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Aplikace matematiky, Vol. 22 (1977), No. 3, 189–198

Persistent URL: http://dml.cz/dmlcz/103692

SVAZEK 22 (1977) APLIKACE MATEMATIKY ČÍSLO 3

SCHRÖDINGER EIGENVALUE PROBLEM FOR THE GAUSSIAN POTENTIAL

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(Received June 28, 1976)

1. INTRODUCTION

Various numerical methods are known by means of which the radial Schrödinger equations with a wide class of potentials are solved. There are two reasons why the investigation of the Schrödinger eigenvalue problem for the attractive Gaussian potential and the general (integer and half-integer) angular momentum is undertaken in this paper. First, we want to derive the explicit equation for the energy of the bound states. Second, the linear homogeneous differential equation which results from the modified Laplace transformation of the Schrödinger equation constitutes an interesting mathematical problem, for one of the complex arguments $\varphi(z)$ of the unknown function is retarded: $|\varphi(z)| < |z| \neq 0$ and at the same time the solution must be analytic in the half-plane $\mathrm{Re}(z) \geqq 0$.

In the monographs on the difference-differential equations [1–3] either the equations with constant coefficients are investigated or the variable z is assumed real or the arguments are shifted by constant values, but a very limited number of eigenvalue problems is solved. Valeev's and Karganyan's investigation [4] is closest to ours, but again it is carried out on the (whole) real axis only and does not concern the eigenvalue problem.

2. MODIFIED LAPLACE TRANSFORMATION OF THE SCHRÖDINGER EQUATION

We want to investigate the solution of the well-known radial Schrödinger equation with the Gaussian potential

$$\chi''(r) - (P^2 - \tfrac{1}{4})\, r^{-2}\, \chi(r) - 4(\varepsilon - a\, e^{-r^2})\, \chi(r) = 0\,, \tag{1}$$

where dimensionless quantities are used. The eigenvalues of energy ε are enforced by the boundary conditions of the finite motion

$$(2)\qquad \chi(r) \equiv r^{P+(1/2)}\,\psi(r) \approx r^{P+(1/2)}\,\text{const.}\quad \text{as}\quad r \to 0^+ \quad\text{and}$$

$$\chi(r) \sim e^{-2\varepsilon^{1/2} r}\,\text{const.}\quad \text{as}\quad r \to \infty\,.$$

In the elementary theory of deuteron [5] the value of quantum number $P = \frac{1}{2}$ is taken, in the hyperspherical-expansion approach to the atomic nuclei P is either integer or half-integer and large in general.

Analogously to the monograph [6] we introduce the modified Laplace transformation

$$(3)\qquad h(s) = \int_0^\infty \mathrm{d}r\, e^{-sr^2}\,\psi(r)\,, \quad \operatorname{Re}(s) \geqq \text{const.}\,.$$

It is related to the usual Laplace transformation

$$(4)\qquad H(s) = 2\int_0^\infty \mathrm{d}r\, r e^{-sr^2}\,\psi(r), \quad \psi(r) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \mathrm{d}s\, e^{sr^2}\,H(s)$$

as follows:

$$(5)\qquad h(s) = \frac{1}{4\pi^{1/2} i}\int_{c-i\infty}^{c+i\infty} \mathrm{d}s'(s - s')^{-1/2}\,H(s')\,,$$

$$H(s) = \frac{1}{2\pi^{1/2} i}\int_{c-i\infty}^{c+i\infty} \mathrm{d}s'(s - s')^{-3/2}\,h(s') \quad (c = \operatorname{Re}(s') < \operatorname{Re}(s)).$$

It preserves the known properties and theorems of the Laplace transformation. Apart from Abel's theorem only the following one [7] is mentioned:

Theorem 2.1. *If the real function $\psi(r)$ has n sign changes in $(0, \infty)$, its transforms $h(s)$ and $H(s)$ (inclusive of the derivatives) have at most n different zero points on the real half-axis $(0, \infty)$.*

