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SUPERSYMMETRY APPROACH AND SHAPE INVARIANCE FOR PSEUDO-HARMONIC POTENTIAL

Ali R. Amani[†], H. Ghorbanpour[‡]

Faculty of Sciences, Department of Physics
Ayatollah Amoli Branch, Islamic Azad University
P.O. Box 678, Amol, Mazandaran, Iran

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In this paper, we have considered supersymmetry algebra for pseudo-harmonic potentials with an arbitrary radial angular momentum. We have obtained the bound states and wave functions by the associated Laguerre differential equation. We have factorized Schrödinger equation for pseudo-harmonic potential in terms of first order differential equations, where these operators can make corresponding partner Hamiltonian. Therefore, by introducing superpotential, we obtained the pseudo-harmonic potential which gives rise to existence of shape invariance condition. In that case, we have calculated supercharge algebras. Finally, we have computed energy eigenvalues for several diatomic molecules.

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1. Introduction

The Schrödinger equation is one of the fundamental wave equations in physics and chemistry. Solutions of Schrödinger equation for some physical potential have important applications in molecular physics, quantum chemistry, nuclear, condensed matter and high energy physics and particle physics. These potentials are such as Hulthén [1], Morse [2], Rosen–Morse [3], pseudo-harmonic [4], Mie [5], Poschl–Teller [6], Kratzer–Fues [7,8] and Woods–Saxon [9]. Application of the aforesaid potentials and Woods–Saxon potential are very useful for describing molecular structures and interaction between a neutron and a heavy nucleus, respectively.

[†] Corresponding author: `a.r.amani@iauamol.ac.ir`

[‡] `hamed.physics2003@gmail.com`

Exact solutions of Schrödinger equations for the potentials are interesting in the fields of material science and condensed matter physics. We note that there are different methods to obtain exact solutions for energy eigenvalues and corresponding wave functions. One of them is the factorization method [10, 11]. It can factorize the Hamiltonian of corresponding system in terms of producing two first order differential operators which are called lowering and raising operators (and *vice versa*). The two obtained Hamiltonians are partners of each other. The method allows classification of problems according to the characteristics involved in the potentials and it is closely related to the supersymmetric quantum mechanics [12, 13].

In quantum mechanics, all of the analytically solvable potentials have a feature which is called shape invariance. In fact, the shape invariance is an integrability condition and an interesting feature of supersymmetric quantum mechanics. This method is an exact and elegant technique for determining the eigenvalues and eigenfunctions of quantum mechanical problems [14, 15].

In this paper, we are going to solve the Schrödinger equation by the pseudo-harmonic potential which includes a centrifugal term. The pseudo-harmonic potential is studied for vibration of polyatomic molecules [16]. This potential has the following form

$$V(r) = V_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2 , \tag{1}$$

where V_0 and r_0 are the bound dissociation energy and the equilibrium intermolecular separation, respectively. We focus on l-wave cases and will obtain eigenvalues and eigenfunction by the factorization method and also achieve the corresponding ladder operators. In order to obtain bound states, we will transform the radial part of Schrödinger equation by a change of variable. Then the transformed equation will be compared to the associated Laguerre polynomial, so that energy eigenvalues and wave function can be obtained. Since the associated Laguerre polynomial is a known function, therefore, we can write the Schrödinger equation in terms of the multiplication two first order equations as the lowering and raising operators.

We have organized the present work as follows. In Sec. 2, we present the general form of Schrödinger equation by the pseudo-harmonic potential. We will obtain the raising and lowering operators with respect to quantum numbers of radial and orbital angular momentum in Sec. 3. In Sec. 4, we discuss supersymmetry approaches and obtain the partner Hamiltonian and shape invariance condition. We will give result and conclusion about energy eigenvalues of the pseudo-harmonic potential for several diatomic molecules in Sec. 5.

