Relativistic solutions for diatomic molecules subject to pseudoharmonic oscillator in arbitrary dimensions

Sami Ortakaya†

Institute of Natural and Applied Sciences, Department of Physics, Erciyes University, 38039 Kayseri, Turkiye

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The exact solutions of the N-dimensional Klein–Gordon equation in the presence of an exactly solvable potential of $V(r) = D_e(r/r_e - r_e/r)^2$ type have been obtained. The N dimensional Klein–Gordon equation has been reduced to a first-order differential equation via Laplace transformation. The exact bound state energy eigenvalues and corresponding wave functions for CH, H_2, and HCl molecules interacting with pseudoharmonic oscillator potential in the arbitrary N dimensions have been determined. Bound state eigenfunctions used in applications related to molecular spectroscopy are obtained in terms of confluent hypergeometric functions.

Keywords: Klein–Gordon equation, Laplace integral transform, bound states

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1. Introduction

Over the last decades, a good few studies have focused on exactly solvable quantum mechanical wave equations. The solutions of the relativistic and nonrelativistic quantum mechanical wave equations with various physical potentials have been regarded as important problems in atomic and molecular quantum mechanics. Due to the mathematical difficulties, Klein–Gordon and Schrödinger-type equations constitute extra-mathematical methods. Recently, the generalizations of these equations to multidimensional space have increased interest in the area of quantum physics. Multidimensional coordinates have been quite extensively used to describe triatomic and diatomic structures.[1–3] The relationship between hydrogen atom and a harmonic oscillator potential in arbitrary dimensions was also studied.[4–6] Moreover, Schrödinger equation in arbitrary high dimensions was investigated by using different methods such as asymptotic iteration method (AIM),[7] exact quantization rule method,[8] Nikiforov–Uvarov method,[9] orthogonal polynomial solution method,[10,11] etc. The solutions of the Klein–Gordon equation with the generalized Hulthén and Kratzer potentials in D dimensions have been also investigated with the AIM.[12,13] The aim of the present paper is to obtain the exact bound satate solutions of the N-dimensional Klein–Gordon equation with pseudoharmonic oscillator-type potential for diatomic molecules. This potential is expressed in the form[14]

$$V(r) = D_e\left(\frac{r}{r_e} - \frac{r_e}{r}\right)^2, \tag{1}$$

where $D_e = \frac{1}{8}K_e r_e^2$ is the dissociation energy with the force constant K_e, and r_e is the equilibrium constant. Pseudoharmonic oscillator potential is generally used for discussion of molecular vibrations. Owing to importance of the pseudoharmonic potential in chemical physics, the quantum systems with this oscillatory-type potential in two dimensions,[15] in three dimensions,[16–20] and in arbitrary dimensions[9,21,22] were also investigated. In this paper, N-dimensional Klein–Gordon equations with pseudoharmonic oscillator potential are solved by the Laplace convolution integral. The various types of problems that can be treated with the Laplace integral transform include ordinary and partial differential equations as well as integral and integro-differential equations.[23] In the quantum mechanics, the solutions of the Schrödinger equation with various potentials such as N-dimensional harmonic oscillator,[24] one-dimensional Morse potential,[25] and Coulomb potential[26,27] have been obtained by Laplace transform with binomial expansion. Besides, the Klein–Gordon equation with ring-shaped oscillator potential was solved via Laplace-convolution integral.[28] The paper is organized as follows: In Section 2, the N-dimensional Klein–Gordon equation is briefly shown. In Section 3, the solutions of the hyperradial Klein–Gordon equation for the pseudoharmonic potential are obtained and the energy eigenvalues of relevant diatomic molecules are calculated. Finally, the last section is devoted to a brief summary and conclusion.

