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NEW METHOD FOR COMPUTATION OF DISCRETE SPECTRUM

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A new method for computation of the discrete spectrum for a certain quantum mechanical problem is presented. The method is based on a transition from the usual boundary value problem to the solution of a first order nonlinear differential equation. The proposed method yields the eigenvalues with the desired numerical accuracy.

I. INTRODUCTION

In quantum mechanics as well as in other fields of physics the following boundary value problem is solved:

A second order differential equation

$$\left(\frac{d^2}{dx^2} - \varkappa^2 - v\right) u = 0\,, \tag{1.1}$$

in which $u = u(x, \varkappa)$ is a function of $x \geqq 0$, is given. The parameter $\varkappa$ is real and the quantity v is a real function of x.

A solution of (1.1) continuous together with its first derivative and satisfying

$$u(0, \varkappa) = 0\,, \tag{1.2}$$

$$u(\infty, \varkappa) = 0 \tag{1.3}$$

is sought.

One may choose

$$\varkappa \geqq 0 \tag{1.4}$$

without a loss of generality.

The function $v(x)$ which is called "potential" has in this paper the form:

$$v(x) = \frac{l(l+1)}{x^2} + v_N(x)\,, \quad l = 0, 1, 2, \ldots, \tag{1.5}$$

$$(1.6) \qquad \lim_{x \to 0_+} x^\nu v_N(x) = \alpha\,, \quad \nu < 2\,, \quad |\alpha| < \infty\,,$$

$$(1.7) \qquad \lim_{x \to \infty} x^\mu v_N(x) = \beta\,, \quad \mu > 2\,, \quad |\beta| < \infty\,.$$

For $x > 0$, $v_N(x)$ is bounded and either continuous or piecewise continuous.

We say that a bound state occurs if a solution of (1.1 – 3) for some eigenvalue of $\varkappa$ exists.

II. SOME FEATURES OF THE SOLUTION $u(x, \varkappa)$

First we shall recall several theorems concerning the solutions of the equation (1.1) and their behaviour.

Theorem 2.1. *If $v(x)$ has the properties given above then there are two solutions $g(x, \varkappa)$ and $h(x, \varkappa)$ for every $\varkappa$, which are continuous together wtth their derivatives for $0 < x < \infty$. For $x \to 0_+$,*

$$(2.1) \qquad g(x, \varkappa) = x^{l+1}[1 + 0(x^\delta)]\,, \quad \delta > 0\,,$$

$$(2.2) \qquad h(x, \varkappa) = x^{-l}[1 + 0(x^\delta)]\,, \quad \delta > 0\,.$$

Theorem 2.1 *is proved in [1] for $l = 0$ and it can be proved for every $l \neq 0$ in full analogy with the case $l = 0$.*

Evidently, only the solution (2.1) satisfies the boundary condition (1.2). One may therefore put

$$(2.3) \qquad u(x, \varkappa) = g(x, \varkappa)$$

and only this solution will be considered in what follows.

Theorem 2.2. *The zeros of $u(x, \varkappa)$ are simple for $0 < x < \infty$.*

Proof. For $0 < x < \infty$ the usual conditions of the existence theorem and uniqueness of the solution of (1.1) are fulfilled. If for some x_0, $0 < x_0 < \infty$, $u(x_0, \varkappa) = 0$ and $u'(x_0, \varkappa) = 0$, then $u(x, \varkappa) = 0$ must hold.

Theorem 2.3 (Sturm). *If $u_i = u(x, \varkappa_i)$, $i = 1, 2$, and $\varkappa_1 > \varkappa_2$ and if a and b are two adjacent zeros of u_1 then there is at least one zero of u_2 in the open interval (a, b).*

The proof can be performed in full analogy with [2].

Theorem 2.4. *If $u_i = u(x, \varkappa_i)$, $i = 1, 2$, and $\varkappa_1 > \varkappa_2$ and if x_1 is the first zero of u_2, $x_1 > 0$, then*

$$u(x, \varkappa_1) > u(x, \varkappa_2)\,, \quad 0 < x < x_1\,.$$

The proof can be done in full analogy with [2].

Theorem 2.5. *If $v(x)$ has the properties given above then for every $\varkappa$ there are two solutions $e_1(x, \varkappa)$ and $e_2(x, \varkappa)$ of (1.1) which for $x \to \infty$ have the form*

$$e_1(x, \varkappa) = e^{\varkappa x}[1 + o(1)], \quad \varkappa > 0, \tag{2.4}$$

$$e_2(x, \varkappa) = e^{-\varkappa x}[1 + o(1)], \quad \varkappa > 0 \tag{2.5}$$

and

$$e_1(x, 0) = x^{l+1}[1 + 0(x^{-\delta})], \quad \delta > 0, \tag{2.6}$$

$$e_2(x, 0) = x^{-l}[1 + 0(x^{-\delta})], \quad \delta > 0. \tag{2.7}$$

The proof for $\varkappa \neq 0$, and $\varkappa = 0$, $l = 0$ is given in [3] and it can be performed for $\varkappa = 0$, $l \neq 0$ in full analogy with [3].

