IOP Conf. Series: Journal of Physics: Conf. Series **865** (2017) 012006 doi:10.1088/1742-6596/865/1/012006

Some applications using the connection between q-deformed harmonic oscillator and symmetric and asymmetric potentials

Ngo Gia Vinh[1], Man Van Ngu[2], Nguyen Tri Lan[3], Luu Thi Kim Thanh[4], Nguyen Thi Dung[5] and Nguyen Ai Viet[3]

[1]Bac Ninh Department of Education and Training, Bac Ninh, Viet Nam
[2]Hung Yen Industrial College, Tu Son, Bac Ninh, Viet Nam
[3]Institute of Physics, Vietnam Academy Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, Viet Nam
[4]Hanoi Pedagogical University No.2, Nguyen Van Linh Str., Vinh Phuc, Viet Nam
[5]Bac Ninh Teacher Training College, 12A Binh Than, Dai Phuc Ward 10, Bac Ninh, Viet Nam

E-mail: ngogiavinh@bacninh.edu.vn

Abstract. In our previous article, the connections between q-deformed harmonic oscillator and the two types of asymmetric (Morse-like) and symmetric (inverse square cosine form) potentials have been investigated. The use of these relations in an inverse way to investigate the properties of q-deformed harmonic oscillators has been proposed. In this work, we explore the possibility of using this approach to study some real physical systems, such as diatomic molecules, phonon, etc.

1. Introduction

Deformed Heisenberg algebras with q-deformed harmonic oscillator have been a subject of intensive investigation and have many useful applications in physics and chemistry [1–7]. The method of q-deformed quantum mechanics was based on the Heisenberg commutation relations for bosons. The main parameter of this method is a real number $q \in [0, 1]$, called deformation parameter, and $q = 1$ is corresponding to the case of in-deformed normal harmonic oscillators.

In the atomic and molecular physics, the interaction between atoms in diatomic and even in polyatomic molecules is usually described by the Morse potential [8–12]. In algebraic approach, the Morse potential can be written in terms of the generators of $SU(2)$ group. The quantum relation between q-deformed harmonic oscillator and the Morse potential was considered in [10], where the anharmonic vibrations in the Morse potential have been described as the levels of q-deformed harmonic oscillator. The extended $SU(2)$ model (q-Morse potential) has been also developed to compare with phenomenological Dunham expansion and experimental data for numbers of diatomic molecules [10].

In our previous works [14–17], considering deformed algebra as mathematical object and atomic effective potential as physical model, we proposed the new representations for q-deformed harmonic oscillator on the base of the physics model potential. In this representation, the potential for normal harmonic oscillation is parabolic with infinity equal-step energy levels. The potentials for q-deformed harmonic oscillation are anharmonic Morse potential (anharmonic

representation) or symmetric Pöschl–Teller potential (symmetric representation). In these case, energy spectra have finite in-equal steps, which are characterized by a maximal step number n_{max}.

In this work, using our developed approach we study some real physical problems: asymmetric representation for diatomic molecules and symmetric representation for phonon in nano structures.

2. Asymmetric representation of q-deformed harmonic oscillator

The Morse potential has the form

$$V(x) = D\left(1 - e^{-k(x-x_0)}\right), \tag{1}$$

where D is the depth, k is the strength, ω is the characterized frequency, and x_0 is the equilibrium position of the Morse potential.

The energy spectrum for Morse potential is

$$E(n) = \hbar\omega\left[\left(n+\frac{1}{2}\right) - \frac{\varepsilon}{2}\left(n+\frac{1}{2}\right)^2 + C_M\right], \tag{2}$$

where n is the vibrational quantum number.

The energy spectrum becomes quadratic if the higher order contribution C_M is neglected. In equation (2), the energy levels are represented by a system of parallel lines that are not equidistant.

$$\frac{E(n)}{\hbar\omega} = \left(n+\frac{1}{2}\right) - \frac{\varepsilon}{2}\left(n+\frac{1}{2}\right)^2. \tag{3}$$

The energy levels of the Morse potential and the corresponding harmonic potential are plotted in Figure 1.

