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Correlations studies in the q-deformed time-dependent Hartree–Fock approximation

S S Avancini, F F de Souza Cruz, D P Menezes and M M Watanabe de Moraes

Depto de Física-Universidade Federal de Santa Catarina, CP 476-88.040-900, Florianópolis-SC, Brazil

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Abstract. In this work we investigate the differences arising in the one-body operator and the correlation parameter when the Lipkin–Meshkov–Glick model is deformed. We calculate these functions exactly and by means of the time-dependent Hartree–Fock approximation (TDHF). We observe that the exact and the TDHF results are much closer to each other in the deformed case.

1. Introduction

Quantum deformed algebras have lately been exploited by several authors in different physical contexts [1]. The final aim of most of these works consists in finding a physical meaning to the deformation procedure and, in this way, to show the range of validity and applicability of models which can be described by these q-algebras [2]. Recently, it has also been shown that when q-deformed coherent states for the $su_q(2)$ (the quantum algebra counterpart of $su(2)$) are introduced in the time-dependent variational principle (TDVP) it yields a generalized Hamiltonian dynamics [3] in complete analogy with the non-deformed case. In a recent work we have analysed the dynamics of the q-deformed Lipkin–Meshkov–Glick (LMG) model [4] in the time-dependent Hartree–Fock approximation (TDHF) [5].

In the present work the q-deformed Lipkin model is used to investigate the differences between the exact evolution in time of a many-particle wavefunction and the evolution which arises from the TDHF equations of motion. The rationale of this study is the very fact that the variational space obtained through the introduction of the deformed coherent states in the TDVP is no longer the usual determinant space.

Several years ago Krieger [6] argued that the relation between the TDHF dynamics and the exact one is by no means clear, since unlike the static case the TDVP cannot warrant that the TDHF wavefunction remains close to the true wavefunction with the evolution of time. According to this idea we may state that if, at any time, the exact wavefunction is a Slater determinant, then the TDHF maximizes the overlap of the Slater determinant with the exact wavefunction in a specific interval of time. In the q-deformed context Krieger's arguments raise some questions since, as stated before, the variational space is no longer the Slater determinant space. The q-deformation brings correlations to the TDHF dynamics and one may wonder whether the enlargement of the variational space and the modifications of the dynamics could create conditions for a possible convergence between the exact and the variational solutions.

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We compare the exact evolution and the TDHF results for a typical value of the q-parameter departing from the initial conditions defined at a fixed energy per particle which corresponds to a particular deformed coherent state.

In order to understand the effects of the correlations we investigate the time evolution of the one-body density ρ and of the correlation parameter Δ defined by $\Delta = \sqrt{\rho^2 - \rho}$, (which is equal to zero for the usual TDHF), when q-deformation is introduced.

For the sake of completeness, we have drawn the trajectories followed by the system, which can be seen in a phase diagram.

2. Exact solutions for the LMG model

The LMG model [4] has often been used because it has many important physical features present in realistic models and at the same time is a relatively simple, non-trivial and exactly solvable model. This model describes a two N-fold degenerate level system with energies $\frac{1}{2}\epsilon$ and $-\frac{1}{2}\epsilon$, respectively. The states in the upper level are denoted by the labels $i = 1, \ldots, N$, the states in the lower level by $-i$.

The many-body LMG Hamiltonian is

$$H = \tfrac{1}{2}\epsilon \sum_{i=1}^{N} \left(a_i^\dagger a_i - a_{-i}^\dagger a_{-i}\right) - \tfrac{1}{2} V \sum_{i,i'=1}^{N} \left(a_i^\dagger a_{i'}^\dagger a_{-i} a_{-i'} + a_{-i}^\dagger a_{-i'}^\dagger a_i a_{i'}\right) \tag{1}$$

where $a_i^\dagger$ ($a_{-i}^\dagger$) creates a fermionic particle in the upper (lower) level, a_i (a_{-i}) annihilates a particle in the upper (lower) level and V is the strength of the interaction. The Hamiltonian in terms of the pseudo-spin operators is given by

$$H = \epsilon J_z - \tfrac{1}{2} V \left(J_+^2 + J_-^2\right) \tag{2}$$

with

$$J_z = \tfrac{1}{2} \sum_{i=1}^{N} \left(a_i^\dagger a_i - a_{-i}^\dagger a_{-i}\right) \qquad J_+ = \sum_{i=1}^{N} a_i^\dagger a_{-i} \qquad J_- = (J_+)^\dagger . \tag{3}$$