The Laplace transform $H(s)$ satisfies the linear differential equation with one advanced argument

$$(6)\qquad s^2 \frac{\mathrm{d}}{\mathrm{d}s} H(s) - (P - 1)\, s\, H(s) + \varepsilon\, H(s) - a\, H(s + 1) + P\,\psi(0) = 0$$

$$(\operatorname{Re}(s) \geqq 0)\,.$$

The investigation is much simplified if instead of $H(s)$ the derivatives

$$(7)\qquad K(s) = \frac{\mathrm{d}^{(P+(1/2))}}{\mathrm{d}s^{(P+(1/2))}}\,h(s) \quad\text{or}\quad K(s) = \frac{\mathrm{d}^P}{\mathrm{d}s^P}\,H(s)$$

are introduced depending whether P is a half-integer or an integer. For both the expressions one obtains the equation

$$(8) \qquad s^2 K'(s) + (P + 1) s K(s) + \varepsilon K(s) - a K(s + 1) = 0 \quad (\mathrm{Re}(s) \geqq 0) .$$

Setting

$$(9) \qquad K(s) = s^{-P-1} e^{\varepsilon/s} Z(s) \quad \text{and} \quad g(s) = as^{-2} \left(\frac{s}{s+1}\right)^{P+1} e^{-\varepsilon/s(s+1)}$$

we transform it into the simple equation

$$(10) \qquad Z'(s) = g(s) Z(s + 1) \quad (\mathrm{Re}(s) \geqq 0) .$$

Its alternative form is

$$(11) \qquad T'(z) = -\varrho(z) T\left(\frac{z}{z+1}\right) \quad (\mathrm{Re}(z) \geqq 0) ,$$

where the notation used is

$$(12) \qquad z = s^{-1}, \; Z(z^{-1}) = T(z) , \quad \varrho(z) = a(1 + z)^{-P-1} e^{-\varepsilon z^2/z+1} .$$

Since the function $T(z)$ is analytic, equation (11) can be easily integrated at the only ordinary (double) point $z = 0$, where both the arguments of the functions $T'(z)$ and $T(z/(z + 1))$ fuse being equal to zero. The integration must, however, point into the interior of the half-plane $\mathrm{Re}(z) \geqq 0$, for the integration path can be then chosen in the way that only the retarded arguments $|t/(1 + t)| \leqq |z|$ i.e. the values of $T(t)$ already calculated are used. Coincidentally, the value of $T(0)$ is determined by the first condition (2) if Abel's theorem [7] is applied:

$$(13) \qquad \begin{aligned} &K(s) \sim s^{-P-1} \text{ const.} \quad \text{and} \quad Z(s) \sim \text{const.} \quad \text{as} \quad s \to \infty , \\ &T(z) \approx \text{const.} \quad \text{as} \quad z \to 0^+ . \end{aligned}$$

The value of the constants used is arbitrary, the resolvent of equation (11) $R(z, \varepsilon) = R(z, 0; \varepsilon)$ is specified by $1 = R(z, z; \varepsilon) = R(0, \varepsilon)$.

Iterating the integrated equation (11) we obtain

$$(14) \qquad R(z, \varepsilon) = 1 - \int_0^z \mathrm{d}t \, \varrho(t) \, R\left(\frac{t}{t+1}, \varepsilon\right) = \sum_{k=0}^{\infty} (-1)^k \delta_k(z, \varepsilon)$$

where $\delta_k(z, \varepsilon)$ are defined by the recursive relations

$$(15) \quad \delta_0(z, \varepsilon) = 1 , \quad \delta_{k+1}(z, \varepsilon) = \int_0^z \mathrm{d}t \, \varrho(t) \, \delta_k\left(\frac{t}{t+1}, \varepsilon\right) \quad (k = 0, 1, \ldots, \infty) .$$

If the absolute value of z is small, $t/(t + 1)$ can be replaced by t and we have

$$(16) \qquad R(z, \varepsilon) \approx e^{-\delta_1(z,\varepsilon)} \approx e^{-az}$$

the last expression being the next approximation. The first approximation could be called automorphic [8], since it assumed virtually that $R(z/(z+1), \varepsilon) \approx R(z, \varepsilon)$. In the same way we get

$$(17) \qquad |R(z, \varepsilon)| \leqq e^{c|z|},$$

where various estimates of the positive constant c can be established, and the series in (14) is absolutely and uniformly convergent for $\mathrm{Re}\,(z) \geqq 0$.

