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ALGEBRAIC APPROACH TO THE MORSE OSCILLATORS

MOHAMMAD R. SETARE

Department of Physics, University of Kurdistan, Sanandaj, Iran

Abstract. In this paper we obtain the ladder operators for the 1D and 3D Morse potential. Then we show that these operators satisfy SU(2) commutation relation. Finally we obtain the Hamiltonian in terms of the $\mathfrak{su}(2)$ algebra.

1. Introduction

In the recent years, Lie algebraic methods have been the subject of interest in many of fields of physics. For example the algebraic methods provide a way to obtain wave functions of polyatomic molecules [15, 16, 18, 20–22]. These methods provide a description to Dunham-type expansions and to force-field variational methods [17]. It is clear that systems displaying a dynamical symmetry can be treated by algebraic methods [1, 2, 19, 23]. For details concerning the ladder operators of quantum systems with some important potentials such as Morse potential the Pöschel-Teller one, the pseudo harmonic one, the infinitely square-well one and other quantum systems we refer to [3–13].

The Morse potential is a solvable potential, hence the interest to deal with it using different approaches, in particular factorization approach [1,4,19]. According to these methods as $\mathfrak{su}(1,1)$ algebra has been found in [4,9,19]. The Morse potential has been studied in terms of SO(2,1) and SU(2) groups [8,13]. In fact SU(2) is the symmetry group associated with the bounded region of the spectrum [12].

In this paper we study the dynamical symmetry for the one and three-dimensional Morse oscillator by another algebraic approach. We establish the creation and annihilation operators directly from the eigenfunctions for this system, and that the ladders operators construct the dynamical algebra $\mathfrak{su}(2)$.

2. Algebraic Method in One-Dimensional Potential

We consider the Schrödinger equation with the Morse potential

$$\left(-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_D(x)\right)\psi_n(x) = E_n\psi_n(x) \tag{1}$$

i.e.,

$$V_D = V_0 (1 - \exp(-ax))^2 \tag{2}$$

and where V_0 and a are constants. By considering the following change of coordinates

$$r = 2\exp(-ax) \tag{3}$$

we obtain

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \left(\frac{1}{4} - \frac{1}{r} - \frac{\varepsilon_n}{r^2}\right)\right)\phi_n(r) = 0$$
(4)

where $\varepsilon_n = \frac{E_n}{V_0}$ and $a^2 = \frac{2M V_0}{\hbar^2}$. From the behavior of the wave functions at the origin and at infinity, we can consider the following ansatz for $\phi_n(r)$

$$\phi_n(r) = Nr^s \exp(-\frac{r}{2}) \, {}_1F_1(-n + \frac{1}{2}, 2n, r) \tag{5}$$

in which

$$s = \sqrt{-\varepsilon_n} := n, \qquad \varepsilon_n = -n^2$$
 (6)

 $_1F_1(-n+\frac{1}{2},2n,r)$ is the hypergeometric function, and N is the normalization factor. From consideration of the finiteness of the wave function (5), it is shown that equation (6) that the general quantum condition is

$$-s + \frac{1}{2} = -m \tag{7}$$

and therefore we can write the wave function as

$$\phi_m(r) = N_m r^s \exp(-\frac{r}{2}) L_m^{2s}(r)$$
 (8)

where the $L_m^{2s}(r)$ are the associated Laguerre polynomials. Here we have used the following relation between hypergeometric functions and Laguerre polynomials

$$L_m^{2s} = \frac{\Gamma(2s+m+1)}{m! \Gamma(2s+1)} {}_{1}F_{1}(-m, 2s+1, r)$$
(9)

and in this way we can obtain the normalization factor N_m that is given by the formula

$$N_m = \sqrt{\frac{m!}{\Gamma(m+2s+1)}}. (10)$$

Now we introduce the ladder operators in the form

$$\hat{L}_{\pm}\phi_{m}(r) = l_{\pm}\phi_{m\pm 1}(r). \tag{11}$$

By considering the following ansatz for ladder operator

$$\hat{L}_{\pm} = A_{\pm}(r)\frac{\mathrm{d}}{\mathrm{d}r} + B_{\pm} \tag{12}$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}r}\phi_m(r) = \frac{s}{r}\phi_m(r) - \frac{1}{2}\phi_m(r) + \frac{m}{r}\phi_m(r) - \frac{m+2s}{r}\frac{N_m}{N_{m-1}}\phi_{m-1}(r).$$
(13)

