The possible conection between q-defomed hamornic oscillator formation and anharmonicity

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Abstract. In our previous article, the connection between q–deformed harmonic oscillation and Morse–like asymmetric potential is investigated. In present work, a possibility of the connection between q-deformed harmonic oscillator and anharmonic symmetric potential is in detail considered. For simplicity, we take the inverse square cosine–hyperbolic form of potential, i.e Pöschl–Teller potential. The relation between the deformation parameter q and the set of parameters of anharmonic symmetric potential was found. The correspondence of two types of connections between q-deformed harmonic oscillator with asymmetric and symmetric potentials are discussed.

1. Introduction
In the last twenty years, quantum group and deformed Heisenberg algebras with q-deformed harmonic oscillator have been a subject of intensive investigation. This approach has found some useful applications in various branches of physics and chemistry [1, 2, 3, 4, 5, 6, 7]. The method of q–deformed quantum mechanics was developed on the base of Heisenberg commutation relation (the Heisenberg algebra) within some typical generalizations. The main parameter of this method is the deformation parameter q which is usually considered to variety in the range $0 < q < 1$, and the models have been constructed that the behaviors of studying objects reduce to theirs conventional counterparts as $q \to 1$.

The Morse potential finds an important role in describing the interaction among atoms in diatomic and even in polyatomic molecules [8, 9, 10, 11, 12, 14] of atomic and molecular physics. Despite its quite simple form, the Morse potential describes very well the vibrations of diatomic molecules. This is because that four–particle complex system (two heavy atomic nuclei with positive charge and two light electrons with negative charge) can be reduced to relative motion of two atomic nuclei in an effective potential which is average Coulomb interaction of nuclei and electron clouds. The Morse–like potential models just work with a simple one-dimensional three-parameter effective potential, and find many applications in condensed matter, bio–physics, nano–science and quantum optics.

The Morse potential in algebraic approach can be written in terms of the generators of $SU(2)$. The quantum relation between q-deformed harmonic oscillator and the Morse potential

was considered in [10], where then 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 this work, by considering deformed algebra as mathematical object and atomic effective potential as physical model, we use this relation in inverse way to investigate properties of q-deformed harmonic oscillator on the base of the Morse potential.

In one hand, the potential of harmonic oscillation is parabolic with infinity equal–step levels. In other hand, we show that the potential of q–deformed harmonic oscillator can be described as Morse-like anharmonic potential with finite unequal–step levels. The relation between the deformation parameter q and the set of parameters of Morse–like anharmonic potential was found. We have also investigated the partition function and some thermodynamic properties of q-deformed harmonic oscillator.

In the our previous work [14] we have shown that mathematical deformation properties can be represented and understood in the language of physical object, which can be described by an anharmonic potential.

The asymmetric representation of deformed harmonic oscillators was investigated in [14] with the Morse potential. And as a further step, in this work we study the symmetric representation of deformed harmonic oscillators with corresponding potential.

2. Harmonic oscillator and q–deformed harmonic oscillator

In q-deformed harmonic oscillator, creation $a^\dagger$ and annihilation a operators of q–deformed harmonic oscillator satisfy the commutation relation

$$[a, a^\dagger]_q = aa^\dagger - qa^\dagger a = 1, \tag{1}$$

where q is deformation parameter taking values in $[0, 1]$.

In the second quantization representation, the Hamiltonian operator of q-deformed harmonic oscillator is written as

$$H = \frac{\omega}{2} \left(aa^\dagger + a^\dagger a \right). \tag{2}$$

As the results of simple algebraic manipulations, energy spectrum of q-deformed harmonic oscillator is obtained as follows

$$E_n = \frac{\omega}{2} \left([n]_q + [n+1]_q \right), \tag{3}$$

where $[n]_q = \frac{1-q^n}{1-q}$ is the q-integer which differs from natural numbers. For very small derivation from unity $\varepsilon = 1 - q$, the energy spectrum becomes quadratic if the higher order contribution $C = O\left((\varepsilon^2)\right)$ is neglected

$$E_n = \hbar\omega \left(n + \frac{1}{2} - \frac{n^2}{2}\varepsilon + C \right). \tag{4}$$

In result (4), the energy levels are represented by a system of parallel lines are not equidistant. The extent depends on the deformation parameter q.