The exponential dependence of the resolvent near $z = 0^+$ can be demonstrated also in the following way. If we denote by $f(t)$ an arbitrary (integrable) function, then it can be directly verified that by differentiating the relation

$$(18) \qquad R(z, \varepsilon) = \exp - \left(\int_0^z \mathrm{d}t\, \varrho(t)\, f(t)\right) \left\{1 - \int_0^z \mathrm{d}t\, \varrho(t) \exp\left(\int_0^t \mathrm{d}s\, \varrho(s) f(s)\right) \left[R\left(\frac{t}{t+1}, \varepsilon\right) - f(t)\, R(t, \varepsilon)\right]\right\}$$

equation (11) is obtained and that both the sides of (18) are also equal to one for $z = 0$. The form of the expression on the right-hand side of (18) is given by a certain transformation and rearrangement of the terms in series (14), the corresponding explicit procedure being specified by function $f(t)$. It applies to the numerical solution of equation (11) in a real neighbourhood of $z = 0^+$, the suitable method being again successive approximations.

If the same approach is applied, the solution (6) reads

$$(19) \qquad H(s) = \mathrm{const.}\; s^{P-1} e^{\varepsilon/s} \sum_{k=0}^{\infty} (-1)^k \alpha_k(s^{-1}, \varepsilon),$$

where

$$(20) \qquad \alpha_0(z, \varepsilon) = \int_0^z \mathrm{d}t\, t^{P-1} e^{-\varepsilon t}, \quad \alpha_{k+1}(z, \varepsilon) = a \int_0^z \mathrm{d}t (1+t)^{P-1} e^{-\varepsilon t^2/(t+1)} \alpha_k\left(\frac{t}{t+1}, \varepsilon\right) \quad (k = 0, 1, \ldots, \infty);$$

the integration must proceed again from the only ordinary point $z = 0$. We prefer, however, the expression which follows from the integration of (7)

$$(21) \qquad H(s) = \mathrm{const.}\; \Gamma^{-1}(P) \int_s^{\infty} \mathrm{d}t\, t^{-P-1} (t - s)^{P-1} e^{\varepsilon/t} R(t^{-1}, \varepsilon)$$

as it is simpler ($\Gamma(P)$ being the well-known Γ-function). Nevertheless, the inversion of the Laplace transformation according to the second formula (4) still remains complicated, the calculation is easily performed for the second approximation (16) only. Using the well-known Hankel's expression [7] for the Γ-function, we get

$$(22) \qquad \psi(r) \approx \mathrm{const.}\; [(a - \varepsilon)^{1/2} r]^{-P} J_P(2(a - \varepsilon)^{1/2} r),$$

where the occurrence of the Bessel function $J_P(z)$ of the P-th order is typical for the description of the interior of a rectangular potential well with a depth a.

Hitherto there was no need for specifying the value of the energy. This means that the continuous spectrum, i.e. the negative values of ε are also admitted in formulae (6–22). The differentiation of the discrete spectrum from the continuous one is due to prescribed asymptotic (2) for the bound states according to which value $H(0)$ given by (4) is finite. Comparing it with the limit of (19) or (21) as $s \to 0^+$ we derive the eigenvalue equation for energy ε. Here the essential singularity must be removed unlike the usual cases, where the quantization of the energy is connected with the removal of poles and branch points only (see e.g. [7]).

3. PROPERTIES OF $R(z, \varepsilon)$ ON THE REAL HALF-AXIS

It is evident from Theorem 2.1 that the most interesting properties of resolvent $R(z, \varepsilon)$ for $\varepsilon \geqq 0$ are concentrated on the real half-axis $\mathrm{Im}\,(z) = 0$, $z \geqq 0$.

Expressions (19), (21) and (9) tend to finite limits as $s \to 0^+$ if the eigenvalue equation for the energy ε is chosen as follows:

$$(23) \qquad \lim_{z \to \infty} R(z, \varepsilon) = \lim_{s \to 0^+} \left\{ \alpha_0^{-1}(s^{-1}, \varepsilon)\, s^{-P+1} e^{-\varepsilon/s} \int_s^\infty dt\, t^{-P-1}(t - s)^{P-1}\, e^{\varepsilon/t} \right.$$
$$\left. R(t^{-1}, \varepsilon) \right\} = \alpha_0^{-1}(\infty, \varepsilon) \lim_{s \to 0^+} \int_0^{s^{-1}} du\, u^{P-1} e^{-\varepsilon u}\, R(s^{-1} - u, \varepsilon) = R(\infty, \varepsilon) = 0\,.$$

