Energy spectrum inverse problem of q-deformed harmonic oscillator and WBK approximation

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Abstract. Using the connection between q-deformed harmonic oscillator and Morse–like anharmonic potential we investigate the energy spectrum inverse problem. Consider some energy levels of energy spectrum of q–deformed harmonic oscillator are known, we construct the corresponding Morse-like potential then find out the deform parameter q. The application possibility of using the WKB approximation in the energy spectrum inverse problem was discussed for the cases of parabolic potential (harmonic oscillator), Morse–like potential (q–deformed harmonic oscillator). so we consider our deformed–three–levels simple model, where the set–parameters of Morse potential and the corresponding set–parameters of level deformations are easily and explicitly defined. For practical problems, we propose the deformed-three-levels simple model, where the set–parameters of Morse potential and the corresponding set-parameters of level deformations are easily and explicitly defined.

1. Introduction

Recently, quantum group and deformed Heisenberg algebras with q–deformed harmonic oscillator have been a subject of intensive investigation. This approach is found some applications in various branches of physics and chemistry [1–6]. The method of q–deformed quantum mechanics was developed on the base of Heisenberg commutation relation (the Heisenberg algebra). The main parameter of this method is the deformation parameter $q \in [0, 1]$.

The Morse potential has an important role in describing the interaction of atoms in diatomic and even polyatomic molecules [7–10] 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) can be reduced to relative motion between two atomic nuclei in an effective potential which is average Coulomb interaction of nuclei and electron clouds. Morse–like potential models just work with a simple one–dimensional three–parameter effective potential, found many applications in condensed matter, biophysics, 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 Morse potential was considered in [8], where then the anharmonic vibrations in Morse potential have been described as the levels of q–deformed harmonic oscillator. The extended SU(2) model (q-Morse potential) also develop to compare with phenomenological Dunham's expansion and experimental data for numbers of diatomic molecules [8, 9]. In this work, considering deformed algebra is mathematical object and atomic effective potential is 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 the our previous works [11, 12] we have shown that the potential of harmonic oscillator is parabolic with infinity equal–step levels, and 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 was found.

In this work, using the connection between q–deformed harmonic oscillator and Morse–like anharmonic potential we investigate the inverse problem of the energy spectrum. Consider some energy levels of energy spectrum of q–deformed harmonic oscillator are known, we construct the corresponding Morse–like potential then find out the deform parameter q and associate with it the new parameter δ characterized the level deformation. The possibility of using the WKB approximation in the energy spectrum inverse problem was discussed for the cases of parabolic potential (harmonic oscillator) and Morse–like potential (q–deformed harmonic oscillator).

2. Semiclassical Wentzel–Kramers–Brillouin WKB method

2.1. Bohr–Sommerfeld quantization conditions

It is well–known that the Bohr–Sommerfeld quantization conditions are a procedure for selecting out certain discrete set of states of a classical integrable motion as allowed states. These are like the allowed orbits of the Bohr model or standing waves of de Broglie of the atom; the system can only be in one of these states, but not in any states in between.

A particle in a one–dimensional potential can be described by the Schrödinger equation:

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial_x^2}+V(x)\right]\psi\left(x\right)=E\psi\left(x\right), \tag{1}$$

where μ is the particle mass, $\hbar$ is the Planck constant.

The semiclassical Wentzel–Kramers–Brillouin WKB method is based on the ansatz

$$\psi\left(x\right)=A\left(x\right)\exp\left[iS\left(x\right)/\hbar\right]. \tag{2}$$

In the limit as $\hbar\to 0$, the action $S(x)$ in the exponential satisfies the Hamilton–Jacobi equation for the action function

$$E=\frac{1}{2\mu}\left(\frac{dS}{dx}\right)^2+V\left(x\right), \tag{3}$$

we have

$$\begin{aligned} S'\left(x\right) &= \tfrac{dS}{dx} \\ &= \sqrt{2\mu\left[E-V\left(x\right)\right]}. \end{aligned} \tag{4}$$

It is then shown that this usually leads to the Bohr–Sommerfeld quantum conditions on periodic orbits

$$\oint dx\,\sqrt{2\mu\left[E-V(x)\right]}=2\pi\hbar\left(n+\frac{1}{2}\right), \tag{5}$$

with $n=0,\,1,2\,,3\,,\ldots$

For one–dimensional problems, the cyclic integral can be replaced by $2\int_{x_1}^{x_2}$, where x_1 and x_2 are the classical turning points of the motion and $E=V(x)$.

