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q-Anharmonic oscillator with quartic interaction

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Abstract. The first order perturbative correction to the energy levels of a boson realization of a q-oscillator due to a quartic term in the potential energy is evaluated. We also discuss the statistical mechanics of q-anharmonic oscillators in the case where the parameter q deviates slightly from unity.

Keywords. Quantum groups; q-oscillators; boson realization; statistical mechanics q.

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1. Introduction

During the recent years quantum groups and quantum algebras have attracted considerable attention among both physicists and mathematicians (see for example Jimbo 1989; Majid 1990). Though a large number of work based on the mathematical aspects of quantum algebras have appeared, direct applications of quantum or q-symmetry to real physical systems are limited. Quantum groups and non-commutative geometry are of relevance to the problem of quantisation of space-time (Ya. Aref'eva and Volovich 1991). It has been argued that physics at the Planck scale may be understood only with the help of noncommutative geometry (Folkert-Muller-Hoissen 1991; Ya. Aref'eva 1991).

The quantum algebras can be viewed as deformations of classical Lie algebras (Drinfeld 1985; Jimbo 1986). They have also been linked to geometries that have non-commutative structures (Wess and Zumino 1990; Zumino 1991). The representation theory of the quantum algebras with a single deformation parameter q has led to the development of q-deformed oscillator algebra (Biedenharn 1989; Macfarlane 1989). The q-oscillators may lead to a new kind of field theory wherein small violations of the Pauli exclusion principle may occur (Greenberg 1991). Recently various implications of q-deformed algebraic structures in some concrete physical models such as squeezed states in quantum optics (Chaichian *et al* 1990; Celeghini *et al* 1991) and molecular vibrations (Chang and Yan 1991a,b,c) have been investigated.

As mentioned above, the q-deformation of harmonic oscillator algebra is a well studied topic, but we know that in real physical systems one cannot dismiss the role of anharmonicity. Here we consider the problem of q-deformations of an anharmonic oscillator in first order perturbation theory and evaluate the correction to energy. The statistical mechanics of q-deformed anharmonic oscillators is also discussed.

2. q-Harmonic oscillator

In order to establish the notation, we summarize here the formulation of q-harmonic oscillator theory (Biedenharn 1989; Macfarlane 1989). The Hamiltonian of a harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 \tag{1}$$

In terms of the creation and annihilation operators a and a^+, (1) reads

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

If a and a^+ satisfy the commutation relation

$$[a, a^+] = 1 \tag{3}$$

and

$$N = a^+ a; \tag{4}$$

then H can be put as

$$H = \hbar\omega(N + \tfrac{1}{2}). \tag{5}$$

The operator N is the number operator. This theory describes what is sometimes called a boson harmonic oscillator (BHO).

The concept of q-deformation can be brought in by introducing the q-creation operator $\bar{a}^+$ and the q-annihilation operator $\bar{a}$ such that they satisfy the following q-commutation relation:

$$[\bar{a}, \bar{a}^+]_q \equiv \bar{a}\bar{a}^+ - q\bar{a}^+ \bar{a} = q^{-\bar{N}} \tag{6}$$

where the number operator $\bar{N}$ is required to satisfy

$$[\bar{a}, \bar{N}] = \bar{a},$$
$$[\bar{a}^+, \bar{N}] = -\bar{a}^+. \tag{7}$$

In this representation, $\bar{N} \neq \bar{a}^+ \bar{a}$. The action of $\bar{a}$ and $\bar{a}^+$ on the Hilbert space with the basis $\{|\bar{n}\rangle\}$, $(\bar{n} = 0, 1, 2, \ldots)$, is described as follows:

$$\bar{a}|\bar{O}\rangle = 0, \quad |\bar{n}\rangle = \frac{(\bar{a}^+)^n |O\rangle}{\sqrt{[\bar{n}]!}},$$
$$\bar{a}^+|\bar{n}\rangle = \sqrt{[\bar{n}+1]}\,|\bar{n}+1\rangle,$$
$$\bar{a}|\bar{n}\rangle = \sqrt{[\bar{n}]}\,|\bar{n}-1\rangle,$$
$$\bar{N}|\bar{n}\rangle = [\bar{n}]|\bar{n}\rangle,$$

where

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}} \tag{8}$$

where $q \in [0,1]$ or is a pure phase.

It is readily seen that as $q \to 1$, these relations coincide with those of the boson oscillator algebra.

