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Analytical Solutions to the D-Dimensional Schrödinger Equation with the Eckart Potential *

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The analytical solutions to the Schrödinger equation with the Eckart potential in arbitrary dimension D is investigated by using the Nikiforov–Uvarov method, and the centrifugal term is treated approximatively with the scheme of Greene and Aldrich. The discrete spectrum is obtained and the wavefunction is expressed in terms of the Jacobi polynomial or the hypergeometric function. Some special cases of the Eckart potential are discussed for D=3, and the resulting energy equation agrees well with that obtained by other methods.

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It is well recognized that the concept of dimensions plays an important role in many areas of physics and the extension of physical problems to higher-dimensional space is of current interest.[1] The exact solutions of both the relativistic and nonrelativistic wave equation with certain physical potential in higher dimensions are remarkably important not only in physics and chemistry, but also in pure and applied mathematics.[2–8] As we know, the exact solutions of the Schrödinger equation for a hydrogen atom and for a harmonic oscillator in three dimensions are an important milestone in quantum mechanics.[9] In recent years, with the interest in high-dimensional field theory,[10] these two common exactly solvable potentials have been thoroughly studied in higher-dimensional space by many researchers.[11–14] Moreover, greater efforts have been devoted to obtaining the solutions of the wave equation in higher-dimensions with some diatomic molecular potentials of exponential-type, such as the Morse,[15] the Rosen–Morse,[16] and the Manning–Rosen potentials.[17] Up to date, several new approaches have been tested on higher-dimensional wave equations. The wavefunction Ansatz method,[18] the exact and proper quantization rules,[17,19] the asymptotic iteration method,[20] the algebraic method[21] and the dimensional scaling method[22] are few among the many methods. On the basis of our recent works,[23,24] in this study we attempt to investigate the analytical solutions of the Schrödinger equation in D-dimensions with the Eckart potential[25] using the Nikiforov–Uvarov (N-U) method.[26]

The original Eckart potential is an exponential-type potential model given by

$$V(r) = -\frac{\eta e^{-\delta r}}{(1-e^{-\delta r})} + \frac{q e^{-\delta r}}{(1-e^{-\delta r})^2}, \tag{1}$$

where η and q describe the depth of potential well, while δ is a positive parameter having dimensions of inverse length and is related to the range of the potential. The Eckart potential has been widely applied in physics[27] and chemical physics.[28] On the other hand, it is found that the Eckart potential and its PT-symmetric version are the special cases of the five-parameter exponential-type potential model.[29,30]

The D-dimensional Schrödinger equation with the spherically symmetric potential $V(r)$ can be obtained in the polar coordinate system with atomic units $\hbar = c = M = 1$, as follows:

$$\Big[-\frac{1}{2}\nabla_D^2 + V(r)\Big]\psi(r, \Omega_{D-1}) = E\psi(r, \Omega_{D-1}), \tag{2}$$

where E and Ω_{D-1} denote the energy and the angular variables $\theta_1, \theta_2, \ldots, \theta_{D-2}, \phi$, respectively, ∇_D^2 is the D-dimensional Laplacian. It is convenient to introduce the hyperspherical coordinates due to the spherical symmetry of the problem, which are

$$\begin{aligned} x_1 &= r\cos\theta_1, \\ x_\alpha &= r\sin\theta_1 \ldots \sin\theta_{\alpha-1}\cos\phi, \ 2 \le \alpha \le D-1, \\ x_D &= r\sin\theta_1 \ldots \sin\theta_{D-2}\sin\phi, \end{aligned} \tag{3}$$

where r is the radius of a D-dimensional sphere, angular variables $\theta_1, \theta_2, \ldots, \theta_{D-2}, \phi$ are the hyperangle, the ranges of the variables are $0 \le r < \infty$, $0 \le \phi \le 2\pi$, $0 \le \theta_k \le \pi$ for $k = 1, 2, \ldots, D-2$. The Laplacian operator in hyperspherical coordinates is

$$\nabla_D^2 = r^{1-D}\frac{\partial}{\partial r}\Big(r^{D-1}\frac{\partial}{\partial r}\Big) - \frac{L^2(\Omega_{D-1})}{r^2}, \tag{4}$$

where

$$\begin{aligned} L^2(\Omega_{D-1}) = &\sum_{i=1}^{D=2}\Big(\prod_{j=1}^{i}\sin\theta_j\Big)^{-2}(\sin\theta_i)^{i+3-D} \\ &\cdot\frac{\partial}{\partial\theta_i}\Big(\sin\theta_i^{D-i-1}\frac{\partial}{\partial\theta_i}\Big) + \Big(\prod_{j=1}^{D-2}\sin\theta_j\Big)^{-2}\frac{\partial^2}{\partial\phi^2}, \end{aligned} \tag{5}$$