The above operators obey the pseudo-spin algebra of $su(2)$. The operators $J_\pm$ are particle–hole and hole–particle excitation operators while J_z is related to the number of excited particle–hole pairs (half the difference between occupied states in the upper and lower levels).

The q-deformed version of the LMG model is obtained through a deformation of the pseudo-spin algebra, as has already been extensively discussed in the literature [2]. All relevant formulae are given in the appendix.

The exact solution of the q-deformed version of this model can be obtained by diagonalizing the Hamiltonian given in (2), in a base $|jm\rangle$, where $j = N/2$ and N is the number of particles involved in the system. Then we obtain the expansion coefficients $\langle m|\psi_i\rangle$ of the eigenstates $|\psi_i\rangle$ in the quasi-spin basis $|m\rangle$, i.e.

$$|\psi_i\rangle = \sum_m |m\rangle\langle m|\psi_i\rangle \qquad H|\psi_i\rangle = E_i|\psi_i\rangle \tag{4}$$

where E_i are the eigenvalues.

The exact time evolution of a general wavefunction $|\varphi_0\rangle$ is easily found to be [6]

$$|\psi(t)\rangle = \sum_{i,m,m'} |m\rangle\langle m|\psi_i\rangle\langle\psi_i|m'\rangle b_{m'}\, \mathrm{e}^{\mathrm{i}[(j+m')\phi - E_i t]} \tag{5}$$

where

$$b_m = \begin{bmatrix} 2j \\ j+m \end{bmatrix}^{1/2} \left(\sin\frac{\theta}{2}\right)^{j+m} \left(\cos\frac{\theta}{2}\right)^{j-m} \frac{1}{\sqrt{bb(\theta)}} \tag{6}$$

$$bb(\theta) = \Pi_{k=0}^{2j-1} \left(\cos^2\frac{\theta}{2} + q^{2k-2j+1}\sin^2\frac{\theta}{2}\right) \tag{7}$$

and

$$\langle m|\varphi_0\rangle = b_m \, \mathrm{e}^{\mathrm{i}(j+m)\phi} . \tag{8}$$

Since we are mainly concerned with the comparison of the exact time evolution with the evolution generated by the TDHF equations, we chose the initial $|\varphi_0\rangle$ as a deformed coherent state throughout this paper. The comparison will be carried out by investigating the time evolution of one-body observables, specifically the one-body density, which may be expressed in matrix form as [6]

$$\rho = \begin{pmatrix} \rho_{p_1} & \cdots & \cdots & \cdots \\ \cdots & \rho_{p_2} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ \cdots & \cdots & \cdots & \rho_{p_N} \end{pmatrix} \tag{9}$$

with

$$\rho_p = \begin{pmatrix} \rho_{pp} & \rho_{p-p} \\ \rho_{-pp} & \rho_{-p-p} \end{pmatrix} \tag{10}$$

where ρ_{pp}, ρ_{p-p}, ρ_{-pp} and ρ_{-p-p} are the particle–particle, particle–hole, hole–particle and hole–hole densities, respectively. The elements of the one-body density at any time can be exactly calculated yielding

$$\rho_{pp} = 1 - \rho_{-p-p} = \langle\psi(t)|a_p^\dagger a_p|\psi(t)\rangle = \tfrac{1}{2} + \sum_m \frac{m}{2j}|f_m|^2 \tag{11}$$

$$\rho_{p-p} = \rho_{-pp}^* = \langle\psi(t)|a_p^\dagger a_{-p}|\psi(t)\rangle = \sum_m f_m g_m^* \sqrt{(j-m)(j+m+1)}/2j \tag{12}$$

where

$$f_m = \sum_i \langle m|\psi_i\rangle d_i \tag{13}$$

$$g_m = \sum_i d_i \langle\psi_i|m+1\rangle \tag{14}$$

$$d_i = \sum_m b_m \, \mathrm{e}^{\mathrm{i}(m\phi - E_i t)} \langle\psi_i|m\rangle . \tag{15}$$

