

# Modified $q$ -deformed Tamm–Dancoff oscillators as a model for vibrations of polyatomic molecule

Won Sang Chung

Received: 27 December 2013 / Accepted: 26 September 2014 / Published online: 4 October 2014  
© Springer International Publishing Switzerland 2014

**Abstract** In this paper we propose the modified  $q$ -deformed bosonic Tamm–Dancoff oscillator algebra and present the Hamiltonian for the modified  $q$ -deformed bosonic Tamm–Dancoff oscillators. We show that this Hamiltonian is equivalent to that of polyatomic molecule.

**Keywords** Modified Tamm–Dancoff oscillator · Polyatomic molecule · Vibration · Angular momentum algebra · Jordan–Schwinger method

## 1 Introduction

One of the most effective methods to approximate an intermediate statistics behavior is to consider deformed boson and deformed fermion systems. Recently, the  $q$ -deformed oscillator systems [1–7] have been applied to many areas of research in physics as well as mathematics. For instance, they have used to understand higher-order effects in the many-body interactions in nuclei [8, 9], and also possible connections between the entanglement characteristics in quantum information theory and the properties of deformed boson systems have been investigated [10, 11].

Historically, the  $q$ -deformed bosonic Tamm–Dancoff oscillator algebra was first introduced in [12], and some of its Hopf algebraic aspects were also discussed in [13]. Therefore, we call them the TD-oscillators model. It should be pointed out that some of the quantum statistical properties of this model with the range  $q < 1$  have been also considered in [14, 15] during the studies on the two-parameter  $p, q$ -deformed oscillators.

---

W. S. Chung (✉)

Department of Physics and Research Institute of Natural Science, College of Natural Science,  
Gyeongsang National University, Jinju 660-701, Korea  
e-mail: mimip4444@hanmail.net

The Hamiltonian usually used for the description of vibrational modes of polyatomic molecule [16] is given by

$$H = \sum_i \hbar w_i \left( n_i + \frac{1}{2} \right) + \hbar \sum_i \frac{\gamma_i}{2} \left( n_i + \frac{1}{2} \right)^2 + \sum_{i < j} \gamma_{ij} \left( n_i + \frac{1}{2} \right) \left( n_j + \frac{1}{2} \right) \tag{1}$$

More specially, the Hamiltonian usually used for the description of vibrational modes of triatomic molecule [17–19] is

$$H = \hbar w_1 \left( n_1 + \frac{1}{2} \right) + \hbar w_2 \left( n_2 + \frac{1}{2} \right) + \frac{\gamma_1}{2} \left( n_1 + \frac{1}{2} \right)^2 + \frac{\gamma_2}{2} \left( n_2 + \frac{1}{2} \right)^2 + \gamma_{12} \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right) \tag{2}$$

The first and third term in this Hamiltonian describe an anharmonic oscillator, the second and fourth term describe another anharmonic oscillator. while the fifth term describes the cross-anharmonicity between them. The energy spectrum of this Hamiltonian is the same as that obtained from solving the Schrödinger equation for the Morse potential [20]. If we assume that atoms 1 and 3 are identical like in a molecule such as CO<sub>2</sub>, the Hamiltonian (2) is then simplified as follows;

$$H = \hbar w \left( n_1 + \frac{1}{2} \right) + \hbar w \left( n_2 + \frac{1}{2} \right) + \frac{\gamma}{2} \left( n_1 + \frac{1}{2} \right)^2 + \frac{\gamma}{2} \left( n_2 + \frac{1}{2} \right)^2 + \gamma_{12} \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right) \tag{3}$$

In this paper we show that the q-deformed Tamm–Dancoff (TD) oscillator algebra is not appropriate for describing a model for vibrations of polyatomic molecule. We modify the TD-oscillator algebra to show that it can explain a model for vibrations of polyatomic molecule.

