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Algebraic approach to the Kratzer potential

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Abstract
In this paper, the energy eigenvalues and the corresponding eigenfunctions are calculated for the Kratzer potential. Then we obtain the ladder operators for the one-dimensional (1D) and 3D Kratzer potential. Finally, we show that these operators satisfy the SU(2) commutation relation.

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1. Introduction

In recent years, Lie algebraic methods have been the subject of interest in many fields of physics. For example the algebraic methods provide a way to obtain wavefunctions of polyatomic molecules [1–5] (for a review of Lie algebraic methods in molecular spectroscopy, see [6]). These methods provide a description to Dunham-type expansions and to force-field variational methods [7]. It is clear that systems displaying a dynamical symmetry can be treated by algebraic methods [8–11]. To see the ladder operators of a quantum system with some important potentials such as the Morse, Pöschl–Teller, pseudo harmonic and infinitely square-well potentials and other quantum systems, refer to [12–14].

We know that the symmetry and degeneracy of the states of a system are associated with each other. For example, a system that possesses rotational symmetry is usually degenerate with respect to the direction of the angular momentum, i.e. with respect to the eigenvalues of a particular component. Beyond the degeneracies arising, say, in rotational symmetry there is the possibility of degeneracies of different origin. Such degeneracies are to be expected whenever the Schrödinger equation can be solved in more than one way, either in different coordinate systems, or in a single coordinate system which can be oriented in different directions. From our present considerations we should expect these degeneracies to be associated with some symmetry, too. The nature of these symmetries is not geometrical. They are called dynamical symmetries, since they are the consequence of particular forms of the Schrodinger equation or of the classical force law.

In this paper, we study the dynamical symmetry for the one-dimensional (1D) and 3D Kratzer potential, by another algebraic approach. The Kratzer potential [15] we consider in this paper has played an important role in the history of molecular and quantum chemistry and it has been so far extensively used to describe molecular structures and interactions [16]. We establish the creation and annihilation operators directly from the eigenfunctions for this system, and that ladder operators construct the dynamical algebra SU(2).

2. The eigenvalue and eigenfunction

We consider the Schrödinger equation with the following Kratzer potential, which is the potential of a diatomic molecule,

$$V(r) = -2D\left[\frac{a}{r} - \frac{1}{2}\left(\frac{a}{r}\right)^2\right], \tag{1}$$

where D and a are constant parameters. Then the 1D Schrödinger equation is

$$\left\{-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - 2D\left[\frac{a}{r} - \frac{1}{2}\left(\frac{a}{r}\right)^2\right]\right\}\psi_m(r) = E_m\psi_m(r). \tag{2}$$

Now we rewrite the above equation in dimensionless form,

$$\left[-\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}}{\mathrm{d}x}\right) - 2\left(\frac{1}{x} - \frac{1}{2x}\right)\right]\psi_m(x) = \varepsilon_m\psi_m(x), \tag{3}$$

where $\hbar^2/2\mathrm{Ma}^2 = \mathrm{D}$, $\varepsilon_m = E_m/D$ and $x = r/a$.

Here, we consider the bound states or states with

$$\varepsilon_m = -s^2, \tag{4}$$

where s is a real number. By considering the wavefunction as

$$\psi_m(x) = \frac{\phi_m(x)}{x}, \tag{5}$$

and using equation (4) we can rewrite equation (3) as

$$\frac{\mathrm{d}^2\phi_m(x)}{\mathrm{d}x^2} + \left(\frac{2}{x} - \frac{1}{x^2} - s^2\right)\phi_m(x) = 0. \tag{6}$$

For simplification we define the new coordinate as $X = 2sx$. The Schrödinger equation (6) in terms of this new coordinate is given by

$$\frac{\mathrm{d}^2\phi_m(X)}{\mathrm{d}X^2} + \left(-\frac{1}{4} + \frac{1}{sX} - \frac{1}{X^2}\right)\phi_m(X) = 0. \tag{7}$$

The solution of the above equation is

$$\phi_m(X) = N_m X^{\frac{1+\sqrt{5}}{2}} \mathrm{e}^{-\frac{X}{2}} L_m^{\sqrt{5}}(X), \tag{8}$$

where the $L_m^{\sqrt{5}}(X)$ are the associated Laguerre polynomials [17], and m is given by

$$m = \frac{1}{s} - \frac{1}{2}(1+\sqrt{5}), \tag{9}$$

from which we have

$$E_m = -D\left(\frac{1}{m+\frac{1}{2}(1+\sqrt{5})}\right)^2, \tag{10}$$

in this case, the energy level is not equidistant. N_m in equation (8) is the normalized factor, to be determined below. By using the following important formula [17]

$$\int_0^\infty \rho^\alpha \mathrm{e}^{-\rho} L_n^\alpha(\rho) L_m^\alpha(\rho)\,\mathrm{d}\rho = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{nm}, \tag{11}$$

we can finally obtain the re-normalized wavefunction $\psi_m(X)$

$$\psi_m(X) = N_m X^{\frac{-1+\sqrt{5}}{2}} \mathrm{e}^{-\frac{X}{2}} L_m^{\sqrt{5}}(X). \tag{12}$$