2. Klein–Gordon equation in hyperspherical coordinates

The N-dimensional Klein–Gordon equation for a diatomic molecule in a spherically symmetric potential is given by[28]

$$-\hbar^2c^2\nabla_N^2\Psi(r,\Omega) + \left(\mu c^2 + \frac{1}{2}S(r,\theta,\varphi)\right)^2\Psi(r,\Omega) = \left(E - \frac{1}{2}V(r,\theta,\varphi)\right)^2\Psi(r,\Omega), \tag{2}$$

where $S(r,\theta,\varphi)$ and $V(r,\theta,\varphi)$ are the scalar and vector potentials respectively. When $S(r,\theta,\varphi) = V(r,\theta,\varphi)$, the Klein–Gordon equation reduces to Schrödinger-type equation; there-

†Corresponding author. E-mail: sami.ortakaya@yahoo.com

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fore, bound state solutions are easily obtained by using well-known mathematical methods. Thus, the N-dimensional Klein–Gordon equation with central equal scalar and vector potentials is given as

$$\left[\nabla_N^2+\frac{E^2-\mu^2c^4}{\hbar^2c^2}-\frac{E+\mu c^2}{\hbar^2c^2}V(r)\right]\Psi(r,\Omega)=0, \tag{3}$$

where $\hbar$, μ, and c are the Planck's constant, the rest mass, and the velocity of light respectively, ∇_N^2 is the Laplacian operator in hyperspherical coordinates, Ω denotes angular variables $\theta_1,\theta_2,\theta_3,\ldots,\theta_{N-2},\varphi$. The Laplacian is written in terms of hyperspherical coordinates as follows:

$$\nabla_N^2=\frac{1}{r^{N-1}}\frac{\partial}{\partial r}r^{N-1}\frac{\partial}{\partial r}-\frac{\boldsymbol{L}_{N-1}^2}{\hbar^2r^2}, \tag{4}$$

where

$$\begin{aligned}\boldsymbol{L}_{N-1}^2 =& -\hbar^2\left[\sum_{k=1}^{N-2}\frac{1}{\sin^2\theta_{k+1}\sin^2\theta_{k+2}\cdots\sin^2\theta_{N-2}\sin^2\varphi}\right.\\ &\times\left(\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k}\right)\\ &\left.+\frac{1}{\sin^{N-2}\varphi}\frac{\partial}{\partial\varphi}\sin^{N-2}\varphi\frac{\partial}{\partial\varphi}\right].\end{aligned} \tag{5}$$

$\boldsymbol{L}_{N-1}^2$ is known as hyperangular momentum operator.[29,30] The N-dimensional Laplacian and hyperangular momentum operator is given in Appendix A. Then, N-dimensional Klein–Gordon equation with central potential can be written as

$$\begin{aligned}&\left[\frac{1}{r^{N-1}}\frac{\partial}{\partial r}r^{N-1}\frac{\partial}{\partial r}-\frac{\boldsymbol{L}_{N-1}^2}{\hbar^2r^2}+\frac{E^2-\mu^2c^4}{\hbar^2c^2}-\frac{E+\mu c^2}{\hbar^2c^2}V(r)\right]\\ &\times\Psi(r,\Omega)=0.\end{aligned} \tag{6}$$

To separate the angular and radial parts of the wave function $\Psi(r,\Omega)$, the following wave function is written as

$$\Psi(r,\Omega)=u(r)Y(\theta_1,\theta_2,\theta_3,\ldots,\theta_{N-2},\varphi).$$

Thus, the Klein–Gordon equation is reduced to the following equations describing the radial and angular motions:

$$\begin{aligned}&\left[\frac{1}{r^{N-1}}\frac{\mathrm{d}}{\mathrm{d}r}r^{N-1}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{E+\mu c^2}{\hbar^2c^2}V(r)+\frac{E^2-\mu^2c^4}{\hbar^2c^2}\right.\\ &\left.-\frac{\ell_{N-1}(\ell_{N-1}+N-2)}{r^2}\right]u(r)=0,\end{aligned} \tag{7}$$

$$\begin{aligned}&\boldsymbol{L}_{N-1}^2Y_{\ell_1,\ldots,\ell_{N-2}}^{\ell_{N-1}}(\theta_1,\ldots,\theta_{N-2},\varphi)\\ &=\ell_{N-1}(\ell_{N-1}+N-2)\hbar^2Y_{\ell_1,\ldots,\ell_{N-2}}^{\ell_{N-1}}(\theta_1,\ldots,\theta_{N-2},\varphi),\end{aligned} \tag{8}$$

where $\ell_{N-1}\equiv\ell=0,1,2,\ldots$. It is well known that the solutions of Eq. (8) is the hyperspherical harmonics.[29,30]