This results from the application of l'Hopital's rule

$$(24) \quad \lim_{s \to 0^+} H(s) = \text{const.}\ \varepsilon^{-1} \left[a e^\varepsilon \sum_{k=0}^{\infty} (-1)^k\, \alpha_k(1, \varepsilon) - 1 \right] = \text{const.}\ \Gamma_{(P)}^{-1} \int_0^\infty dt\,.$$
$$.\, e^{\varepsilon t}\, R(t, \varepsilon)\,,$$
$$\lim_{s \to 0^+} \left[s^{-P-1} e^{\varepsilon/s}\, R(s^{-1}, \varepsilon) \right] = a \varepsilon^{-1} e^\varepsilon\, R(1, \varepsilon)\,.$$

It is worth noting that equation (23) cannot be fulfilled for the repulsive potential, the terms of resolvent series (14) being always positive for a negative depth a and real $z > 0$ according to definitions (12) and (15). This means that then only the continuous spectrum exists in accordance with the expectation.

If z is non-negative and finite, resolvent series (14) represents a transcendental integral function of a complex parameter ε. If $z = \infty$, it is an analytic function in every finite domain of ε with $\mathrm{Re}\,(\varepsilon) > 0$. Hence the function $R(\infty, \varepsilon)$ has a finite number of zero points $\omega_i (i = 1, \ldots, M)$ in any finite interval of real positive values of ε.

Fixing now ε and applying the well-known Rolle's theorem to $R(z, \varepsilon)$ besides equation (11) along the half-axis $z \geqq 0$, we get

Lemma 3.1. *There exist only simple zero points $z_1(\varepsilon) < z_2(\varepsilon) < \ldots < z_n(\varepsilon)$ of resolvent $R(z, \varepsilon)$, if any, on the half-axis $z \geqq 0$ and at most the greatest of them $z_n(\varepsilon) > 1$. Two consecutive zeros $z_i(\varepsilon)$ and $z_{i+1}(\varepsilon)$ obey the inequalities*

$$z_i(\varepsilon) < z_i(\varepsilon)\,[1 - z_i(\varepsilon)]^{-1} < z_{i+1}(\varepsilon)\,. \tag{25}$$

The only simple zero point of derivate $R'(z, \varepsilon)$ which is inserted between them is $z = z_i(\varepsilon)\,[1 - z_i(\varepsilon)]^{-1}$.

According to this lemma every zero point $z_i(\varepsilon)$ can be closed within bounds $k_i^{-1} \leqq z_i(\varepsilon) \leqq (k_i - 1)^{-1}$, where k_i are integers. Because of (25) the inequalities $k_i > k_{i+1}$ then hold, so that we obtain

Lemma 3.2. *In the intervals $I_k = \langle k^{-1}, (k-1)^{-1})$ which are determined by reciprocal integers $k - 1$ and $k > 0$ at most one zero point $z_0(\varepsilon)$ occurs.*

Among the partial sums

$$R_m(z, \varepsilon) = \sum_{k=0}^{m} (-1)^k\, \delta_k(z, \varepsilon)\,, \tag{26}$$

$R_1(z, \varepsilon) = 1 - \delta_1(z, \varepsilon)$ has a special position. Provided $a > P$ and $0 \leqq \varepsilon < \varepsilon_0$, where ε_0 is given by $R_1(\infty, \varepsilon_0) = 0$, it is a decreasing function of z with a simple zero point $s(\varepsilon)$. The series (14) can be rewritten in terms of $R_1(z, \varepsilon)$ as follows:

$$R(z, \varepsilon) = R_1(z, \varepsilon) + \int_0^z \mathrm{d}t_1\, \varrho(t_1) \int_0^{t_1/(t_1+1)} \mathrm{d}t_2\, \varrho(t_2)\, R_1\left(\frac{t_2}{t_2 + 1}, \varepsilon\right) + \ldots \tag{27}$$

$$\ldots + \int_0^z \mathrm{d}t_1\, \varrho(t_1) \int_0^{t_1/(t_1+1)} \mathrm{d}t_2\, \varrho(t_2) \ldots \int_0^{t_{2k-1}/(t_{2k-1}+1)} \mathrm{d}t_{2k}\, \varrho(t_{2k})\, R_1\left(\frac{t_{2k}}{t_{2k} + 1}, \varepsilon\right) + \ldots$$

