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SPECTRAL PROBLEM FOR THE RADIAL SCHRÖDINGER EQUATION WITH CONFINING-TYPE POTENTIALS

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A procedure based on the generalized integral transform method is applied to determining energy spectra for a large class of radial Schrödinger-type equations. This procedure is shown to be usefully employed in a number of known potentials. Moreover, it yields essentially new analytical results for such significant potentials as the Cornell potential important for the hadron physics.

To find a solution of the spectral problem for the Schrödinger equation with spherical symmetric potentials is an important issue of the spectroscopy theory of complex chemical compounds and molecules, as well as of description of baryon resonances [1, 2] and quarkonium mesons [3, 4]. Although any rigorous theoretical justification is absent, the potential models can satisfactorily describe the mass spectra of quarkonium, charmonium and other systems. To model an interaction potential for these systems, the confining-type potentials are usually employed. The latter are exemplified by the Cornell potential with two terms, one describing the quarks Coulomb-type interaction, and the other corresponding to the string potential responsible for confinement.

Energy spectrum calculation for the Schrödinger equation with various types of potentials is a long-standing problem solved by various methods, e.g., by direct calculations under specified boundary conditions imposed on the wave functions, by variational methods, and by various modified combinations of analytical and numerical approaches. The quasiclassical method has been widely employed and well suited for a large class of quantum mechanics problems [5, 6]. A sort of an "intuitive" approach, discussed in [7], is of interest, which is presumably in close relation with a solution of the inverse scattering problem [8].

In the present paper, we developed further the method described in [9, 10] with special consideration of the asymptotic behavior of wave functions at large values of parameter r (which is equivalent to small momenta). Actually, this is a generalization of the integral transform method with a kernel of special form that provides proper asymptotic behavior of wave functions. As it was shown in [9–11], this approach proved to be rather effective in finding low-lying spectral levels. It should be noted that low-lying spectral levels are essential in studying baryon resonances and quarkonium mesons. This allows us to hope that our method may usefully be employed in nuclear spectroscopy problems.

On this basis, we propose here an exact algorithm to reduce the radial Schrödinger equation to the algebraic eigenvalue problem. Solving this problem by the successive approximation method can yield the initial equation spectrum. The procedure proves to be rather simple both for analytical calculations and numerical computation and makes it possible to get some approximate analytical formulas for the lower energy levels that may be employed in discussing qualitative behavior of the spectrum of the model system in question. We notice that the obtained perturbation theory is convergent. The result is of special interest since it points to legitimacy of developed method and its possible application to solving concrete problems.

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As an example, we consider spherical-symmetric "confining" potentials of the form

$$U_k(r) = a^2 r^k - Z/r, \quad a > 0, \quad k = 1, 2, \tag{1}$$

important for the hadron physics applications.

Development of rapidly convergent procedure for the perturbation theory under algebraic symmetry is described in [9]. In the present paper, the method is applied to the case of potentials (1).

We consider the radial part of the Schrödinger equation in the form

$$\left[-\frac{d^2}{dr^2} + U_{\text{eff}}(r)\right] R(r) = \lambda R(r). \tag{2}$$

Let the solution's complete wave function include, along with a radial part, a standard angular function

$$\psi_{nlm}(\mathbf{r}, t) = \frac{R_n(r)}{r} V_{lm}(\theta, \varphi). \tag{3}$$

In this case, the effective potential in (2) takes the well-known form,

$$U_{\text{eff}}(r) = \frac{l(l+1)}{r^2} + U_k(r). \tag{4}$$

If the potential $U_k(r)$ does not contain any negative-power terms higher than r^{-1} (such as in (1)), then the first term in (4) will determine the radial wave function behavior, $R(r) \sim r^{l+1}$, at the origin. Making substitution $R(r) \sim r^{l+1} \cdot F(r)$, where $F(0) \neq 0$, we write the obtained equation in the following form convenient for further transformations:

