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Exact Solution of the Pseudoharmonic Oscillator in the Space of Constant Positive Curvature

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Abstract We present analytically the exact solution of the radial Schrödinger equation with the pseudoharmonic oscillator potential in constant positive curvature representation. Exact bound state eigenfunctions and eigenvalues obtained using factorization method. Finally, energy eigenvalues obtained here compared with the results of the theoretical methods in the limit of flat space.

Keywords Pseudoharmonic oscillator · Constant positive curvature · Eigenfunctions · Eigenvalues

1 Introduction

Solution of Schrödinger equation for three-dimensional anharmonic oscillators has raised a considerable amount of interest due to its wide applications in chemical and molecular physics [1–4]. There are many types of potentials that can be considered as anharmonic type. Mie and pseudoharmonic potentials are major types of them that satisfy the atomic boundary conditions. The pseudoharmonic oscillator potential was first pointed out by Gol'dman et al. 1960 [5]. The pseudoharmonic oscillator potential [6–10] is an anharmonic potential, which, like the harmonic oscillator potential, also allows an exact mathematical treatment. This potential can be used to evaluate the energy spectrum of linear and non-linear systems and molecular vibrations. Solutions of the Schrödinger equation for pseudoharmonic oscillator potential is an interesting subject of chemical physics to explain the characteristics of diatomic molecules. On the other hand, the pseudoharmonic oscillator potential is, in a certain sense, an intermediate potential between the three-dimensional harmonic oscillator

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potential (which is an ideal potential) and the anharmonic potential, as the Morse potential, which is a more realistic potential, in good agreement with the experimental spectroscopical data [11]. It is well established today that the Schrödinger equation is exactly solvable only for several simple types of potentials. In the case, when Schrödinger equation has no exact solution, one can use numerical methods or approximation schemes. There are some approximation methods to solve quantum-mechanical problems such as WKB approximation [12], perturbation theory [13], path integral [14], supersymmetry and shape invariance idea [15]. Another method to solve Schrödinger equation is to represent the problem in higher dimension. Quantum-mechanical problems in spaces of constant positive and negative curvature are the object of interest of researchers since 1940, when Schrödinger [16] was the first to solve the quantum-mechanical problem of the hydrogen atom on the three-dimensional space S_3. In recent years the quantum-mechanical models in the spaces of constant curvature have attracted considerable attention due to their interesting mathematical features as well as the possibility of applications to physical problems. These models based on the geometry of constant curvature are used to describe some problems of nuclear physics [17–19], elementary particle [20] and nanotechnology [21–23]. In this study, we have obtained the exact bound state solutions of the Schrödinger equation for any quantum-mechanical systems describing pseudoharmonic oscillator potential in the space of constant positive curvature. The obtained results are exactly match with the corresponding results in the flat space. Also we applied the presented procedure to explain the characteristics for a few diatomic molecules.

2 Theoretical Calculations

The Schrödinger equation describing the non-relativistic quantum mechanic in the space of constant curvature can be written in the following form

$$H\Psi = \left[-\frac{\hbar^2}{2\mu}\Delta_{LB} + V\right]\Psi = E\Psi, \tag{1}$$

where V is the potential function of the system and Δ_{LB} is the Laplace-Beltrami operator in arbitrary curvilinear coordinates x^i that can be define by

$$\begin{aligned} \Delta_{LB} &= \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\left(\sqrt{g}g^{ik}\frac{\partial}{\partial x^k}\right) \\ ds^2 &= g_{ik}dx^i dx^k \\ g^{ik} &= (g_{ik})^{-1}, \qquad g = \det(g_{ik}). \end{aligned} \tag{2}$$

In this representation the metric tensor has the following form

$$g_{ik} = \frac{1}{1+\frac{r^2}{R^2}}\left[\delta_{ik} + \frac{x_i x_k}{r^2}\left(\frac{1}{1+\frac{r^2}{R^2}} - 1\right)\right], \qquad r^2 = x_i x_i, \tag{3}$$

where R is the curvature radius and Δ_{LB} is defined as

$$\begin{aligned} \Delta_{LB} &= \left(1+\frac{r^2}{R^2}\right)\left[\left(\delta_{ik} + \frac{x_i x_k}{R^2}\right)\frac{\partial^2}{\partial x_i \partial x_k} + \frac{x_i}{R^2}\frac{\partial}{\partial x_i}\right] \\ &= -\left(P_i P_i + \frac{1}{R^2}L_i L_i\right) \end{aligned} \tag{4}$$