2.2. Application of WKB method to the case of harmonic potential

As an example consider the linear harmonic oscillator with

$$V_0\left(x\right)=\frac{1}{2}Kx^2, \tag{6}$$

where K is the spring constant, and

$$x_{1,2}=\pm\sqrt{2E/K}. \tag{7}$$

The quantum condition reads

$$\int_{-\sqrt{2E/k}}^{+\sqrt{2E/k}}dx\sqrt{2\mu\left(E-Kx^2/2\right)}=2\pi\hbar\left(n+\frac{1}{2}\right), \tag{8}$$

which can be solved to give

$$\begin{aligned}E_{0n}&=\hbar\left(n+\tfrac{1}{2}\right)\sqrt{\tfrac{K}{\mu}}\\&=\hbar\omega_0\left(n+\tfrac{1}{2}\right),\end{aligned} \tag{9}$$

where $\omega_0=\sqrt{K/\mu}$. This is one of a small number of cases in which the WKB method gives the exact quantum–mechanical energies.

2.3. Application WKB method to the case of Morse potential

The semiclassical (WKB) method applied to one–dimensional problems with bound states often reduces to the Sommerfeld–Wilson quantization conditions, the cyclic phase–space integrals

$$\oint dx\,\sqrt{2\mu\left[E-V_M(x)\right]}=2\pi\hbar\left(n+\frac{1}{2}\right). \tag{10}$$

It turns out that this formula gives the exact bound–state energies for the Morse oscillator with

$$V_M(x)=D\left[e^{-2k(x-x_0)}-2e^{-k(x-x_0)}\right], \tag{11}$$

where x_0 is the minimum position, D is the depth and k is the width of potential.

The requisite integral can be reduced to

$$2\int_{x_1}^{x_2}dx\,\sqrt{E-V_M(x)}, \tag{12}$$

in which x_1 and x_2 are the classical turning points

$$x_{1,2} = x_0 + \frac{1}{k} \ln \left[\frac{D}{E} \left(-1 \pm \sqrt{1 + \frac{E}{D}} \right) \right]. \tag{13}$$

The integral can be done "by hand", using the transformation, using the transformation $r = \exp\left[k\left(x - x_0\right)\right]$ followed by a contour integration in the complex plane, but can evaluate the integral explicitly, needing only the additional fact that $\ln\left(-1\right) = i\pi$. The result reads

$$\frac{2\pi\sqrt{2\mu}}{k} \left(\sqrt{D} + \sqrt{-E} \right) = 2\pi\hbar \left(n + \frac{1}{2} \right), \tag{14}$$

which can be rewritten

$$\left(\sqrt{D} + \sqrt{-E} \right) = \frac{\hbar k}{\sqrt{2\mu}} \left(n + \frac{1}{2} \right). \tag{15}$$

The above equation can be solved for E to give

$$-E = \left[-\sqrt{D} + \left(n + \frac{1}{2} \right) \frac{k}{\sqrt{2\mu}} \hbar \right]^2. \tag{16}$$

This result is coincided with exact solution (see text book of Landau–Liftshitz: QM).

Denote the highest bound state is $n_{max} = \left[\sqrt{2\mu D}/\left(\hbar k\right)\right]$ where [...] represents the floor, which for positive numbers is simply the integer part.