$$F'' + \frac{2}{r}(l+1)F' + [\lambda - U(r)]F = 0. \tag{5}$$

1. SPECTRAL PROBLEM FOR THE CORNELL POTENTIAL

In potential (1) linear in r, the constant $a^2 > 0$ can be eliminated by simultaneous change of variables in (5), $r \to a^{-2/3} r$, and introduction of dimensionless combinations of parameters, $\lambda^* = \lambda a^{-4/3}$, $z^* = z a^{-2/3}$. A solution of (5) is sought in the form of the series

$$F(r) = \sum_{k=0}^{\infty} \frac{a_k}{f_k} r^k, \quad f_k = \left(\frac{2}{3}\right)^{2k/3} \frac{\Gamma\left(\frac{2k+4l+5}{3}\right)}{\Gamma\left(\frac{4l+5}{3}\right)}. \tag{6}$$

The coefficients f_k are chosen for symmetrization of the Jacobi matrix with coefficients a_k and proper asymptotic behavior of the wave function at infinity, $R(r) \sim \exp\left[-(2/3)r^{3/2}\right]$, which in this case coincides with the asymptotics of the well-known Airy function. Moreover, the chosen form of coefficients allows one to find a proper kernel of the generalized Laplace transform (Mittag–Leffler transform). Substituting (6) into (5), we get the following recurrent relation:

$$\begin{aligned}&(k+2)a_{k+2} - \left(k + 2l + \frac{2}{3}\right) a_{k-1} \\ &+ \left(\frac{2}{3}\right)^{1/3} \frac{z^*}{\Gamma\left(\frac{1}{3}\right)} B\left(\frac{2k+4l+6}{3}; \frac{1}{3}\right) a_{k+1} + \left(\frac{2}{3}\right)^{-1/3} \frac{\lambda^*}{\Gamma\left(-\frac{1}{3}\right)} B\left(\frac{2k+4l+6}{3}; -\frac{1}{3}\right) a_k = 0.\end{aligned} \tag{7}$$

Introducing the generating function $\Phi(w) = \sum_{k=0}^{\infty} a_k w^{2k/3}$ transforms (7) into the integro-differential equation

$$\left[\left(1 - w^2\right)\Phi' - \frac{4l+5}{3} w\Phi\right] + \frac{z^*}{\Gamma\left(\frac{1}{3}\right)} \left(\frac{2}{3}\right)^{4/3} w^{-1/3} I + \frac{\lambda^*}{\Gamma\left(-\frac{1}{3}\right)} \left(\frac{2}{3}\right)^{2/3} w^{1/3} I^* = 0, \tag{8}$$

where

$$I(w) = \int_0^1 dt \cdot t^{(4l+1)/3} (1-t)^{-2/3} \Phi(wt),$$

$$I^*(w) = \int_0^1 dt \cdot t^{(4l+3)/3} (1-t)^{-4/3} \Phi(wt).$$

Isolating explicitly the function pole singularity $\Phi(w) = (1-w^2)^{-(4l-5)/6} H(w)$ at $w = 1$, where $H(w) \equiv x^{(4l+5)/6}(1-x)^{(-4l+2)/3}\overline{\Lambda}(x)$, and carrying out conformal mapping of the complex plane w onto the unit circle $x = \dfrac{1-w}{1+w}$ give the following equation for a new unknown function $\overline{\Lambda}(x)$:

$$x(1-x)\overline{\Lambda}' + \left[\frac{4l+5}{6} + \frac{4l-9}{6}x\right]\overline{\Lambda} = \frac{2^{2/3}z^*}{3^{4/3}\Gamma\left(\frac{1}{3}\right)}(1-x)^{-2/3} I(x) + \frac{\lambda^*}{2^{2/3}3^{2/3}\Gamma\left(-\frac{1}{3}\right)} I^*(x). \qquad (9)$$

Here the integrals I and I^* are related to the function $\overline{\Lambda}(x)$ by the transformations

$$I(x) = \int_x^1 (1-u)\, u^{-2/3} \left(1 - \frac{x}{u}\right)^{-2/3} \overline{\Lambda}(u)\, du,$$

$$I^*(x) = \int_x^1 (1-u)^{5/3} u^{-4/3} \left(1 - \frac{x}{u}\right)^{-4/3} \overline{\Lambda}(u)\, du.$$