3. Physical model for q–deformed harmonic oscillator

In the case of $q = 1 (\varepsilon = 0)$, the energy levels return to non–deformed expression, i.e.

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \tag{5}$$

we obtained the energy levels of the harmonic oscillator, the gaps between the energy levels are constant (Figure 1).
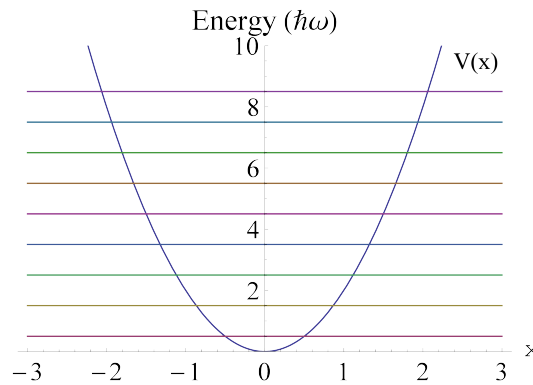

Figure 1. Energy spectrum has infinity equal-step levels form.

In the range of parameter values $0 < q < 1$, the energy levels are represented by a system of parallel lines are not equidistant.

In all previous work, we have studied the deformation parameter q through Morse potential, which is the asymmetric anharmonic potential. In this ongoing one, the deformation parameter q with symmetric anharmonic potential form (Figure 2) will be under consideration.
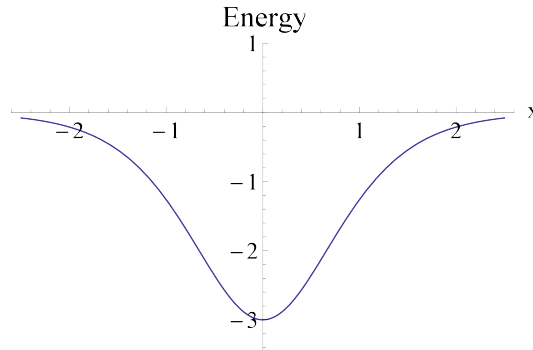

Figure 2. The potential is symmetric anharmonic.

To easily compare potential energy shapes, we observe their appearance on the same coordinate system (Figure 3). The symmetric potential is anharmonic and energy spectrum has finite unequal-step levels, for comparison also plotted harmonic spectrum of corresponding parabolic potential.

4. Symmetric representations

The symmetric potential has an important role in describing the interaction of atoms in diatomic, and even polyatomic molecules. In the case, the symmetric potential is anharmonic, energy spectrum has finite unequal–step levels as presented in the Figure 4, where energy spectrum of symmetric anharmonic and corresponding parabolic potentials are compared.

The symmetric anharmonic potential chosen in study is Pöschl – Teller potential

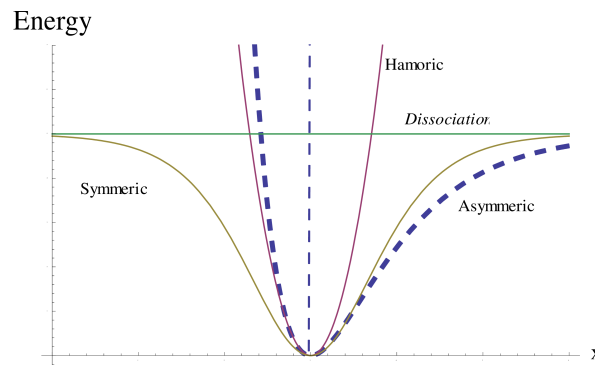$$V_s(x) = -\frac{U_0}{\cosh^2(\alpha x)}, \tag{6}$$