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with $L^2(\Omega_{D-1})$ being a partial differential operator on the unit sphere S^{D-1}, which is called the hyperangular momentum operator or the grand angular momentum operator.[31] This operator is known to fulfill[32]

$$L^2(\Omega_{D-1})Y_\ell^m(\Omega_{D-1}) = \ell(\ell+D-2)Y_\ell^m(\Omega_{D-1}). \quad (6)$$

Since the hyperspherical harmonics $Y_\ell^m(\Omega_{D-1})$ are eigenfunctions of the operator $L^2(\Omega_{D-1})$, we can therefore seek for the solutions of the D-dimensional Schrödinger Eq. (2) in the form

$$\psi(r,\Omega_{D-1}) = R_{n_r,\ell}(r)Y_\ell^m(\Omega_{D-1}). \quad (7)$$

Inserting Eqs. (1) and (7) into Eq. (2), we can obtain the hyperradial component of the D-dimensional Schrödinger equation as

$$\Big[\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{\ell(\ell+D-2)}{r^2} + 2\Big(E + \frac{\eta e^{-\delta r}}{(1-e^{-\delta r})} - \frac{q e^{-\delta r}}{(1-e^{-\delta r})^2}\Big)\Big]R_{n_r,\ell}(r) = 0. \quad (8)$$

If one assigns the hyperradial wavefunction as

$$R_{n_r,\ell}(r) = r^{-(D-1)/2}U_{n_r,\ell}(r). \quad (9)$$

Equation (8) becomes

$$\frac{d^2}{dr^2}U_{n_r,\ell}(r) - \Big[\frac{(D+2\ell-1)(D+2\ell-3)}{4r^2} - \frac{\eta e^{-\delta r}}{1-e^{-\delta r}} + \frac{q e^{-\delta r}}{(1-e^{-\delta r})^2} - 2E\Big]U_{n_r,\ell}(r) = 0. \quad (10)$$

We now give a brief description of the conventional N-U method. For a given potential, the Schrödinger equation could be turned to a generalized hypergeometric equation through an appropriate transformation. Thus this kind of second-order differential equation can be treated effectively by the N-U method. The generalized hypergeometric type equation has the following form

$$\psi''(s) + \frac{\tilde\tau(s)}{\sigma(s)}\psi'(s) + \frac{\tilde\sigma(s)}{\sigma^2(s)}\psi(s) = 0, \quad (11)$$

where the prime denotes the derivative with respect to the argument s, $\tilde\tau(s)$ is a polynomial of degree at most 1, and $\sigma(s)$ and $\tilde\sigma(s)$ polynomials of degree at most 2. Generally speaking, all of solvable quantum problems treated by other methods can be carried out by the present approach. This is only two sides of the same coin.

After using the transformation $\psi(s) = \phi(s)y(s)$ to Eq. (11), we obtain a set of differential equations as follows:

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \quad (12)$$

$$\frac{d}{ds}[\ln\phi(s)] = \frac{\pi(s)}{\sigma(s)},\ \pi(s) = \frac{1}{2}[\tau(s) - \tilde\tau(s)], \quad (13)$$

where the polynomial solutions $y_n(s)$ are given by Rodrigues' formula

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma^n(s)\rho(s)], \quad (14)$$

with a normalized constant B_n and the weight function $\rho(s)$ satisfying a Pearson equation

$$\frac{d}{ds}[\sigma(s)\rho(s)] = \tau(s)\rho(s). \quad (15)$$

The function $\pi(s)$ and the parameter λ are defined as

$$\pi(s) = \frac{\sigma'(s) - \tilde\tau(s)}{2} \pm \sqrt{\Big(\frac{\sigma'(s)-\tilde\tau(s)}{2}\Big)^2 - \tilde\sigma(s) + k\sigma(s)}, \quad (16)$$

$$\lambda = k + \pi'(s). \quad (17)$$

The discriminant of the expression under the square root in the polynomial $\pi(s)$ must be zero, which defines the constant k. Thus a new eigenvalue equation becomes

$$\lambda_n = -n\tau'(s) - \frac{1}{2}n(n-1)\sigma''(s),\ n = 0,1,2,\ldots, \quad (18)$$

where the derivative of $\tau(s) = \tilde\tau(s) + 2\pi(s)$ must be negative.