We have energy spectrum

$$E_n = D \left[\frac{2}{n_{max}} \left(n + \frac{1}{2} \right) - \frac{1}{n_{max}^2} \left(n + \frac{1}{2} \right)^2 - 1 \right], \tag{17}$$

with $n = 0,\, 1, 2\,, 3\,, ...,\, n_{max}$, or

$$\begin{aligned} E_{Mn} &= E_n - D \\ &= \hbar\omega_M \left[\left(n + \tfrac{1}{2} \right) - \tfrac{1}{2n_{max}} \left(n + \tfrac{1}{2} \right)^2 \right], \end{aligned} \tag{18}$$

where ω_M is the Morse frequency, which equals

$$\begin{aligned} \omega_M &= \tfrac{2D}{\hbar n_{max}} \\ &= k\sqrt{\tfrac{2D}{\mu}}, \end{aligned} \tag{19}$$

The values of D, k, and x_0 of diatomic molecules are taken from experiments.

Actually, the Morse experimental parameters are the dissociation parameter D, the fundamental vibrational frequency ω_M, the equilibrium internuclear distance x_0. and the reduced mass $\mu = m_1 m_2/\left(m_1 + m_2\right)$. The exponential parameter is given by $k = \omega_M\sqrt{\mu/2D}$ in appropriate units $k \simeq 1$. The Schrödinger equation for the Morse oscillator is exactly solvable, giving the vibrational eigenvalues

$$\epsilon_M = \omega_M \left(n + \frac{1}{2} \right) - \frac{\omega_M^2}{4D} \left(n + \frac{1}{2} \right)^2, \tag{20}$$

Unlike the harmonic oscillator, the Morse potential has a finite number of bound vibrational levels with $n_{max} \simeq 2D/\omega_M$.

Compare with the Dunham anharmonic parameter relations in the spectroscopy $\chi_e\omega_M = A = k^2/(2D)$and $\omega_M = 2n_{max}A = k\sqrt{2D/\mu}$ we have

$$\chi_e = \frac{k^2}{2D\omega_M} = \frac{k^2}{4D^2}\hbar n_{max} = k\sqrt{\frac{\mu}{2D}} \tag{21}$$

Introduce the energy differences as

$$\Delta E_{Mn} = \hbar\omega_M \left(E_{Mn} - E_{M(n-1)}\right), \tag{22}$$

and for lowest energy levels

$$\Delta E_{M1} = \hbar\omega_M \left(1 - \frac{1}{n_{max}}\right) \Delta E_{M2} = \hbar\omega_M \left(1 - \frac{2}{n_{max}}\right) \Delta E_{M3} = \hbar\omega_M \left(1 - \frac{3}{n_{max}}\right) ... \tag{23}$$

According to our Morse Potential for Deformation model (MPD model) [12], we can define a new deformation parameter q_M, which is satisfied the equation

$$\frac{1}{2n_{max}} = 1 - q_M, \tag{24}$$

we have

$$\Delta E_{M1} = \hbar\omega_M q_M, \, \Delta E_{M2} = \hbar\omega_M \left(2q_M - 1\right), \, \Delta E_{M3} = \hbar\omega_M \left(3q_M - 2\right) ... \tag{25}$$

From the two first equations we obtain the deformation parameter q_M

$$q_M = \frac{1}{2 - \frac{\Delta E_{M2}}{\Delta E_{M1}}}, \tag{26}$$

and the Morse frequency

$$\omega_M = \frac{1}{\hbar}\left(2\Delta E_{M1} - \Delta E_{M2}\right). \tag{27}$$

3. Harmonic approximation for Morse oscillator

In this part we find the harmonic approximation for Morse oscillator.