Figure 3. The harmonic potential, anharmonic potential and symmetric potential.
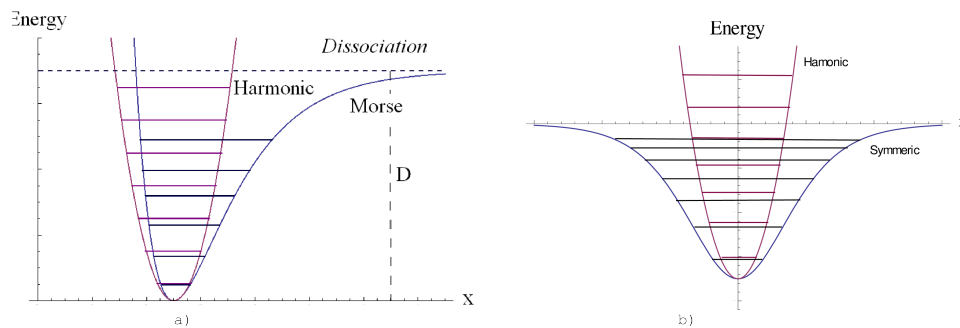

Figure 4. Energy Levels: a) Morse potential and Harmonic potential. b) Symmetric and Harmonic potential.

which is an effective potential with a set of two parameters U_0, α taken from experimental data.

The Schrödinger equation of symmetric anharmonic potential (6) has been exactly and analytically solved [13]. The eigenvalues of this Hamiltonian read

$$E_s = -\frac{\alpha^2 \hbar^2}{8m} \left[-(1 + 2n) + \sqrt{1 + \frac{8U_0}{\alpha^2 \hbar^2}} \right]^2. \tag{7}$$

By introducing new quantity

$$\omega_s = \frac{\alpha^2 \hbar}{2m} \sqrt{1 + \frac{8U_0}{\alpha^2 \hbar^2}}, \tag{8}$$

the energy level of system under consideration can be expressed as

$$E_s = \hbar \omega_s \left[n + \frac{1}{2} - \frac{\varepsilon}{2} \left(n + \frac{1}{2} \right)^2 + C_s \right], \tag{9}$$

where ω_s is the frequency of symmetric oscillator.

Following the tasks presented in our last work [14], the deformation parameter q_s of the given potential is found as

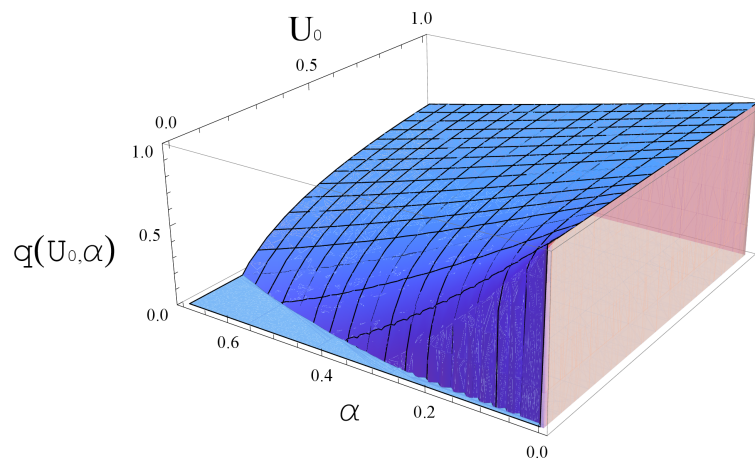$$q_s = 1 - \frac{2}{\sqrt{1 + \frac{8U_0}{\alpha^2 \hbar^2}}}. \tag{10}$$

Figure 5. q-deformed symmetric representation depending parameters U_0, α.

It is obvious that this system has a finite number of energy levels with maximum number $n_{S.max}$

$$n_{S.max} = \left[\frac{1}{(1-q_S)} \right] = \left[\frac{1}{2}\sqrt{1 + \frac{8U_0}{\alpha^2 \hbar^2}} \right], \qquad (11)$$

where the notation $[f]$ is the integer part of the number f.

Using the above relationship, we propose the deformation model (SPD model), based on the symmetric potential, for investigating the properties of q–deformed harmonic oscillator. The main idea is that the role of parabolic potential for harmonic oscillator would be replaced by the symmetric representation potential for q-deformed harmonic oscillation.