Evidently, for $\varkappa > 0$ only the solution $e_2(x, \varkappa)$ satisfies the boundary condition (1.3), for $\varkappa = 0$ again only $e_2(x, 0)$ satisfies (1.3) if $l \neq 0$. If $\varkappa = 0$ and $l = 0$ there is no solution satisfying (1.3), i.e. there is no bound state.

III. TRANSFORMATION OF THE EQUATION (1.1)

We shall deal with the solution of (1.1) which is continuous together with its derivative, satisfies (1.2) and has the form (2.3). By a modified Prüfer's transformation [2] new functions $p(x, \varkappa)$ and $z(x, \varkappa)$ can be introduced:

$$\begin{aligned} u(x, \varkappa) &= p(x, \varkappa) \sin z(x, \varkappa), \\ u'(x, \varkappa) &= (l + 1)\, p(x, \varkappa) \cos z(x, \varkappa). \end{aligned} \tag{3.1}$$

It is shown in [2] that $p(x, \varkappa)$ and $z(x, \varkappa)$ can be defined as continuous functions of x.

With the help of (3.1) one may define

$$p(x, \varkappa) = \sqrt{\left(u^2(x, \varkappa) + \frac{1}{(l + 1)^2}\, u'^2(x, \varkappa)\right)}. \tag{3.2}$$

Then

$$p(x, \varkappa) > 0, \quad 0 < x < \infty \tag{3.3}$$

because Theorem 2.2 holds.

Moreover, for $x \to 0$,

$$p(x, \varkappa) = x^l[1 + 0(x^\delta)], \quad \delta > 0 \tag{3.4}$$

because of Theorem 2.1.

Therefore, for $x \to 0$,

$$z(x, \varkappa) = n\pi + x[1 + 0(x^\delta)], \quad \delta > 0, \tag{3.5}$$

where n is even (see (3.1)).

Without a loss of generality one can put $n = 0$, so that

$$z(x, \varkappa) = x[1 + 0(x^\delta)], \quad \delta > 0, \quad x \to 0. \tag{3.6}$$

Now (3.1) implies

$$\operatorname{tg} z(x, \varkappa) = \frac{(l + 1)\, u(x, \varkappa)}{u'(x, \varkappa)}. \tag{3.7}$$

As the zeros of $u(x, \varkappa)$ are simple (Theorem 2.2) and the function $z(x, \varkappa)$ is continuous,

$$z(x_k, \varkappa) = k\pi \tag{3.8}$$

where $x_k > 0$ is the k-th zero of $u(x, \varkappa)$.

From Eqs. (1.1) and (3.1) we have

$$z' = (l + 1)\cos^2 z - \frac{1}{l + 1}(v + \varkappa^2)\sin^2 z, \tag{3.9}$$

$$\frac{p'}{p} = \frac{1}{2}\left(l + 1 + \frac{v + u^2}{l + 1}\right)\sin 2z. \tag{3.10}$$

It is easy to prove that there is a one to one correspondence between the solution $u(x, \varkappa)$ of (1.1) satisfying (1.2) and the solution $z(x, \varkappa)$ of (3.9) satisfying (3.6).

The exact proof of this statement is based on the fact that the equation (3.10) is linear with respect to $p(x, \varkappa)$ and on the examination of this solution near the origin with regard to the conditions (1.5) and (1.6) imposed on the potential $v(x)$.

Now, we collect the fundamental properties of $z(x, \varkappa)$ which will be useful in what follows:

(i) $z(x, \varkappa)$ is the continuous solution of (3.9) satisfying $z(0, \varkappa) = 0$, $z'(0, \varkappa) = 1$.

(ii) $\varkappa$ is an eigenvalue if

$$\lim_{x \to \infty} \operatorname{tg} z(x, \varkappa) = -(l + 1)/\varkappa \tag{3.11}$$

and it is not an eigenvalue if

$$\lim_{x \to \infty} \operatorname{tg} z(x, \varkappa) = +(l + 1)/\varkappa. \tag{3.12}$$

For $\varkappa = 0$, the right-hand sides of (3.11) and (3.12) assume the value $-\infty$ and $+\infty$, respectively.

Proof. This property is a direct consequence of Theorem 2.5 and of the one to one correspondence between $u(x, \varkappa)$ and $z(x, \varkappa)$.

(iii) Let $z(x, \varkappa)$ be a solution satisfying (i), then for given x_0, $0 < x_0 < \infty$, $z(x_0, \varkappa)$ is a decreasing and continuous function of $\varkappa$.

The proof is given in Appendix A.