3. The construction of ladder operators

The ladder operators can be constructed directly from the wavefunction (12) without introducing any auxiliary variable. We define the ladder operators with the following property

$$\hat{L}_\pm\,\psi_m(X) = l_\pm\,\psi_m(X). \tag{13}$$

We consider the following ansatz for ladder operators

$$\hat{L}_\pm = A_\pm(X)\frac{\mathrm{d}}{\mathrm{d}X} + B_\pm(X). \tag{14}$$

Using the following relations for the first derivative of the associated Laguerre functions

$$\rho\frac{\mathrm{d}}{\mathrm{d}\rho}L_n^\alpha(\rho) = n\,L_n^\alpha(\rho) - (n+\alpha)L_{n-1}^\alpha(\rho), \tag{15}$$

$$\rho\frac{\mathrm{d}}{\mathrm{d}\rho}L_n^\alpha(\rho) = (n+1)\,L_{n+1}^\alpha(\rho) - (n+\alpha+1-\rho)L_n^\alpha(\rho), \tag{16}$$

one can obtain the creation and annihilation operators. Using equation (15) and the action of the differential operator $\mathrm{d}/\mathrm{d}X$ on the wavefunctions (12) we have

$$\left[-X\frac{\mathrm{d}}{\mathrm{d}X} - \frac{X}{2} + m + \left(\frac{-1+\sqrt{5}}{2}\right)\right]\psi_m(X) = (m+\sqrt{5})\frac{N_m}{N_{m-1}}\psi_{m-1}(X), \tag{17}$$

then we obtain

$$\hat{L}_- = \left[-X\frac{\mathrm{d}}{\mathrm{d}X} - \frac{X}{2} + m + \left(\frac{-1+\sqrt{5}}{2}\right)\right], \tag{18}$$

with the following eigenvalue

$$l_- = (m+\sqrt{5})\frac{N_m}{N_{m-1}}. \tag{19}$$

Similarly and using (16) we can write

$$\left[X\frac{\mathrm{d}}{\mathrm{d}X} - \frac{X}{2} + m + \left(\frac{3+\sqrt{5}}{2}\right)\right]\psi_m(X) = (m+1)\frac{N_m}{N_{m+1}}\psi_{m+1}(X). \tag{20}$$

We obtain the following relation for the creation operator

$$\hat{L}_+ = \left[X\frac{\mathrm{d}}{\mathrm{d}X} - \frac{X}{2} + m + \left(\frac{3+\sqrt{5}}{2}\right)\right], \tag{21}$$

where its eigenvalue is given by

$$l_+ = (m+1)\frac{N_m}{N_{m+1}}. \tag{22}$$

We now study the algebra associated with the operators $\hat{L}_-$ and $\hat{L}_+$. Based on equations (18), (19), (21) and (22), we can calculate the commutator $[\hat{L}_-, \hat{L}_+]$

$$[\hat{L}_-, \hat{L}_+]\psi_m(X) = 2l_0\psi_m(X), \tag{23}$$

where we have introduced the eigenvalue

$$l_0 = \left(m + \frac{1+\sqrt{5}}{2}\right). \tag{24}$$

Then we can define the operator

$$\hat{L}_0 = \left(\hat{m} + \frac{1+\sqrt{5}}{2}\right), \tag{25}$$

where the operator $\hat{m}$ is defined by the following relation

$$\hat{m}\psi_m(X) = m\psi_m(X). \tag{26}$$

The operators $\hat{L}_\pm, \hat{L}_0$ satisfy the following commutation relations of the Lie algebra of SU(2)

$$[\hat{L}_-, \hat{L}_+] = 2\hat{L}_0, \quad [\hat{L}_0, \hat{L}_-] = -\hat{L}_-, \quad [\hat{L}_0, \hat{L}_+] = \hat{L}_+. \tag{27}$$

4. Extension to the 3D potential

In this section, we extend the algebraic approach of previous sections to the 3D Kratzer molecular potential. The Schrödinger equation is

$$\left\{-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\hbar^2}{2M}\frac{\hat{L}^2}{r^2}+V(r)\right\}\psi_m(r,\theta,\phi) = E_m\psi_m(r,\theta,\phi). \qquad (28)$$

