{\mu}\left[1 + O\left(\frac{1}{\mu}\right)\right], \qquad 0 \le x \le x_0,$$

$$u(x,\mu) = x^{\mu} e^{-\frac{A_1}{\mu}x}\left[1 + O\left(\frac{1}{\mu^k}\right)\right],$$

where $0 < k < 1,\ x_0 \le x \le \mu^{\frac{3-k}{2}}$, *and, finally,*

$$u(x,\mu) = x^{\mu} e^{-\frac{A}{\mu}x}\left[1 + O\left(\frac{1}{\mu^{\frac{1-3k}{2}}}\right)\right],$$

where $0 < k < \frac{1}{3},\ \mu^{\frac{3-k}{2}} \le x \le \frac{\mu^2}{A_1}\left[1 + \frac{l}{\sqrt{\mu}}\right]\ (l > 0)$.

From Theorem 2 it is easy to obtain:

Corollary. *The inequality holds*

$$\int_0^{p_1\mu^2} x^{-m} u^2(x,\mu)\,dx : \int_0^{p_2\mu^2} u^2(x,\mu)\,dx \le O(r^{2\mu}),$$

where $m \ge 0,\ 0 < p_1 < p < p_2 < \frac{1}{A_1},\ \frac{p_1}{p} e^{A_1(p-p_1)} = r < 1$.

From this corollary, in particular, it follows that

$$\int_0^{p_1\mu^2} \bar{u}^2(x,\mu)\,dx \le O(r^{2\mu}),$$

where $0 < p_1 < p < \frac{1}{A_1},\ \frac{p_1}{p} e^{A_1(p-p_1)} = r < 1$.

Theorem 2 describes the behavior of $u(x,\mu)$ for large μ only on a certain interval of the positive half-axis.

Using the usual methods ([2]) for estimating the solution of a differential equation for large values of x, it is easy to characterize the behavior of $u(x,\mu)$ for $x \gg \mu^2$.

The following two theorems describe the behavior of the minimizing eigenfunction on the entire half-axis.

Theorem 3. The minimizing normalized eigenfunction $\bar{u}(x,\mu)$ satisfies the relation

$$\left\|\bar{u}(x,\mu)-c(\mu_1)e^{-\frac{A_1}{\mu_1}x}\right\|^2 \leqslant O\left(\frac{1}{\mu^3}\right),$$

where

$$\mu_1=\frac{1+\sqrt{(2\mu-1)^2-8A_2}}{2},\qquad c(\mu_1)=\left[\int_0^\infty x^{2\mu_1}e^{-\frac{2A_1}{\mu_1}x}\,dx\right]^{-\frac{1}{2}}.$$

Theorem 4. The minimizing normalized eigenfunction $\bar{u}(x,\mu)$ satisfies the relation

$$\left\|u(x,\mu)-c(\mu)x^{\mu}e^{-\frac{A_1}{\mu}x}\right\|^2 \leqslant O\left(\frac{1}{\mu}\right),$$

where

$$c(\mu)=\left[\int_0^\infty x^{2\mu}e^{-\frac{2A_1}{\mu}x}\,dx\right]^{-\frac{1}{2}}.$$

Let us note that Theorems 3 and 4 are obtained from Theorem 1 and the following lemma:

Lemma. Let A be a self-adjoint operator such that the leftmost point of its spectrum, λ_1, is an isolated point of multiplicity 1. Then, for a function y ($\|y\|=1$) belonging to the domain of definition of A, the inequality

$$\|y-\alpha_1 y_1\| \leqslant \frac{(Ay,y)-\lambda_1}{m},\qquad \|y_1\|=1,$$

holds, where y_1 is the normalized eigenfunction corresponding to the number λ_1; m is the distance from the point λ_1 to the remaining part of the spectrum; $\alpha_1=(y,y_1)$ satisfies the inequalities

$$1\geqslant|\alpha_1|\geqslant 1-\frac{(Ay,y)-\lambda_1}{m}.$$

The validity of this lemma is easily established if one uses the spectral decomposition of the operator A.

Theorem 5. Let $\varphi_1(\mu)$ and $\varphi_2(\mu)$ be the minimum functions of two boundary-value problems, and suppose that

$$q_1(x)-q_2(x)=\frac{A_m}{x^m}+O\left(\frac{1}{x^{m+1}}\right),\qquad x\geqslant x_0,\quad m>1;$$

then the equality

$$\varphi_1(\mu) = \varphi_2(\mu) - \frac{2A_m A_1^m}{\mu^{2m}} + O\left(\frac{1}{\mu^{2m+\frac{1}{2}}}\right)$$

holds.

Using Theorem 5, one can refine Theorem 1 in the following way:

Theorem 6. If the potential $q(x)$ has the form:

$$q(x) = \frac{A_1}{x} + \frac{A_2}{x^2} + \frac{A_3}{x^3} + O\left(\frac{1}{x^4}\right), \qquad x \geqslant x_0,$$

then the equality holds

$$\varphi(\mu) = -\frac{A_1^2}{\mu^2} - \frac{4A_2 A_1^2}{\mu^4} - \frac{4A_2^2 A_1^2 + 2A_3 A_1^3}{\mu^6} + O\left(\frac{1}{\mu^{13/2}}\right).$$

2. The following problem seems important to us:
   to determine whether the minimum function $\varphi(\mu)$ uniquely determines the potential $q(x)$, and to give a method for constructing $q(x)$ from $\varphi(\mu)$.

Theorems 1-6 allow one to draw certain, although only preliminary, conclusions.

Theorem 7. *Let the minimum functions $\varphi_1(\mu)$ and $\varphi_2(\mu)$ be such that*

$$\varphi_1(\mu) = \varphi_2(\mu) + O\left(\frac{1}{\mu^m}\right),$$

where $m = 1, 2, \ldots$.
If the corresponding potentials $q_1(x)$ and $q_2(x)$ are analytic functions, regular at infinity, then

$$\varphi_1(\mu) = \varphi_2(\mu), \qquad q_1(x) = q_2(x).$$

Let us note that the theorem remains valid also in the case when the equality

$$\varphi_1(\mu) = \varphi_2(\mu) + o\left(\frac{1}{\mu^m}\right), \qquad m = 1, 2, \ldots,$$

holds only for some sequence of points $\mu_1, \mu_2, \mu_3, \ldots \to \infty$, and this sequence may depend on m.

Thus, analytic potentials are determined uniquely by means of $\varphi(\mu)$.

From Theorem 6 it is clear how to find the first three coefficients (A_1, A_2, A_3) of the expansion of $q(x)$ at infinity, if the function $\varphi(\mu)$ is known.

Odessa Institute
of the Food and Refrigeration Industry

Received
1 VII 1961

REFERENCES

1. L. Schiff, *Quantum Mechanics*, IL, 1959.

2. M. A. Naimark, *Linear Differential Operators*, 1954.

3. S. G. Mikhlin, *Variational Methods in Mathematical Physics*, 1957.

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