From definition of Morse potential easy to see that

$$\frac{dV_M(x)}{dx} = V_M^{(1)}(x) = D\left[-2ke^{-2k(x-x_0)} - 2ke^{-k(x-x_0)}\right], \tag{28}$$

and

$$\frac{d^2V_M(x)}{dx^2} = V_M^{(2)}(x) = D\left[4k^2e^{-2k(x-x_0)} - 2k^2e^{-k(x-x_0)}\right], \tag{29}$$

so

$$V_M(x_0) = -D, \, V_M^{(1)}(x_0) = 0, \, V_M^2(x_0) = 2Dk^2. \tag{30}$$

Using the Taylor series expansion around $x = x_0$, we found harmonic approximation potential for Morse oscillator

$$V_H(x) \simeq V_M(x_0) + V_M^{(1)}(x_0)(x - x_0) + \frac{1}{2}V_M^{(2)}(x_0)(x - x_0)^2 = -D + Dk^2(x - x_0)^2, \quad (31)$$

with the spring constant $K'/2 = Dk^2$and corresponding harmonic frequency $\omega_H = \sqrt{K'/\mu} = k\sqrt{2D/\mu}$. We have the relation

$$\omega_i = k_i\sqrt{2D_i/\mu}, \quad (32)$$

where $i = M, H, 0$.

4. Inverse problem of deformed harmonic oscillator

Suppose that the 3 first energy levels E_0, E_1, E_2 are known, so we have two energy separations Δ_2 and Δ_2

$$\Delta_1 = E_1 - E_0,\ \Delta_2 = E_2 - E_1. \quad (33)$$

Define the deformation parameter q

$$q = \frac{1}{2 - \frac{\Delta_2}{\Delta_1}}, \quad (34)$$

the oscillation frequency ω_q

$$\omega_q = \frac{1}{\hbar}(2\Delta_1 - \Delta_2), \quad (35)$$

The highest bound state N_q is

$$N_q = [1/2(1 - q)] = \left[\frac{(2 - \Delta_2/\Delta_1)}{2(1 - \Delta_2/\Delta_1)}\right], \quad (36)$$

where [...] represents the integer part.

If $\Delta_2 < \Delta_1$, then $0 < q < 1$, $N_q = /2(1 - q)$, we have the case of deformed harmonic oscillator with finite unequal-step levels, which can be characterized by a Morse-like potential

$$V_{Mq}(x) = D_q\left[e^{-2k_q(x-x_0)} - 2e^{-k_q(x-x_0)}\right]. \quad (37)$$

with the energy deep D_q

$$D_q = \frac{\hbar\omega_q}{(1 - q)} = \frac{(2\Delta_1 - \Delta_2)^2}{(\Delta_1 - \Delta_2)}, \quad (38)$$

The exponential parameter k_q

$$k_q = \omega_q\sqrt{\frac{\mu}{2D_q}} = \sqrt{1 - q}\sqrt{\frac{\omega_q\mu}{2\hbar}} = \frac{1}{\hbar}\sqrt{\frac{\mu}{2}(\Delta_1 - \Delta_2)}. \quad (39)$$

The corresponding parabolic potential $V_{Hq}(x)$ with the oscillation frequency $\omega_q = \frac{1}{\hbar}(2\Delta_1 - \Delta_2) = k_q\sqrt{2D_q/\mu}$ is

$$V_{Hq}(x) = -D_q + \frac{K_q}{2}(x - x_0)^2 = -D_q + \frac{1}{2}\mu\omega_q^2(x - x_0)^2. \quad (40)$$

If the separations are equal $\Delta_2 = \Delta_1$, then $q = 1$, $N = \infty$, we have the case of harmonic oscillator with infinite equal-step levels, which can be characterized by a parabolic potential $V_{H1}(x)$ with the oscillation frequency $\omega_1 = k_1\sqrt{2D_1/\mu}$