3. Energy eigenvalues and corresponding wave functions

The hyperradial Klein–Gordon equation for the pseudo-harmonic potential is written as follows:

$$\begin{aligned}&\left[\frac{1}{r^{N-1}}\frac{\mathrm{d}}{\mathrm{d}r}r^{N-1}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{E+\mu c^2}{\hbar^2c^2}D_{\mathrm{e}}\left(\frac{r^2}{r_{\mathrm{e}}^2}+\frac{r_{\mathrm{e}}^2}{r^2}-2\right)\right.\\ &\left.+\frac{E^2-\mu^2c^4}{\hbar^2c^2}-\frac{\ell(\ell+N-2)}{r^2}\right]u(r)=0.\end{aligned} \tag{9}$$

If we use the following abbreviations

$$\begin{aligned}\kappa^2&=\left(\frac{E^2-\mu^2c^4}{\hbar^2c^2}+2D_{\mathrm{e}}\frac{E+\mu c^2}{\hbar^2c^2}\right)r_{\mathrm{e}}^2,\\ \gamma^2&=\frac{E+\mu c^2}{\hbar^2c^2}D_{\mathrm{e}}r_{\mathrm{e}}^2,\quad x=\left(\frac{r}{r_{\mathrm{e}}}\right)^2,\end{aligned} \tag{10}$$

equation (9) takes the following form

$$\begin{aligned}&x\frac{\mathrm{d}^2u(x)}{\mathrm{d}x^2}+\frac{N}{2}\frac{\mathrm{d}u(x)}{\mathrm{d}x}+\frac{1}{4}(\kappa^2-\gamma^2x)u(x)\\ &-\frac{\Lambda(\Lambda+N-2)}{4x}u(x)=0,\end{aligned} \tag{11}$$

where

$$\Lambda=1-\frac{N}{2}+\sqrt{\left(\ell+\frac{N}{2}-1\right)^2+\gamma^2}, \tag{12}$$

$$\Lambda(\Lambda+N-2)=\gamma^2+\ell(\ell+N-2), \tag{13}$$

$$\ell_{N-1}\equiv\ell=0,1,2,\ldots \tag{14}$$

If we consider the asymptotic behavior of the function $u(x)$ as $x\to0$ and $x\to\infty$ reasonably physical wave function is expressed as

$$u(x)=x^{\Lambda+(N-2)/2}\mathrm{e}^{-(\gamma/2)x}\phi(x), \tag{15}$$

where $\phi(x)$ is a function to be determined. When we use the reasonably physical solution which is given in Eq. (15), the equation (11) cannot be reduced by means of the Laplace transformation. Therefore, we must take a new mathematical solution of the form

$$u(x)=x^{\sigma}f(x), \tag{16}$$

where σ is a constant, $f(x)$ is a function which is given as

$$f(x)=x^{\Lambda+(N-2)/2-\sigma}\mathrm{e}^{-(\gamma/2)x}\phi(x).$$

When equation (16) is inserted into Eq. (11), we have

$$\begin{aligned}&x\frac{\mathrm{d}^2f(x)}{\mathrm{d}x^2}+\left(\frac{N}{2}+\sigma\right)\frac{\mathrm{d}f(x)}{\mathrm{d}x}+\frac{1}{4}\left[(\kappa^2-\gamma^2x)\right.\\ &\left.-\frac{1}{x}\left(4\sigma^2-4\sigma+2N\sigma-\Lambda(\Lambda+N-2)\right)\right]f(x)=0.\end{aligned} \tag{17}$$

If we apply the Laplace integral transform to Eq. (17), this equation cannot be reduced to first-order differential equation due to containing the polynomial term,

$$\frac{1}{4x}\left[4\sigma^2-4\sigma+2N\sigma-\Lambda(\Lambda+N-2)\right].$$

When we neglect this polynomial term, we should have

$$\sigma=\pm\frac{\Lambda+N-2}{2}. \tag{18}$$

If we choose $\sigma=(\Lambda+N-2)/2$, the function $u(x)$ given in Eq. (16) diverges for $x\to\infty$. This case is not acceptable physically. Then, we have to choose $\sigma=-(\Lambda+N-2)/2$ so that,

$$u(x)=x^{-(\Lambda+N-2)/2}f(x), \tag{19}$$

and hence equation (17) becomes

$$x\frac{\mathrm{d}^2f(x)}{\mathrm{d}x^2}+\left(2-\Lambda-\frac{N}{2}\right)\frac{\mathrm{d}f(x)}{\mathrm{d}x}+\frac{1}{4}(\kappa^2-\gamma^2x)f(x)=0. \tag{20}$$