We can decompose the wave equation as

$$\psi_m(r,\theta,\phi)=R_m(r)Y_l(\theta,\phi), \qquad (29)$$

then by the action of operator $\hat{L}^2$ on the $Y_l(\theta,\phi)$ we obtain

$$\hat{L}^2\,Y_l(\theta,\phi)=l(l+1)\,Y_l(\theta,\phi), \qquad (30)$$

therefore the radial wavefunction $R_m(r)$ satisfies the following equation

$$\left\{-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right)+\frac{\hbar^2}{2M}\frac{l(l+1)}{r^2}+V(r)\right\}R_m(r)=E_m\,R_m(r). \qquad (31)$$

Similar to what we have done in section 2, we can rewrite the above equation in dimensionless form

$$\left\{-\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}}{\mathrm{d}x}\right)+\frac{l(l+1)}{x^2}-\left(\frac{2}{x}-\frac{1}{x^2}\right)\right\}R_m(x)=\varepsilon_m\,R_m(x), \qquad (32)$$

where $x=r/a$, $\varepsilon_m=E_m/D$ and $\hbar^2 2Ma^2=D$. Now we take the radial wavefunction in the new form

$$R_m(x)=\frac{\phi_m(x)}{x}. \qquad (33)$$

Substitution of the above expression into equation (32) allows us to obtain

$$\frac{\mathrm{d}^2\phi_m(x)}{\mathrm{d}x^2}+\left(-s^2+\frac{2}{x}-\frac{1+l(l+1)}{x^2}\right)\phi_m(x)=0, \qquad (34)$$

where $s^2=-\varepsilon_m$. Defining the new variable $X=2sx$, equation (34) can be re-arranged as

$$\frac{\mathrm{d}^2\phi_m(X)}{\mathrm{d}X^2}+\left(-\frac{1}{4}+\frac{1}{sX}-\frac{1+l(l+1)}{X^2}\right)\phi_m(X)=0. \qquad (35)$$

The solutions of the above equation are

$$\phi_m(X)=N_m X^{\left(\frac{1+\sqrt{5+4l(l+1)}}{2}\right)}\,\mathrm{e}^{-\frac{X}{2}}\,L_m^{\sqrt{5+4l(l+1)}}(X), \qquad (36)$$

where N_m is the normalized factor. Defining $\alpha=\sqrt{5+4l(l+1)}$, we can write the radial wavefunction $R_m(X)$ as

$$R_m(X)=N_m X^{\left(\frac{-1+\alpha}{2}\right)}\,\mathrm{e}^{-\frac{X}{2}}\,L_m^{\alpha}(X). \qquad (37)$$

Making use of equations (15) and (16), similar to the previous section we obtain the following relation for the creation and annihilation operators

$$\hat{L}_+=X\frac{\mathrm{d}}{\mathrm{d}X}-\frac{X}{2}+m+\frac{3+\alpha}{2}, \qquad (38)$$

$$\hat{L}_-=-X\frac{\mathrm{d}}{\mathrm{d}X}-\frac{X}{2}+m+\frac{-1+\alpha}{2}, \qquad (39)$$

with the following eigenvalues respectively

$$l_+=(m+1)\frac{N_m}{N_{m+1}}, \qquad (40)$$

$$l_-=(m+\alpha)\frac{N_m}{N_{m-1}}, \qquad (41)$$

Now we can obtain the algebra associated with the operators $\hat{L}_+$ and $\hat{L}_-$. Using the results ((38), (40)) and ((39), (41)) we have

$$[\hat{L}_-,\hat{L}_+]R_m(X)=2\left(m+\frac{1+\sqrt{5+4l(l+1)}}{2}\right)R_m(X), \qquad (42)$$

where we have introduced the eigenvalue

$$l_0=m+\frac{1+\sqrt{5+4l(l+1)}}{2}. \qquad (43)$$

We can define the operator

$$\hat{L}_0=\left(\hat{m}+\frac{1+\sqrt{5+4l(l+1)}}{2}\right), \qquad (44)$$

where $\hat{m}$ is the number operator with the property

$$\hat{m}\,R_m(X)=m\,R_m(X). \qquad (45)$$

The operator $\hat{L}_0$, $\hat{L}_-$ and $\hat{L}_+$ thus satisfy the commutation relation

$$[\hat{L}_-,\hat{L}_+]=2\hat{L}_0,\quad [\hat{L}_0,\hat{L}_-]=-\hat{L}_-,\quad [\hat{L}_0,\hat{L}_+]=\hat{L}_+, \qquad (46)$$

which correspond to SU(2) Lie algebra.

5. Conclusion

In this paper, we have calculated the exact bound-state energy eigenvalues and the corresponding eigenfunctions of the exactly solvable Kratzer potential. We have shown that the energy level is not equidistant in this case. Then we have obtained the raising and lowering operators for the 1D and 3D Kratzer potentials. We have shown that SU(2) is the dynamical group associated with the bounded region of the spectrum.

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