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Q-Deformed Harmonic Oscillator and Morse-like Anharmonic Potential

Ngo Gia Vinh¹, Man Van Ngu², Nguyen Tri Lan³, Luu Thi Kim Thanh⁴ and Nguyen Ai Viet³

¹Bac Ninh Department of Education and Training, Bac Ninh Province, Vietnam

²Hung Yen Industrial College, Hung Yen Province, Vietnam

³Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan Str., Ba Dinh, Hanoi, Vietnam

⁴Hanoi Pedagogical University No.2, Vinh Phuc Province, Vietnam

E-mail: vinhphongvan@gmail.com

Abstract. Connection between q -deformed harmonic oscillator and Morse-like anharmonic potential is investigated. It is well known that the potential of harmonic oscillator is parabolic. We have shown that the potential of q -deformed harmonic oscillator could be a Morse-like anharmonic potential. The relation between the deformation parameter q and the set of parameters of Morse-like anharmonic potential was found. We also investigated the partition function and some thermodynamic properties of q -deformed harmonic oscillator.

1. Introduction

Recently, quantum group and deformed Heisenberg algebras with q -deformed harmonic oscillator have been a subject of intensive investigation. This approach has found a number of applications in various branches of physics and chemistry [1–7]. In context, the method of q -deformed quantum mechanics was developed on the base of Heisenberg commutation relation i.e. the Heisenberg algebra. The main parameter in this method is the deformation parameter q varying in the range $0 < q < 1$, and the models have been constructed so that the physical behaviours of studying objects reduce to theirs standard counterparts as $q \rightarrow 1$.

In other hand, the well-known Morse and Morse-like potentials have an important role in describing the interaction of atoms in diatomic and even polyatomic molecules [8–12] in 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) could be reduced to relative motion between two atomic nuclei in an effective potential which is an average Coulomb interaction of nuclei and electron clouds. 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.

In algebraic approach, the Morse potential models would be rewritten in terms of the generators of $SU(2)$. The quantum relation between q -deformed harmonic oscillator and Morse potential has been considered in many literature such as in [10], where then the anharmonic vibrations of Morse potential have been described as the levels of q -deformed harmonic oscillators.



The extended $SU(2)$ model (the q -Morse potential) was also developed to compare with phenomenological Dunhams expansion and experimental data for numbers of diatomic molecules [10, 11].

In this work, deformed algebra under consideration is mathematical object and atomic effective potential is physical model, we use this relation in inverse way: investigate properties of q -deformed harmonic oscillator on the base of the Morse potential.

The potential of harmonic oscillator is parabolic with infinity equal-step levels. We will show that the potential of q -deformed harmonic oscillator might 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 has been found. Based on this relation, we investigate thermodynamics of q -deformed harmonic oscillator such as the partition function and some derivative properties.

2. Harmonic Oscillator ($q = 1$)

In the term of first quantization representation, the Hamiltonian of harmonic oscillator is

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2, \quad (1)$$

where m and ω are the mass and frequency of oscillator, respectively. \hat{x} and $\hat{p} = -i\hbar\frac{d}{dx}$ are the coordinate and momentum operators, which satisfy the commutation relation $[\hat{x}, \hat{p}] = -i\hbar$.

In the second quantization representation, the Hamiltonian of harmonic oscillator is rewritten as

$$H_0 = \frac{\hbar\omega}{2} (a_0 a_0^\dagger + a_0^\dagger a_0), \quad (2)$$

where a_0^\dagger and a_0 are creation and annihilation operators, which satisfy the commutation relation

$$[a_0, a_0^\dagger] = 1. \quad (3)$$

Energy spectrum of harmonic oscillator has the form

$$E_{0n} = \frac{\hbar\omega}{2} (2n + 1), \quad (4)$$

where $n = 0, 1, 2, 3, \dots$ are the integers.

Note that for harmonic oscillator case, potential $V(x) = \frac{1}{2}m\omega^2x^2$ is parabolic, and energy spectrum has infinite equal-step levels as presented in the fig. 1.