P_i and L_i satisfy the following commutation relations

$$P_i = -i\left[\frac{\partial}{\partial x_i} + \frac{x_i x_k}{R^2}\frac{\partial}{\partial x_k}\right], \qquad [P_i, x_l] = -i\left(\delta_{il} + \frac{x_i x_l}{R^2}\right)$$
$$L_i = -i\epsilon_{ijk} x_j \frac{\partial}{\partial x_k}, \qquad [L_i, x_l] = -i\epsilon_{ijk} x_j. \tag{5}$$

The three-dimensional space of constant positive curvature can also be realized geometrically on the three-dimensional sphere S_3 of the radius R, embedded into the four-dimensional Euclidean space (i.e on the hypersurface),

$$\eta_0^2 + \eta_i \eta_i = R^2, \tag{6}$$

where η_0 and η_i are the Euclidean coordinates of the ambient space $\Re^4$. The coordinates η_i define in the region $\eta_i \eta_i \leq R^2$. η_i $(i = 0,\ 1,\ 2,\ 3)$ relate to the coordinates x_i of the tangent space by the following relations

$$\eta_i = \frac{x_i}{\sqrt{1 + \frac{r^2}{R^2}}} \tag{7}$$

$$\eta_0 = \frac{R}{\sqrt{1 + \frac{r^2}{R^2}}}. \tag{8}$$

The pseudoharmonic potential in the three-dimensional space can be shown by [6–10]:

$$V(r) = \frac{1}{8} k r_0^2 \left(\frac{r}{r_0} - \frac{r_0}{r}\right)^2, \tag{9}$$

where k and r_0 are the force and equilibrium intermolecular separation parameters, respectively. This potential in the space of constant positive curvature reduce to the following symmetric function,

$$V(r) \equiv V(\eta) = v_0\left[\frac{R^2(\eta_1^2 + \eta_2^2 + \eta_3^2)}{r_0^2 \eta_0^2} + \frac{r_0^2 \eta_0^2}{R^2(\eta_1^2 + \eta_2^2 + \eta_3^2)} - 2\right], \tag{10}$$

where $v_0 = \frac{1}{8} k r_0^2$ is the dissociation energy between two atoms in a solid. For any central potential $V(\tau)$, the Schrödinger equation admits following separation of variables in hyperspherical coordinates

$$\begin{aligned} \eta_0 &= R\cos\tau \\ \eta_1 &= R\sin\tau\sin\theta\cos\phi \\ \eta_2 &= R\sin\tau\sin\theta\sin\phi \\ \eta_3 &= R\sin\tau\cos\theta, \end{aligned} \tag{11}$$

where $\tau, \theta \in [0,\ \pi]$ and $\phi \in [0,\ 2\pi]$. So, the pseudoharmonic oscillator potential (10) in spherical system transform to,

$$V(\tau) = v_0\left[\frac{R^2\tan^2\tau}{r_0^2} + \frac{r_0^2}{R^2\tan^2\tau} - 2\right]. \tag{12}$$

After separation of variables in (1) we obtain the following quasiradial equation

$$\frac{1}{\sin^2\tau}\frac{d}{d\tau}\sin^2\tau\frac{dR(\tau)}{d\tau}+\frac{2\mu}{\hbar^2}\left[R^2E-\frac{\hbar^2}{2\mu}\frac{l(l+1)}{\sin^2\tau}-R^2V(\tau)\right]R(\tau)=0. \qquad (13)$$

After substituting for potential, this relation reduce to,

$$\frac{1}{\sin^2\tau}\frac{d}{d\tau}\sin^2\tau\frac{dR(\tau)}{d\tau}+\frac{2\mu R^2}{\hbar^2}\left[E+\left(2+\frac{r_0^2}{R^2}\right)v_0\right]R(\tau)$$

$$-\frac{2\mu}{\hbar^2}\left[\frac{\hbar^2}{2\mu}\frac{l(l+1)+\frac{2\mu r_0^2}{\hbar^2}v_0}{\sin^2\tau}+\frac{R^4v_0}{r_0^2}\tan^2\tau\right]R(\tau)=0. \qquad (14)$$

Application of the following transformation

$$W(\tau)=\sin\tau R(\tau) \qquad (15)$$

reduce this equation to the well known Pöschl-Teller type

$$\frac{d^2W(\tau)}{d\tau^2}+\left[\epsilon-\frac{K^2-\frac{1}{4}}{\cos^2\tau}-\frac{(L+\frac{1}{2})^2-\frac{1}{4}}{\sin^2\tau}\right]W(\tau)=0, \qquad (16)$$

where K, L and ϵ are

$$K^2=\frac{2\mu R^4v_0}{\hbar^2r_0^2}+\frac{1}{4}$$

$$L=\frac{1}{2}\left[-1+\sqrt{(2l+1)^2+\frac{8\mu r_0^2v_0}{\hbar^2}}\right] \qquad (17)$$

$$\epsilon=\frac{2\mu R^2}{\hbar^2}E+\frac{2\mu}{\hbar^2}\left(r_0^2+2R^2-\frac{R^4}{r_0^2}\right)v_0+1.$$