According to the general theory [9, 12], required asymptotic behavior of the wave function is realized only if $x = 0$ is a regular point of the function $\overline{\Lambda}(x)$. In this case these solutions can be sought as a series in nonnegative powers of x,

$$\overline{\Lambda}(x) = \sum_{k=0}^{\infty} A_k x^k. \qquad (10)$$

Calculating I and I^* with the help of the direct and inverse Mellin integral transform results in the following recurrent relation for the coefficients A_k:

$$\left(n + \frac{2}{3}l + \frac{5}{6}\right) A_n - \left(n - \frac{2}{3}l + \frac{1}{2}\right) A_{n-1} = \overline{z} \sum_{k=0}^{\infty} F_{nk} A_k + \overline{\lambda} \sum_{k=0}^{\infty} G_{nk} A_k. \qquad (11)$$

Here

$$F_{nk} = \frac{1}{n!} \sum_{m=0}^{n} C_n^m \left[\frac{\Gamma\left(n-m+\frac{2}{3}\right)}{\Gamma\left(\frac{2}{3}\right)}\right] \left[\frac{\Gamma\left(m+\frac{2}{3}\right)}{\Gamma\left(\frac{2}{3}\right)}\right] \left[\frac{\Gamma\left(k-m+\frac{1}{3}\right)}{\Gamma\left(\frac{1}{3}\right)}\right] \left[\frac{\Gamma\left(\frac{7}{3}\right)}{\Gamma\left(k-m+\frac{7}{3}\right)}\right],$$

$$G_{nk} = \frac{1}{n!} \left[\frac{\Gamma\left(\frac{7}{3}\right)}{\Gamma\left(k-n+\frac{7}{3}\right)}\right] \left[\frac{\Gamma\left(n+\frac{4}{3}\right)}{\Gamma\left(\frac{4}{3}\right)}\right] \left[\frac{\Gamma\left(k-n-\frac{1}{3}\right)}{\Gamma\left(-\frac{1}{3}\right)}\right]$$

are the semi-infinite matrices, $\overline{\lambda} = 5 \cdot 2^{-5/3} \cdot 3^{-2/3} \cdot a^{-4/3} \cdot \lambda \cdot \Gamma\left(\frac{2}{3}\right) / \Gamma\left(\frac{1}{3}\right)$ and $\overline{z} = 2^{-4/3} 3^{2/3} a^{-2/3} z / \Gamma\left(\frac{1}{3}\right)$ are the parameters. Then we continue seeking the approximate energy eigenvalues λ_n by introducing a cutoff on the dimension of matrices $\hat{F}$, $\hat{G}$ up to $(N+1) \times (N+1)$, where $N = 0, 1, 2, \ldots$. The resulting $N+1$ eigenvalues λ_n, $n = 0, 1, 2, \ldots, N$, define positions of the spectral problem first levels. Larger N give smaller errors. In this case, the first levels accuracy is considerably higher.

We illustrate the convergence rate of the above procedure on an example of exactly solvable problem. In a particular case of $z = 0$ and $l = 0$, the spectrum eigenvalues for the spherical linear-type potential $U_{\text{eff}} = r$ are obtained from expression (11). As is well known, they coincide with the corresponding zeros of the Airy function [12]. In the second iteration ($N = 1$), the approximate value of the ground state energy, $\lambda_0(N=1) = 2.3377$, differs from the exact one (the first zero of the Airy function), $\lambda_0^{\text{exact}} = 2.3381$, by

0.017%. We notice, however, that for large values of z higher approximations in N should be used. The above-mentioned function of parameters a and z is yet qualitatively correctly reproduced even at $N = 0, 1, 2$. For instance, at $N = 0$, the radial ground state for the potential of the given type is:

$$\lambda_{0,l}^{(N=0)} = 1.742a^{4/3}\left(l + \frac{5}{4}\right) - 2.415a^{2/3}z. \tag{12}$$