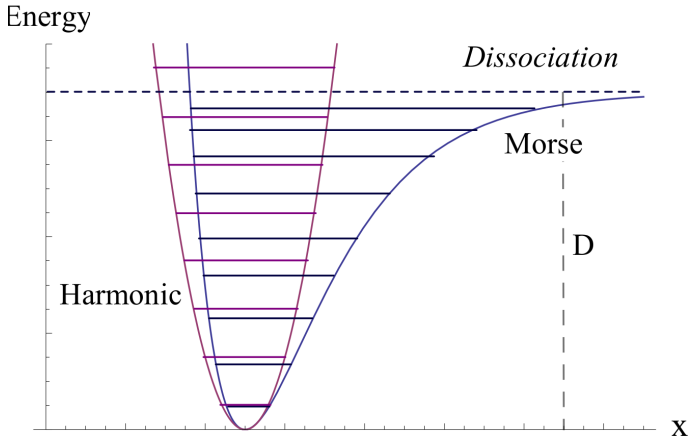

Figure 1. The energy levels Morse potential and harmonic potential.

3. Asymmetric representation and diatomic molecules

The energy spectrum of diatomic molecules with phenomenological Dunham quadratic expansion is

$$E(n) = hc\omega_e \left(n + \frac{1}{2}\right) - hc\omega_e x_e \left(n + \frac{1}{2}\right)^2 + ..., \tag{4}$$

where $\omega_e = \frac{\omega}{2\pi c}$, ω is frequency, c is the speed of light in vacuum and n is the vibrational quantum number. The Dunham vibrational molecular ω_e, $\omega_e x_e$ are obtained by fitting the potential curve to the experimental spectral data, $\omega_e x_e \ll \omega_e$ [10].

If the expansion (4) is truncated to the quadratic term, one obtains essentially the discrete spectrum of the Morse potential

$$E(n) = hc\omega_e \left[\left(n + \frac{1}{2}\right) - x_e \left(n + \frac{1}{2}\right)^2\right], \tag{5}$$

or

$$\frac{E(n)}{hc\omega_e} = \left(n + \frac{1}{2}\right) - x_e \left(n + \frac{1}{2}\right)^2. \tag{6}$$

Comparing the coefficients in the expressions (3) and (6), we can express the parameter-set of the Morse potential via the Dunham parameters, the depth D is

$$D = \frac{\omega_e}{4x_e}, \tag{7}$$

and the strength k equals

$$k = \sqrt{\frac{4\pi c}{\hbar}\mu\omega_e x_e}. \tag{8}$$

Setting $k_0 = \sqrt{\frac{4\pi c}{\hbar}\mu\omega_e}$ we get

$$k = k_0\sqrt{x_e}. \tag{9}$$

The q-deformed parameter can be expressed via x_e

$$q = 1 - 2x_e, \tag{10}$$

and the values of largest number n_{max} is

$$n_{max} = \left[\frac{1}{1-q}\right]. \tag{11}$$

The experimental value of the Dunham constant x_e of diatomic molecules are taken from [10], and the corresponding our calculated values of q, D/ω_e, $k/k_0, \mathrm{n}_{max}$ are presented in Table 1 and in Figures 2-5.

Diatomic molecules	$x_e.10^{-2}$	q	$\frac{D}{\omega_e}$	$\frac{k}{k_0}$	n_{max}
AgBr	2.4613	0.950774	10.1572	0.1569	20
HF	2.1764	0.956472	11.4869	0.1475	22
AgCl	2.1352	0.957296	11.7085	0.1461	23
NaH	1.74179	0.965164	14.3531	0.1320	28
AlH	1.73217	0.965357	14.4328	0.1316	28
BO	0.884985	0.982300	28.2491	0.0941	68
CO	0.617701	0.987646	40.4727	0.0786	80
SnO	0.528665	0.989427	47.2889	0.0727	94
KCl	0.32143	0.993571	77.7774	0.0567	155
KBr	0.30303	0.993939	82.5001	0.0550	165

Table 1. The values of the parameters of diatomic molecules.