3.1. Energy eigenvalues

The Laplace integral transform of the function $f(x)$ is given by[23]

$$\mathscr{L}[f(x)] = F(s) = \int_0^\infty \mathrm{e}^{-sx} f(x)\mathrm{d}x. \tag{21}$$

Applying this transform to Eq. (20) we have

$$\left(s^2 - \frac{\gamma^2}{4}\right)\frac{\mathrm{d}F(s)}{\mathrm{d}s} = \left[\frac{\kappa^2}{4} - \left(\Lambda + \frac{N}{2}\right)s\right]F(s). \tag{22}$$

The solution of Eq. (22) is easily obtained as

$$\begin{aligned} F(s) &= A\left(s+\frac{\gamma}{2}\right)^{-(\kappa^2/4\gamma)-(2\Lambda+N)/4} \\ &\times \left(s-\frac{\gamma}{2}\right)^{(\kappa^2/4\gamma)-(2\Lambda+N)/4}, \end{aligned} \tag{23}$$

where A is the constant of integration. If $F(s) = \mathscr{L}[f(x)]$,

$$\lim_{x\to\infty} f(x) = \lim_{s\to 0} sF(s), \tag{24}$$

where s is real. This condition is known as "terminal value theorem".[23] According to this condition, because of the fact that the function $u(x)$ converges for $x \to \infty$, $[\kappa^2/(4\gamma)] - (2\Lambda + N)/4$ is not a negative value. Then, we must take

$$\frac{\kappa^2}{4\gamma} - \frac{2\Lambda+N}{4} = n, \quad (n = 0,1,2,\ldots). \tag{25}$$

From Eq. (25), the bound state energy eigenvalues is obtained as follows:

$$\begin{aligned} &\sqrt{\frac{(E_{n\ell}+\mu c^2)r_\mathrm{e}^2}{4D_\mathrm{e}\hbar^2c^2}(E_{n\ell}-\mu c^2+2D_\mathrm{e})} \\ &= 2n+1+\sqrt{\left(\ell+\frac{N}{2}-1\right)^2+\frac{(E_{n\ell}+\mu c^2)}{\hbar^2c^2}D_\mathrm{e}r_\mathrm{e}^2}, \end{aligned} \tag{26}$$

where $n, \ell = 0, 1, 2, \ldots$.

In the nonrelativistic limit, applying the following transformation

$$E_{n\ell} - \mu c^2 \to E_\mathrm{nonrel}, \quad E_{n\ell} + \mu c^2 \to 2\mu c^2,$$

we obtain the nonrelativistic rovibrational energy spectrum as follows:

$$\begin{aligned} E_{n\ell} &= -2D_\mathrm{e} + \sqrt{\frac{2\hbar^2 D_\mathrm{e}}{\mu r_\mathrm{e}^2}}(2n+1) \\ &+ \sqrt{\frac{2\hbar^2 D_\mathrm{e}}{\mu r_\mathrm{e}^2}\left(\ell+\frac{N}{2}-1\right)^2+4D_\mathrm{e}^2}, \quad (n,\ell=0,1,2,\ldots). \end{aligned} \tag{27}$$

We can calculate the relativistic vibrational energy spectrum using the parameters given in Table 1 for CH, H_2, and HCl diatomic molecules. The explicit values of the relativistic and nonrelativistic vibrational energies of these diatomic molecules for $n = 1$, $\ell = 0$ values (1s state) are given in Table 2.

Table 1. Spectroscopic parameters of diatomic molecules in the ground electronic state. The data in this table are taken from Refs. [31]–[33]. The unit a.u. is the abbreviation for atomic unit.