The q-analogue harmonic oscillator Hamiltonian (Biedenharn 1989) is

$$\bar{H} = \frac{\bar{p}^2}{2m} + \frac{1}{2} m\omega^2 \bar{q}^2. \tag{9}$$

Defining the two operators $\bar{a}$ and $\bar{a}^+$ as in the case of the BHO

$$\begin{aligned} \bar{p} &= i\sqrt{\left(\frac{m\hbar\omega}{2}\right)}(\bar{a} - \bar{a}^+), \\ \bar{q} &= \sqrt{\left(\frac{\hbar}{2m\omega}\right)}(\bar{a} + \bar{a}^+), \end{aligned} \tag{10}$$

the Hamiltonian $\bar{H}$ can be rewritten as

$$\bar{H} = \frac{\hbar\omega}{2}(\bar{a}\bar{a}^+ + \bar{a}^+\bar{a}). \tag{11}$$

The Hamiltonian $\bar{H}$ is diagonal in the eigenstates $|\bar{n}\rangle$ and the eigenvalue equation reads

$$\begin{aligned} \bar{H}|\bar{n}\rangle &= \frac{\hbar\omega}{2}(\bar{a}\bar{a}^+ + \bar{a}^+\bar{a})|\bar{n}\rangle \\ &= \frac{\hbar\omega}{2}([\bar{n}+1] + [\bar{n}])|\bar{n}\rangle. \end{aligned} \tag{12}$$

This implies that the Hamiltonian $\bar{H}$ can be put as

$$\bar{H} = \frac{\hbar\omega}{2}([\bar{N}+1] + [\bar{N}]) \tag{13}$$

The eigenvalues and eigenstates of $\bar{H}$ are q-dependent. Let us look for a situation in which the eigenstates of $\bar{H}$ are q-independent (Polychronakos 1990), i.e. $|\bar{n}\rangle = |n\rangle$ where $|n\rangle$ are the eigenstates of the BHO Hamiltonian and in this situation $\bar{N} = N$. The corresponding creation and annihilation operators are related to those of the BHO by

$$\begin{aligned} \bar{a}^+ &= a^+\sqrt{\left(\frac{[N+1]}{N+1}\right)}, \\ a &= a\sqrt{\left(\frac{[N]}{N}\right)}. \end{aligned} \tag{14}$$

This scheme is usually known as the boson realization of the q-algebra and the eigenvalue equation (12) becomes

$$\bar{H}|n\rangle = \frac{\hbar\omega}{2}([N+1] + [N])|n\rangle. \tag{15}$$

3. *q*-Anharmonic oscillator

With the preliminaries introduced in the preceding section, we take up the q-analogue anharmonic oscillator described by the Hamiltonian

$$\bar{H}_{\mathrm{AH}} = \frac{\bar{p}^2}{2m} + \frac{1}{2}m\omega^2\bar{q}^2 + \frac{\lambda}{4!}\bar{q}^4. \tag{16}$$

In the boson realization, the Hamiltonian becomes

$$\begin{aligned}\bar{H}_{\mathrm{AH}} = {} & \frac{\hbar\omega}{2}([N+1]+[N]) + \frac{\lambda}{4!}\left(\frac{\hbar}{2m\omega}\right)^2\{[N+2][N+1] \\ & + [N+1][N+1] + 2[N+1][N] + [N][N] \\ & + [N][N-1]\} + \ldots \end{aligned} \tag{17}$$

where we have indicated by dots those terms that do not contribute to $\langle n|\bar{H}_{\mathrm{AH}}|n\rangle$.

When $q \to 1$, $\bar{H}_{\mathrm{AH}}$ becomes the Hamiltonian of the ordinary anharmonic oscillator (Parisi 1988). If we introduce a parameter η such that $\eta = \log q$ where η is purely real or imaginary, then (17) can be put as

$$\begin{aligned}\bar{H}_{\mathrm{AH}} = {} & \frac{\hbar\omega}{2}\left(\frac{\sinh(N\eta) + \sinh(N+1)\eta}{\sinh(\eta)}\right) \\ & + \frac{\lambda}{4!}\left(\frac{\hbar}{2m\omega}\right)^2 \frac{1}{(\sinh\eta)^2}\{\sinh(N+2)\eta\sinh(N+1)\eta \\ & + \sinh(N+1)\eta\sinh(N+1)\eta + 2\sinh(N+1)\eta\sinh(N\eta) \\ & + \sinh(N\eta)\sinh(N\eta) + \sinh(N\eta)\sinh(N-1)\eta\} + \ldots \end{aligned} \tag{18}$$

