The statistical distribution of (q, R)-deformed crystal lattice vibration for generic atomic string

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Abstract. The deformed oscillators formalism plays a useful role in the study of physical models. Specifically, many variants of deformed oscillators have been used to study of the quantum optics, condensed matter physics, etc ... In this paper we construct a (q, R)-deformed crystal lattice vibration for generic atomic string and calculate statistical distribution of this vibration. This is a fundament for study of crystal lattice vibration, which would give a base for a new quantization proceduce.

1. Introduction

The study of q-quantum algebras and their oscillator representation [1, 2, 3, 4, 5, 6] is a direction of actual character in theoretical physics. They find application in many problems such as quantum inverse scattering theory, exactly solvable model in statistical mechanics, rational conformal field theory, two-demensional field theory with fractional statistics, etc. The algebraic structure of quantum group can be formally described as a deformation, depending on one or more parameters of the classical Lie algebras [7, 8]. In the special limiting cases of these parameters the quantum algebra reduce to the ordinary Lie algebras. Especially the oscillator representation of quantum algebras has proved to be powerful for the study of the quantum optics, condensed matter physics, etc.

The R-deformed Heisenberg algebra, which is the deformation involving the reflection operator $R(R^2 = 1)$, was introduced by Vasiliev [9] in the context of the higher spin algebras. The (q, R)-deformed Heisenberg algebra is combined the q-deformed algebra with the R-deformed, which may be described as a deformation, depending on q-parameter and reflection operator $R(R^2 = 1)$ of the ordinary Lie algebra.

The above mentioned arguments have encouraged us to consider the possibility for the application of the quantum group concepts to the problem in the theory of solid physics.

Our aim here is to construct a (q, R)-deformed crystal lattice vibration for generic atomic string, consider a statistical distribution in view of this vibration.

2. The (q, R)-deformed crystal lattice vibration for generic atomic string

In this section, we are using the result in our previous paper [10] to construct a (q, R)-deformed crystal lattice vibration for generic atomic string.

The Hamiltonian of the crystal lattice vibration for generic atomic string can be expressed following form:

$$H = \sum_{k \in BZ_1} \left(\frac{p_k^2}{2m} + \frac{1}{2} m\omega^2 (k)\, x_k^2 \right), \tag{1}$$

where k is wave vector and $\sum_{k \in BZ_1}$ is a sum on k, which is one in first Brillouin zone, the x_k is extended coordinate of atom in order k and the p_k is correspondent momentum of generic atomic string.
The creation and annihilation operators, which are to correspond to waved vector k, are form

$$\begin{aligned} b_k^\dagger &= \tfrac{1}{\sqrt{2\hbar\omega(k)}} \left(\sqrt{m}\omega (k)\, x_k - \tfrac{i}{\sqrt{m}} p_k \right) \\ b_k &= \tfrac{1}{\sqrt{2\hbar\omega(k)}} \left(\sqrt{m}\omega (k)\, x_k + \tfrac{i}{\sqrt{m}} p_k \right). \end{aligned} \tag{2}$$

The coordinate and momentum operators can be expressed in creation and annihilation operators $b^\dagger, b$ as:

$$\begin{aligned} x_k &= \sqrt{\tfrac{\hbar}{2m\omega(k)}} \left(b_k + b_k^\dagger \right) \\ p_k &= -i \sqrt{\tfrac{\hbar m\omega(k)}{2}} \left(b_k - b_k^\dagger \right). \end{aligned} \tag{3}$$

Using equations (1) and (3), one obtains the Hamiltonian of the crystal lattice vibration for generic atomic string in following form:

$$H = \sum_{k \in BZ_1} \frac{\hbar\omega (k)}{2} \left(b_k b_k^\dagger + b_k^\dagger b_k \right). \tag{4}$$

The creation (annihilation) operator $b_k^\dagger\,(b_k)$ of the equation (4) satisfy the commutation relation:

$$b_k b_k^\dagger - b_k^\dagger b_k = 1. \tag{5}$$

The (q, R)-deformed crystal lattice vibration can be considered as nonlinear crystal lattice vibration which its frequency depending on amplitude. Using the analogical method in the work [11] we calculated a frequency depending on amplitude, such as:

$$W_{q\nu} (k) = \left\{ \frac{\cosh\left(\hbar b b^\dagger\right)}{\sinh \hbar} + \frac{\hbar e^{\hbar b b^\dagger}}{e^\hbar - 1} \nu \right\} \omega (k).$$

Instead of amplitude dependence of frequency the Hamiltonian could be rewritten in the form of standard Hamiltonian as:

$$H = \sum_{k \in BZ_1} \frac{\hbar\omega (k)}{2} \left(a_k a_k^\dagger + a_k^\dagger a_k \right), \tag{6}$$

where the creation (annihilation) operator $a_k^\dagger\,(a_k)$ and the number operators N_k of the (q, R)-deformed crystal lattice vibration satisfy the commutation relations:

$$\begin{aligned} a_k a_{k'}^\dagger - q a_{k'}^\dagger a_k &= q^{-N_k} \delta_{k,k'} + \nu R \\ [a_k, a_{k'}] &= 0 \\ [N_k, a_{k'}] &= -a_k \delta_{k,k'} \\ \left[N_k, a_{k'}^\dagger \right] &= a_{k'}^\dagger \delta_{k,k'}, \end{aligned} \tag{7}$$

with R is reflection operator satisfying the following commutation relations:

$$Ra_k^\dagger + a_k^\dagger R = Ra_k + a_k R = 0, \tag{8}$$

and frequence is now not depending on the amplitude.
The (q,R)-deformed state vectors in Fock space are

$$|n_k\rangle_{q\nu} = \frac{\left(a_k^\dagger\right)^{n_k}}{\sqrt{[n_k]_{q\nu}!}}|0\rangle_{q\nu}, \tag{9}$$

where $|0\rangle_{q\nu}$ is the ground state satisfying the following conditions:

$$\begin{array}{ll} a_k|0\rangle_{q\nu} & = 0 \\ \langle 0 \mid 0\rangle_{q\nu} & = 1 \\ N_k|0\rangle_{q\nu} & = 0 \\ R|0\rangle_{q\nu} & = r|0\rangle_{q\nu} \\ r & = \pm 1, \end{array} \tag{10}$$

using the notations:

$$\begin{array}{ll} [n_k]_q & = \frac{q^{n_k}-q^{-n_k}}{q-q^{-1}} \\ [n_k]_{q\nu} & = [n_k]_q + \frac{q^{n_k}-(-1)^{n_k}}{q-1}\nu \\ [n_k]_{q\nu}! & = [n_k]_{q\nu}.[n_k-1]_{q\nu}...\,[1]_{q\nu}. \end{array} \tag{11}$$

Let $|n_k\rangle_{q\nu}$ be the eigenstates of the oscillator number operator

$$N_k|n_k\rangle_{q\nu} = n_k|n_k\rangle_{q\nu}. \tag{12}$$

From (7) one sees that: The action of operators $a_k^\dagger$ and a_k on the eigenstates $|n_k\rangle_{q\nu}$ can be chosen as

$$\begin{array}{l} a_k^\dagger|n_k\rangle_{q\nu} = \sqrt{[n_k+1]_{q\nu}}|n_k+1\rangle_{q\nu} \\ a_k|n_k\rangle_{q\nu} = \sqrt{[n_k]_{q\nu}}|n_k-1\rangle_{q\nu}. \end{array} \tag{13}$$

The energy spectrum of (q,R)-deformed crystal lattice vibration of generic atomic string is given by

$$\begin{array}{cl} H|n_k\rangle_{q\nu} & = E_{n_k}|n_k\rangle_{q\nu} \\ \sum\limits_{k\in BZ_1} \frac{\hbar\omega(k)}{2}\left(a_k a_k^\dagger + a_k^\dagger a_k\right)\frac{\left(a_k^\dagger\right)^{n_k}}{\sqrt{[n_k]_{q\nu}!}}|0\rangle_{q\nu} & = E_{n_k}|n_k\rangle_{q\nu}, \end{array}$$

where

$$E_{n_k} = \sum_{k\in BZ_1}\frac{\hbar\omega\,(k)}{2}\left\{[n_k+1]_{q\nu} + [n_k]_{q\nu}\right\}. \tag{14}$$

Hence, the energy spectrum E_{n_k} of the (q,R)-deformed crystal lattice vibration for generic atomic string have been depended on deformed parameters in the formulation (14).

3. The Green function for (q, R)-deformed crystal lattice vibration for generic atomic string

The Green function for (q, R)-deformed crystal lattice vibration for generic atomic string is defined as the statistical distribution of $\left(a_k^\dagger a_k\right)$

$$\left\langle a_k^\dagger a_k \right\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-N_k\beta\omega(k)}a_k^\dagger a_k\right), \tag{15}$$

where Z is the partition function

$$\begin{aligned} Z &= \mathrm{Tr}\left(e^{-N_k\beta\omega(k)}\right) \\ &= \sum_{n_k}^{\infty} {}_{q\nu}\left\langle n_k|e^{-N_k\beta\omega(k)}|n_k\right\rangle_{q\nu}, \end{aligned} \tag{16}$$

which could be used to determine the thermodynamic properties of the system, $\beta = \frac{1}{kT}$, $\omega(k)$ is one particle-oscillator energy. The trace most be taken over a complete set of states.
The calculations based on the equation (9) give the following results:

$$\left\langle a_k^\dagger a_k \right\rangle = \frac{\left(e^{\beta\omega}-1\right)}{\left(e^{\beta\omega}-q\right)}\left\{\frac{1}{e^{\beta\omega}-q^{-1}} + \frac{\nu}{e^{\beta\omega}+1}\right\}.$$

In the limit $q \to 1$ and $\nu \to 0$, this gives

$$\left\langle a_k^\dagger a_k \right\rangle = \frac{1}{e^{\beta\omega}-1},$$

which is just the usual Bose-Einstein formulae.

4. Conclusion

In this work, we present the results of our primary calculations which have been performed on the model of (q, R)-deformed crystal lattice vibration that can be realized by several symmetric and asymmetric potentials in solid systems such as Rogers-Szegö and Stieltjes-Wigert polynomials. The most important properties of potentials in the solid systems are the finite number of energy levels and the non-equal steps between energy levels that would not be described by the model of harmonic oscillators, however, that are possible to transform into the model of (q, R)-deformed harmonic oscillators by one-to-one mapping. Our results provide the initial powerful tools to study Einstein and Debye solid models to obtain thermodynamic quantities such as Einstein and Debye temperatures, specific heat, thermal conductivity, electrical conductivity and resistivity with $q \neq 1$ that will be calculated in next works.
Our results have shown that it is possible to apply q-deformation in condensed matter physics and to investigate the causes of other factors within materials in definition of q-deformation.

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