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LETTER TO THE EDITOR

Simple applications of q-bosons

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Abstract

A deformation of the harmonic oscillator algebra associated with the Morse potential and the $SU(2)$ algebra is derived using the quantum analogue of the anharmonic oscillator. We use the quantum oscillator algebra or q-boson algebra, which is a generalization of the Heisenberg–Weyl algebra obtained by introducing a deformation parameter q. Further, we present a new algebraic realization of the q-bosons, for the case of q being a root of unity, which corresponds to a periodic structure described by a finite-dimensional representation. We show that this structure represents the symmetry of a linear lattice with periodic boundary conditions.

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1. Introduction

Algebraic models have been used very successfully in nuclear and molecular physics and have led to new insights into the nature of complex many-body systems [1–3]. The methods combine Lie algebraic techniques, describing the interatomic interactions, with discrete symmetry techniques associated with the global symmetry of the atoms and molecules in complex compounds. In the framework of the algebraic model [2], the anharmonic effects of the local interactions are described by substituting the local harmonic potentials by a Morse-like potential. The Morse potential, which is associated with the $SU(2)$ algebra, leads to a deformation of the harmonic oscillator algebra.

In this Letter we derive the above-mentioned deformation using the quantum analogue of the anharmonic oscillator. We describe the anharmonic vibrations as anharmonic q-bosons. Their algebra, known as quantum oscillator algebra HW_q or q-boson algebra, has been introduced in [4–6], and is a generalization of the Heisenberg–Weyl algebra obtained by introducing a deformation parameter q. A change of parametrization leads naturally to

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Lie-algebraic approximations of the general q-deformation. In particular, we present a new algebraic realization of the q-boson algebra, for the case of q being a root of unity, which corresponds to a periodic structure described by a finite-dimensional representation. We show that this structure generates a group isomorphic to the symmetry group of a linear lattice with periodic boundary conditions.

2. Algebraic model

In the algebraic model [2], the one-dimensional Morse Hamiltonian is written in terms of the generators of $SU(2)$,

$$H_{\mathrm{M}} = \frac{A}{4}(\hat{\mathcal{N}}^2 - 4\hat{J}_Z^2) = \frac{A}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ - \hat{\mathcal{N}}) \tag{1}$$

where A is a constant. The eigenstates, $|[\mathcal{N}], v\rangle$, correspond to the $U(2) \supset SU(2)$ symmetry-adapted basis, where $\mathcal{N}$ is the total number of bosons fixed by the potential shape, and v is the number of quanta in the oscillator, $v = 1, 2, \ldots, [\frac{\mathcal{N}}{2}]$.

The anharmonic effects are described by anharmonic boson operators [2],

$$\hat{b} = \frac{\hat{J}_+}{\sqrt{\mathcal{N}}} \qquad \hat{b}^\dagger = \frac{\hat{J}_-}{\sqrt{\mathcal{N}}} \qquad \hat{v} = \frac{\hat{\mathcal{N}}}{2} - \hat{J}_z \tag{2}$$

where $\hat{v}$ is the Morse phonon operator with an eigenvalue v. The operators satisfy the commutation relations,

$$[\hat{b}, \hat{v}] = \hat{b} \qquad [\hat{b}^\dagger, \hat{v}] = -\hat{b}^\dagger \qquad [\hat{b}, \hat{b}^\dagger] = 1 - \frac{2\hat{v}}{\mathcal{N}}. \tag{3}$$

For an infinite potential depth, $\mathcal{N} \to \infty$, $[\hat{b}, \hat{b}^\dagger] \to 1$, giving the usual boson commutation relations associated with the harmonic oscillator.

The Morse Hamiltonian can be written in terms of the anharmonic bosons $\hat{b}$ and $\hat{b}^\dagger$,

$$H_{\mathrm{M}} \sim \tfrac{1}{2}(\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b}) \tag{4}$$

which corresponds to vibrational energies

$$\varepsilon_v = \hbar\omega_0 \left(v + \frac{1}{2} - \frac{v^2}{\mathcal{N}} \right) \tag{5}$$

where ω_0 is the harmonic oscillator frequency. When $\mathcal{N} \to \infty$, the Morse potential cannot be distinguished from the harmonic potential.

The algebraic model has been developed to analyse molecular vibrational spectra [2,3,7–11]. It provides a systematic procedure for studying vibrational excitations in a simple form by describing the stretching and bending modes in a unified scheme based on $SU(2)$ algebra which incorporates the anharmonicity at the local level.