3. q -Deformed Harmonic Oscillator

Creation a^\dagger and annihilation a operators of q -deformed harmonic oscillator satisfy the deformed commutation relation with parameter q [8] as

$$\begin{aligned} [a, a^\dagger]_q &= aa^\dagger - qa^\dagger a \\ &= 1, \end{aligned} \quad (5)$$

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

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

$$H = \frac{\omega}{2} (aa^\dagger + a^\dagger a), \quad (6)$$

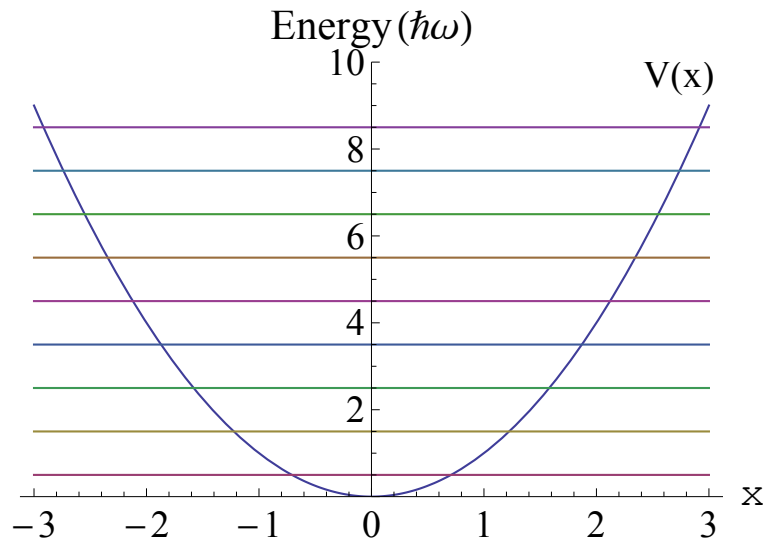


Figure 1. For harmonic oscillator case, the potential is parabolic, and energy spectrum has infinite equal-step levels.

Energy spectrum of q -deformed harmonic oscillator correspondingly takes the form

$$E_n = \frac{\omega}{2}([n] + [n + 1]), \quad (7)$$

where $[n] = (1 - q^n) / (1 - q)$ denotes the q -integer which differs from natural numbers. For small derivation from unity $\varepsilon = 1 - q$, the energy spectrum become quadratic if the higher order contribution $O(\varepsilon^2)$ is neglected

$$E_n = \hbar\omega \left(n + \frac{1}{2} - \frac{n^2}{2}\varepsilon + O(\varepsilon^2) \right). \quad (8)$$

4. Morse-like Anharmonic Potential

The Morse potential has an important role in describing the interaction of atoms in diatomic, and even polyatomic molecules. Obviously, the Morse potential is anharmonic, and has finite unequal-step level energy spectrum as presented in the fig. 2 where for comparison the harmonic spectrum of corresponding parabolic potential is also plotted. The so-called Morse-like potential is an effective potential with a set of three parameters (D, d, x_e) taken from experiment

$$V_x = D \left(1 - e^{-d(x-x_e)} \right)^2, \quad (9)$$

where x_e is the minimum position, D is the depth of the well, and d is the width of potential. In practice, these parameters are determined from experimental data, D is dissociation energy, and d is restitution constant in the harmonic approximation model as shown in the fig. 2.

The one-dimensional Morse Hamiltonian for oscillator with mass M can be rewritten in term of the generators of $SU(2)$ and reads