Parameter	CH	H_2	HCl
$D_\mathrm{e}/\mathrm{cm}^{-1}$	31838.082	38300	37255.00
μ/a.u.	0.929931	0.50391	0.98010
r_e/Å	1.11980	0.74160	1.27460

Table 2. $N = 3$ dimensional relativistic and nonrelativistic vibrational energies of 1s states for relevant diatomic molecules in the ground electronic state.

	CH	H_2	HCl
$E_\mathrm{nonrel.}$/eV	0.16868	0.38037	0.15606
$E_\mathrm{rel.}$/MeV	866.232	469.393	912.965

3.2. Radial eigenfunctions

The inverse Laplece integral transform of the function $F(s)$ yields the function $f(x)$. Namely,

$$f(x) = \mathscr{L}^{-1}[F(s)].$$

Inserting Eq. (25) into Eq. (23), we should have

$$F(s) = A\left(s+\frac{\gamma}{2}\right)^{-\beta}\left(s-\frac{\gamma}{2}\right)^{-\alpha}, \tag{28}$$

where

$$\alpha = -n, \quad \beta = n + \Lambda + \frac{N}{2}. \tag{29}$$

In order to find the inverse Laplace transformation of $F(s)$, firstly we find[23]

$$\begin{aligned} \mathscr{L}^{-1}\left[\left(s+\frac{\gamma}{2}\right)^{-\beta}\right] &= g(x) = \frac{x^{\beta-1}\mathrm{e}^{-\gamma x/2}}{\Gamma(\beta)}, \\ \mathscr{L}^{-1}\left[\left(s-\frac{\gamma}{2}\right)^{-\alpha}\right] &= h(x) = \frac{x^{\alpha-1}\mathrm{e}^{\gamma x/2}}{\Gamma(\alpha)}. \end{aligned} \tag{30}$$

Then,

$$f(x) = \mathscr{L}^{-1}[F(s)] = A(g*h)(x), \tag{31}$$

where $(g*h)(x)$ is given by integral expression

$$(g*h)(x) = \int_0^x g(x-\tau)h(\tau)\mathrm{d}\tau. \tag{32}$$

Hence, $f(x)$ becomes

$$f(x) = \frac{A}{\Gamma(\alpha)\Gamma(\beta)}\mathrm{e}^{-\gamma x/2}\int_0^x (x-\tau)^{\beta-1}\tau^{\alpha-1}\mathrm{e}^{-\gamma\tau}\mathrm{d}\tau. \tag{33}$$

The integral expression yields[34]

$$\begin{aligned} f(x) &= \frac{A}{\Gamma(\alpha+\beta)}\mathrm{e}^{-\gamma x/2}x^{\alpha+\beta-1}{}_1\mathrm{F}_1(\alpha,\alpha+\beta,\gamma x), \\ &= \frac{A}{\Gamma(\Lambda+N/2)}\mathrm{e}^{-\gamma x/2}x^{\Lambda+N/2-1}{}_1\mathrm{F}_1\left(-n,\Lambda+\frac{N}{2},\gamma x\right). \end{aligned} \tag{34}$$

Substituting Eq. (34) into Eq. (19) the hyperradial wavefunction is obtained as follows:

$$u(x) = C_1 x^{\Lambda/2} \mathrm{e}^{-\gamma x/2} {}_1\mathrm{F}_1\Big(-n, \Lambda + \frac{N}{2}, \gamma x\Big), \tag{35}$$

where $C_1 = A/[\Gamma(\Lambda + N/2)]$. Making use of the relation between the generalized Laguerre polynomials and the confluent hypergeometric functions,[35]

$${}_1\mathrm{F}_1(-n, p+1, z) = \frac{n!\Gamma(p+1+n)}{\Gamma(p+1)} L_n^p(z), \tag{36}$$

we can rewrite Eq. (35) as

$$\begin{aligned} u_{n\ell}(x) &= C_2 x^{\Lambda/2} \mathrm{e}^{-\gamma x/2} L_n^{\Lambda+N/2-1}(\gamma x), \\ u_{n\ell}(r) &= C_2 r^{\Lambda} \exp\Big(-\frac{\gamma}{2r_\mathrm{e}^2} r^2\Big) L_n^{\Lambda+N/2-1}\Big(\frac{\gamma}{r_\mathrm{e}^2} r^2\Big), \end{aligned} \tag{37}$$

where C_2 is the normalization constant determined from $\int_0^\infty |u(r)|^2 r^{N-1} \mathrm{d}r = 1$. Applying the orthogonality condition of Laguerre polynomials, the normalization constant can be determined as follows:

$$C_2 = \sqrt{\frac{2n!\gamma^{\Lambda+N/2}}{r_\mathrm{e}^{N+2\Lambda}\big(n+\Lambda+N/2-1\big)!}}. \tag{38}$$