In above proposed model, every given value of deformation parameter q_S in the interval from zero to unity, $q_S \in [0, 1]$, can be described by a symmetric potential with the largest number $n_{S.max}$ determined by the expression (11). Here, we note the well–defined one–to–one correspondence between q_S and $n_{S.max}$. The values of largest number depending on deformation parameter q_S and on parameters of material system are plotted in figure 6 and in figure 7.
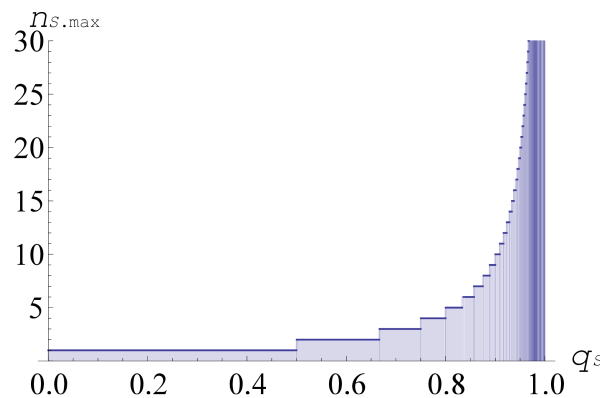

Figure 6. The values of largest number $n_{S.max}$ depending on deformation parameter q_S.
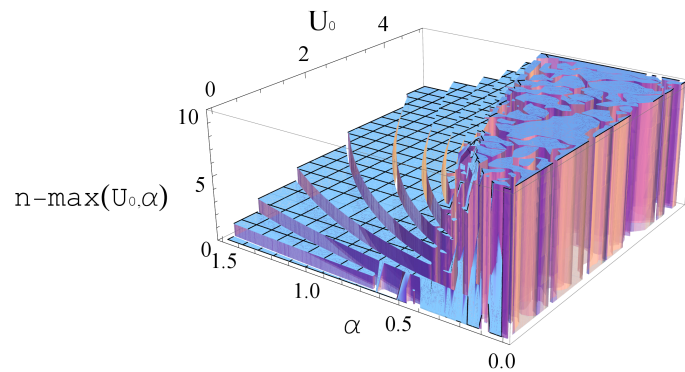
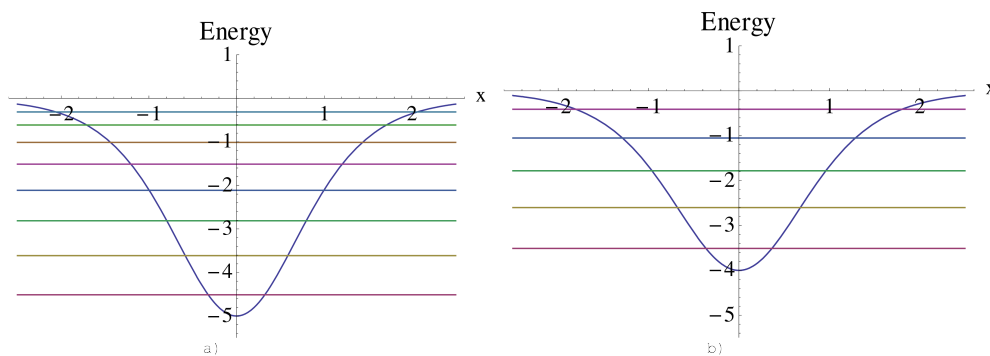**Figure 7.** The values of largest number $n_{S.max}$ depending on given input parameters U_0, α.

Figure 8. Dependence of number of energy levels on U_0 while α is fixed ($\alpha = 1$), a) $U_0 = 5$, b) $U_0 = 4$.
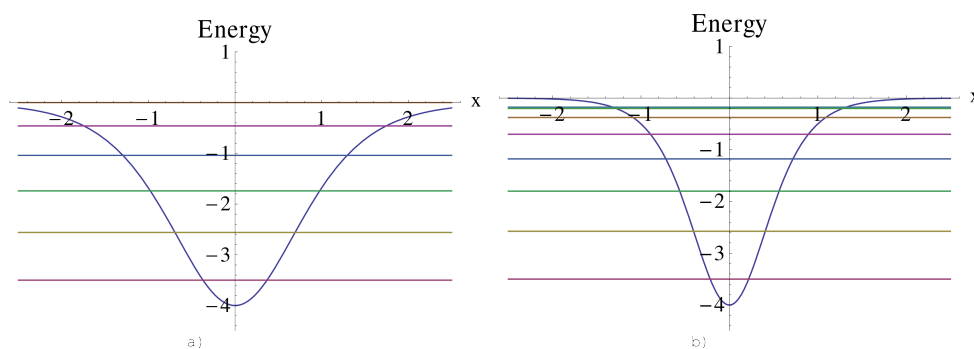

Figure 9. Dependence of number of energy levels on α while U_0 is fixed ($U_0 = 4$), a) $\alpha = 1.2$, b) $\alpha = 1.8$.