Since our main interest is the analysis of the extent of correlations we give here the expression of the one-body density fluctuation Δ.

$$\Delta^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \rho^2 - \rho . \tag{16}$$

The parameter Δ is a measure of how much a particular many-body state differs from a Slater determinant and, in the non-deformed case, its time evolution can give us information about how the exact dynamics drives the states out of the Slater determinant space [6]. For that reason this parameter is extremely useful in the study of the correlations introduced by the q-deformation either for the exact or for the TDHF dynamics. When $q \to 1$, all formulae which appear in [6] are recovered from the ones above.

We then utilize the above equations to perform the exact calculation where we have used the eigenvectors and eigenvalues obtained from the deformed Hamiltonian in a deformed basis. Our results are discussed in the last section of this work.

3. TDHF solutions

In order to apply the deformed TDVP formalism developed so far to the Lipkin model, we use the definition of the q-analogues of the $su(2)$ coherent states as given in the appendix.

The deformed Lipkin density Hamiltonian in this basis can be written as

$$\mathcal{H}(z,\bar{z}) = \frac{\langle z|H/\epsilon|z\rangle}{\langle z|z\rangle} = \frac{\langle z|J_z|z\rangle}{\langle z|z\rangle} - \frac{\chi}{2[N]}\frac{\langle z|J_+^2 + J_-^2|z\rangle}{\langle z|z\rangle}$$
$$= -\tfrac{1}{2}N + z\bar{z}\sum_{k=0}^{N-1}\left(\frac{1}{q^{N-1-2k} + z\bar{z}}\right) - \tfrac{1}{2}\chi[N-1](z^2+\bar{z}^2)\frac{[1(+)z\bar{z}]^{N-2}}{[1(+)z\bar{z}]^N} \qquad (17)$$

where $\chi \equiv V[N]/\epsilon$.

The Lagrangian density becomes

$$\mathcal{L}(z,\bar{z}) = \frac{\mathrm{i}}{2}\left(\dot{\bar{z}}\frac{\partial}{\partial\bar{z}} - \dot{z}\frac{\partial}{\partial z}\right)\ln\langle z|z\rangle - \mathcal{H}(z,\bar{z})\,. \qquad (18)$$

Introducing the Lagrangian in the action functional

$$\mathcal{S} = \int \mathcal{L}(z,\bar{z})\,\mathrm{d}t \qquad (19)$$

and performing the variation $\delta\mathcal{S} = 0$ in the space spanned by the deformed coherent states, we obtain the following equations of motion:

$$\dot{z} = \frac{\mathrm{i}}{g(z,\bar{z})}\frac{\partial\mathcal{H}}{\partial\bar{z}} \qquad (20)$$

and

$$\dot{\bar{z}} = \frac{-\mathrm{i}}{g(z,\bar{z})}\frac{\partial\mathcal{H}}{\partial z} \qquad (21)$$

where

$$g(z,\bar{z}) = \frac{\partial^2}{\partial z\partial\bar{z}}\ln\langle z|z\rangle = \sum_{k=0}^{2j-1}\frac{q^{2k-2j+1}}{(1+q^{2k-2j+1}z\bar{z})^2}\,. \qquad (22)$$

To recover the same parametrization of the deformed coherent states utilized in the exact time evolution of last section, we parametrize z as $z = \tan\left(\frac{\theta}{2}\right)\mathrm{e}^{\mathrm{i}\phi}$ where $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$. With this parametrization, (17) becomes

$$\mathcal{H}(\theta,\phi) = -\frac{N}{2} + \sin^2\frac{\theta}{2}B_N(\theta) - \frac{\chi}{4}\sin^2\theta\cos 2\phi\, C_N(\theta) \qquad (23)$$

with

$$B_N(\theta) = \sum_{k=0}^{N-1}\frac{1}{q^{N-1-2k}\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}} \qquad (24)$$

$$C_N(\theta) = \frac{[N-1]}{\left(\cos^2\frac{\theta}{2} + q^{-N+1}\sin^2\frac{\theta}{2}\right)\left(\cos^2\frac{\theta}{2} + q^{N-1}\sin^2\frac{\theta}{2}\right)}\,. \qquad (25)$$