$$V_{H1}(x) = -D + \frac{1}{2}\mu\omega_1^2(x - x_0)^2. \quad (41)$$

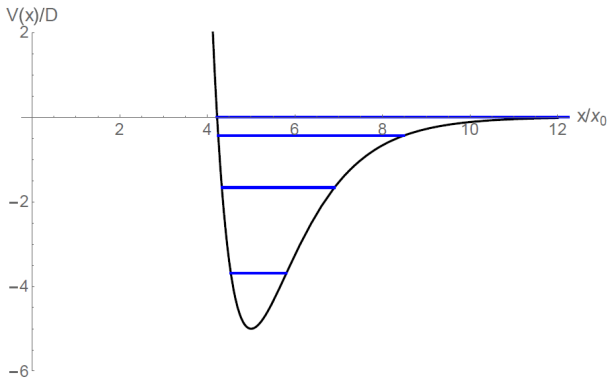

Figure 1. Morse potential

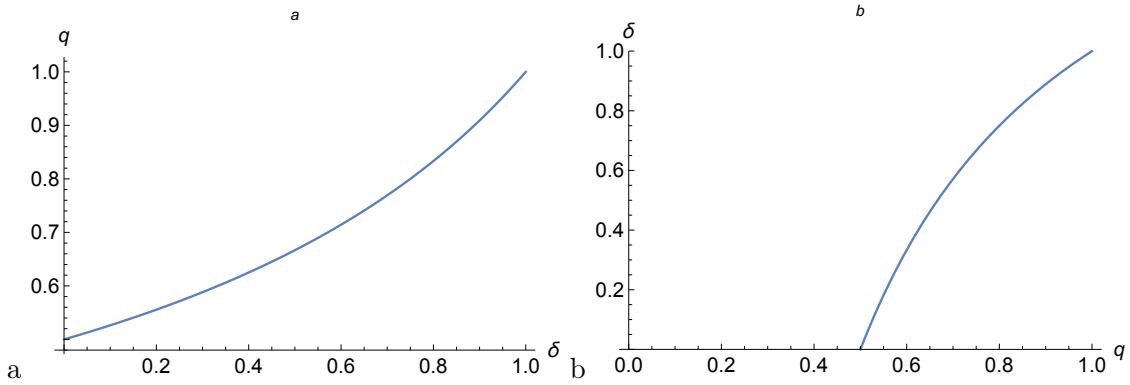

Figure 2. The relation between q and δ: a) q on δ, and b) δ on q.

5. Model example

Consider the first three energy levels E_0, E_1, $E_2$are known, we define two parameters $\Delta_1 = E_1 - E_0$, and $\Delta_2 = E_2 - E_1$. Introduce the ratio parameter δ as the main parameter of our model

$$\delta = \Delta E_2/\Delta E_1 = \Delta\varepsilon_2/\Delta\varepsilon_1. \tag{42}$$

For the case of Morse oscillator $0 < \delta < 1$, example three levels Morse oscillator is presented in the figure 1. For the case of harmonic potential $\delta = 1$.

Taking also two values r_0 and $k_0 = (1/\hbar)\sqrt{\Delta_1\mu/2}$ are the equilibrium distance and imaginary impulse of anharmonic Morse oscillator (with q=1 is harmonic case), we will express all physical values via the energy difference $\{\Delta_1, \delta\}$or deformation$\{\Delta_1, q\}$set parameters.

We have the deformation parameter q

$$q = \frac{1}{2-\delta} \longleftrightarrow \delta = 2 - \frac{1}{q}, \tag{43}$$

the relation between q and δ are presented in the Fig. 2a and 2b

The value n_{max} is

$$N = n_{max} = \left[\frac{(2-\delta)}{2\,(1-\delta)}\right] = \left[\frac{1}{2\,(1-q)}\right], \tag{44}$$

where [...]is the integer part, and are presented in the figure 3 as a functions on δ (upper steps), and on q (lower steps).

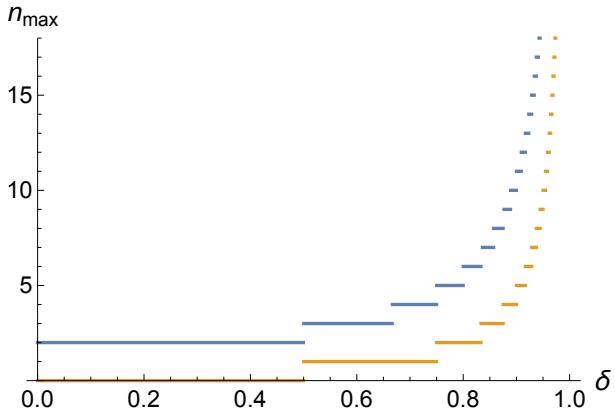

Figure 3. The relation value n_{max} on δ (upper steps), and on q (lower steps).

