Int J Theor Phys (2009) 48: 607–610
DOI 10.1007/s10773-008-9833-8

Oscillator Representation for Pseudoharmonic Potential

Nail Sh. Ussembayev

Received: 4 January 2008 / Accepted: 14 August 2008 / Published online: 23 August 2008

Abstract Oscillator representation method is applied to obtain the bound state energy eigenvalues and the corresponding eigenfunctions of the n-dimensional Schrödinger equation for the pseudoharmonic potential with arbitrary angular momentum.

Keywords Oscillator representation method · Schrödinger equation · Pseudoharmonic potential · Energy levels · Wave functions

1 Introduction

Many physically interesting and important quantum-mechanical models are described by potentials for which we do not have analytical solutions of the Schrödinger equation. This has led to the development of many numerical, approximate methods such as WKB, $1/N$-expansion, etc. Nevertheless, the understanding of the physical situation, in some sense, relies upon exactly solvable potentials like Coulomb, harmonic oscillator, and some others. These potentials have been deeply studied in n-dimensional space and investigating the dependence of the solutions upon the n-dimensional space has recently attracted much attention.

The Coulomb force occurs in nature, whereas the harmonic oscillator is an approximate model, which works for small oscillations, but is inappropriate to use to describe anharmonic systems. The pseudoharmonic potential is used to study the anharmonicity of diatomic molecules, and might be considered as a potential with behavior between exactly solvable harmonic oscillator and nonlinear anharmonic models. The energy levels and eigenfunctions of the pseudoharmonic potential were determined for any angular momentum by means of several techniques. For example, by use of the Nikiforov-Uvarov method in [1], by ansatz method in [2], exact polynomial eigensolutions were given in [3], path-integral solution was given in [4].

N.S. Ussembayev (✉)
Department of Physics, Indiana University, Bloomington, IN, USA
e-mail: nussemba@indiana.edu

In the present paper, the oscillator representation method [5], the alternative effective method of solving the non-relativistic Schrödinger equation is applied for the n-dimensional spherically symmetric pseudoharmonic potential:

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

where r_0 is the equilibrium intermolecular separation and V_0 is the dissociation energy between two atoms.

The pseudoharmonic potential has wide applications in various fields of physics and chemistry such as molecular physics, solid state physics, chemical physics and in the study of carbon nanotubes and nanowires [6–9].

2 Pseudoharmonic Potential in the Oscillator Representation

The n-dimensional Schrödinger equation for the radial function $R(r)$ is

$$\frac{1}{r^{n-1}} \frac{d}{dr} \left(r^{n-1} \frac{dR}{dr} \right) - \frac{l(l+n-2)}{r^2} R + \frac{2m}{\hbar^2} \left[E - V_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2 \right] R = 0, \tag{1}$$

where $r^2 = \sum_{i=1}^{n} x_i^2$. To match with asymptotic behavior of the radial wave function near the origin and as $r \to \infty$ we introduce the substitutions

$$r = q^{2\rho} \text{ and } R(r) = q^{2\rho s(l)} \Phi(q),$$

where $s(l)$ and ρ are some parameters to be determined. Under this change of variables (1) transforms into

$$\frac{d^2\Phi}{dq^2} + \frac{1 + 2\rho(n-2) + 4\rho s}{q} \frac{d\Phi}{dq} + \frac{4\rho^2(s^2 + (n-2)s - l(l+n-2))}{q^2} \Phi + \frac{8m\rho^2}{\hbar^2} \left[E - V_0 \left(\frac{q^{2\rho}}{r_0} - \frac{r_0}{q^{2\rho}} \right)^2 \right] q^{4\rho-2} \Phi = 0. \tag{2}$$

We require the term with q^{-2} in (2) to be equal to zero. This can be done by setting $\rho = 1/2$ and the quadratic equation for $s(l)$ to be:

$$s^2 + (n-2)s - l(l+n-2) - \frac{2m V_0 r_0^2}{\hbar^2} = 0.$$

Hence, (2) simplifies to the form:

$$\frac{d^2\Phi}{dq^2} + \frac{n + 2s - 1}{q} \frac{d\Phi}{dq} + \frac{2m}{\hbar^2} \left[E + 2V_0 - \frac{V_0}{r_0^2} q^2 \right] \Phi = 0. \tag{3}$$

If one defines the radial Laplacian operator in the d-dimensional space as $\Delta_d = \frac{d^2}{dq^2} + \frac{d-1}{q} \frac{d}{dq}$, then it can be easily seen that (3) corresponds to the harmonic oscillator with frequency $\omega = \sqrt{\frac{2V_0}{mr_0^2}}$ in $d = n + 2s$ dimensional space:

$$\left(\frac{\hat{p}^2}{2m} + \frac{m\omega^2 q^2}{2} - E - 2V_0 \right) \Phi = 0, \tag{4}$$

where $\hat{p}^2 = \sum_{j=1}^{d} \hat{p}_j^2$ and $q^2 = \sum_{j=1}^{d} q_j^2$.