## 2 TD-oscillators as a model for vibrations of polyatomic molecule

The TD-oscillator algebra is defined as

$$aa^\dagger - qa^\dagger a = q^N, \quad [N, a^\dagger] = a^\dagger, \quad [N, a] = -a, \tag{4}$$

If we introduce the ground state  $|0\rangle$  satisfying  $a|0\rangle = 0$ , we have the following Fock representation

$$N|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \dots$$

$$a^\dagger|n\rangle = \sqrt{(n+1)q^n}|n+1\rangle, \quad a|n\rangle = \sqrt{nq^{n-1}}|n-1\rangle, \tag{5}$$

where we used the relation

$$a^\dagger a = \{N\}_q = Nq^{N-1} \quad (6)$$

The algebra (4) was shown to have a Hopf algebra structure with the comultiplication, antipode and counit [7]. Coupling two of TD-oscillators, we can obtain the following Hamiltonian

$$H = w \left[ a_1^\dagger a_1 q^{N_2} + a_2^\dagger a_2 q^{N_1} \right] \quad (7)$$

where we set  $\hbar = 1$ . The relevant eigenvalues of the Hamiltonian (7) are

$$E(n_1, n_2) = w \{n_1 + n_2\}_q \quad (8)$$

When  $q$  is real, we can set  $q = e^\tau$ . The energy eigenvalues given in Eq. (8), including terms up to  $\tau^2$ , can be written as

$$E(n_1, n_2) = w \left[ n_1 + n_2 + (n_1 + n_2)(n_1 + n_2 - 1)\tau + \frac{\tau^2}{2}(n_1 + n_2)(n_1 + n_2 - 1)^2 + \dots \right] \quad (9)$$

This construction can be easily generalized to the case of  $M$  coupled TD-oscillators. The Hamiltonian then reads

$$H = w \sum_{i=1}^M a_i^\dagger a_i q^{\sum_{l=1}^M N_l - N_i} \quad (10)$$

and its relevant energy eigenvalues are

$$E(n_1, n_2, \dots, n_M) = w \{n_1 + n_2 + \dots + n_M\}_q \quad (11)$$

The energy eigenvalues (9) can be written as

$$E(n_1, n_2) = w \left[ 2\tau - 1 + (1 - 3\tau) \left( n_1 + \frac{1}{2} \right) + (1 - 3\tau) \left( n_2 + \frac{1}{2} \right) + \tau \left( n_1 + \frac{1}{2} \right)^2 + \tau \left( n_2 + \frac{1}{2} \right)^2 + 2\tau \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right) + \dots \right] \quad (12)$$

Comparing Eq. (12) with Eq. (3), we have  $\tau = 0$ , which implies  $q = 0$ . Thus, TD-oscillators cannot explain a model for vibrations of polyatomic molecule

### 3 Modified TD-oscillators as a model for vibrations of polyatomic molecule

In this section we consider the modified TD-oscillator algebra defined as

$$aa^\dagger - q^\mu a^\dagger a = q^{\mu N + \mu - 1}, \quad [N, a^\dagger] = a^\dagger, \quad [N, a] = -a, \quad (13)$$

where  $q, \mu$  are real. If we introduce the ground state  $|0\rangle$  satisfying  $a|0\rangle = 0$ , we have the following Fock representation

$$N|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \dots$$

$$a^\dagger|n\rangle = \sqrt{(n+1)q^{\mu n + \mu - 1}}|n+1\rangle, \quad a|n\rangle = \sqrt{nq^{\mu n - 1}}|n-1\rangle, \quad (14)$$

where we used the relation

$$a^\dagger a = \{N\}_{q,\mu} = Nq^{\mu N - 1} \quad (15)$$

Coupling two of modified TD-oscillators, we can obtained the following Hamiltonian

$$H = w \left[ a_1^\dagger a_1 q^{\mu N_2} + a_2^\dagger a_2 q^{\mu N_1} \right] \quad (16)$$