At $N = 1$, two sets of levels corresponding to the ground and the first excited radial state are obtained,

$$\bar{\lambda}_{0,l}^{(N=1)} = q - \sqrt{\frac{D}{4}}, \quad \bar{\lambda}_{1,l}^{(N=1)} = q + \sqrt{\frac{D}{4}}, \tag{13}$$

where

$$q = \frac{13}{18}l - \frac{157}{168}\overline{z} + \frac{172}{144},$$
$$\frac{D}{4} = q^2 - \left(\frac{31}{36}l + \frac{113}{144} - \frac{13}{12}\overline{z}\right)\left(\frac{7}{12}l + \frac{77}{48} - \frac{35}{42}\overline{z}\right) + \left(\frac{1}{12}l + \frac{11}{48} - \frac{11}{42}\overline{z}\right)\left(\frac{49}{36}l + \frac{49}{144} - \frac{7}{12}\overline{z}\right).$$

At $N = 2$, solutions of the cubic equation correspond to the three radial quantum numbers, 0, 1, and 2.

It should be mentioned that satisfactory accuracy of the above analytical expressions can be obtained in the limited range of parameters $z < z_{\max}(N)$, $a < a_{\max}(N)$, where the boundary values increase with the cutoff index of infinite matrix N. The boundary values can be estimated within the specified error only numerically. Convergence of this method is determined by the initial differential operator compactness, and its rate is high enough for carrying out numerical calculations without application of any substantial computer resources.

2. SPECTRAL PROBLEM FOR POTENTIAL $U_2(R)$

As in the previous case, the coefficient at the leading power of r of potential $U_2(r)$ can be eliminated by the substitution $r \to r/\sqrt{a}$, $z^* = Z/\sqrt{a}$, $\lambda^* = \lambda/a$.

Analogous arguments easily lead to an equation similar to (9),

$$x(1-x)\overline{\Lambda}' + \left[\left(\frac{l}{2} + \frac{3}{4} - \frac{\lambda}{4}\right) + \left(\frac{l}{2} - \frac{3}{4} - \frac{\lambda}{4}\right)x\right]\overline{\Lambda} = \frac{1}{2}\overline{z}\,I(x), \tag{14}$$

$$I(x) = \int_x^1 u^{-1/2}\left(1 - \frac{x}{u}\right)^{-1/3}\overline{\Lambda}(u)\,du, \qquad \overline{z} = \frac{Z^*}{\sqrt{2}\Gamma\left(\frac{1}{2}\right)},$$

and the recurrent relation for the expansion coefficients of the function $\overline{\Lambda}(x) = \sum_{k=0}^{\infty} A_k x^k$ takes the form

$$\left(n + \frac{l}{2} + \frac{3}{4} - \frac{\lambda}{4}\right)A_n - \left(n - \frac{l}{2} - \frac{1}{4} - \frac{\lambda}{4}\right)A_{n-1} = \overline{z}\sum_{k=0}^{\infty} F_{nk}A_k,$$
$$F_{nk} = \frac{1}{2n!}\left[\frac{\Gamma\left(n + \frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}\right]\left[\frac{1}{k - n + \frac{1}{2}}\right]. \tag{15}$$

In particular, at $\overline{z} = 0$, formula (15) reproduces exactly the spectrum of an ordinary spherical-symmetric harmonic oscillator, $\lambda_n = (4n + 2l + 3)a = 2a(N_m + 3/2)$, where N_m is the principal quantum number. Hence the zero approximation for arbitrary z gives

$$\lambda_{0,l}^{(N=0)} = a(2l + 3) - \sqrt{\frac{8a}{\pi}}z. \tag{16}$$

The results obtained can be compared with the experimental charmonium and bottomonium spectra. Basing on this comparison, the running coupling constant can be determined. Preliminary estimates show

that, in contrast to other models which need several variables to establish a correspondence between the Schrödinger equation spectra and parameters, the present calculations need only a single parameter, the running coupling constant. Thus we hope that the proposed technique can also be applied to calculations with actual systems.

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