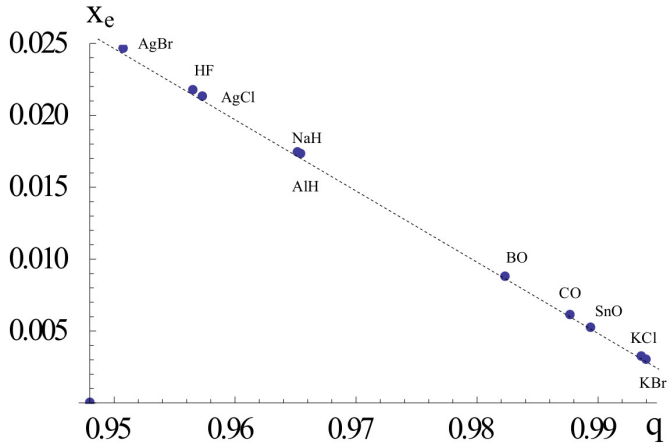

Figure 2. The dependence of x_e on q of some diatomic molecules.

From Figures 2-5 we can conclude that among the investigated here diatomic molecules, the most deformed diatomic molecule is AgBr with the deformation parameter q_{AgBr} =0.950774, and the less deformed diatomic molecule is KBr with the deformation parameter q_{KBr} =0.993939. All real diatomic molecules have very small deformation with $0.95 < q < 1$.

4. Symmetric representation of q-deformed harmonic oscillator

In the work [17] we have studied the deformation parameter q through Pöschl – Teller potential

$$V_s(x) = -\frac{U_0}{\cosh^2(\alpha x)}. \tag{12}$$

This potential is a symmetric anharmonic potential and has in-equal-step quadratic energy spectrum with the largest number n_{max} as above.

The energy levels of symmetric potential and harmonic potential are shown in Figure 6.

In the next session, we use this potential to study the phonon problem.

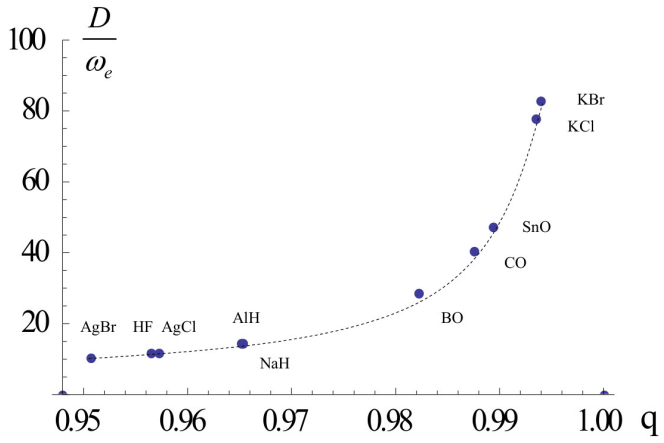

Figure 3. The dependence of $\frac{D}{\omega_e}$ on q of some diatomic molecules.

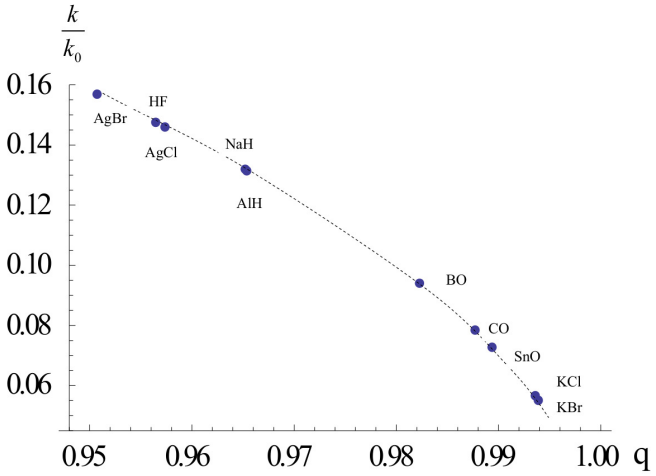

Figure 4. The dependence of $\frac{k}{k_0}$ on q of some diatomic molecules.

5. Symmetric representation and phonon in 1D atomic chain

It is well known that, phonon in the solids can be treated as a boson gas. For simplicity we take the case of 1D atomic lattice and study the deformation effect of phonon in this system.