2. Fundamentals of Schrödinger equation

The complete Schrödinger equation written for a diatomic molecule with nuclei mass of m_1 and m_2 in three dimensions is as follows

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2+V(r)\right)\Psi_{nlm}(r,\theta,\phi)=E\Psi_{nlm}(r,\theta,\phi)\,, \tag{2}$$

where $\hbar$, $\mu^{-1}=m_1^{-1}+m_2^{-1}$, $V(r)$ and E are Planck's constant, reduced mass, spherical potential and energy eigenvalue of a quantum system, respectively. The radial part of the wave function $R_{nl}(r)$ is defined by relation of $\Psi_{nlm}(r,\theta,\phi)=R_{nl}(r)Y_{lm}(\theta,\phi)$. In that case, the radial Schrödinger equation is written by

$$\frac{d^2R_{nl}(r)}{dr^2}+\frac{2}{r}\frac{dR_{nl}(r)}{dr}-\frac{l(l+1)}{r^2}R_{nl}(r)+\frac{2\mu}{\hbar^2}(E_{nl}-V_{\mathrm{eff}})R_{nl}(r)=0\,, \tag{3}$$

where $V_{\mathrm{eff}}=V(r)+\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}$, and also n and l are radial and orbital angular momentum quantum numbers, respectively. By inserting the pseudo-harmonic potential (1) in Eq. (3), the radial part of wave function yields to

$$\frac{d^2R_{nl}(r)}{dr^2}+\frac{2}{r}\frac{dR_{nl}(r)}{dr}+\frac{2\mu}{\hbar^2}\left(E_{nl}-V_0\left(\frac{r}{r_0}-\frac{r_0}{r}\right)^2-\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right)R_{nl}(r)=0\,. \tag{4}$$

In order to solve Eq. (4), we use a change of variable as $x=r^2$, we can rewrite Eq. (4) with respect to variable x in the following form

$$\begin{aligned}&\frac{d^2R_{nl}(x)}{dx^2}+\frac{3}{2x}\frac{dR_{nl}(x)}{dx}\\&+\frac{\mu}{\hbar^2x^2}\left(-\frac{V_0}{2r_0^2}x^2+\tfrac{1}{2}\left(E_{nl}+2V_0\right)x-\tfrac{1}{2}\left(V_0r_0^2+\frac{\hbar^2}{2\mu}l(l+1)\right)\right)R_{nl}(x)=0\,.\end{aligned} \tag{5}$$

By using the method of separation of variables, the function $R_{nl}(x)$ is written in terms of multiplication an arbitrary function $u(x)$ and the associated Laguerre function $L_{n,l}^{\alpha,\beta}(x)$ as $R_{nl}(x)=u(x)\,L_{n,l}^{\alpha,\beta}(x)$. In that case, Eq. (5) is written as

$$\begin{aligned}&L_{n,l}^{''\alpha,\beta}(x)+\left(\frac{2u'}{u}+\frac{3}{2x}\right)L_{n,l}^{'\alpha,\beta}(x)\\&+\left(\frac{u''}{u}+\frac{3}{2x}\frac{u'}{u}-\frac{\mu V_0}{2\hbar^2r_0^2}+\frac{\mu}{2\hbar^2x}\left(E_{nl}+2V_0\right)-\frac{\mu}{2\hbar^2x^2}\left(V_0r_0^2+\frac{\hbar^2}{2\mu}l(l+1)\right)\right)\\&\times L_{n,l}^{\alpha,\beta}(x)=0\,,\end{aligned} \tag{6}$$

where the prime exhibits derivative with respect to variable x. The associated Laguerre differential equation is

$$L''^{\alpha,\beta}_{n,l}(x)+\frac{1+\alpha-\beta x}{x}\,L'^{\alpha,\beta}_{n,l}(x)+\left[\left(n-\frac{l}{2}\right)\frac{\beta}{x}-\frac{l}{2x^2}\left(\alpha+\frac{l}{2}\right)\right]L^{\alpha,\beta}_{n,l}(x)=0\,, \tag{7}$$

and we note that the Rodrigues representation of associated Laguerre equation is

$$L^{\alpha,\beta}_{n,l}(x)=\frac{a_{n,l}(\alpha,\beta)}{x^{\alpha+\frac{l}{2}}\,e^{-\beta x}}\left(\frac{d}{dx}\right)^{n-l}\left(x^{n+\alpha}\,e^{-\beta x}\right), \tag{8}$$

where $a_{n,l}$ is the normalization coefficient, and can be written as

$$a_{n,l}(\alpha,\beta)=(-1)^l\sqrt{\frac{\beta^{(\alpha+l+1)}}{\Gamma(n-l+1)\,\Gamma(n+\alpha+1)}}\,. \tag{9}$$