To solve Eq. (10), one can consider the following approximation scheme of Greene and Aldrich for centrifugal term[33]

$$\frac{1}{r^2} \approx \frac{\delta^2 e^{-\delta r}}{(1-e^{-\delta r})^2}. \quad (19)$$

By introducing a new variable $x = e^{-\delta r}$, Eq. (10) with (19) can be re-arranged as

$$\frac{d^2U_{n_r,\ell}(x)}{dx^2} + \frac{(1-x)}{x(1-x)}\frac{dU_{n_r,\ell}(x)}{dx} + \frac{1}{x^2(1-x)^2}\big[-(\varepsilon^2+\omega^2)x^2 + (2\varepsilon^2+\omega^2-\gamma^2)x - \varepsilon^2\big]U_{n_r,\ell}(x) = 0. \quad (20)$$

In comparison with Eq. (11), we obtain the relations

$$\tilde\tau(x) = 1-x, \sigma(x) = x(1-x),$$
$$\tilde\sigma(x) = -(\varepsilon^2+\omega^2)x^2 + (2\varepsilon^2+\omega^2-\gamma^2)x - \varepsilon^2, \quad (21)$$

where

$$\varepsilon^2 = -\frac{2E}{\lambda^2},\ \ \omega^2 = \frac{2\eta}{\lambda^2},$$
$$\gamma^2 = \frac{2q}{\lambda^2} + \frac{(D+2\ell-1)(D+2\ell-3)}{4}. \quad (22)$$

Substituting them into Eq. (16), we have

$$\pi(x) = \frac{-x}{2} \pm \frac{1}{2}\sqrt{ax^2+bx+c}, \quad (23)$$

where the parameters are given by

$$a = \frac{1}{4} + \varepsilon^2 + \omega^2 - k,$$
$$b = k - 2\varepsilon^2 - \omega^2 + \gamma^2, \quad c = \varepsilon^2. \tag{24}$$

The constant k can be determined by setting the discriminate of expression under the square root in Eq. (23) to zero, i.e., $\Delta = b^2 - 4ac = 0$. After simple manipulations, we find

$$k_\pm = \omega^2 - \gamma^2 \pm \varepsilon\sqrt{1+4\gamma^2}. \tag{25}$$

Using them, we are able to find four possible solutions for $\pi(x)$ as follows:

$$\pi(x) = \begin{cases} -\frac{x}{2} \pm \frac{1}{2}[(2\varepsilon + \sqrt{1+4\gamma^2})x - 2\varepsilon] \\ \quad \text{for } k = k_+, \\ -\frac{x}{2} \pm \frac{1}{2}[(2\varepsilon - \sqrt{1+4\gamma^2})x - 2\varepsilon] \\ \quad \text{for } k = k_-. \end{cases} \tag{26}$$

To make the first derivative of $\tau(x) = \tilde{\tau}(x) + 2\pi(x)$ negative, we must select the most suitable form of the $\pi(x)$ as

$$\pi(x) = -\frac{x}{2} - \frac{1}{2}[(2\varepsilon - \sqrt{1+4\gamma^2})x - 2\varepsilon],$$
$$\text{for } k_- = \omega^2 - \gamma^2 - \varepsilon\sqrt{1+4\gamma^2}. \tag{27}$$

According to Eqs. (17) and (18), we can calculate the values of the parameters λ and λ_{n_r} as

$$\lambda = \omega^2 - \gamma^2 - \frac{1}{2}(1+2\varepsilon)(1+\sqrt{1+4\gamma^2}),$$
$$\lambda_{n_r} = n_r(1 + n_r + 2\varepsilon + \sqrt{1+4\gamma^2}). \tag{28}$$

Using the fact that $\lambda = \lambda_{n_r}$, we obtain the energy levels as

$$E_{n_r} = -\frac{\lambda^2}{2}\Big[\omega^2 - \gamma^2 - \frac{1}{4} - \Big(n_r + \frac{1}{2}\Big)\Big[\Big(n_r + \frac{1}{2}\Big) + \sqrt{1+4\gamma^2}\Big]\Big]^2 \times [(2n_r+1) + \sqrt{1+4\gamma^2}]^{-\frac{1}{2}}, \tag{29}$$

which gives the approximate energy spectrum of the Eckart potential in D-dimensions. However, when $D = 3$, $\gamma^2 = 2q/\lambda^2 + \ell(\ell+1) = L(L+1)$, and