The relevant eigenvalues of the Hamiltonian (16) are

$$E(n_1, n_2) = w\{n_1 + n_2\}_{q,\mu} \quad (17)$$

The energy eigenvalues given in Eq. (17), including terms up to  $\tau^2$ , can be written as

$$E(n_1, n_2) = w \left[ n_1 + n_2 + (n_1 + n_2)\{\mu(n_1 + n_2) - 1\}\tau + \frac{\tau^2}{2}(n_1 + n_2)\{\mu(n_1 + n_2) - 1\}^2 + \dots \right] \quad (18)$$

The energy eigenvalues (18) can be written as

$$E(n_1, n_2) = w \left[ (1 + \mu)\tau - 1 + (1 - (2\mu + 1)\tau) \left( n_1 + \frac{1}{2} \right) + (1 - (2\mu + 1)\tau) \left( n_2 + \frac{1}{2} \right) + \tau\mu \left( n_1 + \frac{1}{2} \right)^2 + \tau\mu \left( n_2 + \frac{1}{2} \right)^2 + 2\tau\mu \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right) + \dots \right] \quad (19)$$

Comparing Eq. (19) with Eq. (3), we have  $\mu = -1/2$ , which implies that the modified TD-oscillators can explain a model for vibrations of polyatomic molecule. This

construction can be easily generalized to the case of  $M$  coupled TD-oscillators. The Hamiltonian then reads

$$H = w \sum_{i=1}^M a_i^\dagger a_i q^\mu \sum_{l=1}^M N_l - \mu N_i \quad (20)$$

and its relevant energy eigenvalues are

$$E(n_1, n_2, \dots, n_M) = w\{n_1 + n_2 + \dots + n_M\}_{q, \mu} \quad (21)$$

In this case, if we choose  $\mu = -1/M$ , the Hamiltonian (20) describes a vibrational model of molecules consisting  $M$  atoms.

#### 4 Angular momentum algebra related to the modified TD-oscillator algebra

In this section, we will discuss the angular momentum algebra related to the modified TD-oscillator algebra. Let us introduce the Jordan–Schwinger realization of this algebra as follows:

$$J_+ = a_1^\dagger a_2, \quad J_- = a_1 a_2^\dagger, \quad J_3 = \frac{N_1 - N_2}{2}, \quad \mathcal{L} = \frac{N_1 + N_2}{2}, \quad (22)$$

where is a total number operator satisfying

$$[\mathcal{L}, J_3] = [\mathcal{L}, J_\pm] = 0 \quad (23)$$

and  $J_3$  and  $\mathcal{L}$  are hermitian. Then we have the following commutation relations:

$$[J_+, J_-] = 2J_3 q^{2\mu\mathcal{L} + \mu - 2}, \quad [J_3, J_\pm] = \pm J_\pm, \quad (24)$$

where  $J_-$  is an hermitian adjoint operator of  $J_+$ . The representation of this algebra is given by

$$\begin{aligned} J_3 |n_1, n_2\rangle &= \frac{1}{2}(n_1 - n_2) |n_1, n_2\rangle, & \mathcal{L} |n_1, n_2\rangle &= \frac{1}{2}(n_1 + n_2) |n_1, n_2\rangle, \\ J_- |n_1, n_2\rangle &= \sqrt{q^{\mu(n_1+n_2)+\mu-2} n_1 (n_2 + 1)} |n_1 - 1, n_2 + 1\rangle \\ J_+ |n_1, n_2\rangle &= \sqrt{q^{\mu(n_1+n_2)+\mu-2} (n_1 + 1) n_2} |n_1 + 1, n_2 - 1\rangle \end{aligned} \quad (25)$$

By introducing

$$n_1 = j + m, \quad n_2 = j - m \quad (26)$$

and

$$|j, m\rangle \equiv |j + m, j - m\rangle = |n_1, n_2\rangle, \quad (27)$$

we have the following representation:

$$\begin{aligned}
 J_3|\widetilde{j}, \widetilde{m}\rangle &= m|\widetilde{j}, \widetilde{m}\rangle, \quad \mathcal{L}|\widetilde{j}, \widetilde{m}\rangle = j|\widetilde{j}, \widetilde{m}\rangle \\
 J_-|\widetilde{j}, \widetilde{m}\rangle &= \sqrt{q^{2\mu j + \mu - 2}(j + m)(j - m + 1)}|\widetilde{j}, \widetilde{m} - 1\rangle \\
 J_+|\widetilde{j}, \widetilde{m}\rangle &= \sqrt{q^{2\mu j + \mu - 2}(j + m + 1)(j - m)}|\widetilde{j}, \widetilde{m} + 1\rangle
 \end{aligned}
 \tag{28}$$