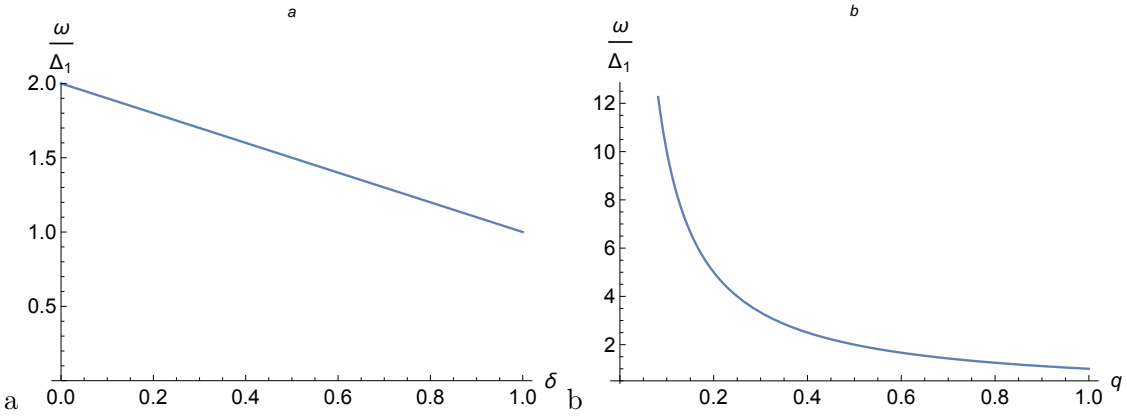

Figure 4. The frequency ω/Δ_1 : a) on δ, and b) on q.

The frequency

$$\frac{\omega}{\Delta_1} = 2 - \delta = \frac{1}{q}, \tag{45}$$

and its values are presented in the figure 4 as a functions of (blue), and on q (yellow).
The energy deep D_q

$$\frac{D_q}{\Delta_1} = \frac{(2-\delta)^2}{(1-\delta)} = \frac{1}{q}\left[\frac{1}{(1-q)}\right], \tag{46}$$

are ploted in the figure 5.
The imaginary momentum-like width (effective mass) k_q

$$\frac{k_q}{k_0} = \sqrt{1-\delta} = \sqrt{\frac{1}{q} - 1}, \tag{47}$$

are presented in the figure 6.
We found the Morse-like potential

$$U_M(\chi) = \frac{V_M}{\hbar\omega_0} = \frac{(2-\delta)^2}{(1-\delta)}\left[e^{-2a(\chi-1)\sqrt{1-\delta}.} - 2e^{-a(\chi-1)\sqrt{1-\delta}}\right], \tag{48}$$

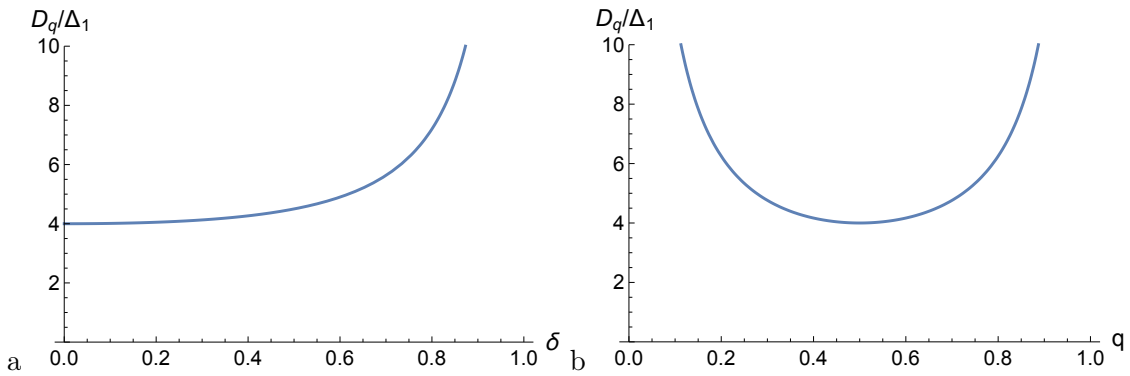

Figure 5. The energy deep of Morse potential D_q/Δ_1: a) on δ, and b) on q.