Consequently, the normalized hyperradial wave function is obtained as

$$\begin{aligned} u_{n\ell}(r)7 \;=\; & \sqrt{\frac{2n!\gamma^{\Lambda+N/2}}{r_\mathrm{e}^{N+2\Lambda}\Big(n+\Lambda+N/2-1\Big)!}} r^{\Lambda} \\ & \times \exp\Big(-\frac{\gamma}{2r_\mathrm{e}^2} r^2\Big) L_n^{\Lambda+N/2-1}\Big(\frac{\gamma}{r_\mathrm{e}^2} r^2\Big) \end{aligned} \tag{39}$$

with

$$\gamma^2 = \frac{E+\mu c^2}{\hbar^2 c^2} D_\mathrm{e} r_\mathrm{e}^2, \quad \Lambda = 1 - \frac{N}{2} + \sqrt{\Big(\ell + \frac{N}{2} - 1\Big)^2 + \gamma^2}.$$

4. Discussion and conclusion

In this paper, the exact solutions of the N-dimensional Klein–Gordon equation with pesudoharmonic potential for diatomic molecules are obtained by means of Laplace integral transformation. An integral transfom approach, i.e. the Laplace integral transform method, to calculate the relativistic rovibrational eigenvalues and eigenfunctions is also presented. N-dimensional exact bound state energy is obtained via initial-value theorem. Laplace transformation is tested by calculating the vibrational energies of CH, H_2, and HCl molecules. The $3D$-relativistic energy eigenvalues ($N = 3$ dimensional energy spectrum) for pseudoharmonic oscillator have been shown for $\ell = 0$ states with $r_\mathrm{e} = 1.2$, $\mu = 1.5$ values in Fig. 1. It can be seen from Fig. 1, that the energy eigenvalue E_{00} reaches zero at the critical value at the critical value $D_\mathrm{e} = 0.62$ and the energy eigenvalues become negative for larger D_e values. Likewise, E_{10} and E_{20} become zero for the critical values of $D_\mathrm{e} = 3.54$ and $D_\mathrm{e} = 5.78$, respectively. It has been also proved that in the nonrelativistic limit $c \to \infty$, where c is the speed of light, solutions of the Klein–Gordon system converge to those of the Schrödinger system.

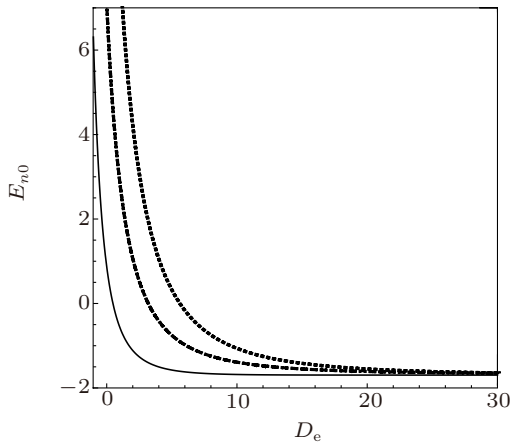


Fig. 1. In atomic units ($\hbar = 1$, $c = 1$), the relativistic $3D$-vibrational energy spectrum for molecular particles. The quantum states are considered as $n = 0, \ell = 0$ (solid line), $n = 1$, $\ell = 0$ (dashed line), and $n = 2$, $\ell = 0$ (dotted line).

The corresponding wave functions are determined by Laplace convolution integral. Moreover, the normalized corresponding eigenfunctions of the $3D$-pseudoharmonic oscillator are given with ($n = 0$, $\ell = 0$), ($n = 1$, $\ell = 0$), and ($n = 2$, $\ell = 0$) states as shown in Fig. 2.