The symmetry of the d-dimensional Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 q^2}{2}$ in which both the coordinates q_j and operators $\hat{p}_j$ exist as the sums of squares suggests to introduce the complex conjugate operators

$$\hat{a}_j = \frac{m\omega q_j + i\,\hat{p}_j}{\sqrt{2m\hbar\omega}} \quad \text{and} \quad \hat{a}_j^\dagger = \frac{m\omega q_j - i\,\hat{p}_j}{\sqrt{2m\hbar\omega}}.$$

Then we have

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 q^2}{2} = \sum_{j=1}^{d} \left(\frac{\hat{p}_j^2}{2m} + \frac{m\omega^2 q_j^2}{2} \right) = \frac{\hbar\omega}{2} \sum_{j=1}^{d} \left(\hat{a}_j \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_j \right).$$

From the relation $\hat{p}_i q_j - q_j \hat{p}_i = -i\hbar\delta_{ij}$ there follows $\hat{a}_j \hat{a}_j^\dagger - \hat{a}_j^\dagger \hat{a}_j = 1$. Thus, the above Hamiltonian can be written as

$$\hat{H} = \hbar\omega \sum_{j=1}^{d} \hat{a}_j^\dagger \hat{a}_j + \frac{\hbar d\omega}{2} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{d}{2} \right).$$

In oscillator representation method the radial excitations with zero angular momentum are defined in the following form:

$$|n_r\rangle = c_{n_r} (\hat{a}^\dagger \hat{a}^\dagger)^{n_r} |0\rangle, \quad \text{where } c_{n_r}^{-2} = 4^{n_r} \frac{\Gamma(d/2 + n_r)}{\Gamma(d/2)} n_r!$$

and the ground state wave function is

$$|0\rangle = \left(\frac{\omega}{\pi} \right)^{d/4} \prod_{j=1}^{d} e^{-\frac{\omega}{2} q_j^2} = \left(\frac{\omega}{\pi} \right)^{d/4} e^{-\frac{\omega}{2} q^2}.$$

Using this we can find the radial excitations for (4):

$$\hat{H}\Phi_{n_r} = \hat{H}|n_r\rangle = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{d}{2} \right) |n_r\rangle = \hbar\omega \left(2n_r + \frac{d}{2} \right) \Phi_{n_r} = (E_{n_r} + 2V_0)\Phi_{n_r}.$$

From the latter simple algebraic equation with known ω and d we can finally determine the energy levels:

$$E_{n_r} = -2V_0 + \frac{\hbar}{r_0} \sqrt{\frac{2V_0}{m}} \left[1 + 2n_r + \sqrt{\left(l + \frac{n-2}{2} \right)^2 + \frac{2mV_0 r_0^2}{\hbar^2}} \right].$$

To obtain the wave functions we rewrite the coordinates q_j in the form:

$$q_j = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}_j + \hat{a}_j^\dagger \right) = \sqrt{\frac{\hbar}{m\omega}} Q_j$$

and similarly,

$$\hat{p}_j = \frac{1}{i} \sqrt{\frac{\hbar m\omega}{2}} \left(\hat{a}_j - \hat{a}_j^\dagger \right) = \sqrt{\frac{m\omega}{\hbar}} P_j = \frac{\sqrt{\hbar m\omega}}{i} \frac{\partial}{\partial Q_j}.$$

Thus, $\hat{a}_j^\dagger$ becomes

$$\hat{a}_j^\dagger = \frac{1}{\sqrt{2}}\left(Q_j - \frac{\partial}{\partial Q_j}\right).$$

Now taking into account the above listed expressions for radial excitations and the ground state wave function we obtain:

$$R_{n_r,l} \sim q^{s(l)}(\hat{a}^\dagger\hat{a}^\dagger)^{n_r}|0\rangle = q^{s(l)}\left[\frac{1}{2}\left(Q_j - \frac{\partial}{\partial Q_j}\right)\left(Q_j - \frac{\partial}{\partial Q_j}\right)\right]^{n_r} e^{-\frac{\omega}{2}q^2}.$$

3 Conclusions

The aim of this manuscript was to present a different approach to determine the arbitrary angular momentum solutions of the n -dimensional Schrödinger equation. With this purpose, the original n-dimensional Schrödinger equation was modified to the differential equation with Gaussian asymptotic behavior at large distances by the change of the variables. The modified Schrödinger equation was recognized with harmonic oscillator in the $(n + 2s)$-dimensional space. Thus, the angular momentum l was absorbed by the dimension $d = n + 2s(l)$ of that space. Finally, using the formalism of the creation $\hat{a}^\dagger$ and annihilation operators $\hat{a}$, the energy levels and the corresponding wave functions of the reduced problem were calculated.

In the oscillator representation method there is no need to deal with solving hypergeometric type second order differential equations or to use special functions as in Nikiforov-Uvarov, ansatz and other methods. The bound state energy eigenvalues can be calculated by solving simple algebraic equations which one obtains after reducing the original problem to the harmonic oscillator and using the ladder operators.

References

1. Sever, R., et al.: J. Math. Chem. **43**, 2 (2008)
2. Oyewumi, K., et al.: Int. J. Theor. Phys. **47**, 4 (2008)
3. Ikhdair, S., Sever, R.: Int. J. Mol. Struct. (Theochem.) **806**, 155 (2007)
4. Erkoc, S., Sever, R.: Phys. Rev. A **37**, 2687 (1988)
5. Dineykhan, M., et al.: Oscillator Representation in Quantum Mechanics. Springer, New York (1995)
6. Maitland, G., et al.: Intermolecular Forces. Oxford University Press, Oxford (1987)
7. Shigeru, A.: J. Math. Chem. **41**, 3 (2007)
8. Chakraborty, T.: Commun. Cond. Mat. Phys. **16**, 35 (1992)
9. Ashoori, R.: Nature **379**, 413 (1996)