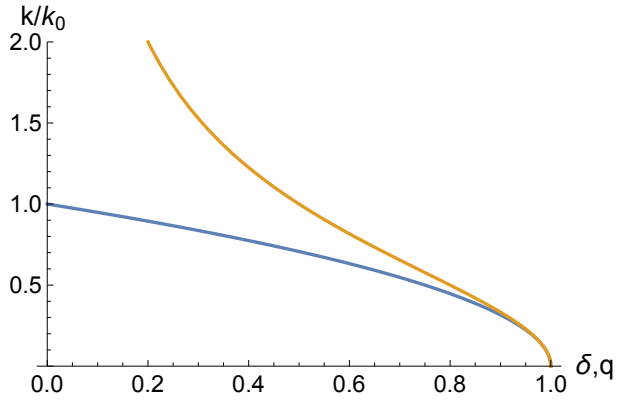

Figure 6. The parameter k_q of Morse potential on δ (upper curve), and on q (lower curve).

where $\chi = x/x_0$, $a = k_0 x_0$, and the corresponding harmonic potential

$$U_H(\chi) = \frac{V_H}{\hbar\omega_0} = -\frac{(2-\delta)^2}{(1-\delta)} + \frac{1}{2}(2-\delta)^2 \mu x_0^2 (\chi - 1)^2 . \tag{49}$$

The Morse potential U_M and the corresponding harmonic potential U_H are presented in the figure 7.

The energy spectrum of Morse potential is

$$\varepsilon_n = \frac{E_n}{\triangle_1} = (2-\delta)\left[\left(n+\frac{1}{2}\right) - \frac{1}{2n_{max}}\left(n+\frac{1}{2}\right)^2\right],\ n = 0,\ 1, 2, 3, ...,\ n_{max}, \tag{50}$$

with first four levels

$$\begin{aligned}
\varepsilon_0 &= (2-\delta)\left(\frac{1}{2} - \frac{1}{8n_{max}}\right), \\
\varepsilon_1 &= (2-\delta)\left(\frac{3}{2} - \frac{9}{8n_{max}}\right), \\
\varepsilon_2 &= (2-\delta)\left(\frac{5}{2} - \frac{25}{8n_{max}}\right), \\
\varepsilon_3 &= (2-\delta)\left(\frac{7}{2} - \frac{49}{8n_{max}}\right),
\end{aligned} \tag{51}$$

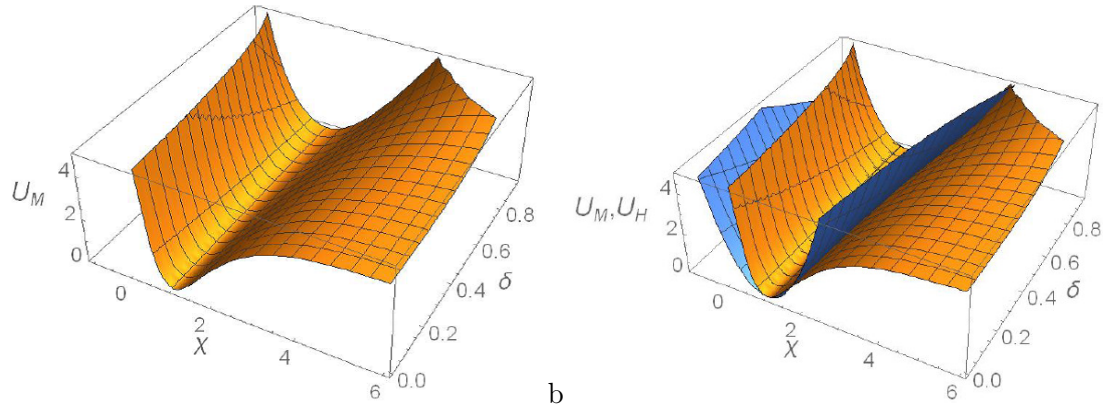

Figure 7. a) The Morse potential U_M and b) with the corresponding harmonic potential U_H