(iv) If $z(x_0, \varkappa) > k\pi$, $k = 0, 1, 2, \ldots$, for some $x_0 > 0$, then $z(x, \varkappa) > k\pi$ for every $x \in (x_0, \infty)$.

Proof. Suppose that there is $x_1 > x_0$ for which $z(x_1, \varkappa) \leqq k\pi$. Then the continuity of $z(x, \varkappa)$ implies that there is such x_2, $x_0 < x_2 \leqq x_1$, for which $z(x_2, \varkappa) = k\pi$ and $z(x, \varkappa)$ is decreasing in x_2. But this is a contradiction with the equation (3.8) which yields

$$z'(x_2, \varkappa) = l + 1 > 0 . \tag{3.13}$$

(v) Let $\varkappa \neq 0$ and let $x_0(\varkappa)$ be such that $\varkappa^2 + v(x) \geqq 0$ for every $x > x_0$. If $z(x_1, \varkappa) < < (2k + 1)\pi/2$, $k = 0, 1, 2, \ldots$, for $x_1 > x_0$, then $z(x, \varkappa) < \frac{1}{2}(2k + 1)\pi$ for every $x \in (x_1, \infty)$.

The proof is done again by contradiction and with the help of the fact that if $x_2 \geqq x_0$ is such that

$$z(x_2, \varkappa) = (2k + 1)\pi/2 , \quad x_2 \geqq x_0 ,$$

then the inequality

$$z'(x_2, \varkappa) = -(\varkappa^2 + v(x_2))/(l + 1) \leqq 0 \tag{3.14}$$

holds.

(vi) $z(x, \varkappa) < \pi/2$ for $\varkappa$ great enough.

Proof is based on the properties (iii) and (v).

(vii) $z(x, \varkappa)$ is bounded.

Proof. If $z(x, \varkappa)$ were not bounded, the limits (3.11) or (3.12) would not exist.

If the function $z(x, \varkappa)$ has the properties (i)–(vii), the following existence theorem holds:

Theorem 3.1. *If $k\pi < z(x, \varkappa_0) < (k + 1)\pi$, $k = 0, 1, 2, \ldots$, for some $\varkappa = \varkappa_0$ and for all x larger than some $x_0 > 0$, then there are either $k + 1$ or k eigenvalues of $\varkappa$. Their number is $k + 1$ if $\varkappa_0$ is an eigenvalue and their number is k if $\varkappa_0$ is not an eigenvalue.*

The proof is given in Appendix B.

Theorem 3.1 has several consequences:

1. If $k\pi < z(x, 0) < (k + 1)\pi$ for some k, $k = 0, 1, 2, \ldots$, and for all x larger than some x_0, then to the potential $v(x)$ $k + 1$ or k eigenvalues (bound states) correspond. The number of eigenvalues is $k + 1$ if $z(x, 0) > (2k + 1)\pi/2$ for $x > x_0 \geqq 0$ and their number is k if $z(x, 0) < (2k + 1)\pi/2$ for $x > x_0 \geqq 0$.

To prove this statement one has to use (3.11) or (3.12), i.e., if $\varkappa = 0$ is an eigenvalue then

(3.15) $$\lim_{x \to \infty} \operatorname{tg} z(x, 0) = -\infty$$

if $\varkappa = 0$ is not an eigenvalue then

(3.16) $$\lim_{x \to \infty} \operatorname{tg} z(x, 0) = +\infty$$

and in both cases

(3.17) $$\lim_{x \to \infty} z(x, 0) = (2k + 1)\,\pi/2 \,.$$

2. The eigenvalues form a decreasing and finite set

(3.18) $$\varkappa_0 > \varkappa_1 > \varkappa_2 > \ldots > \varkappa_k > \ldots > \varkappa_n \geqq 0$$

and the eigenfunction corresponding to $\varkappa_k$ has k zeros. For the proof one has to apply (iii) from which we see that two different functions $z(x, \varkappa)$ corresponding to two different values of $\varkappa$ have only one common point, i.e. $x = 0$. Then, from (iii) we get that the functions $z(x, \varkappa)$ are ordered and Theorem 3.1 defines the relation between $\varkappa = \varkappa_k$ and the number of zeros of $u(x, \varkappa_k)$.

3. The function $z(\infty, \varkappa)$ is discontinuous. The discontinuity points of $z(\infty, \varkappa)$ are just the eigenvalues $\varkappa_0, \varkappa_1, \ldots, \varkappa_k$.

The proof is based on (i) and (3.11), (3.12) and Theorem 3.1 itself. (See also Appendix B).

IV. NUMERICAL APPLICATIONS

From the point of view of analysis the computation of eigenvalues of a discrete spectrum is straightforward. For the given function $v(x)$ (1.5) one integrates the equation (3.9) from zero to infinity for $\varkappa = 0$. Then, using (3.17), i.e.