For 1D atomic chain, $n_{max} = L/a$ where a is the inter-atomic distance, L is the chain-length. Usually in real crystals $a \simeq 5$Å, and if L is very short (of few nanometers) we have only small n_{max}.

We apply symmetric representation of q–deformed harmonic oscillator for phonon in the 1D atom chain with standard relation between the deformation parameter q and n_{max}: $n_{max} = \left[\frac{1}{1-q}\right]$.

For the case of long chains (a large-sized structures) $L \gg a$, $n_{max} \to \infty$, $q \to 1$, deformation effect is very small and we can use the Einstein-Debye cut-off frequency: $\omega_E = \omega_0$, $n_{max} = \frac{L}{a} \gg 1$.

For the inverse case of very short chain $n_{max} = L/a = [1/(1-q)]$. For example $L = 5nm$,

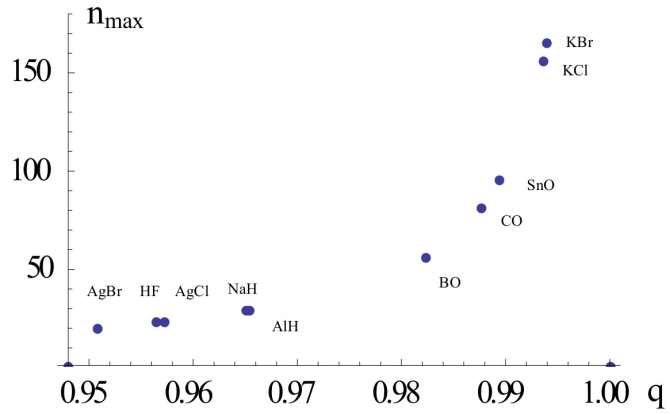

Figure 5. The dependence of n_{max} on q of some diatomic molecules.

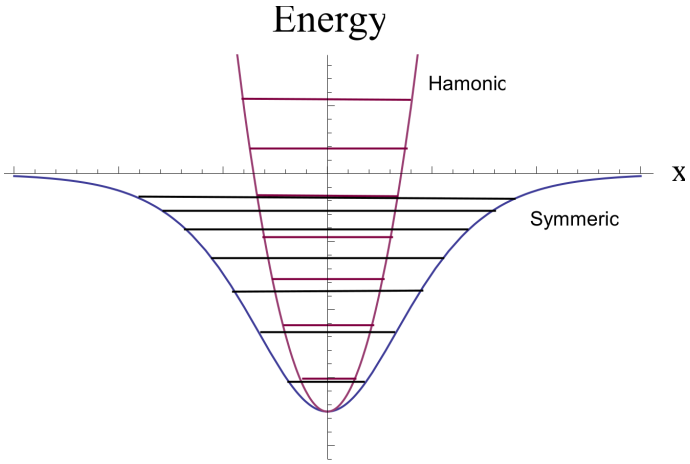

Figure 6. Energy levels of symmetric and harmonic potential.

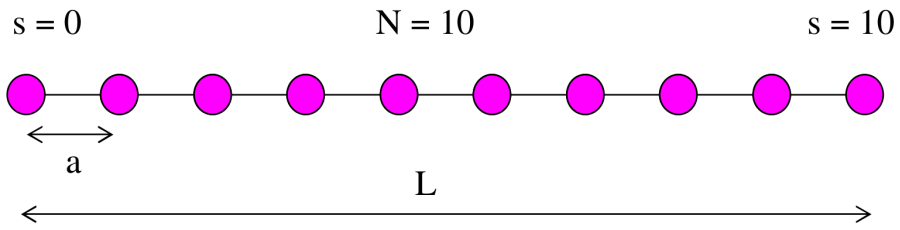

Figure 7. Model of 1D atomic lattice.

$n_{max} = 10$, the deformation parameter is $q \sim 0.9$. We conclude that for nano size chains the deformation effect is important.