Further on, we can rewrite the above equation as

$$\left(-r\frac{\mathrm{d}}{\mathrm{d}r} + (s+m) - \frac{r}{2}\right)\phi_m(r) = (m+2s)\frac{N_m}{N_{m-1}}\phi_{m-1}(r)$$
 (14)

in order to obtain the operator

$$\hat{L}_{-} = -r\frac{d}{dr} + (s+m) - \frac{r}{2} \tag{15}$$

with eigenvalues

$$l_{-} = \sqrt{m(m+2s)}. (16)$$

Similarly one can obtain

$$\hat{L}_{+} = r \frac{\mathrm{d}}{\mathrm{d}r} + (s+m+1) - \frac{r}{2}, \qquad l_{+} = \sqrt{(m+1)(m+2s+1)}.$$
 (17)

Now, using relation (7) we have for the ladder operators

$$\hat{L}_{-} = -r\frac{\mathrm{d}}{\mathrm{d}r} + (2m + \frac{1}{2}) - \frac{r}{2}, \qquad \hat{L}_{+} = r\frac{\mathrm{d}}{\mathrm{d}r} + (2m + \frac{3}{2}) - \frac{r}{2}$$
 (18)

with eigenvalues

$$l_{-} = \sqrt{m(3m+1)}, \qquad l_{+} = \sqrt{(m+1)(3m+2)}.$$
 (19)

Now, we obtain the algebra associated with the operators \hat{L}_{-} , \hat{L}_{+} . Using equation (11, 16, 17) we can calculate their commutator

$$[\hat{L}_{-}, \hat{L}_{+}]\phi_{m} = 2(m+s+\frac{1}{2}).$$
 (20)

Now, we define the operator \hat{L}_0 as

$$\hat{L}_0 = 2(\hat{m} + s + \frac{1}{2}) \tag{21}$$

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

$$\hat{m}\phi_m(r) = m\phi_m(r) \tag{22}$$

and therefore one can rewrite the eigenvalues of \hat{L}_0 as

$$l_0 = 2(m+s+\frac{1}{2})\tag{23}$$

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

$$[\hat{L}_{-}, \hat{L}_{+}] = 2\hat{L}_{0}, \qquad [\hat{L}_{0}, \hat{L}_{-}] = -\hat{L}_{-}, \qquad [\hat{L}_{0}, \hat{L}_{+}] = \hat{L}_{+}.$$
 (24)

Then we notice that in terms of the $\mathfrak{su}(2)$ algebra the hamiltonian has following form

$$\hat{\mathcal{H}} = -\frac{V_0}{16}\hat{L}_0^2 \tag{25}$$

with eigenvalues

$$E_n = -\frac{V_0}{4}(2m+1)^2. (26)$$

Using equations (6), (7) we can rewrite the eigenvalues as

$$E_n = -\frac{V_0}{4}(2s)^2 = -V_0 n^2 \tag{27}$$

which is consistent with the definition of E_n in equation (1), where $\varepsilon_n = \frac{E_n}{V_0}$, and ε_n given by equation (6).

3. Three-Dimensional Morse Potential

In this section we extend the algebraic approach of previous section to the threedimensional Morse potential. The Morse potential in three-dimension is

$$V(r) = V_0(\exp(-2ar) - 2\exp(-ar))$$
(28)

and therefore the radial part of the Hamiltonian given by

$$H = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r}\right) + V_0(\exp(-2ar) - 2\exp(-ar)). \tag{29}$$

Now by using x = ar the above equation can be rewriten in the dimensionless form

$$H = -\frac{\hbar^2 a^2}{2M} \left(\frac{\partial^2}{\partial x^2} + \frac{2}{x} \frac{\partial}{\partial x}\right) + V_0(\exp(-2x) - 2\exp(-x)). \tag{30}$$

If in the Schrödinger equation

$$\hat{H}\Psi_m(x) = E_m \Psi_m(x) \tag{31}$$

we take $\frac{\hbar^2 a^2}{2M} = V_0$, $\frac{E_m}{V_0} = \varepsilon_m$, then we have

$$\left(-\left(\frac{\partial^2}{\partial x^2} + \frac{2}{x}\frac{\partial}{\partial x}\right) + \left(\exp(-2x) - 2\exp(-x)\right)\right)\Psi_m(x) = \varepsilon_m\Psi_m(x).$$
 (32)