3. Anharmonic q-bosons

The anharmonic bosons of the previous section may be obtained as an approximation of the so-called q-bosons [4–6], which enter the Heisenberg–Weyl q-algebra HW_q given by the following commutation relations:

$$[a, a^\dagger] = q^{\hat{n}} \qquad [\hat{n}, a] = -a \qquad [\hat{n}, a^\dagger] = a^\dagger \tag{6}$$

where q is in general a complex number. This number is called the deformation parameter since the boson commutation relations of the harmonic oscillator may be recovered for the value $q = 1$.

For the general analysis of the system (6) it is useful to know operators which are diagonalizable. Such an operator is the Casimir operator which for HW_q can be written in the form

$$\mathcal{C} = aa^\dagger + a^\dagger a - \frac{q^{\hat{n}+1} + q^{\hat{n}} - 2}{q-1}. \tag{7}$$

Checking that:

$$[\mathcal{C}, a] = [\mathcal{C}, a^\dagger] = [\mathcal{C}, \hat{n}] = 0 \tag{8}$$

is straightforward. Thus, a possible Hamiltonian is

$$H = \frac{1}{2}(aa^\dagger + a^\dagger a) = \frac{1}{2}\mathcal{C} + \frac{1}{2}\frac{q^{\hat{n}+1} + q^{\hat{n}} - 2}{q-1}. \tag{9}$$

The anharmonic bosons (3) may be obtained from the q-bosons (6) for real values of q close to 1. Namely, let $q < 1$ and $p \equiv 1/(1-q)$, so that $q = 1 - 1/p$ and

$$q^{\hat{n}} = \left(1 - \frac{1}{p}\right)^{\hat{n}}. \tag{10}$$

The harmonic limit is recovered for $p \to \infty$ in this parametrization.

Further, assuming that $1/p \ll 1$ and neglecting the terms of order $1/p^2$ and higher, we obtain

$$q^{\hat{n}} = 1 - \frac{\hat{n}}{p}. \tag{11}$$

If we now substitute the approximation for $q^{\hat{n}}$ from equation (11) in the commutation relations (6) and identify the parameter p with $\mathcal{N}/2$, $\hat{n}$ with $\hat{v}$ and the creation and annihilation operators $a, a^\dagger$, with $b, b^\dagger$, we recover the $SU(2)$ anharmonic relations (3). We can now explain the meaning of this approximation. In a sense, the form (3) of the $SU(2)$ commutation relations can be considered as a deformation of the usual (harmonic oscillator) commutation relations, with $\mathcal{N} = 2p$ being the deformation parameter. The form of (11) and (3) indicates that for the low-lying levels of the Hamiltonian (9) the spectrum corresponds to (5), the Morse eigenvalues. More generally, one may consider the parametrization (11) to mean that, up to order $1/p$, the HW_q algebra contracts to $SU(2)$. Although the range covered by the full Morse eigenvalue (3) is not consistent with the expansion (11), the approximation is useful nevertheless to provide a physical interpretation for p or q in terms of the Morse anharmonicity parameter [2].

For $q \leqslant 1$, we thus retrieve the case of low-energy harmonic and anharmonic vibrations in molecules and solids. The quantum parameter q (or the related parameter p) would naturally appear in all vibration-related properties such as infrared and Raman spectroscopy, partition functions, specific heat and thermal expansions [7, 12–15]. The case of $q > 1$ is also very interesting as it is related to Bose–Einstein condensation and superfluidity [16,17]. Under these conditions one may define a new parameter $S \equiv 1/(q-1)$ and the approximation equivalent to (11), leads to the noncompact $SU(1,1)$ algebra. This case is currently under investigation.

4. q-bosons at roots of unity

4.1. Finite-dimensional systems

In the previous section we considered the system given by (6) for real values of the deformation parameter. But it may be very interesting also in the case when the deformation parameter

q is a root of unity. The reason is that in that case we can also define finite-dimensional representations. Note that this case is not related to the bosonic relations (3).