$$H_M = \frac{\hbar\omega_M}{2} (bb^\dagger + b^\dagger b), \quad (10)$$

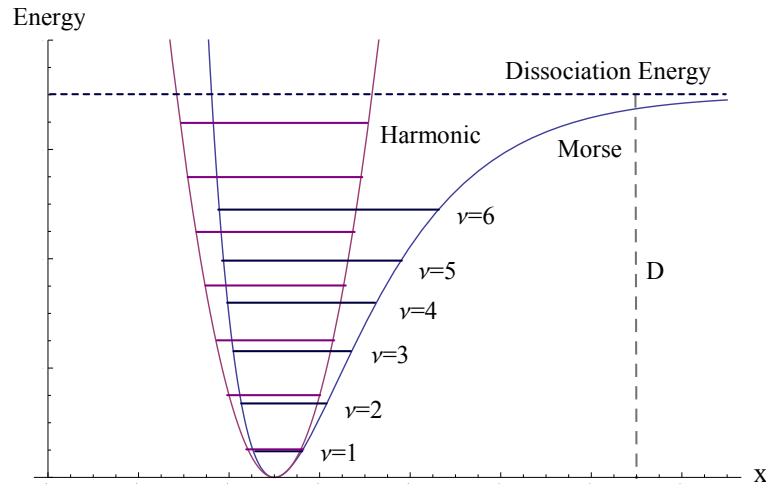


Figure 2. The Morse potential is anharmonic and energy spectrum has finite unequal-step levels, for comparison, the harmonic spectrum of corresponding parabolic potential is also plotted.

where b^\dagger and b are creation and annihilation operators, which satisfy the commutation relations

$$[b, b^\dagger] = 1 - \frac{2\hat{\nu}}{N}, \quad (11)$$

$$[b, \hat{\nu}] = b, \quad (12)$$

$$[b^\dagger, \hat{\nu}] = -b^\dagger, \quad (13)$$

where $\hat{\nu}$ is the Morse phonon operator with an eigenvalue. The value of N depends on the depth D and the width d of the Morse potential

$$N = \left(\frac{8Dd^2}{\hbar^2} \right)^{1/2} - 1, \quad (14)$$

and the frequency of Morse oscillator equals to

$$\omega_M = \left(\frac{2D}{md^2} \right)^{1/2}. \quad (15)$$

Energy spectrum of Morse oscillator is

$$E_{M\hat{\nu}} = \hbar\omega_M \left(\nu + \frac{1}{2} - \frac{\nu^2}{N} \right). \quad (16)$$

where $\nu = 1, 2, 3, \dots, \nu_{\max}$ is the quanta number. The largest value $\nu_{\max} = [N/2]$, here $[f]$ is the integer part of f . When $N \rightarrow \infty$, then $[b, b^\dagger] \rightarrow 1$ giving the usual boson commutation relations, we come back to case of harmonic oscillator with parabolic potential and infinity equal-step energy levels.

5. Relation between q -deformed harmonic oscillator and Morse anharmonic vibrations

Compare the energy spectrum of q -deformed harmonic oscillator (8) and those of Morse oscillator (16), neglecting the higher order contribution $O(\varepsilon^2) = O((1-q)^2)$, we realize the relations

$$\begin{aligned}\omega_M &\leftrightarrow \omega, \\ \nu &\leftrightarrow n, \\ \varepsilon &\leftrightarrow 1 - q.\end{aligned}\tag{17}$$

This is the relation between q -deformed harmonic oscillator and Morse anharmonic vibrations. The changing energy spectrum from linear to quadratic form caused by deformations of commutation relations in the mathematical algebraic approach, while in case of Morse potential in atomic and molecular physics by anharmonic vibrations.

6. Morse potential for deformation model (MPD model)

Using the relation (17), we propose MPD model for investigation properties of q -deformed harmonic oscillator based on the Morse potential. The main idea is that the role of parabolic potential for harmonic oscillator will be replaced by the Morse anharmonic potential for q -deformed harmonic oscillator. In our proposed model, every given value of deformation parameter q in the interval from zero to unity $q \in [0, 1]$ can be described by the Morse anharmonic potential with the largest number n_{\max}

$$n_{\max}(q) = \left[\frac{1}{(1-q)} \right].\tag{18}$$

where here $[f]$ is the integer part of f . We note here the well-defined one-to-one corresponding between q and n_{\max} . The values of largest number n_{\max} depending on deformation parameter q are plotted in the fig. 3.