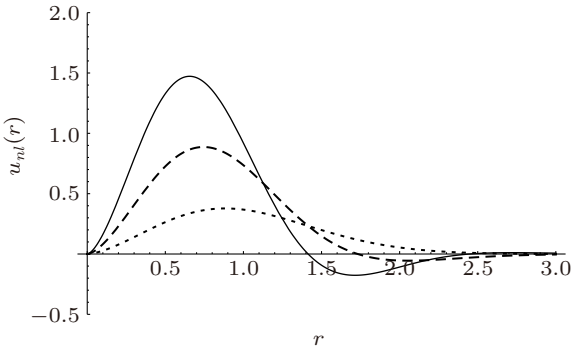


Fig. 2. In atomic units ($\hbar = 1$, $c = 1$), the $3D$-relativistic wavefunctions of the molecular particle under pseudoharmonic oscillator potential. Here, $u_{00}(r)$ (dotted line), $u_{10}(r)$ (dashed line), and $u_{20}(r)$ (solid line) are displayed.

Appendix A

A.1. Hyperangular momentum operator

The Cartesian coordinates is given in terms of the hyperspherical coordinates $\theta_1, \theta_2, \theta_3, \ldots, \theta_{N-2}, \varphi$ by[7]

$$\begin{aligned} x_1 &= r\cos\theta_1 \sin\theta_2 \sin\theta_3 \cdots \sin\theta_{N-2} \sin\varphi, \\ x_2 &= r\sin\theta_1 \sin\theta_2 \sin\theta_3 \cdots \sin\theta_{N-2} \sin\varphi, \\ x_3 &= r\cos\theta_2 \sin\theta_3 \sin\theta_4 \cdots \sin\theta_{N-2} \sin\varphi, \\ x_4 &= r\cos\theta_3 \sin\theta_4 \sin\theta_5 \cdots \sin\theta_{N-2} \sin\varphi, \\ &\vdots \\ x_j &= r\cos\theta_{j-1} \sin\theta_j \sin\theta_{j+1} \cdots \sin\theta_{N-2} \sin\varphi, \end{aligned}$$

$$3 \le j \le N-1,$$
$$x_N = r\cos\varphi, \tag{A1}$$

where

$$N = 3,4,5\ldots,\ \ 0 \le r \le \infty,\ \ 0 \le \theta_1 \le 2\pi,\ \ 0 \le \theta_1 \le 2\pi,$$
$$j = 2,3,\ldots,N-1.$$

The scale factors for N-dimensional sphere is written as follows:

$$h_k^2 = \sum_{j=1}^{N}\left(\frac{\partial x_j}{\partial\theta_k}\right)^2, \tag{A2}$$
$$h_0 = 1,$$
$$h_1 = r\sin\theta_2\sin\theta_3\sin\theta_4\cdots\sin\theta_{N-2}\sin\varphi,$$
$$h_2 = r\sin\theta_3\sin\theta_4\sin\theta_5\cdots\sin\theta_{N-2}\sin\varphi,$$
$$h_3 = r\sin\theta_4\sin\theta_5\sin\theta_6\cdots\sin\theta_{N-2}\sin\varphi,$$
$$\vdots$$
$$h_k = r\sin\theta_{k+1}\sin\theta_{k+2}\sin\theta_{k+3}\cdots\sin\theta_{N-2}\sin\varphi,$$
$$h_{N-2} = r\sin\varphi,$$
$$h_{N-1} = r \tag{A3}$$

for $N = 3,4,5,\ldots$, and $1 \le k \le N-1$. The generalized angular momentum and momentum operator components are given by

$$L_{ij} = x_i p_j - x_j p_i, \quad i = 1,2,\ldots,j-1; \quad j = 2,3,\ldots,N,$$
$$p_k = -\mathrm{i}\hbar\frac{\partial}{\partial x_k} = -\mathrm{i}\hbar\left[\sum_{j=0}^{N-2}\left(\frac{\partial\theta_j}{\partial x_k}\frac{\partial}{\partial\theta_j}\right) + \frac{\partial\varphi}{\partial x_k}\frac{\partial}{\partial\varphi}\right]$$
$$= -\mathrm{i}\hbar\left[\sum_{j=0}^{N-2}\frac{1}{h_j^2}\left(\frac{\partial x_k}{\partial\theta_j}\frac{\partial}{\partial\theta_j} + \frac{\partial x_k}{\partial\varphi}\frac{\partial}{\partial\varphi}\right)\right]. \tag{A4}$$