One regular solution of this equation (at points $\tau=0$ and $\tau=\frac{\pi}{2}$) have the following form

$$R_{nL}^{\lambda}(\tau)=C_{nL}^{\lambda}(\sin\tau)^L(\cos\tau)^{\lambda}{}_2F_1\left(-n,n+L+\lambda+2;\ L+\frac{3}{2};\ \sin^2\tau\right), \qquad (18)$$

where

$$\lambda=K-\frac{1}{2}=\frac{1}{2}\left(-1+\sqrt{\frac{8\mu R^4v_0}{\hbar^2r_0^2}+1}\right). \qquad (19)$$

Normalization condition of wave function, $R_{nL}^{\lambda}(\tau)$ satisfy the following integral

$$R^3\int_0^{\frac{\pi}{2}}\sin^2\tau|R_{nL}^{\lambda}(\tau)|^2d\tau=1. \qquad (20)$$

Using the formulas

$${}_2F_1\left(-n,\ n+a+b+1;\ a+1;\ \frac{1-y}{2}\right)=\frac{n!\Gamma(a+1)}{\Gamma(n+a+1)}P_n^{(a,b)}(y), \qquad (21)$$

$$P_n^{(a,b)}(y)=\frac{(-1)^n}{2^n n!}(1-y)^{-a}(1+y)^{-b}\frac{d^n}{dx^n}\big[(1-y)^{a+n}(1+y)^{b+n}\big], \tag{22}$$

with $P_n^{(a,b)}(y)$ as Jacobi polynomials, and considering,

$$\int_{-1}^{1}(1-y)^a(1+y)^b\big\{P_n^{(a,b)}(y)\big\}^2 dy=\frac{2^{a+b+1}}{2n+a+b+1}\frac{\Gamma(n+a+1)\Gamma(n+b+1)}{n!\Gamma(n+a+b+1)}. \tag{23}$$

it is easy to obtain the normalization constant

$$C_{nL}^{\lambda}=\sqrt{\frac{2(2n+L+\lambda+2)\Gamma(n+L+\lambda+2)\Gamma(n+L+\frac{3}{2})}{R^3[\Gamma(L+\frac{3}{2})]^2\Gamma(n+\lambda+\frac{3}{2})(n)!}}. \tag{24}$$

Also, the energy eigenvalues, E_{nL}^{λ} are given by

$$E_{nL}^{\lambda}=\frac{\hbar^2}{2\mu R^2}\left[-\frac{4\mu}{\hbar^2}\left(R^2 v_0+\frac{r_0^2}{2}\right)+(2n+L+1)(2n+L+3)+2\lambda\left(2n+L+\frac{3}{2}\right)\right]. \tag{25}$$

In the contraction limit $R\rightarrow\infty$, $\tau\rightarrow 0$ and $\tau\sim r/R$, where r is the radius vector in the three-dimensional flat space, we obtain

$$\begin{aligned}\lim_{R\longrightarrow\infty}E_{nL}^{\lambda}&=\frac{\hbar^2}{2\mu}\left[-\frac{4\mu v_0}{\hbar^2}+2\sqrt{\frac{2\mu v_0}{\hbar^2 r_0^2}}\left(2n+L+\frac{3}{2}\right)\right]\\&=-2v_0+\frac{\hbar}{r_0}\sqrt{\frac{2v_0}{\mu}}\left[2n+1+\sqrt{\frac{2\mu r_0^2 v_0}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]\end{aligned} \tag{26}$$