The level difference $\Delta\varepsilon_n$ are

$$\Delta\varepsilon_n = \varepsilon_{n+1} - \varepsilon_n, \tag{52}$$

and for some lowest levels

$$\Delta\varepsilon_1 = (2-\delta)\left(1 - \frac{1}{n_{max}}\right), \Delta\varepsilon_2 = (2-\delta)\left(1 - \frac{2}{n_{max}}\right), \Delta\varepsilon_3 = (2-\delta)\left(1 - \frac{3}{n_{max}}\right) ... \tag{53}$$

In the harmonic limit $\delta \to 1$,$q \to 1$, $n_{max} \to \infty$, we have $\varepsilon_0 \to 1/2$,$\varepsilon_1 \to 3/2$,$\varepsilon_2 \to 5/2$, ... and $\Delta\varepsilon_1 \to 1$,$\Delta\varepsilon_2 \to 1$,$\Delta\varepsilon_3 \to 1$, ...

In the strong deformation limit $\delta \to 0$, $q \to 1/2$, $n_{max} \to 1$ (see the figure 3), we remain only two levels $\varepsilon_0 \to 2\,(1/2 - 1/16) = 0.875$, $\varepsilon_1 \to 2\,(3/2 - 9/16) = 1.875$, and $\Delta\varepsilon_1 \to 1$, $\Delta\varepsilon_2 \to 0$.

In general, for Morse like potential in WKB approximation the classical turning points are defined by the expression

$$\chi_{1,2}\,(n) = 1 + \frac{1}{k_0 x_0} Ln\left[\frac{D}{E\,(n)}\left(-1 \pm \sqrt{1 + \frac{E\,(n)}{D}}\right)\right]. \tag{54}$$

Given energy spectra $E\,(n)$, we define $\chi_{1,2}\,(n)$, so and Morse–like potential.

6. Discussion

In this work using the model proposed in [12] with the defined connection between q-deformed harmonic oscillator and Morse–like anharmonic potential, we investigate the energy spectrum inverse problem. Consider some lowest levels of energy spectrum of q-deformed harmonic oscillator are known, we construct the corresponding Morse-like potential with well defined deform parameter q and also new level deformation parameter δ. The possibility of using the WKB approximation in the energy spectrum inverse problem was discussed for both cases of parabolic potential (harmonic oscillator) and Morse-like potential (q-deformed harmonic oscillator).

Some most important relations between the set-parameters $\{\Delta_1, \delta, q\}$ of level deformations and set-parameters $\{D, k, x_0\}$ of Morse potential are derived explicitly. In the week-deform limit $\delta \to 1$,$q \to 1$; $n_{max} \to \infty$, we back to the harmonic case with many unique step levels. In the strong-deform limit $\delta \to 0$, $q \to 1/2$; $n_{max} \to 1$, we go to the two-levels problem, where only the ground $(n = 0)$ and first $(n = 1)$ levels can be existed and the other $(n \geq 2)$ levels are collapsed.

In principal, with a given energy spectra $E(n)$ we can define the classical turning points $\chi_{1,2}(n)$ and then construct the effective potential by using the WKB approximation, but it is a inverse-like problem and usually difficult to solve. In practical, because for many problems of atom and molecular physics, quantum optics, condensed matter, ... only the ground and one or two first excited levels are considered, so we propose to use our deformed-three-levels simple model, where the set-parameters of Morse potential and the corresponding set-parameters of level deformations are easily and explicitly defined.

Our level deformation model might be useful in investigation the problem of entanglement entropy, when the environment or vacuum effects are taken in to account. This will be studied in the our next work.

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