Before proceeding further, we consider a restriction in the basis of the algebra, namely, we may use only the operator $K \equiv q^{\hat{n}}$ but not $\hat{n}$, the reason being that the Casimir operator depends only on $q^{\hat{n}}$. The commutation relations are then

$$[a, a^\dagger] = K \qquad K\, a = q^{-1}\, a\, K \qquad K\, a^\dagger = q\, a^\dagger\, K. \tag{12}$$

We start with the generic case for the deformation parameter. Let $|\rangle$ be the vacuum which is annihilated by the operators lowering the boson number and is an eigenvector of the number operator:

$$a\,|0\rangle = 0 \qquad K\,|\rangle = q^{\nu}|0\rangle \qquad (\text{or } \hat{n}|\rangle = \nu|0\rangle) \tag{13}$$

where ν for the moment is an arbitrary complex number. The states of the system are built by applying the operators raising the boson number:

$$|k\rangle \equiv (a^\dagger)^k\,|0\rangle. \tag{14}$$

The action of the algebra on the basis $|k\rangle$ is

$$\begin{aligned} K|k\rangle &= q^{\nu+k}|k\rangle \\ a\,|k\rangle &= q^{\nu}\,\frac{q^k - 1}{q - 1}\,|k-1\rangle \\ a^\dagger\,|k\rangle &= |k+1\rangle. \end{aligned} \tag{15}$$

We denote this representation space by V_ν. Clearly, for generic deformation parameter q, V_ν is infinite dimensional.

The only way to have a finite-dimensional representation is to suppose that q is a nontrivial root of unity, i.e. $q^N = 1$ for some natural number $N > 1$. In this case we have

$$a\,|N\rangle = q^{\nu}\,\frac{q^N - 1}{q - 1}\,|N-1\rangle = 0. \tag{16}$$

Then all states $|k\rangle$ with $k \geqslant N$ form an infinite-dimensional invariant subspace, which we denote by I_ν. Indeed, K is diagonal, $a^\dagger$ raises the boson number of $|k\rangle$ and the lowering operator a has $|N\rangle$ as a boundary for its action, since it annihilates this state. Now, we obtain a finite-dimensional representation space as the following factor-space:

$$F_\nu = V_\nu / I_\nu. \tag{17}$$

The space F_ν is N dimensional.

Another way to obtain a finite-dimensional space is by noting that the above structure is periodic. To see this we consider the states $|k + mN\rangle$ for fixed $k < N$ and for all non-negative integer m. Then we have

$$\begin{aligned} K|k+mN\rangle &= q^{\nu+k+mN}|k\rangle = q^{\nu+k}|k\rangle \\ a\,|k+mN\rangle &= q^{\nu}\frac{q^{k+mN} - 1}{q - 1}\,|k+mN-1\rangle = q^{\nu}\frac{q^k - 1}{q - 1}\,|k+mN-1\rangle \\ a^\dagger\,|k+mN\rangle &= |k+mN+1\rangle \end{aligned} \tag{18}$$

i.e., the action of the algebra on all states $|k + mN\rangle$ (for fixed k) coincides.

Thus, we can identify these states between themselves and it is enough to consider the states $|k\rangle$ with $k < N$. Let us denote these identified states by $|\tilde{k}\rangle$, $k = 0, \ldots, N-1$. They form a finite-dimensional representation space $\tilde{F}_\nu$ which has the same dimension as F_ν. The action of the algebra on these states is

$$\begin{aligned} K\,|\tilde{k}\rangle &= q^\nu |\tilde{k}\rangle \\ a\,|\tilde{k}\rangle &= q^\nu \frac{q^k - 1}{q - 1}\,\widetilde{|k-1\rangle} \\ a^\dagger\,|\tilde{k}\rangle &= \widetilde{|k+1\rangle} \qquad k < N - 1 \\ a^\dagger\,\widetilde{|N-1\rangle} &= |\tilde{0}\rangle \end{aligned} \tag{19}$$

where in the last line we have used the identification of $|\tilde{N}\rangle$ with $|\tilde{0}\rangle$.

We have thus obtained an interesting finite-dimensional system. In this system the boson number lowering operator acts in the usual way (in particular, it annihilates the vacuum state $|\tilde{0}\rangle$), but the boson raising operator acts cyclically. In particular, it has a non-zero action on all states. Another interesting feature is that the vacuum state may be obtained not only by the action of the lowering operator but also by the action of the raising operator producing a jump from $\widetilde{|N-1\rangle}$ to $|\tilde{0}\rangle$. One realization of this operator is a two-level system, obtained for $N = 2$ (equivalent to $q = -1$). For $N > 2$, systems with finite number of levels and population inversion, are illustrations of possible action of these operators.

4.2. Application to linear lattice with periodic boundary conditions

For large N, periodicity of the type decribed above appears in crystals. We will show that it represents the periodic boundary conditions, first proposed by Born and von Kármán [18]. The periodic boundary conditions are imposed on the translational symmetry, which strictly speaking is a property of an infinite crystalline lattice, to allow its use for finite crystals. The boundary conditions require that every energy eigenfunction $\phi(\boldsymbol{r})$ is periodic,

$$\phi(\boldsymbol{r}) = \phi(\boldsymbol{r} + N\boldsymbol{t}) \tag{20}$$

where $\boldsymbol{r}$ is the position vector, $\boldsymbol{t}$ is the vector of primitive translations and N is a large positive number.