$$L = -\frac{1}{2} \pm \sqrt{2q/\lambda^2 + (\ell + 1/2)^2}, \tag{30}$$

where ℓ is the orbital angular momentum quantum number, and L is defined as the deformed orbital angular momentum quantum number. After some simple manipulations, we have

$$E_{n_r} = -\frac{1}{8}\Big[\frac{2\eta}{\lambda(n_r + L + 1)} - \lambda(n_r + L + 1)\Big]^2, \tag{31}$$

which is in agreement with those obtained by the other methods.[23,34] From Eq. (1), it can be found that when q=0, the Eckart potential reduces to the Hulthén potential and the corresponding study has been carried out by another researcher.[35]

We are now in the position to find the wave functions $U_{n_r,\ell}(x)$. By solving Eqs. (13) and (15), and using Eqs. (21) and (27), we obtain

$$\phi(x) = x^\varepsilon(1-x)^{\mu/2}, \ \rho(x) = x^{2\varepsilon}(1-x)^{\mu-1}, \tag{32}$$

where

$$\mu = 1 + \sqrt{1+4\gamma^2}. \tag{33}$$

Substituting $\rho(x)$ into Eq. (14) allows us to obtain the polynomials $y_{n_r}(x)$ as follows:

$$y_{n_r}(x) = B_{n_r} x^{-2\varepsilon}(1-x)^{1-\mu} \cdot \frac{d^{n_r}}{dx^{n_r}}[x^{n_r+2\varepsilon}(1-x)^{n_r+\mu-1}]. \tag{34}$$

This function is very similar to the definition of the Jacobi polynomials except for an unimportant factor[36]

$$P_n^{(\alpha,\beta)}(z) = \frac{(-1)^n}{2^n n!}(1-z)^{-\alpha}(1+z)^{-\beta} \cdot \frac{d^n}{dz^n}[(1-z)^{n+\alpha}(1+z)^{n+\beta}]. \tag{35}$$

If set $z = 1 - 2x$, we can obtain $y_{n_r}(x) \approx P_{n_r}^{(\alpha,\beta)}(1-2x)$, where $\alpha = 2\varepsilon$, $\beta = \mu - 1$. Thus the wavefunction $U_{n_r,\ell}(x) = \phi(x)y_{n_r}(x)$ can be expressed as

$$U_{n_r,\ell}(x) \approx x^\varepsilon(1-x)^{\mu/2}P_{n_r}^{(2\varepsilon,\mu-1)}(1-2x). \tag{36}$$

By using the relation between the hypergeometric function and the Jacobi polynomials[36]

$$P_n^{(\alpha,\beta)}(z) = \frac{\Gamma(n+1+\alpha)}{n!\Gamma(1+\alpha)}{}_2F_1\Big(-n, n + \alpha + \beta + 1; \alpha + 1; \frac{1-z}{2}\Big), \tag{37}$$

the wave function $U_{n_r,\ell}(x)$ is rewritten as

$$U_{n_r,\ell}(x) = C'_{n_r} x^\varepsilon(1-x)^{\mu/2}{}_2F_1(-n_r, n_r + 2\varepsilon + \mu - 1; 2\varepsilon + 1; x), \tag{38}$$

where C'_{n_r} is a normalization constant. Finally, the hyperradial component of the D-dimensional Schrödinger equation with the Eckart potential is obtained as follows:

$$R_{n_r,\ell}(r) = C'_{n_r} r^{-(\frac{D-1}{2})}e^{-\varepsilon\alpha r}(1-e^{-\alpha r})^{\mu/2} \cdot {}_2F_1(-n_r, n_r + 2\varepsilon + \mu - 1; 2\varepsilon + 1; e^{-\alpha r}). \tag{39}$$

In summary, we have investigated the D-dimensional Schrödinger equation with the Eckart potential analytically. To solving the corresponding hyperradial equation, the N-U method is used and the

centrifugal term is approximated with the scheme of Greene and Aldrich. The discrete spectrum of the bound states is obtained and the wavefunctions are expressed in terms of the Jocobi polynomial or the hypergeometric function. We find that this potential reduces to the Hulthén potential when parameter $q = 0$. It is also found that when $D = 3$, the D-dimensional Schrödinger equation with the Eckart potential is transformed into that of the arbitrary ℓ-wave solutions of the Eckart potential in three dimensions, and the resulting energy equation is in good agreement with those obtained by other methods.

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