Introducing

$$\Psi_m(x) := \frac{\Phi_m(x)}{x} \tag{33}$$

we can rewrite equation (32) as

$$\left(-\frac{\partial^2}{\partial x^2} + (\exp(-2x) - 2\exp(-x))\right)\Phi_m(x) = \varepsilon_m \Phi_m(x)$$
 (34)

which is the one-dimensional Morse potential problem from the previous section. The solutions of the above equation are

$$\Phi_m(\rho) = N_m \rho^s \exp(-\frac{\rho}{2}) L_m^{2s}(\rho)$$
(35)

in which $\rho:=2\exp(-x)$ and N_m is again the normalization factor. Then we obtain the following relation for the functions $\Psi_m(\rho)$

$$\Psi_m(\rho) = N_m \frac{\rho^s e^{-\frac{\rho}{2}}}{\ln \frac{2}{\rho}} L_m^{2s}(\rho).$$
 (36)

Since $0 \le x \le +\infty$, then, $0 \le \rho \le 2$, we obtain the normalization factor from the formula

$$N_m^2 \int_0^2 \left(\frac{\rho^s e^{-\frac{\rho}{2}}}{\ln \frac{2}{\rho}} L_m^{2s}(\rho) \right)^2 d\rho = 1.$$
 (37)

Now we want to obtain the ladder operators and for this purpose we use the relation given in [14]

$$\rho \frac{\mathrm{d}}{\mathrm{d}\rho} L_n^{\alpha}(\rho) = n L_n^{\alpha}(\rho) - (n+\alpha) L_{n-1}^{\alpha}(\rho)$$
(38)

$$\rho \frac{d}{d\rho} L_n^{\alpha}(\rho) = (n+1) L_{n+1}^{\alpha}(\rho) - (n+\alpha+1-\rho) L_n^{\alpha}(\rho)$$
 (39)

where $L_n^{\alpha}(\rho)$ are the associated Laguerre function. By the action of the differential operator $\frac{\mathrm{d}}{\mathrm{d}\rho}$ on the wave functions (36) and using equation (38)

$$\left(\rho \frac{\mathrm{d}}{\mathrm{d}\rho} - (s+m) + \frac{\rho}{2} - \frac{1}{\ln\frac{2}{\rho}}\right) \Psi_m(\rho) = -(m+2s) \frac{N_m}{N_{m-1}} \Psi_{m-1}(\rho) \quad (40)$$

we can define the lowering operator

$$\hat{L}_{-} = -\rho \frac{\mathrm{d}}{\mathrm{d}\rho} + (s+m) - \frac{\rho}{2} + \frac{1}{\ln\frac{2}{\rho}}$$
(41)

with eigenvalues

$$l_{-} = (m+2s)\frac{N_m}{N_{m-1}}. (42)$$

Now we proceed to find the corresponding creation operators. Here we should make use of equation (39)

$$\left(\rho \frac{\mathrm{d}}{\mathrm{d}\rho} + (s+m+1) - \frac{\rho}{2} - \frac{1}{\ln\frac{2}{\rho}}\right) \Psi_m(\rho) = (m+1) \frac{N_m}{N_{m+1}} \Psi_{m+1}(\rho) \tag{43}$$

Then, we can define the operator

$$\hat{L}_{+} = \rho \frac{\mathrm{d}}{\mathrm{d}\rho} + (s+m+1) - \frac{\rho}{2} - \frac{1}{\ln\frac{2}{\rho}}$$
(44)

which has as eigenvalues

$$l_{+} = (m+1)\frac{N_{m}}{N_{m+1}}. (45)$$

Now we investigate the algebra associated with the operators \hat{L}_+ , \hat{L}_- . Based on the equations (40, 42) and(43, 45) we can calculate their commutator $[\hat{L}_-, \hat{L}_+]$

$$[\hat{L}_{-}, \hat{L}_{+}]\Psi_{m}(\rho) = 2(m+s+\frac{1}{2})\Psi_{m}(\rho)$$
(46)

suggesting to introduce the eigenvalues

$$l_0 = 2(m+s+\frac{1}{2}). (47)$$

In this way, we can define the operator

$$\hat{L}_0 = (\hat{m} + s + \frac{1}{2}). \tag{48}$$

The operators \hat{L}_+ , \hat{L}_- , \hat{L}_0 satisfy the commutation relations

$$[\hat{L}_{-}, \hat{L}_{+}] = 2\hat{L}_{0}, \qquad [\hat{L}_{0}, \hat{L}_{-}] = -\hat{L}_{-}, \qquad [\hat{L}_{0}, \hat{L}_{+}] = \hat{L}_{+}.$$
 (49)

4. Conclusion

In this paper we have obtained the raising and lowering operators for the 1D and 3D Morse potentials. We have shown that SU(2) is the dynamical group associated with the bounded region of the spectrum. Also we have obtained the Hamiltonian and eigenvalues of the Hamiltonian in terms of the $\mathfrak{su}(2)$ algebra.