It is shown that the total number of energy levels rapidly grows up when q tends to unity. In the limit of weak deformation $q \to 1$, $n_{max} \to \infty$. In contrast, when q tends to 0.5 only one level

can be found, i.e. in the strong deformation limit $q \to 1/2$, $n_{\max} \to 1$. The actual working range of deformation parameter q is not to be in $q \in [0,1]$, but in more narrow half range $0.5 < q < 1$, where the physical system has more than one energy level.

The last but not least, the main parameters of harmonic, q–deformed harmonic, symmetric and asymmetric potentials are compared in Table 1.

	Harmonic	q-deformed Harmonic	Asymmetric	Symmetric
Potential	$-\frac{1}{2}kx^2$		$D\left(1-e^{-k(x-x_0)}\right)$	$-\frac{U_0}{\cosh^2(\alpha x)}$
ε	0	$1-q$	$\frac{\hbar k}{\sqrt{2mD}}$	$\frac{2}{\sqrt{1+\frac{8mU_0}{\alpha^2\hbar^2}}}$
Frequency	$\sqrt{k/m}$	$\hbar\omega$	$\hbar\sqrt{\frac{2D}{mk^2}}$	$\frac{\alpha^2\hbar^2}{2m}\sqrt{1+\frac{8mU_0}{\alpha^2\hbar^2}}$
q	1	$1-\varepsilon$	$1-\frac{\hbar k}{\sqrt{2mD}}$	$1-\frac{2\alpha\hbar}{\sqrt{\alpha^2\hbar^2+8mU_0}}$
n_{max}	∞	$\left[\frac{1}{(1-q)}\right]$	$\left[\sqrt{\frac{8Dk^2}{\hbar^2}}-1\right]$	$\left[\frac{1}{2}\sqrt{1+\frac{8mU_0}{\alpha^2\hbar^2}}\right]$

Table 1. Comparison of asymmetric and symmetric representations.

5. Discussion

Comparing the energy spectrum of q-deformed harmonic oscillator (4) and energy spectrum of symmetric anharmonic potential (7) and neglecting the higher order contribution $O\left((\varepsilon^2)\right) = O\left(\left((1-q)^2\right)\right)$, we realize the relations

$$\omega_s \leftrightarrow \omega, \tag{12}$$

$$\frac{2}{N} \leftrightarrow \varepsilon. \tag{13}$$

This is the relation between q-deformed harmonic oscillator and symmetric anharmonic vibrations, providing the analogy of q–deformation and symmetric anharmonicity. The change of energy spectrum from linear to quadratic form is reasoned by deformations of commutation relations in the mathematical algebraic approach, while in case of the symmetric potential by appearance of periodic distribution of atoms or molecules.

The main results of this work are the consequences of the expression of energy levels (7), on which we proposed a new symmetric potential deformation SPD model for investigating properties of q-deformed harmonic oscillator via the symmetric potential (6). Instead of parabolic potential for harmonic oscillation, the symmetric anharmonic potential is used to study the q-deformed harmonic oscillation, and as it is expected, the mathematical deformation properties now would be described and understood in the language of physical anharmonic behaviors.

In our proposed SPD model, q-deformed harmonic oscillator can be described by the corresponding symmetric Pöschl–Teller potential. With every given value of deformation parameter in the interval $q_S \in [0,1]$, we would determine the largest number $n_{S.max}$ and the deformed energy spectrum $E_q(n)$ of q–deformed harmonic oscillation.

In one hand, the asymmetric representation of deformed harmonic oscillators by using a symmetric Morse potential [14] can be applied to describe interaction between two atoms molecules, where the space among them is clearly non–symmetric. In other hand, the possible applications of symmetric representation for deformed harmonic oscillators are atomic chain, symmetric atoms, where the space is translationally symmetric. This models could be expanded and generalized to investigate many other physical problems such as composite bosons with deformation which is the topic of our ongoing research.

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