(4.1) $$z(\infty, 0) = (2k + 1)\,\pi/2$$

one determines the number of eigenvalues. When this is known, one integrates again the equation (3.9) for various and increasing values of $\varkappa$ until all eigenvalues are obtained from the corresponding discontinuities of the function $z(\infty, \varkappa)$ – (see consequence 3, Sec. III).

In practice one usually cannot integrate to infinity. Nevertheless, the new method yields accurate results.

Actual calculation is based on the proved properties of the function $z(x, \varkappa)$. In principle, to assure accuracy a certain x_{max} as an upper limit of integration must be determined.

If there is such an x_{max}, $0 < x_{max} < \infty$, that

$$\varkappa^2 + v(x) \geqq 0 \quad x \geqq x_{max} \tag{4.2}$$

one can use the properties (iv) and (v) of $z(x, \varkappa)$ (Sec. III). Now, suppose (4.2) is fulfilled. If

$$k\pi < z(x_{max}, \varkappa) < (2k + 1)\,\pi/2\,, \quad \text{for some} \quad k = 0, 1, 2, \ldots, \tag{4.3}$$

then the function $z(x, \varkappa)$ remains in the strip $(k\pi, (2k + 1)\,\pi/2)$ for all $x > x_{max}$. Further, we apply the property (iii) and choose two values of $\varkappa$, say $\varkappa_1 > \varkappa_2$, and the corresponding $x_{max}(\varkappa_2)$.

Let

$$k\pi < z(x_{max}, \varkappa_2) < (2k + 1)\,\pi/2\,, \quad \text{for some} \quad k = 1, 2\,. \tag{4.4}$$

(Notice that the value $k = 0$ would indicate immediately: there is no bound state) and

$$(k - 1)\,\pi < z(x_{max}, \varkappa_1) < (2k - 1)\,\pi/2 \tag{4.5}$$

then the eigenvalue $\bar{\varkappa}$ certainly satisfies the inequality

$$\varkappa_2 < \bar{\varkappa} < \varkappa_1\,. \tag{4.6}$$

In principle, there are no bounds on $\varkappa_1$ and $\varkappa_2$. If for some $\varkappa_i$, $i = 1, 2$, $z(x_{max}, \varkappa_i) \in \in ((2k - 1)\,\pi/2, k\pi)$ then we can replace x_{max} by $x'_{max} > x_{max}$ and again use (4.6) to achieve the desired accuracy.

For $\varkappa \neq 0$, x_{max} defined in (4.2) always exists.

For practical applications of the equation (4.1), which is important for the determination of the number of eigenvalues, one can find also a corresponding x_{max}. We are dealing now with the case $\varkappa = 0$ and we limit the discussion to two actually important cases.

If for $x \geqq x_{max} > 0$

$$\frac{l(l + 1)}{x^2} + v_N(x) \geqq 0\,, \quad l = 0, 1, 2, \ldots \tag{4.7}$$

then the following assertions hold:

a) If $z(x_{max}, 0) \in (k\pi, (2k + 1)\,\pi/2)$, the number of eigenvalues is k.

This conclusion follows from the properties (iv) and (v) of the function $z(x_{max}, 0)$ and from (3.17).

b) If $z(x_{max}, 0) \in ((2k - 1)\,\pi/2, k\pi)$ and $z'(x_{max}, 0) \geqq 0$ then the number of eigenvalues is k.

This statement is due to the properties (iv) and (v) and to Eqs. (3.7) and (3.9).

c) If $z(x_{max}, 0) \in ((2k - 1)\pi/2, k\pi)$ and $z'(x_{max}, 0) < 0$ then the number of eigenvalues is either k or $k - 1$.

To prove this conclusion one has to use again (iv), (v) and (3.17).

If $l = 0$ and

$$v_N(x) \leqq 0 \tag{4.8}$$

for $x \geqq x_0$, $x_0 \geqq 0$ the condition (1.7) implies that there exists such x_{max} that

$$v_N(x) \geqq -\frac{3}{16x^2} \tag{4.9}$$

for all $x > x_{max}$. Let us denote by $z_{up}(x, 0)$ the solution of (3.9) with the actual potential $v_N(x)$ replaced by $-3/(16x^2)$ for $x_{max} < x < \infty$. Then we have

$$\begin{aligned} z_{up}(x, 0) &= z(x, 0), \quad 0 \leqq x \leqq x_{max}, \\ z_{up}(x, 0) &\geqq z(x, 0), \quad x > x_{max}. \end{aligned} \tag{4.10}$$

The relation (4.10) can be proved on the basis of (4.9) in full analogy with the proofs of Lemmas A1 and A2 from Appendix A.

From the solution of (1.1) and with the help of (3.7) we get

$$\operatorname{tg} z_{up}(x, 0) = 4x \frac{c_1 \sqrt{(x)} + c_2}{3c_1 \sqrt{(x)} + c_2}, \quad x > x_{max} \tag{4.11}$$

and from (3.9)

$$z'(x, 0) \geqq 0, \quad z'_{up}(x, 0) \geqq 0, \quad x > x_{max}. \tag{4.12}$$

In (4.11), c_1 and c_2 are fixed real numbers.