and

$$\begin{aligned}&\lim_{R\longrightarrow\infty}R_{nL}^{\lambda}(\tau)\\&\quad=\frac{(\frac{2\mu v_0}{\hbar^2 r_0^2})^{\frac{L}{4}+\frac{3}{8}}}{\Gamma(L+\frac{3}{2})}\sqrt{\frac{2\Gamma(n+L+\frac{3}{2})}{n!}}e^{\sqrt{\frac{\mu v_0}{2\hbar^2 r_0^2}}r^2}\, r^L\,{}_1F_1\left(-n,L+\frac{3}{2};\sqrt{\frac{2\mu v_0}{\hbar^2 r_0}}^{2}\right)\\&\quad=\frac{(\frac{2\mu v_0}{\hbar^2 r_0^2})^{\frac{1}{4}+\frac{1}{8}\sqrt{(2l+1)^2+\frac{8\mu r_0^2 v_0}{\hbar^2}}}}{\Gamma(1+\frac{1}{2}\sqrt{(2l+1)^2+\frac{8\mu r_0^2 v_0}{\hbar^2}})}\sqrt{\frac{2\Gamma(n+1+\frac{1}{2}\sqrt{(2l+1)^2+\frac{8\mu r_0^2 v_0}{\hbar^2}})}{n!}}e^{\sqrt{\frac{\mu v_0}{2\hbar^2 r_0^2}}r^2}\\&\qquad\times r^{\frac{1}{2}[-1+\sqrt{(2l+1)^2+\frac{8\mu r_0^2 v_0}{\hbar^2}}]}\,{}_1F_1\left(-n,1+\frac{1}{2}\sqrt{(2l+1)^2+\frac{8\mu r_0^2 v_0}{\hbar^2}};\sqrt{\frac{2\mu v_0}{\hbar^2 r_0}}^{2}\right).\end{aligned} \tag{27}$$

These results for the energy spectrum and the normalized spherical radial wave function exactly coincide with corresponding solutions in ordinary three-dimensional flat space [24]. The calculated energy eigenvalue using associated parameters for N_2, CO, NO and CH molecules of Table 1 in the state ($n=0$, $l=0$) and ($l=0$, n) as a function of curvature radius, R shown in Figs. 1 and 2, respectively. As we see, from Figs. 1 and 2 by increasing R, the energy eigenvalues decreases to a constant limit that expected.

Table 1 Reduced masses and spectroscopically determined properties of N_2, CO, NO and CH molecules in the ground electronic state [25]

Parameters	N_2	CO	NO	CH
v_0 (in cm^{-1})	96288.03528	87471.42567	64877.06229	31838.08149
r_0 (in Å)	1.0940	1.1282	1.1508	1.1198
μ (in amu)	7.00335	6.860586	7.468441	0.929931

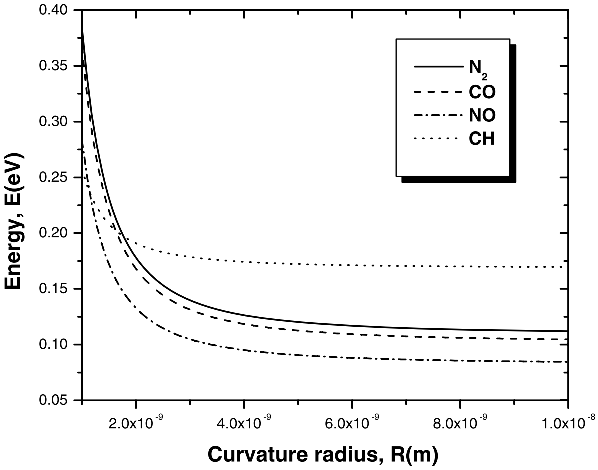

Fig. 1 The graph of the dependence E $(n = 0, l = 0)$ on R for N_2, CO, NO and CH molecules

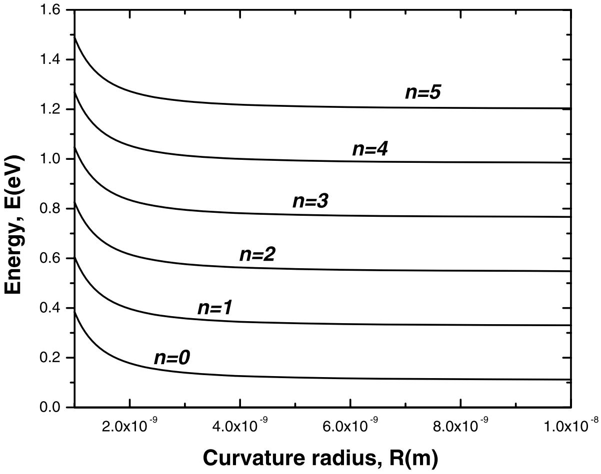

Fig. 2 The graph of the dependence E $(n, l = 0)$ on R for N_2 molecule

3 Conclusion

In this paper, the eigenfunctions and eigenvalues of the Schrödinger equation with a pseudo-harmonic oscillator in the space of constant positive curvature are obtained. The binding energy of N_2, CO, NO and CH molecules have been calculated using this approach. By applying to limit of large R, all results obtained in the present paper lead to the corresponding results in the flat space. This fact may be considered as a good check of the correctness of our calculations.

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