In order to obtain eigenvalues and eigenfunction, we compare second and third terms respectively in Eqs. (6) and (7). The result is

$$u(x)=x^{\frac{\alpha}{2}-\frac{1}{4}}\,e^{-\frac{\beta}{2}x}\,, \tag{10}$$

and

$$\alpha = l+\sqrt{\frac{2\mu V_0 r_0^2}{\hbar^2}+\left(l+\tfrac{1}{2}\right)^2}\,, \tag{11}$$

$$\beta^2 = \frac{2\mu V_0}{\hbar^2 r_0^2}\,, \tag{12}$$

$$-\frac{\beta(\alpha+1)}{2}+\frac{\mu}{2\hbar^2}(E+2V_0)=\left(n-\frac{l}{2}\right)\beta\,. \tag{13}$$

Finally, we can obviously obtain the radial part of wave function and the energy eigenvalue for the pseudo-harmonic potential as the following form

$$R_{nl}(r) = r^{\alpha+\frac{1}{2}}\,e^{-\frac{\beta}{2}r^2}\,L^{\alpha,\beta}_{n,l}(r)\,, \tag{14}$$

$$E_{nl} = -2V_0+\sqrt{\frac{2V_0}{\mu}}\frac{\hbar}{r_0}\left[2n-l+\alpha+1\right]\,. \tag{15}$$

From Eqs. (14) and (15) we can write wave function and energy eigenvalue in terms of n and l. Also we realize that energy eigenvalue depend on the equilibrium intermolecular separations.

3. Ladder operators of the pseudo-harmonic potential

In this section, we are going to find raising and lowering operators for the pseudo-harmonic potential. The operators help us factorize second order equation in terms of the first order equations. By using corresponding operators, we can obtain shape invariance condition. Then, we can write the associated Laguerre differential equation (7) with respect to l as the following form [16]

$$\begin{aligned} A_l^+(x)A_l^-(x)L_{n,l}^{\alpha,\beta}(x) &= (n-l+1)\beta L_{n,l}^{\alpha,\beta}(x)\,, \\ A_l^-(x)A_l^+(x)L_{n,l-1}^{\alpha,\beta}(x) &= (n-l+1)\beta(n+\alpha)L_{n,l-1}^{\alpha,\beta}(x)\,, \end{aligned} \tag{16}$$

where the differential explicit forms of the operators $A_l^+(r)$ and $A_l^-(r)$ are, respectively

$$\begin{aligned} A_l^+(x) &= \sqrt{x}\frac{d}{dx} - \frac{l-1}{2\sqrt{x}}\,, \\ A_l^-(x) &= -\sqrt{x}\frac{d}{dx} - \frac{2\alpha+l-2\beta x}{2\sqrt{x}}\,. \end{aligned} \tag{17}$$

The equations (16) may be written as the raising and lowering relations

$$\begin{aligned} A_l^+(x)L_{n,l-1}^{\alpha,\beta}(x) &= \sqrt{(n-l+1)\beta}L_{n,l}^{\alpha,\beta}(x)\,, \\ A_l^-(x)L_{n,l}^{\alpha,\beta}(x) &= \sqrt{(n-l+1)\beta}L_{n,l-1}^{\alpha,\beta}(x)\,. \end{aligned} \tag{18}$$

Now, in order to obtain the operators, we can factorize the associated Laguerre differential equation by raising and lowering operators with respect to the parameters l and n as follows [16, 17]

$$A_{n,l}^+(r)A_{n,l}^-(r)L_{n,l}^{\alpha,\beta}(r) = (n-l)(n+\alpha)L_{n,l}^{\alpha,\beta}(r)\,, \tag{19}$$

$$A_{n,l}^-(r)A_{n,l}^+(r)L_{n-1,l}^{\alpha,\beta}(r) = (n-l)(n+\alpha)L_{n-1,l}^{\alpha,\beta}(r)\,, \tag{20}$$

where

$$A_{n,l}^+(x) = x\frac{d}{dx} - \beta\,x + \frac{2n+2\alpha-l}{2}\,, \tag{21}$$

$$A_{n,l}^-(x) = -x\frac{d}{dx} + \frac{2n-l}{2}\,. \tag{22}$$

By comparing the associated Laguerre differential equation and Schrödinger equation with the pseudo-harmonic potential, we will obtain raising and lowering operators in terms of the parameters n and l as the following form

$$A_{n,l}^+(r) = \frac{r}{2}\frac{d}{dr} - \beta\,r^2 + \frac{2n+2\alpha-l}{2}\,, \tag{23}$$

$$A_{n,l}^-(r) = -\frac{r}{2}\frac{d}{dr} + \frac{2n-l}{2}\,. \tag{24}$$

The operators help us have bound states for the aforesaid system.