Substituting the q-deformed LMG Hamiltonian in (20) and (21) and performing the required manipulations, we obtain

$$\dot{\theta} = \frac{\chi}{g(\theta)} \cos^4 \frac{\theta}{2} \sin\theta \sin 2\phi C_N(\theta) \tag{26}$$

and

$$\dot{\phi} = -1 + \frac{\chi}{4g(\theta)} \cos^2 \frac{\theta}{2} \operatorname{cotan} \frac{\theta}{2} \cos 2\phi \sin 2\theta C_N(\theta) \times \left(1 + \frac{1}{4[N-1]} \sin^2\theta (2 - q^{N-1} - q^{-N+1}) C_N(\theta)\right). \tag{27}$$

As mentioned in the last section, we also have to calculate the TDHF time evolution of the one-body density matrix elements defined in (9) and (10). The matrix elements can be written in terms of the parameters,

$$\rho_{pp} = 1 - \rho_{-p-p} = \frac{\langle z|a_p^\dagger a_p|z\rangle}{\langle z|z\rangle} = \frac{1}{2} + \frac{[2j]!}{N\langle z|z\rangle} \sum_m \frac{m}{[j-m]![j+m]!} (\tan^2\theta/2)^{j+m} \tag{28}$$

$$\rho_{p-p} = \rho^*_{-pp} = \frac{\langle z|a_p^\dagger a_{-p}|z\rangle}{\langle z|z\rangle} = \frac{[2j]!}{N\langle z|z\rangle} \times \sum_m \frac{1}{[j-m-1]![j+m]!} \sqrt{\frac{j(j+1) - m(m+1)}{[j+m+1][j-m]}} (\tan^2\theta/2)^{2j+2m+1} \tag{29}$$

and its time evolution is simply given by the equations of motion above. The parametrization in terms of θ and ϕ is convenient since it is the same as the traditional representations of TDHF equation in the non-deformed case. Since the equations of motion (equations (26) and (27)) are generalized Hamiltonian equations, the TDHF time evolution can be seen as trajectories in a phase space θ and ϕ. Other representations can also be obtained, and an interesting one, which has been introduced by the authors of [6], directly relates the phase-space variables to the one-body density elements.

$$\beta = 1 - 2\rho_{pp} \qquad \gamma = \frac{\rho^2_{p-p} - \rho^2_{-pp}}{2\mathrm{i}\rho_{pp}\rho_{-p-p}}. \tag{30}$$

In the non-deformed case this parametrization corresponds to a canonical transformation of the θ, ϕ pair. We will show some trajectories in the (β, γ) plane in the next section.

The correlation parameter Δ is also obtained for the TDHF approximation where (16) and the above operators for ρ_{pp} and ρ_{p-p} are used. Our results are considered in the next section.

4. Results and conclusions

In sections 2 and 3 we have calculated the one-body density operator ρ and the correlation parameter Δ for the exact case and the TDHF approximation. We have plotted these functions versus time in figures 1 and 2.

We have studied both possibilities for χ, i.e. we have chosen one value for $\chi < 1$ and another one for $\chi > 1$, $\chi = 1$ being the critical point where the non-deformed Lipkin model shows a phase transition.

For $\chi = 0.7$, we have fixed as our initial condition $E/N = -0.304$ MeV and for $\chi = 2.5$, we have fixed $E/N = -0.271$ MeV.