Now it is evident:

a) if $z(x_{max}, 0) \in ((2k - 1)\pi/2, k\pi)$ then the number of eigenvalues is just k;

b) if $z(x_{max}, 0) \in (k\pi, (2k + 1)\pi/2)$ then the number of eigenvalues is either k or $k + 1$.

We demonstrate this method, which has been already applied to compute actual and quite complicated problems [4], on a simple example.

In (1.5) we put

$$v_N(x) = -40\frac{e^{-x}}{x}. \tag{4.13}$$

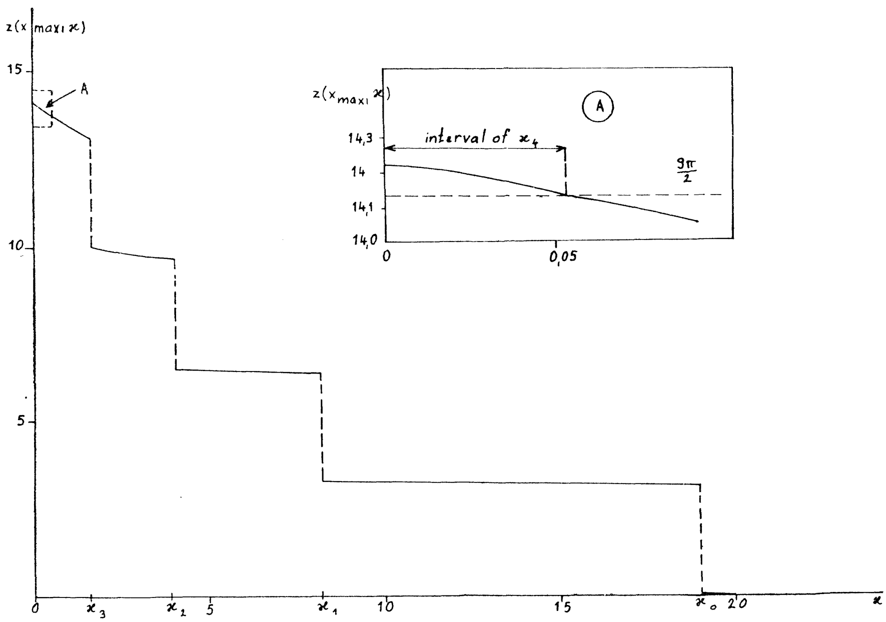
If we choose $x_{max} = 20$ the conditions (4.7) for $l \neq 0$ and (4.9) for $l = 0$ are well satisfied.

The numerical integration of the equation (3.9) for $v_N(x)$ (4.13) and for $\varkappa = 0$, $l = 0$ gives

$$z(x_{max}, 0) \doteq 14{\cdot}224.$$

Thus the number of eigenvalues equals five.

The integration of the equation (3.9) for non-zero $\varkappa$ yields the function $z(x_{max}, \varkappa)$ as a function of $\varkappa$ and this is presented in Fig. 1.



The function $z(x_{max}, \varkappa)$, $x_{max} = 20$, has very sharp slope near the eigenvalues $\varkappa_i$, $i = 0, 1, 2, 3$ and it defines the interval in which the smallest eigenvalue $\varkappa_4$ lies — A.

The curve has extremely sharp slope in the neighbourhood of the eigenvalues with the exception of the smallest eigenvalue $\varkappa_4$ for $l = 0$. The corresponding eigenvalues are tabulated in Tab. I; they are given with an error $\pm 0{\cdot}01$. The value of $\varkappa_4$ for $l = 0$ has been determined for greater x_{max} then 20 (see the discussion after (4.6)).

Table I.

	$l = 0$	$l = 1$	$l = 2$	$l = 3$
$\varkappa_0$	19.02	8.03	3.67	—
$\varkappa_1$	9.09	3.55	1.12	—
$\varkappa_2$	3.94	1.44	—	—
$\varkappa_3$	1.58	—	—	—
$\varkappa_4$	0.04	—	—	—

For $l = 1, 2$ and 3 we proceed in complete analogy with $l = 0$. There are only three bound states for $l = 1$, only two for $l = 2$ and none for $l = 3$, there are no bound states for $l > 3$.

CONCLUSION

A new approach to the problem of discrete spectrum belonging to the operator defined by (1.1), (1.2) and (1.3) is given. It is suitable for numerical treatment and leads to a quick and reliable computation of the spectrum.

The method is based on the transformation of the original linear second order differential equation (1.1) to a non-linear first order differential equation (3.9) for a certain function $z(x, \varkappa)$.