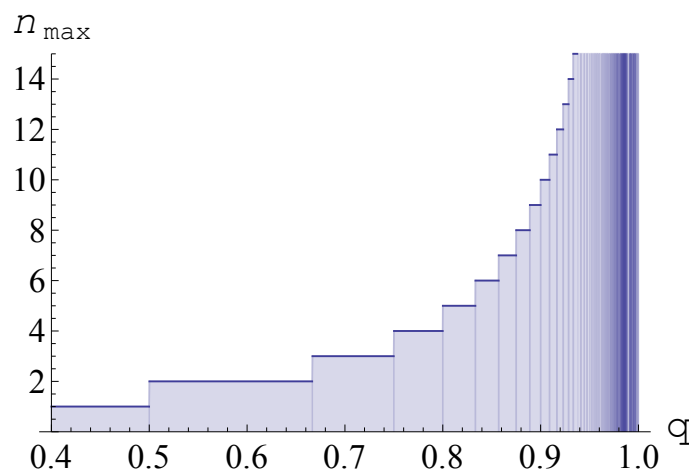


Figure 3. The values of largest number depend on deformation parameter q .

We could see that the total level number rapidly grown up when q tends to unity. In the limit of weak deformation $q \rightarrow 1$, $n_{\max} \rightarrow \infty$. In contrast, when q tends to 0.5 only one level can exist. In strong deformation limit $q \rightarrow 1/2$, $n_{\max} \rightarrow 1$. Consequently, the actual working range of deformation parameter q is not in whole range $q \in [0, 1]$, but only in more narrow half range

q	$0 < q < 0.5$	$0.5 < q < 0.66$	$0.66 < q < 0.75$	$0.75 < q < 0.8$...	$q \rightarrow 1$
n_{\max}	0	1	2	3	...	$n_{\max} \rightarrow \infty$

Table 1. Some first values of deformation parameter q and n_{\max} largest number.

$0.5 < q < 1$.

With a given value of deformation parameter q , the energy spectrum of deformed harmonic oscillator is well-defined

$$E_q(n) = \hbar\omega \left(n + \frac{1}{2} - \frac{n^2}{2n_{\max}} \right), \tag{19}$$

where $n = 1, 2, 3, \dots, n_{\max}$.

Energy spectrum of deformed harmonic oscillator is well-defined and now has finite unequal-step form. In the fig. 4, four lowest energy levels ($n = 1, 2, 3, 4$) and two higher levels ($n = 10, 20$) of deformed harmonic oscillator depending on deformation parameter q are showed.