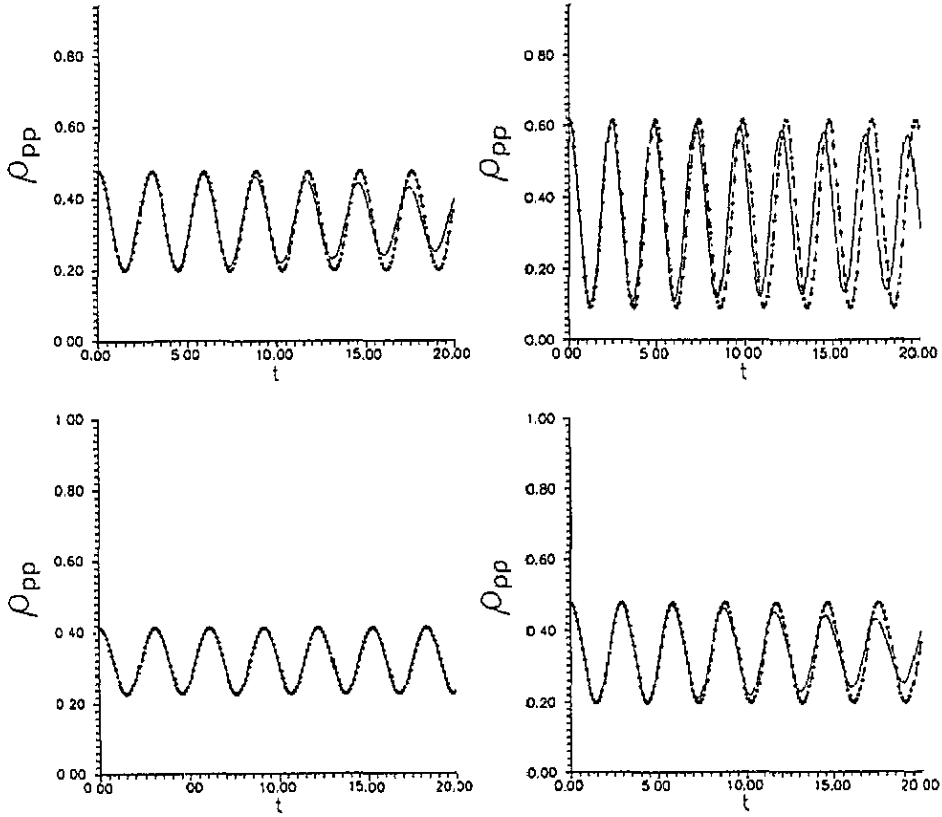

Figure 1. The evolution in time of ρ_{pp} is shown for $q = 1$ in the upper figures and for $q = 1.08$ in the lower figures. The figures on the left have been calculated with $\chi = 0.7$ and on the right with $\chi = 2.5$. The full curve stand for the exact calculation and the curves with crosses for the TDHF calculation.

In figure 1 we show the evolution in time of ρ_{pp} for $q = 1$ in the upper figures and for $q = 1.08$ in the lower figures. The figures on the left have been calculated with $\chi = 0.7$ and on the right with $\chi = 2.5$. Comparing the exact and the TDHF evolution in time of ρ_{pp} for $q = 1$, which is the case investigated in [6], we obtain reasonable results, which improve considerably when we look at the results obtained for $q = 1.08$. This is true either for $\chi = 0.7$ or for $\chi = 2.5$.

In figure 2 we have plotted Δ versus time for the exact case and the TDHF approximation for $q = 1$ in the upper figures and for $q = 1.08$ in the lower figures. The figures on the left have once again been calculated with $\chi = 0.7$ and on the right with $\chi = 2.5$.

Notice that for $q = 1$ the TDHF result is always equal to zero. For $q \neq 1$ we can see that even for the initial state we have correlations clearly indicating that the coherent deformed state is not a Slater determinant. It is interesting to note that in the TDHF approximation the Δ oscillates close to the initial value, while in the exact case we can have a large increase in fluctuations. When the q-parameter increases the amplitude of the oscillating fluctuations decreases for the two cases and again we obtain results closer to each other. Those results seem to indicate that the increasing deformation affects the dynamics in such a way that we have no more correlations than those introduced kinematically by the initial coherent state.