An analogue of the Levinson Theorem [1] is proved for this function, i.e., its value for $x = \infty$ and $\varkappa = 0$ determines the number of eigenvalues of the given operator.*) A proof that this function as a function of $\varkappa \in (0, \infty)$ for $x = \infty$ is discontinuous just at the points at which $\varkappa$ is equal to its eigenvalue, is also given.

Thus, the usual tedious and complicated problem of searching for eigenfunctions and eigenvalues simultaneously, as for example in the Ritz variational method, is replaced by an almost trivial integration of the equation for the function $z(x, \varkappa)$.

It has been shown that the eigenvalues can be determined easily with the desired accuracy.

Other numerical results not presented here indicate that the proposed method can be applied also in some cases in which the number of eigenvalues is not limited. We have in mind especially the potentials decreasing to zero slower than $1/x^2$ for $x \to \infty$.

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*) This theorem was given also on the basis of Eq. (3.9) by F. Calogero [6].

Theorem. *If $z(x, \varkappa)$ is a solution of (3.9) satisfying $z(0, \varkappa) = 0$, $z'(0, \varkappa) = 1$ then for a given x_0, $0 < x_0 < \infty$, $z(x_0, \varkappa)$ is a decreasing and continuous function of $\varkappa$.* The proof is divided in four parts:

Lemma A.1. *If $\varkappa_1 > \varkappa_2$ and if z_1 and z_2 are solutions of*

$$z_1' = (l+1)\cos^2 z_1 - \frac{\varkappa_1^2 + v}{l+1}\sin^2 z_1\,, \tag{A.1}$$

$$z_2' = (l+1)\cos^2 z_2 - \frac{\varkappa_2^2 + v}{l+1}\sin^2 z_2$$

satisfying the initial conditions given above, then $z_1(x) < z_2(x)$ for $x \to 0$, $x > 0$.

Proof. We start from a solution of (1.1)

$$u_1'' - \varkappa_1^2 u_1 - v u_1 = 0\,,$$

$$u_2'' - \varkappa_2^2 u_2 - v u_2 = 0\,.$$

By substraction and integration

$$u_2 u_1' - u_1 u_2' = (\varkappa_1^2 - \varkappa_2^2)\int_0^x u_1 u_2 \,\mathrm{d}x \tag{A.2}$$

and by (3.7),

$$u_{1,2}' \operatorname{tg} z_{1,2} = (l+1)\, u_{1,2}\,. \tag{A.3}$$

Substituting (A.3) in (A.2) we have

$$\frac{1}{l+1}\, u_1' u_2' (\operatorname{tg} z_2 - \operatorname{tg} z_1) = (\varkappa_1^2 - \varkappa_2^2)\int_0^x u_1 u_2 \,\mathrm{d}x\,.$$

The behaviour of $u(x, \varkappa)$ for $x \to 0$ is known from Theorem 2.1 and definition (2.3). In this region $u_{1,2} > 0$, $u_{1,2}' > 0$, so that $z_2 > z_1$.

Lemma A.2. *If $\varkappa_1 > \varkappa_2$ and if z_1 and z_2 are solutions of (A.1) satisfying the given initial conditions, then $z_1(x) < z_2(x)$.*

Proof. Suppose there is $x_0 > 0$ for which $z_1(x_0) = z_2(x_0)$, then

$$\frac{\mathrm{d}}{\mathrm{d}x}(z_2 - z_1)\big|_{x=x_0} = (\varkappa_1^2 - \varkappa_2^2)\frac{1}{l+1}\sin^2 z_1\big|_{x=x_0}\,. \tag{A.4}$$

Consider the smallest $x_0 > 0$, i.e. $z_2 - z_1 \neq 0$ for x, $0 < x < x_0$. If $z_1(x_0) \neq k\pi$, $k = 1, 2, \ldots$, then Lemma A.2 is proved, because $z_2 - z_1$ is an increasing function at the point x_0 and this is a contradiction with Lemma A.1.

The case $z_1(x_0) = z_2(x_0) = k\pi$, $k = 1, 2, \ldots$, cannot occur: in the opposite case

$$u_1(x_0) = 0$$

(see (3.1)) and Theorem 2.3 of Sturm states that for x, $0 < x < x_0$, at least one zero of u_2 must exist. Thus, u_2 has more zeros than u_1 in the corresponding interval, so that

$$z_1(x_0) \neq z_2(x_0)\,.$$

Lemma A.3. *Let $\varkappa_0$ be given, $0 < \varkappa_0 < \infty$. There is such an $a(\varkappa_0)$ that for every x_0, $0 < x_0 < a(\varkappa_0)$, the function $z(x_0, \varkappa)$ is continuous at the point $\varkappa_0$.*