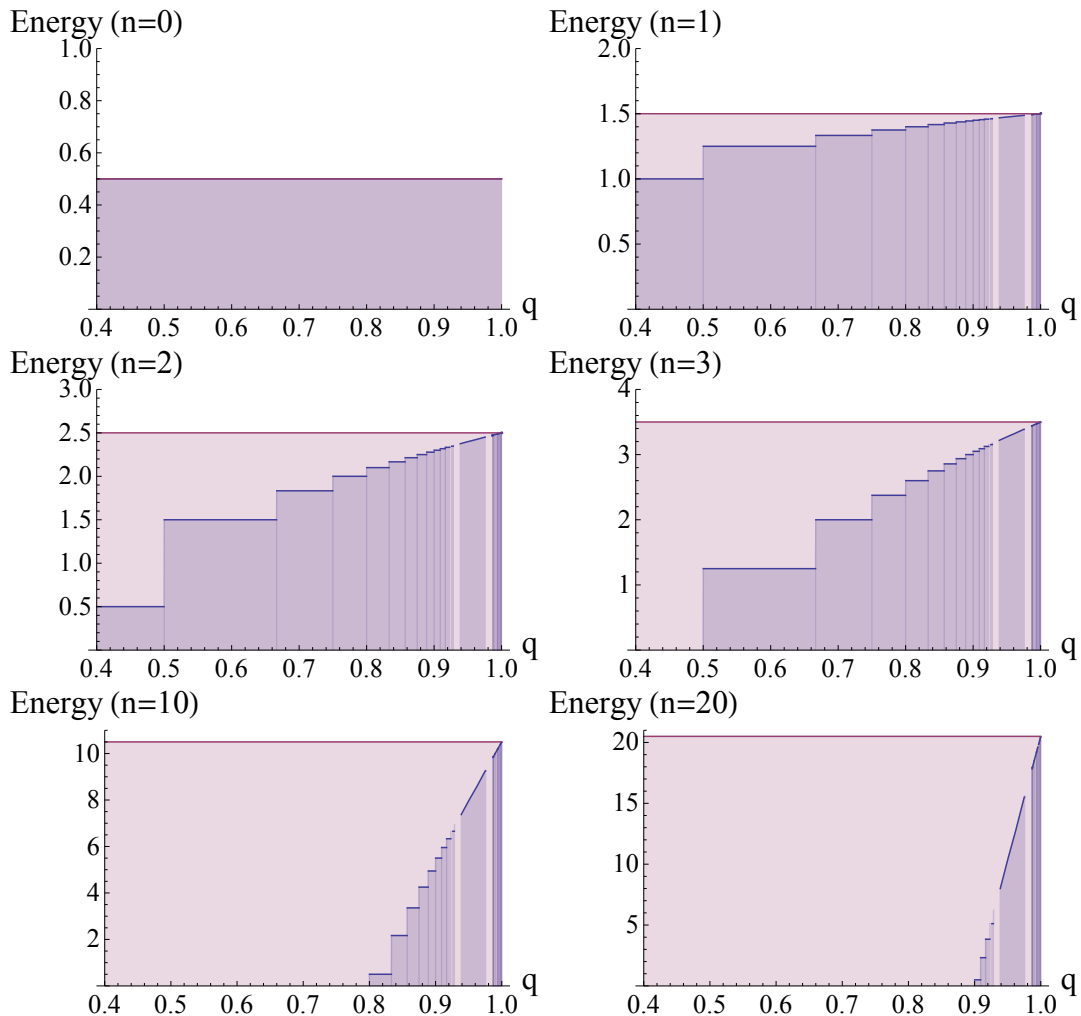


Figure 4. Four lowest energy levels ($n = 1, 2, 3, 4$) and two higher levels ($n = 10, 20$) of deformed harmonic oscillator depending on deformation parameter q .

Higher levels can be occurred when deformation parameter q is very closed to one. The lowest level $n = 1$ occurs if $q = 0.5$, below that point $q < 0.5$ we remain only level $n = 0$ with vacuum oscillation energy $\hbar\omega/2$.

Energy spectrum of deformed harmonic oscillator depends on deformation parameter q and largest number n_{\max} are expressed in the fig. 5. As shown in table 1, begin at $q = 0.5$ we have

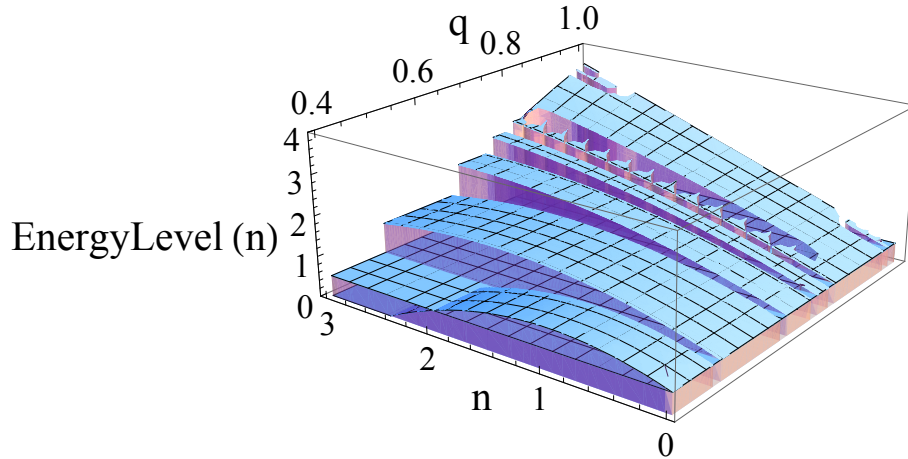


Figure 5. Energy spectrum of q -deformed harmonic oscillator and largest number n_{\max} .

one level, at $q = 0.66$ two levels, at $q = 0.75$ three levels, $q = 0.8$ four levels ... and number of energy levels rapidly grown up when q tends to one. In the weak deformation limit $q \rightarrow 1$, $n_{\max} \rightarrow \infty$ we get back the case of harmonic oscillator with infinite equal-step levels.