Finally, we have plotted trajectories in the (β, γ) phase space, the points defined by

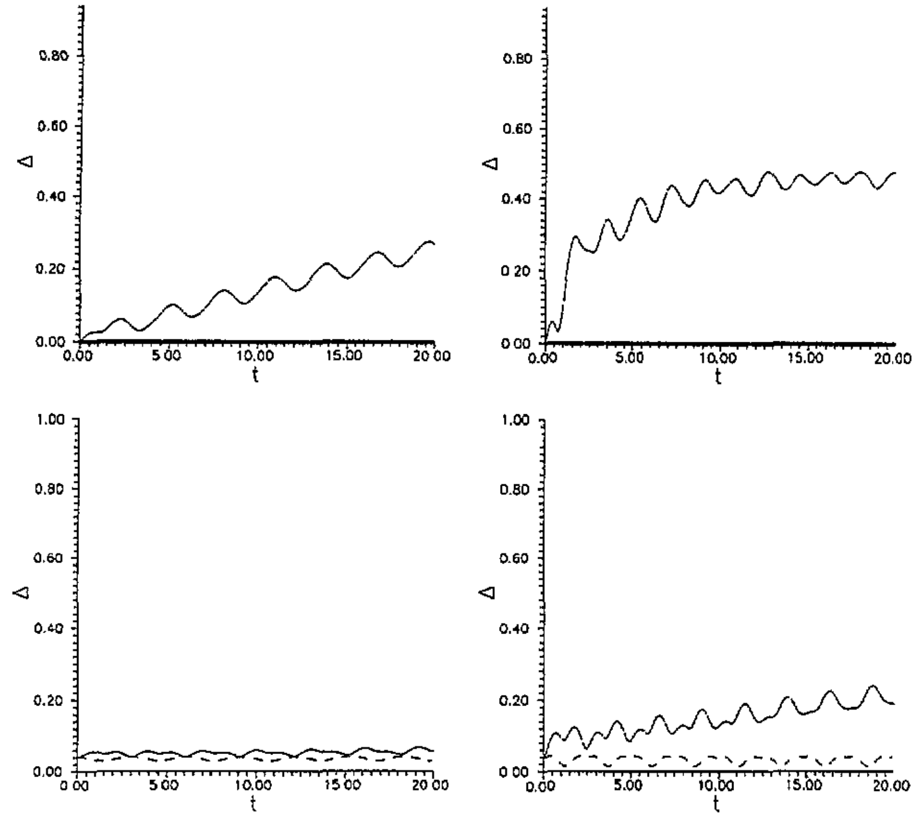

Figure 2. Δ is plotted versus time for the exact case (full curve) and the TDHF approximation (broken curve) for $q = 1$ in the upper drawings and for $q = 1.08$ in the lower drawings. The figures on the left have been calculated with $\chi = 0.7$ and on the right with $\chi = 2.5$. Notice that for $q = 1$ the TDHF result is always equal to zero.

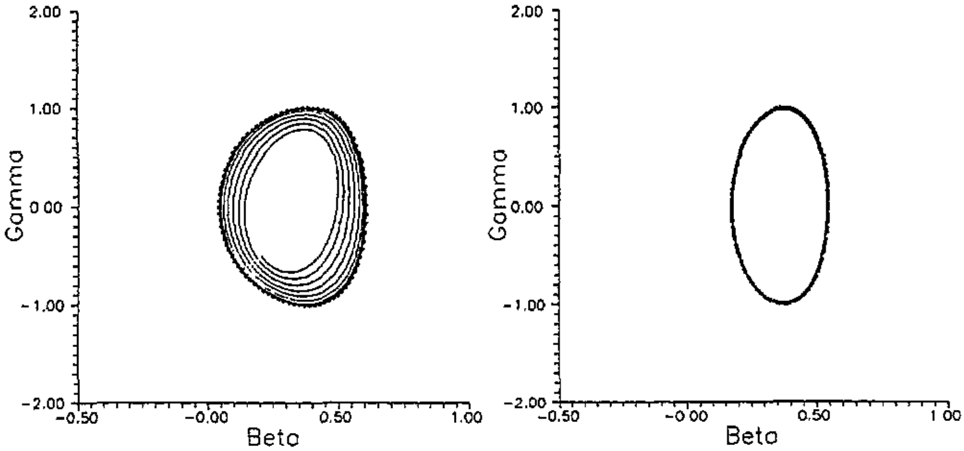

Figure 3. γ is plotted in function of β for $\chi = 0.7$. In the left part of the figure ($q = 1$), the full curve stands for the exact case and the line with crosses for the TDHF result. In the right part $q = 1.08$ and the exact and TDHF results coincide.