References

- [1] Arima A. and Iachello F., *Interacting Boson Model of Collective States. I-The Vibrational Limit*, Ann. Phys. **99** (1976) 253–317.
- [2] Cooper I., An Iintegrated Approach to Ladder and Shift Operators for the Morse Oscillator, Radial Coulomb and Radial Oscillator Potentials, J. Phys. A: Math. & Gen. **26** (1993) 1601–1623.
- [3] Dong S., *Algebraic Approach to the Morse Potential and Its Coherent States*, Z. Phys. Chem. **216** (2002) 103–108.
- [4] Dong S., *The SU*(2) *Realization for the Morse Potential and Its Coherent States*, Can. J. Phys. **80** (2002) 129–139.
- [5] Dong S. H., *The Realization of Dynamic Group for the Pseudoharmonic Oscillator*, Appl. Math. Lett. **16** (2003) 199–203.
- [6] Dong S. H., Realization of the Dynamical Group for the Generalized Laguerre Functions, Computer and Mathematics with Application 47 (2004) 1035–1039.
- [7] Dong S. and Dong S. H., A Realization of Dynamic Group for an Electron in a Uniform Magnetic Field, Int. J. Mod. Phys. E 11 (2002) 265–271.

- [8] Dong S. and Dong S. H., *An Alternative Approach to Study the Dynamical Group for the Modified Poschl-Teller Potential*, Czech. J. Phys. **52** (2002) 753–764.
- [9] Dong S., Lemus R. and Frank A., *Ladder Operators for the Morse Potential*, Int. J. Quan. Chem. **86** (2002) 433–439.
- [10] Dong S. H and Lemus R., *Ladder Operators for the Modified Pöschl-Teller Potential*, Int. J. Quan. Chem. **86** (2002) 265–272.
- [11] Dong S. and Ma Z., *The Hidden Symmetry for a Quantum System with an Infinitely Deep Square-Well Potential*, Am. J. Phys. **70** (2001) 520–521.
- [12] Dong S. and Ma Z., *Algebraic Approach to the Pseudoharmonic Oscillator in 2D*, Int. J. Mod. Phys. E **11** (2002) 155–160.
- [13] Dong S. H., Sun G. and Tang Y., *The Hidden Symmetry for a Quantum System with a Poschl-Teller-Like Potential*, Int. J. Mod. Phys. E **12** (2003) 809–816.
- [14] Gradshteyn I. and Ryzhik I., *Tables of Integrals, Series and Products*, 5th Edn., Academic Press, New York 1994.
- [15] Iachello F. and Ibrahim M., *Analytic and Algebraic Evaluation of Franck-Condon Overlap Integrals*, J. Phys. Chem. A **102** (1998) 9427–9432.
- [16] Iachello F. and Levine R., *Algebraic Theory of Molecules*, Oxford Univ. Press, New York 1995.
- [17] Iachello F. and Oss S., *Algebraic Approach to Molecular Spectra: Two-Dimensional Problems*, J. Chem. Phys. **104** (1996) 6956–6963.
- [18] Iachello F. and Oss S., *Model of N Coupled Anharmonic Oscillators and Applications to Octahedral Molecules*, Phys. Rev. Lett. **66** (1991) 2976–2979.
- [19] Perelomov A., Generalized Coherent States and their Applications, Springer, New York 1985.
- [20] Roosmalen O., Benjamin I. and Levine R., A Unified Algebraic Model Description for Interacting Vibrational Modes in ABA Molecules, J. Chem. Phys. 81 (1984) 5986–5997.
- [21] Roosmalen O., Dieperink A. and Iachello F., *A Dynamic Algebra for Molecular Rotation-Vibraion Spectra of Complex Molecules*, Chem. Phys. Lett. **85** (1982) 32–36.
- [22] Roosmalen O., Iachello F., Levine R. and Dieperink A., Algebraic Approach to Molecular Rotation-Vibration Spectra. II. Triatomic Molecules, J. Chem. Phys. 79 (1983) 2515–2536.
- [23] Wybourne R., Classical Groups for Physicists, Wiley, New York 1974.