Hence we conclude

Lemma 3.3. *$R(z, \varepsilon)$ is a positive, bounded and decreasing function for $0 \leqq z \leqq s(\varepsilon)$ and its first zero $z_1(\varepsilon) > s(\varepsilon)$. The simplest bounds are*

$$1 \geqq \mathrm{e}^{-\delta_1(z,\varepsilon)} \geqq R(z, \varepsilon) \geqq 1 - \int_0^z \mathrm{d}t\, \varrho(t)\, \mathrm{e}^{-\delta_1(t/(t+1),\varepsilon)} \geqq R_1(z, \varepsilon)\,, \tag{28}$$
$$0 \leqq z \leqq z_1(\varepsilon)\,.$$

They follow immediately from equation (11) and the properties of $R(z, \varepsilon)$ in the given interval.

Corollary 3.3.1. *$R(z, \varepsilon) > 0$ for any $z \geqq 0$ and $\varepsilon \geqq \varepsilon_0$.*

Since relation (15) can be transformed into the inequality

$$\delta_{k+1}(z, \varepsilon) < \delta_1\left(\frac{z}{1 + kz}, \varepsilon\right) \delta_k(z, \varepsilon)\,, \tag{29}$$

we have

Lemma 3.4. *Functions* $\delta_{k+p}(z, \varepsilon)$ $(p = 0, 1, \ldots, \infty)$ *form a positive decreasing sequence if* $z(1 + kz)^{-1} \leqq s(\varepsilon)$.

Function $s(\varepsilon)$ increases monotonically in the interval $\langle 0, \varepsilon_0)$, so that the inverse function $\varepsilon(s)$ can be defined. It maps each of the intervals $I_k = \langle k^{-1}, (k - 1)^{-1})$ into the interval $E_k = \langle \varepsilon_k, \varepsilon_{k-1})$, where bounds ε_k are the solutions of equation $R_1(k^{-1}, \varepsilon_k) = 0$. Whilst the greatest bound ε_0 has been determined by this equation, the lowest bound of ε is, naturally, zero, so that the lowest interval for the corresponding zero points $s(\varepsilon)$ is $I_N = \langle s(0), (N - 1)^{-1})$. Number N is given either by the integer $s^{-1}(0)$ or by its integer parts as follows:

$$(30) \quad N = 1 + [s^{-1}(0)] = 1 + \left[\left\{\left(1 - \frac{P}{a}\right)^{-1/P} - 1\right\}^{-1}\right] \leqq 1 + a \quad (a > P);$$

hence every $k \leqq N$.

In view of Lemma 3.4 the properties of the alternating series

$$(31) \qquad \Delta_n(z, \varepsilon) = (-1)^n \{R(z, \varepsilon) - R_{n-1}(z, \varepsilon)\} = \sum_{p=0}^{\infty} (-1)^p \, \delta_{n+p}(z, \varepsilon)$$

are described by the following

Lemma 3.5. *Series* $\Delta_{n+p}(z, \varepsilon)$ $(p = 0, 1, 2, \ldots)$ *are positive, bounded and increasing functions for* $z > 0$ *and* $\varepsilon \geqq \varepsilon_n$.

The number and location of the zero points of $R(z, \varepsilon)$ can be estimated by means of Lemmas 3.3, 3.4 and 3.1 which lead to

Proposition 3.6. *Provided* $\varepsilon \in E_n$, *the maximum number of zero points of* $R(z, \varepsilon)$ *on the real half-axis is* n. *Then they are located in the intervals*

$$(32) \qquad (n - i + 1)^{-1} < z_i(\varepsilon) < (n - i)^{-1} \quad (i = 1, \ldots, n).$$

Proposition 3.7. *Let* e'_n *and* e_n *be two values of parameter* ε *for which the resolvent* $R(z, \varepsilon)$ *has* n *zero points. Suppose that* $z_n(e'_n) \leqq 1$ *and* $z_n(e_n) > 1$. *Then*

$$(33) \qquad z_i(e_n) < (n - i)^{-1}, \quad z_i(e'_n) < (n - i + 1)^{-1} \quad \text{for} \quad i = 1, \ldots, n - 1$$

and $e'_n < \varepsilon_n$, $e_n < \varepsilon_{n-1}$.