Figure 1. The linear lattice.

Consider the classic example of a linear lattice of identical particles with periodic boundary conditions (figure 1). The equilibrium positions of the particles are given by

$$\boldsymbol{t}_n = n\boldsymbol{t} \qquad n = 0, 1, \ldots, N - 1 \tag{21}$$

and the periodic boundary condition requires

$$\boldsymbol{t}_N \equiv \boldsymbol{t}_0 \equiv \boldsymbol{0}. \tag{22}$$

The symmetry operations of the linear lattice form a cyclic finite group of order N with a generator, the primitive translation $\{E|\boldsymbol{t}\}$. Here, the Seitz notation is used to represent a translation and E is the identity, $E \equiv \{E|0\}$.

The nth element of the group is

$$\{E|t\}^n = \{E|\boldsymbol{t}_n\} \qquad n = 1, 2, \ldots, N - 1. \tag{23}$$

The product of two elements of the group is an element of the group

$$\{E|t_m\}\{E|t_n\} = \{E|t_{m+n}\} \qquad m, n = 1, 2, \ldots, N-1 \tag{24}$$

where $m + n \equiv (m + n) \pmod N$. The identity is

$$\{E|\boldsymbol{t}\}^N \equiv \{E|\boldsymbol{t}_0\} \equiv \{E|\boldsymbol{0}\}. \tag{25}$$

Now, we can show that the generator $\{E|\boldsymbol{t}\}$ is isomporphic to the raising operator $a^\dagger$. Using the action (19) of the operator $a^\dagger$ on the states $|\tilde{k}\rangle$, one can verify that

$$(a^\dagger)^n|\tilde{k}\rangle = |\widetilde{(k+n)\,(\mathrm{mod}\,N)}\rangle \qquad n = 0, 1, \ldots, N-1 \tag{26}$$

and thus

$$(a^\dagger)^m(a^\dagger)^n = (a^\dagger)^{(m+n)\,(\mathrm{mod}\,N)} \qquad m, n = 0, 1, \ldots, N-1. \tag{27}$$

Also,

$$(a^\dagger)^N|\tilde{k}\rangle = (a^\dagger)^k a^\dagger (a^\dagger)^{N-k-1}|\tilde{k}\rangle = (a^\dagger)^k a^\dagger|\widetilde{N-1}\rangle = (a^\dagger)^k|\tilde{0}\rangle = |\tilde{k}\rangle \tag{28}$$

which gives the identity

$$(a^\dagger)^N = E. \tag{29}$$

Thus, the symmetry group of the lattice with periodic boundary conditions is isomorphic to the finite cyclic group of order N with a generator, the operator $a^\dagger$. This group can be used with the other symmetry operations of one-dimensional crystalline or polymer Hamiltonians. To recall, the periodic boundary conditions [19, 20] determine the number of allowed wavevector states in the Brillouin zone model and imply additional selection rules on certain frequencies. The boundary conditions can be generalized for the three-dimensional case by introducing raising operators for each dimension.

The deformation at roots of unity, discussed in this section, imposes in a natural way a periodicity on the boundaries of a finite lattice, which makes its symmetry compatible with the translational symmetry of the corresponding infinite lattice.

5. Conclusion

The application of a q-algebra to physical problems is often hampered by a lack of an appropriate interpretation for the deformation parameters and often applications are carried out where generalization to q-deformed versions of well known models are made with no simple interpretation.

In this Letter we have shown, on the one hand, that a reparametrization of the deformed algebras (where the classical limit corresponds to $p \to \infty$ in our example) leads to a natural next order of approximation for the q-system. The $1/p$ approximation of the HW_q example considered in this Letter leads to the $SU(2)$ algebra and to an interpretation of p in terms of the Morse potential anharmonicity. Such an approximation may be very useful for the analysis of other systems in a similar fashion.

On the other hand, we have presented in section 4 a new application of the HW_q algebra when q is a root of unity, which gives a periodic structure described by a finite-dimensional representation. We have shown that the raising operator belonging to this structure generates a group isomorphic to the symmetry group of a linear lattice with periodic boundary conditions. The latter may provide a useful framework for the deformation of crystalline or polymer Hamiltonians.

To conclude, we stress that simple approximations and specific realizations of q-algebras, such as the ones discussed in this Letter, may shed some light on the role of these mathematical constructs and open new ways to their physical interpretation.

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