Let us choose $\varkappa_0$, $0 < \varkappa_0 < \infty$, and a fixed δ_1, $0 < \delta_1 < \varkappa_0$. Let us denote by $x_1' > 0$ the first zero of $u(x, \varkappa_0 - \delta_1)$ and by $x_1'' > 0$ the first zero of $u(x, \varkappa_0 + \delta_1)$; by Theorem 2.4, $x_1' < x_2'$. For $\varkappa$ and x_0 satisfying

$$\varkappa_0 - \delta_1 < \varkappa < \varkappa_0 + \delta_1\,,$$

$$0 < x_0 < x_1'\,,$$

Theorem 2.4 leads to $u(x_0, \varkappa) \neq 0$
and

$$u(x_0, \varkappa_0 - \delta_1) < u(x_0, \varkappa) < u(x_0, \varkappa_0 + \delta_1)\,.$$

By using (3.7) and (A.2) we get easily

$$(l + 1)\, u(x_0, \varkappa)\, u(x_0, \varkappa_0) \left[\operatorname{cotg} z(x_0, \varkappa) - \operatorname{cotg} z(x_0, \varkappa_0)\right] =$$

$$= (\varkappa^2 - \varkappa_0^2) \int_0^{x_0} u(x, \varkappa)\, u(x, \varkappa_0)\, \mathrm{d}x$$

and with the help of the above derived inequalities we can establish an estimate:

$$(l + 1) \left|\operatorname{cotg} z(x_0, \varkappa) - \operatorname{cotg} z(x_0, \varkappa_0)\right| \leqq |\varkappa - \varkappa_0|\, (2\varkappa_0 + \delta_1)\,.$$

$$\cdot \frac{1}{\left|u(x_0, \varkappa_0)\, u(x_0, \varkappa_0 - \delta_1)\right|} \int_0^{x_0} \left|u(x, \varkappa + \delta_1)\right| \left|u(x, \varkappa_0)\right| \mathrm{d}x \equiv |\varkappa - \varkappa_0|\, A(x_0, \delta_1, \varkappa_0)\,.$$

Thus, Lemma A.3 is proved, because $z(x_0, \varkappa) < \pi$ for the admissible x_0 with $a(\varkappa_0) \equiv x_1'$.

Lemma A.4. *The function $z(x_0, \varkappa)$ is continuous at the point $\varkappa_0$ for any x_0, $0 < x_0 < \infty$ and the given $\varkappa_0$.*

This Lemma is a consequence of Lemma A.3 and of the standard theorems about continuity of solutions of the differential equation with respect to the boundary condition and to the parameter (see e.g. [5], Theorem 14.11 p. 241 and Remark 18.4.14 p. 329).

Theorem. *If $z(x, \varkappa)$ is a solution of (3.9) satisfying $z(0, \varkappa) = 0$, $z'(0, \varkappa) = 1$ and if for some $\varkappa = \bar{\varkappa}$ and every x, larger than some x_0,*

$$k\pi < z(x, \bar{\varkappa}) < (k + 1)\pi, \quad k = 0, 1, 2, \dots,$$

holds, then there are either $k + 1$ or k eigenvalues. Their number is $k + 1$ if $\bar{\varkappa}$ is an eigenvalue and k if it is not.

Proof. Let $\varkappa_{\text{crit}}$ be defined as follows:

$$\varkappa_{\text{crit}} = \inf\{\varkappa > \bar{\varkappa} \mid z(x, \varkappa) < k\pi \text{ for } x \in \langle 0, \infty)\}.$$

From this definition and from the property (iii) of the function $z(x, \varkappa)$ we obtain

$$z(x, \varkappa) < k\pi$$

for *every* $\varkappa > \varkappa_{\text{crit}}$. Similarly $z(x, \varkappa) > k\pi$ for all x larger than some x_0 if $\varkappa > \varkappa_{\text{crit}}$.

We say that $z(x, \varkappa)$ is of the 1st kind if for some x $z(x, \varkappa) > k\pi$; in the opposite case it is said to be of the 2nd kind.

Next we prove that $z(x, \varkappa_{\text{crit}})$ is of the 2nd kind, i.e. $z(x, \varkappa_{\text{crit}}) < k\pi$ for every x, $0 < x < \infty$. If $z(x, \varkappa_{\text{crit}})$ were of the 1st kind, then $z(x_1, \varkappa_{\text{crit}}) > k\pi$ for some x_1.

Then, it follows from (ii) that there is $\varkappa > \varkappa_{\text{crit}}$ such that $z(x_1, \varkappa) > k\pi$. This is a contradiction with the definition of $\varkappa_{\text{crit}}$.

