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q-Anharmonic oscillator with quartic interaction

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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

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1. Introduction

During the very 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 works 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 (Zhe Chang and Hong Yan 1991a,1991b,1991c) 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 summarise here the formulation of the theory of the q-harmonic oscillator (Biedenharn 1989, Macfarlane 1989). The Hamiltonian of a harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 \qquad (1)$$

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

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

If a and a^+ satisfy the commutation relation

$$[a,a^+] = 1 \qquad (3)$$

and

$$N = a^+a \; ; \qquad (4)$$

then H can be put as

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

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:

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

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

$$[\bar{a}, \bar{N}] = \bar{a}$$
$$[\bar{a}^+ ,N] = -\bar{a}^+ \qquad (7)$$

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,...), is described as follows:

$$\bar{a}|\bar{0}\rangle = 0, \qquad |\bar{n}\rangle = \frac{(\bar{a}^{+})^{n}|0\rangle}{\sqrt{[\bar{n}]!}}$$

$$\bar{a}^{+}|\bar{n}\rangle = \sqrt{[\bar{n}+1]}\ |\bar{n}+1\rangle$$

$$\bar{a}\ |\bar{n}\rangle = \sqrt{[\bar{n}]}\ |\bar{n}-1\rangle$$

$$\bar{N}\ |\bar{n}\rangle = [\bar{n}]\ |\ \bar{n}\ \rangle$$

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:

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

$$\bar{q} = \sqrt{\left(\frac{\hbar}{2m\omega}\right)}\ (\bar{a} + \bar{a}^{+})$$

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

$$\bar{H}\ |\bar{n}\ \rangle = \frac{\hbar\omega}{2}(\bar{a}\ \bar{a}^{+} + \bar{a}^{+}\bar{a})|\bar{n}\rangle$$

$$= \frac{\hbar\omega}{2}([\bar{n} + 1] + [\bar{n}])\ |\ \bar{n}\ \rangle \tag{12}$$

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), ie $|\bar{n}\rangle = |n\rangle$ 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

$$\bar{a}^{+} = a^{+}\sqrt{\left(\frac{[N+1]}{N+1}\right)}$$

$$a = a\sqrt{\left(\frac{[N]}{N}\right)} \tag{14}$$

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

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

In the boson realization, the Hamiltonian becomes

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

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

When $q \to 1$, $\bar{H}_{AH}$ 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

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

When $q \to 1$, ie $\eta \to o$, 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

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

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

Again one can see that as $q \to 1$, $\bar{H}_{AH}$ 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 $\langle n|\bar{H}_{AH}|n\rangle$ 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:

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

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

$$Z = \sum_n \langle n| e^{-\beta \bar{H}} |n\rangle$$

$$\approx \sum_n \langle n| e^{-\beta H_o}(1-\beta(\frac{\eta^2}{3!} H_1 + H')|n\rangle$$

$$= Z_o(1-\beta(\frac{\eta^2}{3!}\langle H_1\rangle + \langle H'\rangle)) \qquad (21)$$

where $Z_o = \sum_n \langle n| e^{-\beta H_o}|n\rangle$ and $\langle H_1\rangle$ and $\langle H'\rangle$ are the thermal averages of H_1 and H' respectively:

$$\langle H_1\rangle = \frac{\sum_n \langle n|H_1 e^{-\beta H_o}|n\rangle}{\sum_n \langle n|e^{-\beta H_o}|n\rangle}$$

$$= \frac{\hbar\omega}{2} \frac{\sum_n (n^3+(n+1)^3 - (2n+1)) e^{-\beta\hbar\omega(n+1/2)}}{\sum_n e^{-\beta\hbar\omega(n+1/2)}}$$

$$= -\frac{\hbar\omega}{2} - \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} + \hbar\omega (\sinh(\beta\hbar\omega)g(\beta\hbar\omega) \qquad (22)$$

where

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

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

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

$$= \frac{\lambda\hbar^2}{32m^2\omega^2}(\coth(\frac{\beta\hbar\omega}{2}))^2 \qquad (23)$$

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

$$Z \approx Z_o(1- \frac{\eta^2}{3!} \beta(-\frac{\hbar\omega}{2} - \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} +$$

$$\hbar\omega \sinh(\beta\hbar\omega) g(\beta\hbar\omega)) - \frac{\beta\lambda\hbar^2}{32m^2\omega^2}(\coth(\frac{\beta\hbar\omega}{2}))^2) \qquad (24)$$

In the limit $q \to 1$, the expression for Z 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):

$$e^{-\beta\Omega} = Z,$$

$$S = \beta^2(\frac{\partial\Omega}{\partial\beta}), \qquad U = \frac{S}{\beta} + \Omega \qquad (25)$$

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

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

where

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

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

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

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 1991 a,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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