Because  $J_+|\widetilde{j}, j\rangle = J_-|\widetilde{j}, -j\rangle = 0$ , the representation is bounded below and above and the possible value of  $m$  is given by

$$m = -j, -j + 1, -j + 2, \dots, j - 2, j - 1, j
 \tag{29}$$

So we have the finite dimensional Fock space. Applying  $J_+$  to the lowest state  $|\widetilde{j}, -j\rangle$   $2j + 1$  times, we have

$$(J_+)^{2j+1}|\widetilde{j}, -j\rangle = 0,
 \tag{30}$$

and applying  $J_-$  to the highest state  $|\widetilde{j}, j\rangle$   $2j + 1$  times, we have

$$(J_-^\dagger)^{2j+1}|\widetilde{j}, j\rangle = 0
 \tag{31}$$

### 5 Conclusion

In this paper we found that the  $q$ -deformed Tamm–Dancoff oscillator algebra was not appropriate for describing a model for vibrations of polyatomic molecule. Thus, we modified the TD-oscillator algebra by introducing one more parameter  $\mu$  and showed that it could explain a model for vibrations of polyatomic molecule. Finally, using Jordan–Schwinger method, we presented the angular momentum algebra related to the modified TD-oscillator algebra.

**Acknowledgments** This work was supported by the Gyeongsang National University Fund for Professors on Sabbatical Leave, 2006.

### References

1. M. Jimbo, Lett. Math. Phys. **10**, 63 (1985)
2. M. Jimbo, Lett. Math. Phys. **11**, 247 (1986)
3. V. Drinfeld, in *Proceedings of International Congress of Mathematicians* (Berkeley, 1986), p. 78
4. M. Arik, D. Coon, J. Math. Phys **17**, 524 (1976)
5. A. Macfarlane, J. Phys. A **22**, 4581 (1989)
6. L. Biedenharn, J. Phys. A **22**, L873 (1990)
7. W. Chung, K. Chung, S. Nam, C. Um, Phys. Lett. A **183**, 363 (1993)
8. K.D. Sviratcheva, C. Bahri, A.I. Georgieva, J.P. Draayer, Phys. Rev. Lett. **93**, 152501 (2004)
9. A. Ballesteros, O. Civitarese, F.J. Herranz, M. Reboiro, Phys. Rev. C **66**, 064317 (2002)
10. M.C. Tichy, F. Mintert, A. Buchleitner, J. Phys. B At. Mol. Opt. Phys. **44**, 192001 (2011)
11. A.M. Gavrilik, Y.A. Mishchenko, Phys. Lett. A **376**, 1596 (2012)

12. K. Odaka, T. Kishi, S. Kamefuchi, J. Phys. A Math. Gen. **24**, L591 (1991)
13. S. Chaturvedi, V. Srinivasan, R. Jagannathan, Mod. Phys. Lett. A **8**, 3727 (1993)
14. A.M. Gavrilik, A.P. Rebesh, Mod. Phys. Lett. A **22**, 949 (2007)
15. A.M. Gavrilik, A.P. Rebesh, Mod. Phys. Lett. B **25**, 1150030 (2012)
16. G. Herzberg, *Molecular Spectra and Molecular Structure*, vol. 3 (Van Nostrand, Toronto, 1979)
17. M. Kellman, J. Chem. Phys. **81**, 389 (1984)
18. M. Kellman, Chem. Phys. Lett. **113**, 489 (1985)
19. M. Kellman, J. Chem. Phys. **83**, 3843 (1985)
20. F. Iachello, S. Oss, Phys. Rev. Lett. **66**, 2976 (1991)