7. Deformed partition function

We define the deformed partition function Z_q of deformed harmonic oscillator depending on deformation parameter q as follows

$$Z_q = \sum_{n=0}^{n_{\max}} \exp\left(-\frac{E_q(n)}{k_B T}\right) \quad (20)$$

where k_B is the Boltzmann constant.

With a given value of deformation parameter q , the corresponding values of largest number n_{\max} and energy spectrum $E_q(n)$ of deformed harmonic oscillator are well-defined so deformed partition function Z_q also is well-defined by expression (20).

Using the correspondence between q and n_{\max} , the values of deformed partition function Z_q depend on temperature T for some first low lying levels $n_{\max} = 0, 1, 2, 4, 6$ and one high level $n_{\max} = 30$ are presented in the fig. 6.

If the given value of deformation parameter q in the range $0 < q < 0.5$ then $n_{\max} = 0$, only one level of vacuum oscillation remains and its partition function is a constant with temperature $Z_q = 1$ as in fig. 6. For large values of q closed to one $0 < q < 1$, n_{\max} might have a large value, so we can approximate take the sum analytically. By doing that we found an explicit expression of Z_q , and it rapidly tends to the partition function of harmonic oscillator when $q \rightarrow 1$. For medium q values $0.5 < q < 0.9$, the values of n_{\max} are in the range $1 < n_{\max} < 9$ so the analytical summation is impossible, and we can treat the problem numerically only.

From the deformed partition function Z_q we can derive other related thermodynamic deformed functions such as deformed mean energy, deformed specific heat, the mean number of deformed boson and deformed statistic functions.

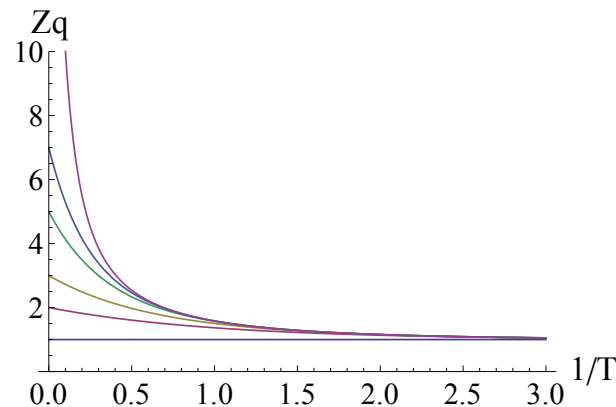


Figure 6. Values of deformed partition function Z_q depend on temperature T for some first low lying levels $n_{\max}=0, 1, 2, 4, 6$ and one high level $n_{\max} = 30$.

8. Discussion

The main results of this work are obtained by using the relation (17). We proposed a new Morse potential for deformation MPD model for investigating properties of q -deformed harmonic oscillator via the Morse potential. The main idea is that the role of parabolic potential for harmonic oscillator can be replaced by the Morse anharmonic potential for q -deformed harmonic oscillator, so that mathematical deform properties can be described and understood in the language of physical anharmonic behaviours.

In our proposed MPD model, q -deformed harmonic oscillator can be described by the corresponding to Morse anharmonic potential. With every given value of deformation parameter q in the interval $q \in [0, 1]$, we can explicitly define the largest number n_{\max} and the deformed energy spectrum $E_n(q)$ of q -deformed harmonic oscillator.

We have also shown that with a given value of deformation parameter q , the deformed partition function Z_q is also well-defined.

Some explicit properties of larges number n_{\max} , deformed energy spectrum $E_q(n)$, and deformed partition function Z_q depending on deformation parameter q are studied for further investigation of other related thermodynamic deformed functions and applications.

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