(30). The one-body densities defining the points of the trajectories are calculated through the exact (equations (11) and (12)) and TDHF (equations (28) and (29)) time evolution.

In figure 3 we observe the trajectories followed by the system when $\chi = 0.7$. In the upper part of the figure ($q = 1$), the full curve stands for the exact case and the curve with crosses stands for the TDHF results. In the lower part of figure 3 we have $q = 1.08$ and the exact and TDHF results coincide. We observe that the dispersion present in the $q = 1$ case disappears when deformation is introduced. For $\chi = 2.5$ we obtain similar patterns but the dispersion, although decreasing, remains in the deformed case. The trajectories are very instructive since as long as the variables (β, γ) depend on all the matrix elements of ρ, the agreement obtained between the exact and TDHF solutions strongly suggests that, for some energy per particle, the q-deformation maximizes the overlap between the variational solution and the exact one.

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Appendix

Here, we introduce some important quantities related to the $su_q(2)$ algebra, whose generators obey the following commutation relations:

$$[J_+, J_-] = [2J_z] \qquad [J_z, J_\pm] = \pm J_\pm \tag{A.1}$$

where

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}} \tag{A.2}$$

and q is the deformation parameter such that when $q \to 1$, $[x] = x$. The above operators, when applied to a basis $|jm\rangle$ of the carrier space V^j of the representation T^j of $su_q(2)$, yield

$$J_z|jm\rangle = m|jm\rangle$$

$$J_\pm|jm\rangle = \sqrt{[j \mp m][j \pm m + 1]}|jm \pm 1\rangle$$

with $m = -j, -j+1, \ldots, j$ and $j = 0, 1/2, 1 \ldots$.

The q-analogues of the $su(2)$ coherent states [7] are given by

$$|z\rangle = e_q^{\bar{z}J_+}|j - j\rangle \tag{A.3}$$

where the q-exponential is given by

$$e_q^x = \sum_{n=0}^{\infty} \frac{x^n}{[n]!} \tag{A.4}$$

with $[m]! = [m][m-1]\ldots[1]$. Notice that $|z\rangle$ is a state belonging to the $su_q(2)$ space V^j and its normalization is

$$\langle z|z\rangle = [1(+)z\bar{z}]^{2j} = \prod_{k=0}^{2j-1}(1 + q^{2k-2j+1}z\bar{z}) \tag{A.5}$$

where j is related to the number of particles N considered in the system and the q-binomial is given by

$$[a(\pm)b]^m = \sum_{k=0}^{m} \begin{bmatrix} m \\ k \end{bmatrix} a^{m-k}(\pm b)^k$$

where

$$\begin{bmatrix} m \\ k \end{bmatrix} = \frac{[m]!}{[m-k]![k]!} . \tag{A.6}$$

We also need to define the $su_q(2)$ operators in the Bargmann space [9]:

$$\begin{aligned} \langle z|J_z|\psi\rangle &= \left(z\frac{\partial}{\partial z} - j\right)\langle z|\psi\rangle \\ \langle z|J_+|\psi\rangle &= \left(-q^{-2j}z^2 D_z + [2j]zL_{q^{-1}}\right)\langle z|\psi\rangle \\ \langle z|J_-|\psi\rangle &= D_z\langle z|\psi\rangle \end{aligned} \tag{A.7}$$

where $|\psi\rangle$ is an arbitrary state in the space V^J and

$$D_z f(z) = \frac{f(qz) - f(q^{-1}z)}{(q - q^{-1})z}$$

is the q-derivative and

$$L_{q^{-1}} f(z) = f(q^{-1}z) .$$

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