Now

$$\lim_{x \to \infty} z(x, \varkappa) = k\pi - \operatorname{arctg} \frac{l + 1}{\varkappa} \tag{B.1}$$

or

$$\lim_{x \to \infty} z(x, \varkappa) = (k - 1)\pi + \operatorname{arctg} \frac{l + 1}{\varkappa} \tag{B.2}$$

if

$$(k - 1)\pi < z(x, \varkappa) < k\pi.$$

If $\varkappa = \varkappa_{\text{crit}}$ only (B.1) is possible and at the same time

$$\lim_{x \to \infty} z(x, \varkappa) < (k - 1)\pi + \frac{\pi}{2}, \quad \varkappa > \varkappa_{\text{crit}}. \tag{B.3}$$

To prove it let us suppose that for $\varkappa = \varkappa_{\text{crit}}$ (B.2) holds, i.e.

$$A = (k - 1)\pi + \operatorname{arctg} \frac{l + 1}{\varkappa_{\text{crit}}} < (k - 1)\pi + \frac{\pi}{2}.$$

Therefore, there is x_0 such that for every $x_1 > x_0$,

$$z(x_1, \varkappa_{\text{crit}}) < A + \varepsilon_0 < (k - 1)\pi + \frac{\pi}{2}.$$

Because of (iii) there is a $\varkappa < \varkappa_{\text{crit}}$ such that

$$z(x_1, \varkappa) < (k - 1)\pi + \frac{\pi}{2}.$$

It is easy to see that x_1 can be chosen so large as to guarantee the property (v). The function $z(x, \varkappa)$ cannot then be greater than $(k - 1)\pi + \frac{1}{2}\pi$ so that $z(x, \varkappa) > k\pi$. This is again a contradiction with the definition of $\varkappa_{\text{crit}}$ and so (B.1) for $\varkappa = \varkappa_{\text{crit}}$ must hold.

To prove (B.3), let us suppose that there is $\varkappa > \varkappa_{\text{crit}}$ such that

$$\lim_{x \to \infty} z(x, \varkappa) > (k - 1)\pi + \frac{\pi}{2},$$

i.e.

$$\lim_{x \to \infty} z(x, \varkappa) = k\pi - \operatorname{arctg} \frac{l + 1}{\varkappa}.$$

Then

$$\lim_{x \to \infty} z(x, \varkappa) > \lim_{x \to \infty} z(x, \varkappa_{\text{crit}})$$

and this implies that from some x

$$z(x, \varkappa) > (x, \varkappa_{\text{crit}}).$$

But this is excluded by the definition of $\varkappa_{\text{crit}}$. It has been proved that there is one eigenvalue, i.e. (see (ii))

$$\varkappa_{\text{crit}} = \varkappa_{k-1},$$

and it has been shown that

$$(k - 1)\pi < \lim_{x \to \infty} z(x, \varkappa_{\text{crit}}) < k\pi.$$

Therefore the same proof can be repeated with the substitution of $\bar{\varkappa} \to \varkappa_{k-1}$. Thus we prove that there are just k eigenvalues in the open interval $(\bar{\varkappa}, \varkappa_M)$:

$$\bar{\varkappa} < \varkappa_{k-1} < \varkappa_{k-2} < \ldots < \varkappa_0 < \varkappa_M.$$

If $\lim_{\chi \to \infty} z(x, \bar{\varkappa}) > k\pi + \frac{1}{2}\pi$ then $\bar{\varkappa} = \varkappa_M$ is the $(k + 1)$-th eigenvalue.

Remark. The properties of $\varkappa_{\text{crit}}$ and the relation (B.3) leads to the conclusion that the function

$$g(\varkappa) = \lim_{x \to \infty} z(x, \varkappa)$$

is discontinuous at the point $\varkappa = \varkappa_{\text{crit}}$ and the discontinuity is equal to π.

Souhrn

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NOVÁ METODA VÝPOČTU DISKRÉTNÍHO SPEKTRA RADIÁLNÍHO SCHRÖDINGEROVA OPERÁTORU

V práci je předložena nová metoda výpočtu vlastních hodnot radiálního Schrödingerova operátoru $-d^2/dx^2 + v(x)$, $x \geqq 0$. Tato třída je vymezena m.j. požadavkem, aby pro $x \to 0_+$, resp. $x \to +\infty$ se potenciál $v(x)$ choval jako $x^{-2+\varepsilon}$, resp. $x^{-2-\varepsilon}$, $\varepsilon \geqq 0$.

Schrödingerova rovnice se Prüferovou transformací převede na nelineární diferenciální rovnici prvního řádu (3.9) pro funkci $z(x, \varkappa)$ ($\varkappa$ – parametr) a ukáže se, že hledané vlastní hodnoty jsou body nespojitosti funkce $z(\infty, \varkappa)$. Kromě toho z průběhu funkce $z(x_{max}, \varkappa)$ (kde x_{max} je hodnota „dostatečně veliká" a v textu specifikovaná), obdržíme disjunktní intervaly, z nichž každý obsahuje právě jednu vlastní hodnotu a jejichž délka se zmenšuje se vzrůstem x_{max}.

Výpočet vlastních hodnot předloženou metodou je podstatně kratší a méně náročný na strojní čas než jinými známými metodami.

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