Inequalities (33) follow immediately from Lemma 3.1. Using Lemma 3.3 and the definition of values ε_n we get the last inequalities. Since $n^{-1} = s(\varepsilon_n) < z_1(\varepsilon_n)$ according to Lemma 3.3 and $z_n(\varepsilon_n) > z_1(\varepsilon_n)[1 - (n - 1) z_i(\varepsilon_n)] > 1$ according to (25) we add

Corollary 3.7.1. *The bound* ε_n *belongs to the class of values* e_n *introduced by Proposition* 3.7.

According to Proposition 3.6 and Definition (30) the maximum number of zero points on the whole i.e. $M' \leqq N$ is to be expected if parameter ε belongs to the interval $E_N = \langle 0, \varepsilon_{N-1})$. From the Implicit Functions Theorem we can infer that the functions

$z_i(\varepsilon)$ have the derivatives of all orders in some intervals $(0, h_i)$. Since the partial derivative

$$\left[\frac{\partial}{\partial z} R(z, \varepsilon)\right]_{z=z_i(\varepsilon)} = -\left[\varrho(z)\, R\left(\frac{z}{1+z}, \varepsilon\right)\right]_{z=z_i(\varepsilon)} \tag{34}$$

equals to zero if and only if $z_i(\varepsilon) = \infty$ owing to Lemma 3.1, the limits of the upper bounds h_i are to be found among the eigenvalues of (23) $\omega_1 > \omega_2 > \ldots > \omega_n > \ldots \ldots (\varepsilon_0 > \omega_1)$. The other possibility, that there exist intervals (h_i', h_i'') whose both bounds tend to limits given by two different eigenvalues $\omega_{n'} \neq \omega_{n''}$, will be excluded. In this case at least two values ε' and $\varepsilon''(>\varepsilon')$ can be taken such that $z_i(\varepsilon') = z_i(\varepsilon'')$. Investigating the difference of the functions $R(z, \varepsilon')$ and $R(z, \varepsilon'')$ by means of Rolle's theorem and their derivatives at $z = z_i(\varepsilon') = z_i(\varepsilon'')$ and passing to limits $\omega_{n'}$ and $\omega_{n''}$ respectively, we deduce that $R(1, \omega_{n'}) = 0$; this contradicts $R(\infty, \omega_{n'}) = 0$. At the same time we have shown, in fact that the eigenvalues ω_n are simple.

Now, we let ε decrease from a value ε_0 at which $R(\infty, \varepsilon_0) > 0$ in accordance with Corollary 3.3.1, to the greatest eigenvalue of (23), ω_1. At this value the first branch $z_1(\varepsilon)$ of zero points of $R(z, \varepsilon)$ is introduced; no further zero point occurs until the parameter ε is reduced to the next greatest eigenvalue ω_2. Since ω_1 is also the greatest value among the values of class e_1 of Proposition 3.7 and Corollary 3.7.1 holds, it belongs to the interval E_1. At the second eigenvalue ω_2 which is less than ε_1 owing of the same proposition the second branch $z_2(\varepsilon)$ of zero points appears. Further on, the foregoing procedure is repeated. When ε passes from the bound ε_n to ε_{n+1} the number of zero points of $R(\infty, \varepsilon)$ increases by one. This procedure stops at some ω_M in E_M where $M = M' \leqq N$.

We conclude our consideration by stating

Theorem 3.8. *The eigenvalue equation $R(\infty, \varepsilon) = 0$ has M simple positive solutions $\omega_n(n = 1, \ldots, M)$, where $M \leqq N$ and N is given by equation (30). The eigenvalues ω_n are closed within the intervals E_n and the resolvent $R(z, \omega_n)$ has n nodes (inclusive of the zero point* at $z = \infty$).

In the theory of the eigenvalue problem (1) and (2) (see e.g. [9]) level ordering number n of eigenvalue ω_n gives the number of nodes of the corresponding eigensolution $\chi_n(r)$ if the zero point at $r = \infty$ is, again, included. Consequently, Theorem 2.1 is realized to its maximum extent.