For $k = 1,2,3,\ldots,N-1$ values, the k-components of angular momentum operator is defined as

$$\boldsymbol{L}_k^2 = \sum_{j=2}^{k+1}\sum_{i=1}^{j-1}\boldsymbol{L}_{ij}^2,$$
$$\boldsymbol{L}_1^2 = -\hbar^2\frac{\partial^2}{\partial\theta_1^2},$$
$$\boldsymbol{L}_2^2 = -\hbar^2\left[\frac{1}{\sin\theta_2}\frac{\partial}{\partial\theta_2}\sin\theta_2\frac{\partial}{\partial\theta_2} - \frac{\boldsymbol{L}_1^2}{\hbar^2\sin^2\theta_2}\right],$$
$$\boldsymbol{L}_3^2 = -\hbar^2\left[\frac{1}{\sin^2\theta_3}\frac{\partial}{\partial\theta_3}\sin^2\theta_3\frac{\partial}{\partial\theta_3} - \frac{\boldsymbol{L}_2^2}{\hbar^2\sin^2\theta_3}\right],$$
$$\boldsymbol{L}_4^2 = -\hbar^2\left[\frac{1}{\sin^3\theta_4}\frac{\partial}{\partial\theta_4}\sin^3\theta_4\frac{\partial}{\partial\theta_4} - \frac{\boldsymbol{L}_3^2}{\hbar^2\sin^2\theta_4}\right],$$
$$\vdots$$
$$\boldsymbol{L}_k^2 = -\hbar^2\left[\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k} - \frac{\boldsymbol{L}_{k-1}^2}{\hbar^2\sin^2\theta_k}\right],$$
$$\vdots$$
$$\boldsymbol{L}_{N-1}^2 = -\hbar^2\left[\frac{1}{\sin^{N-2}\varphi}\frac{\partial}{\partial\varphi}\sin^{N-2}\varphi\frac{\partial}{\partial\varphi} - \frac{\boldsymbol{L}_{N-2}^2}{\hbar^2\sin^2\varphi}\right]. \tag{A5}$$

Thus, N-dimensional angular momentum operator is obtained as follows:

$$\boldsymbol{L}_{N-1}^2 = -\hbar^2\left[\sum_{k=1}^{N-2}\frac{1}{\sin^2\theta_{k+1}\sin^2\theta_{k+2}\ldots\sin^2\theta_{N-2}\sin^2\varphi}\right.$$
$$\times\left(\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k}\right)$$
$$\left.+\frac{1}{\sin^{N-2}\varphi}\frac{\partial}{\partial\varphi}\sin^{N-2}\varphi\frac{\partial}{\partial\varphi}\right]. \tag{A6}$$

A.2. N-dimensional Laplacian operator

The Laplacian in hyperspherical coordinates is given by

$$\nabla_N^2 = \sum_{k=0}^{N-1}\frac{1}{h}\frac{\partial}{\partial\theta_k}\left(\frac{h}{h_k^2}\frac{\partial}{\partial\theta_k}\right), \tag{A7}$$

where

$$h = \prod_{j=0}^{N-1} = r^{N-1}\sin\theta_2\sin^2\theta_3\sin^3\theta_4\cdots\sin^{N-2}\varphi. \tag{A8}$$

When equations (A2) and (A8) are inserted into Eq. (A7), we obtain

$$\nabla_N^2 = \frac{1}{r^{N-1}}\frac{\partial}{\partial r}r^{N-1}\frac{\partial}{\partial r}$$
$$+\frac{1}{r^2}\left[\sum_{k=1}^{N-2}\frac{1}{\sin^2\theta_{k+1}\sin^2\theta_{k+2}\cdots\sin^2\theta_{N-2}\sin^2\varphi}\right.$$
$$\times\left(\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k}\right)$$
$$\left.+\frac{1}{\sin^{N-2}\varphi}\frac{\partial}{\partial\varphi}\sin^{N-2}\varphi\frac{\partial}{\partial\varphi}\right]. \tag{A9}$$

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