When $q \to 1$, i.e. $\eta \to 0$, we can regain the usual result, and therefore we will consider the case of η being very small. For sufficiently small values of η, (18) can be further simplified as

$$\begin{aligned}\bar{H}_{\mathrm{AH}} \approx {} & \frac{\hbar\omega}{2}(2N+1) + \frac{\eta^2}{3!}\frac{\hbar\omega}{2}((N+1)^3 + N^3 - (2N+1)) \\ & + \frac{\lambda}{4!}\left(\frac{\hbar}{2m\omega}\right)^2(6N^2+6N+3) + \frac{\eta^2}{3!}\frac{\lambda}{4!}\left(\frac{\hbar}{2m\omega}\right)^2(10N^4 + 24N^3 \\ & + 52N^2 + 38N + 16) + \ldots \end{aligned} \tag{19}$$

$$= H_0 + \frac{\eta^2}{3!}H_1 + H' + \frac{\eta^2}{3!}H'' + \ldots$$

Again one can see that as $q \to 1$, $\bar{H}_{\mathrm{AH}}$ is reduced to the Hamiltonian of the boson anharmonic oscillator (Parisi 1988). The quartic anharmonic corrections (to first order in λ) to the energy levels of the boson realization of the q-oscillator follow at once by calculating $\langle n|\bar{H}_{\mathrm{AH}}|n\rangle$ where $|n\rangle$'s are the unperturbed eigenstates.

4. Statistical mechanics of q-anharmonic oscillators

Very recently, Neskovic and Urosevic (1991) have studied the statistical mechanics of q-deformed harmonic oscillators. We will discuss below, the statistical mechanics of q-deformed anharmonic oscillators. The quantity which is of prime importance in the study of thermodynamics of systems is the partition function

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta H} \tag{20}$$

where $\beta = 1/kT$ and H is the Hamiltonian of the system. In the case of an assembly of q-anharmonic oscillators. H is given by (19). We consider a boson realization in which the $|n\rangle$ are the eigenstates of H_0 – the Hamiltonian of the unperturbed harmonic oscillator. η and λ will be assumed to be very small. Hence in this perturbative approach in partition function for the q-deformed anharmonic oscillators is expressed in the form

$$\begin{aligned} Z &= \sum_n \langle n|\mathrm{e}^{-\beta \bar{H}_{AH}}|n\rangle, \\ &\approx \sum_n \left\langle n \middle| \mathrm{e}^{-\beta H_0}\left(1 - \beta\left(\frac{\eta^2}{3!}H_1 + H'\right)\right) \middle| n \right\rangle, \\ &= Z_0\left(1 - \beta\left(\frac{\eta^2}{3!}\langle H_1\rangle + \langle H'\rangle\right)\right), \end{aligned} \tag{21}$$

where $Z_0 = \Sigma_n \langle n|\mathrm{e}^{-\beta H_0}|n\rangle$ and $\langle H_1\rangle$ and $\langle H'\rangle$ are the thermal averages of H_1 and H' respectively:

$$\begin{aligned} \langle H_1\rangle &= \frac{\sum_n \langle n|H_1\,\mathrm{e}^{-\beta H_0}|n\rangle}{\sum_n \langle n|\mathrm{e}^{-\beta H_0}|n\rangle}, \\ &= \frac{\hbar\omega}{2}\, \frac{\sum_n (n^3 + (n+1)^3 - (2n+1))\,\mathrm{e}^{-\beta\hbar\omega(n+1/2)}}{\sum_n \mathrm{e}^{-\beta\hbar\omega(n+1/2)}}, \\ &= -\frac{\hbar\omega}{2} - \frac{\hbar\omega}{\mathrm{e}^{\beta\hbar\omega} - 1} + \hbar\omega\,(\sin\mathrm{h}(\beta\hbar\omega) g(\beta\hbar\omega)), \end{aligned} \tag{22}$$

where

$$g(\beta\hbar\omega) = \frac{\mathrm{e}^{3\beta\hbar\omega} + 4\,\mathrm{e}^{2\beta\hbar\omega} + \mathrm{e}^{\beta\hbar\omega}}{(\mathrm{e}^{\beta\hbar\omega} - 1)^4}$$

$$\langle H'\rangle = \frac{\sum_n \langle n|H'\mathrm{e}^{-\beta H_0}|n\rangle}{\sum_n \langle n|\mathrm{e}^{-\beta H_0}|n\rangle}$$

$$= \frac{\lambda \hbar^2}{32 m^2 \omega^2} \frac{\sum_{n=0}^{\infty} [(2(n+1)^2 - 2n - 1) e^{-\beta\hbar\omega(n+1/2)}]}{\sum_{n=0}^{\infty} e^{-\beta\hbar\omega}(n+1/2)}$$

$$= \frac{\lambda \hbar^2}{32 m^2 \omega^2} \left(\coth\left(\frac{\beta\hbar\omega}{2} \right) \right)^2. \tag{23}$$