4. The supersymmetry approaches for pseudo-harmonic potential

In this section, we are going to discuss the supersymmetry for pseudo-harmonic potential. In that case, the matrix supersymmetry for Hamiltonian is given by

$$H = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix} , \tag{25}$$

where we can write H_1 and H_2 as the factorization operators

$$H_1 = A^+ A\,, \tag{26}$$

$$H_2 = A\,A^+\,. \tag{27}$$

On the other hand, we can write V_1 and V_2 as

$$V_1(r) = W^2(r) + \frac{\hbar}{\sqrt{2m}} W^{'}(r)\,, \tag{28}$$

$$V_2(r) = W^2(r) - \frac{\hbar}{\sqrt{2m}} W^{'}(r)\,, \tag{29}$$

where $W(r)$ is called superpotential. By using ladder operators (23), (24), (26) and (27), we can obtain the partner Hamiltonian as the following form

$$\begin{aligned} H_1 &= -\frac{r^2}{4}\frac{d^2}{dr^2} - \frac{r}{4}\left[1+2\alpha-2\beta r^2\right]\frac{d}{dr} - \left[\frac{(2n-l)}{2}\right] \\ &\quad \times\beta r^2 + \frac{(2n-l)(2n+2\alpha-l)}{4}\,, \end{aligned} \tag{30}$$

$$\begin{aligned} H_2 &= -\frac{r^2}{4}\frac{d^2}{dr^2} - \frac{r}{4}\left[1+2\alpha\right]\frac{d}{dr} + \left[1-\frac{(2n-l)}{2}\right] \\ &\quad \times\beta r^2 + \frac{(2n-l)(2n+2\alpha-l)}{4}\,. \end{aligned} \tag{31}$$

Now, we can write the superpotential in terms of angular quantum numbers l as

$$W(r) = \frac{\beta r}{2} - \frac{\alpha+4l+1}{4r}\,. \tag{32}$$

In that case, by using Eqs. (28), (29), we have

$$\begin{aligned} V_1(r) &= \frac{\beta^2 r^2}{4} - \frac{\alpha\beta}{4} - \beta l - \frac{\beta}{4} + \frac{\alpha^2+8\alpha l+2\alpha+16l^2+8l+1}{16r^2} \\ &\quad + \frac{\hbar}{\sqrt{2m}}\left[\frac{2\beta r^2+\alpha+4l+1}{4r^2}\right], \end{aligned} \tag{33}$$

$$\begin{aligned} V_2(r) &= \frac{\beta^2 r^2}{4} - \frac{\alpha\beta}{4} - \beta l - \frac{\beta}{4} + \frac{\alpha^2+8\alpha l+2\alpha+16l^2+8l+1}{16r^2} \\ &\quad - \frac{\hbar}{\sqrt{2m}}\left[\frac{2\beta r^2+\alpha+4l+1}{4r^2}\right]. \end{aligned} \tag{34}$$

The shape invariance condition will be as $V_1(l) - V_2(l+1) = 2\beta$ when $\hbar = 2m = 1$. The supercharges are written by

$$Q = \begin{pmatrix} 0 & 0 \\ A_n & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ -\frac{r}{2}\frac{d}{dr} + \frac{2n-l}{2} & 0 \end{pmatrix}, \tag{35}$$

$$Q^{\dagger} = \begin{pmatrix} 0 & A_n^{\dagger} \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \frac{r}{2}\frac{d}{dr} - \beta r^2 + \frac{2n+2\alpha-l}{2} \\ 0 & 0 \end{pmatrix}. \tag{36}$$