6. Conclusion

In our previous works considering deformed algebra as mathematical object and atomic effective potential as physical model, we proposed a new representation for q-deformed harmonic oscillator on the base of a physical model potential. In this representation, the potential for normal

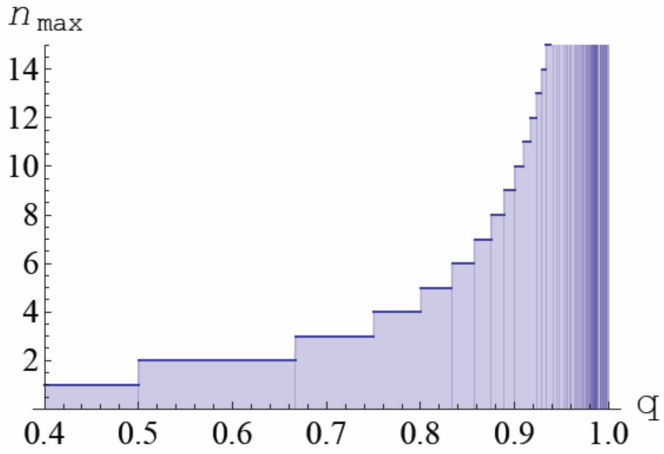

Figure 8. The values of the largest numbers n_{max} depending on deformation parameter q.

harmonic oscillation is parabolic with infinity equal-step energy levels. The potentials for q-deformed harmonic oscillation are asymmetric Morse potential (asymmetric representation) or symmetric Pöschl–Teller potential (symmetric representation). In these cases, energy spectra have finite in-equal steps, which are characterized by a maximal step number n_{max}.

In this work, using our developed approach we study some real physical problems: asymmetric representation for diatomic molecules and symmetric representation for phonon in nano structures.

We prove that the anharmonic potential deformation representation works well for the case of diatomic molecules. The physical parameters for diatomic molecules depending on deformation parameter q are plotted in Figures 2-5 with well determined curves. From those figures we can see that among the investigated here diatomic molecules, the most deformed diatomic molecule is AgBr with the deformation parameter q_{AgBr} =0.950, and the less deformed diatomic molecule is KBr with the deformation parameter q_{KBr} =0.993. All investigated real diatomic molecules have very small deformation of $0.95 < q < 1$.

We applied the symmetric potential deformation representation for phonon problem in very short atomic chain of nanometer length. We found that for 1D atomic nano chains the deformation effect of phonon is important.

Our developed approach with deformed potentials should be useful in investigating other physics problems. This will be the subject of our next work.

Acknowledgments

This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2015.42.

References

[1] Eremin V V and Meldianov A A 2008 *arXiv:0810.1967v1*
[2] Mirzrahi S S, Camargo J P and Dodonov V V 2004 *J. Phys.* A **37** 3707
[3] Abe S 2009 *Phys. Rev.* E **79** 041116
[4] Lavagno A and Swamy P P 2010 *Physica* A **389** 993
[5] Algin A, Senay M 2012 *Phys. Rev.* E **85** 041123
[6] Andrade F M and Silva E O 2013 *Phys. Lett.* B **719** 467
[7] Tkachuck V M 2013 *Phys. Rev.* A **86**, 062112
[8] Angelova M and Franck A 2005 *Phys. Atom. Nuclei* **68** 1689-1697
[9] Dong S H, Lemus R and Frank A 2002 *J. Quant. Phys.* **86** 433

[10] Angelova M, Dobrev V and Frank A 2004 *Eur. Phys. J.* D **31** 27
[11] Kaplan I G 2003 *Handbook of Molecular Physics and Quantum Chemistry* (Wiley)
[12] Lima E F and Hornos J E M 2005 *J. Phys.* B **38** 815
[13] Landau L D and Lifshitz E M 1991 *Course of Theoretical Physics* Vol. 3
[14] Vinh N G, Ngu M V, Lan N T, Viet N A and Thanh L T K 2015 *J. Phys.: Conf. Ser.* **627** 012022
[15] Ngu M V, Vinh N G, Lan N T, Viet N A and Thanh L T K 2015 *J. Phys.: Conf. Ser.* **627** 012021
[16] Vinh N G, Ngu M V, Lan N T, Viet N A and Thanh L T K 2016 *J. Phys.: Conf. Ser.* **726** 012018
[17] Ngu M V, Vinh N G, Lan N T, Viet N A and Thanh L T K 2016 *J. Phys.: Conf. Ser.* **726** 012017