Thus we find the partition function of the q-deformed anharmonic oscillators as

$$Z \approx Z_0 \left(1 - \frac{\eta^2}{3!} \beta \left(\frac{-\hbar\omega}{2} - \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} + \hbar\omega \sinh(\beta\hbar\omega) g(\beta\hbar\omega) \right) \right.$$
$$\left. \frac{-\beta\lambda\hbar^2}{32 m^2 \omega^2} \left(\coth\left(\frac{\beta\hbar\omega}{2} \right) \right)^2 \right). \tag{24}$$

In the limit $q \to 1$, the expression for Z thus turns out to be the same as that of a boson anharmonic oscillator (Parisi 1988).

A knowledge of the partition function enables one to evaluate other thermodynamic quantities such as the grand canonical potential Ω, the internal energy U and the entropy S which are defined by the following relations (Feynman 1972)

$$e^{-\beta\Omega} = Z, \quad S = \beta^2 \left(\frac{\partial \Omega}{\partial \beta} \right), \quad U = \frac{S}{\beta} + \Omega. \tag{25}$$

The partition function given by (24) will be rewritten as

$$Z \approx Z_0 \left(1 + \frac{\eta^2}{3!} \beta U_1 + \frac{\lambda\beta}{4!} U_2 \right),$$

where

$$U_1 = U_0 - \hbar\omega \sinh(\beta\hbar\omega) g(\beta\hbar\omega),$$

$$U_0 = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1},$$

$$U_2 = -\frac{3\hbar^2}{4 m^2 \omega^2} \left(\coth\left(\frac{\beta\hbar\omega}{2} \right) \right)^2,$$

The grand canonical potential Ω is then

$$\Omega = \Omega_0 - \frac{\eta^2}{3!} U_1 - \frac{\lambda}{4!} U_2 \tag{26}$$

where

$$\Omega_0 = -\frac{1}{\beta} \log Z_0.$$

The entropy S of the system is

$$S = S_0 - \frac{\eta^2}{3!} \beta^2 \frac{\partial U_1}{\partial \beta} - \frac{\lambda}{4!} \beta^2 \frac{\partial U_2}{\partial \beta} \tag{27}$$

where

$$S_0 = \beta^2 \frac{\partial \Omega_0}{\partial \beta},$$

$$\frac{\partial U_1}{\partial \beta} = \frac{(\hbar\omega)^2}{2} 3! \left(\frac{e^{4\beta\hbar\omega} + 3e^{3\beta\hbar\omega} - 3e^{2\beta\hbar\omega} - e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^5} \right)$$

$$\frac{\partial U_2}{\partial \beta} = \frac{3\hbar^3}{4m^2\omega} \coth\frac{(\beta\hbar\omega)}{2} \left(\operatorname{cosech}\left(\frac{\beta\hbar\omega}{2}\right)\right)^2.$$

The internal energy U of the system is given by

$$U = U_0 - \frac{\eta^2}{3!}\left(U_1 + \beta\frac{\partial U_1}{\partial \beta}\right) - \frac{\lambda}{4!}\left(U + \beta\frac{\partial U_2}{\partial \beta}\right). \tag{28}$$

5. Concluding remarks

We have investigated the energy spectrum of a q-quartic anharmonic oscillator using first order perturbation theory and a boson realization of the unperturbed q-oscillator eigenstates. The evaluation of the partition function and various thermodynamic quantities carried out in this paper is expected to be of relevance to investigations of anharmonic effects in q-deformed versions of molecular and condensed matter systems. It has been argued that the q-deformation of the harmonic oscillator can absorb the anharmonicity effects in molecular vibrational spectra (Bonatsos *et al* 1991; Chang and Yan 1991a,b,c). The effect of anharmonicity is well studied both in classical and quantum physics. In the present work we have studied the q-version of the anharmonic oscillator, but the relevance of such a study will be clear only when it is applied to some real physical systems. A possible scenario where anharmonicity considerations might be applicable is lattice dynamics. This aspect is currently under investigation.

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