So the following commutation relations are set between partner Hamiltonian and supercharges as

$$[H, Q] = \left[H, Q^{\dagger}\right] = 0\,, \tag{37}$$

$$\left\{Q, Q^{\dagger}\right\} = H\,, \qquad \{Q, Q\} = \left\{Q^{\dagger}, Q^{\dagger}\right\} = 0\,. \tag{38}$$

We note that the supercharges satisfy an anti-commutation and are responsible for the degeneracy. The ground states of H are

$$|0\rangle = \psi_0(r) = \begin{pmatrix} \phi_0^{(1)}(r) \\ \phi_0^{(2)}(r) \end{pmatrix}, \tag{39}$$

where

$$A\phi_0^{(1)} = 0 \to \phi_0^{(1)} = N \exp\left(-\int^{r} W(y)dy\right), \tag{40}$$

$$A^{\dagger}\phi_0^{(2)} = 0 \to \phi_0^{(2)} = N \exp\left(\int^{r} W(y)\,dy\right). \tag{41}$$

For unbroken supersymmetry

$$Q\,|0\rangle = Q^{\dagger}\,|0\rangle = 0\,|0\rangle\,. \tag{42}$$

Thus, by the following relationship

$$[H, Q] = \left[H, Q^{\dagger}\right] = 0 \tag{43}$$

ground state energy must be zero and ground state wave function for the matrix Hamiltonian should be

$$\psi_0(x) = \begin{pmatrix} \phi_0^{(1)}(r) \\ 0 \end{pmatrix}. \tag{44}$$

5. Result and summary

In this paper, we have discussed the solution of the Schrödinger equation with pseudo-harmonic potential. In that case, we have solved the radial part of Schrödinger equation with the method of separation of variable. By using the factorization method and comparison the corresponding system with associated Laguerre differential equation, we have obtained energy eigenvalues and wave function. The raising and lowering operators have calculated with respect to parameters n and l by supersymmetry approach. By computing the partner Hamiltonian of system, the shape invariance condition has been satisfied with respect to parameters radial quantum numbers n and angular quantum numbers l.

TABLE I

Reduced masses and spectroscopically determined properties of N_2, CO, NO and CH diatomic molecules in the ground electronic state [18].

Parameters	N_2	CO	NO	CH
V_0 (cm^{-1})	96288.03528	87471.42567	64877.06229	31838.08149
r_0 (A°)	1.0940	1.1282	1.1508	1.1198
μ (a.m.u.)	7.00335	6.860586	7.468441	0.929931

TABLE II

Calculated energy eigenvalues of the pseudo-harmonic potential for N_2, CO, NO and CH diatomic molecules with different values of n and l in terms of *ev*.

State (n)	l	N_2	CO	NO	CH
0	0	0.10918388	0.10195674	0.08250941	0.168677587
1	0	0.32742695	0.30575052	0.24742256	0.505136594
1	1	0.32792565	0.30622921	0.24784519	0.508720344
2	0	0.54567002	0.50954431	0.41233572	0.841595601
2	1	0.54616872	0.51002300	0.41275835	0.845179351
2	2	0.54716612	0.51098035	0.41360357	0.852341983
4	0	0.98215615	0.91713188	0.74216202	1.514513616
4	1	0.98265486	0.91761058	0.74258465	1.518097366
4	2	0.98365226	0.91856792	0.74342988	1.525259997
4	3	0.98514826	0.92000386	0.74469762	1.535991786
4	4	0.98714277	0.92191830	0.74638779	1.550278259
5	0	1.20039923	1.12092567	0.90707518	1.850972616
5	1	1.20089794	1.12140436	0.90749781	1.854556373
5	2	1.20189533	1.12236171	0.90834303	1.861719004
5	3	1.20339133	1.12379765	0.90961078	1.872450793
5	4	1.20538584	1.12571208	0.91130094	1.886737266
5	5	1.20787877	1.12810490	0.91341341	1.904559241

Now we are going to compute eigenvalues energy for the system. Therefore, from Eq. (15) and Table I we can calculate the binding energy for any angular momentum l in Table II. The energy eigenvalues have been written for several diatomic molecules such as N_2, CO, NO and CH. Table II shows us by increasing level n the energy of diatomic molecules increase, also by increasing l increase energy of diatomic molecules in a similar n.

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