4. APPROXIMATION OF THE EIGENVALUE EQUATION

Aiming at a more applicable form of the eigenvalue equation (23) we rewrite the expression (31) in an alternative form

$$\Delta_n(z, \varepsilon) = \int_0^z \mathrm{d}t_1\, \varrho(t_1) \int_0^{t_1/(t_1+1)} \mathrm{d}t_2\, \varrho(t_2) \ldots \int_0^{t_{n-1}/(t_{n-1}+1)} \mathrm{d}t_n\, \varrho(t_n)\, R\left(\frac{t_n}{t_n+1}, \varepsilon\right). \tag{35}$$

Looking for the energy eigenvalue from the interval E_n we may substitute the resolvent by its approximate expression (16) and (28) respectively, since its argument in (35) is always less than $1/n$. Then the approximate eigenvalue equation reads

$$R_{n-1}(\infty, \varepsilon) + (-1)^n \int_0^\infty \mathrm{d}t_1\, \varrho(t_1) \int_0^{t_1/(t_1+1)} \mathrm{d}t_2\, \varrho(t_2) \ldots \ldots \int_0^{t_{n-1}/(t_{n-1}+1)} \mathrm{d}t_n\, \varrho(t_n) \exp\left[-\delta_1\left(\frac{t_n}{t_n+1}, \varepsilon\right)\right] = 0 . \tag{36a}$$

The eigenvalues which are larger than the bound ε_{n-1} evidently satisfy this equation, too. If they are calculated from it, the corrected values are obtained in comparison with those following from the equations with lower n's. The simplest equation corresponds to the ground-state energy:

$$1 = \int_0^\infty \mathrm{d}t\, \varrho(t) \exp\left[-\delta_1\left(\frac{t}{t+1}, \varepsilon\right)\right]; \tag{36b}$$

thus this ε lies in $(\omega_1, \varepsilon_0)$ according to inequalities (28).

5. CONCLUDING REMARKS

In conclusion we want to emphasize some important points of the preceding considerations.

The simplification which has arisen from the introduction of functions (7) instead of the Laplace transform (4) is best seen by comparing the expressions (15) and (20) and from (23). The point $z = 0$ is the only one where equation (11) can be integrated in the same way as an ordinary differential equation (without the retarded argument).

The considerations of Part 3 rest upon the general properties of the function $\varrho(t)$. Consequently, they hold also for a wider class of $\varrho(t)$ than that given by the special expression in (12).

From the point of view of equation (8) it would be attractive to replace its last term by

$$K(s+1) \approx K(s) + K'(s) \tag{37}$$

in an effort to obtain an improved approximation (16) and the corresponding expression (22). This simplification makes an immediate integration of (8) possible. After having removed the improper branch point the infinite energy spectrum of the shifted harmonic oscillator with length $2^{-1/2}a^{-1/4}$ is obtained. The inverse Laplace transform is the known harmonic-oscillator wavefunction which exhibits also the defects of the approximation (37), its asymptotic being completely different from the expression (2). These facts confirm the well-known experience [1, 7] that intuitive approximaations of the type (37) are usually wrong. Here it is worth noting that while the approximate expressions can be easily inverted, the explicit inversion of the complete Laplace transform under investigation is a problem by itself.

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Souhrn

SCHRÖDINGERŮV PROBLÉM VLASTNÍCH HODNOT PRO GAUSSŮV POTENCIÁL

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Radiální Schrödingerova rovnice s přitažlivým Gaussovým potenciálem a s obecným (celým nebo polocelým) orbitálním momentem se transformuje s pomocí modifikované Laplaceovy transformace na lineární homogenní diferenciální rovnici prvního řádu s jedním „retardovaným" argumentem. Protože argumenty splývají v (jediném) bodě $z = 0$, kde jsou rovny nule, je možné tuto rovnici řešit iterací. Nespojité spektrum se odlišuje od spojitého spektra uloženou okrajovou podmínkou při $z = \infty$, která také vede k explicitní rovnici pro vlastní hodnoty energie. Vlastnosti resolventy se podrobně vyšetřují na reálné poloose a diskutují se různá přiblížení.

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