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Compositeness effects in the Bose–Einstein condensation

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Abstract

Small deviations from purely bosonic behaviour of trapped atomic Bose–Einstein condensates are investigated with the help of the quon algebra, which interpolates between bosonic and fermionic statistics. A previously developed formalism is employed to obtain a generalized version of the Gross–Pitaevskii equation. The depletion of the amount of condensed atoms for the case of repulsive forces between atoms in the trap can be accounted for by a universal fitting of the deformation parameter.

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1. Introduction

In many physical problems one has to deal with a large number of identical particles that are not of fundamental character but which are known to be composed by a bound system of several fermions. Examples include systems of identical atoms, molecules or nuclei. If the number of 'fundamental' fermions contained in the composite particle is odd, it is a fermion, otherwise it is a boson. In many situations the internal structure of the composite particle can be ignored and the system as a whole treated as a collection of interacting or noninteracting point-like particles. This is the case for instance, in the theories of Bose–Einstein condensation (BEC) of trapped bosonic gases [1]. Another example is provided by electron–hole bosonic states in semiconductors, called excitons [2]. In such systems, the bosons have internal structure and finite size, i.e., they are composite bosonic particles. The rationale for neglecting the internal structure of the atoms in atomic BEC is that one is dealing with a very dilute system in the trap. The low-density regime makes it very improbable that the internal structures of the atoms overlap in the trap, since the average distance between atoms in typical condensates is several times the size of an atom. For excitons, the situation is not as favourable as in atomic BEC and effects of the internal structure of the bosons might play an important role [2]. A departure from the purely bosonic behaviour of the atoms in a trap might occur in situations where the central density of the condensate grows beyond some critical value.

The aim of the present paper is to set up a framework to evaluate the departure from purely bosonic behaviour of a BEC of composite particles. A complete theory aimed at such a task should include all the possible degrees of freedom for the constituent particles, which is in general highly prohibitive from the computational point of view. In the present paper, we use a phenomenological approach, making use of the concept of *quons* [3]. Quons are particles that are neither bosons, nor fermions, and the quon creation and annihilation operators obey a particular algebra that interpolates between Fermi and Bose algebras. The quon algebra is in fact a deformation of the Fermi and Bose algebras, and is such that when a parameter (q) runs from -1 and +1, it interpolates between the Fermi and Bose algebras.

Recently, a systematic way to build a many-body quon state has been discussed [3, 4] and a general formula for a normalized many-quon symmetric state [4] has been found. The developed formalism was then applied to simple physical systems for which a comparison to the more usual quantum algebra [5] results was made. The formalism and applications involving the antisymmetric subspace (fermion-like particles) were also considered [6].

The use of the symmetric subspace, and q close enough to +1, allows us to describe in a very natural way the departure from purely bosonic behaviour of systems of composite bosons. In section 2, we present a brief discussion on the description of a composite boson built from two non-identical fermions and provide a connection with the quon algebra. In order to apply such ideas to the BEC in trapped gases, we derive in section 3 a quonic version of the Gross–Pitaeviskii (GP) equation, which we denote qGP. In the limit of $q = 1$, the qGP equation reduces to the usual GP equation, widely used in the literature [1]. Then, in section 4 we present some numerical results in order to estimate the effects implied by our model in BEC with trapped atoms. Conclusions and future perspectives are presented in section 5.

2. Relation between composite particles and quons

Most of the results found in this section were discussed in detail in [4, 7], so we present below the main equations and ideas. Let us consider a composite boson state with quantum number α as a bound state of two distinct fermions

$$A_\alpha^\dagger|0\rangle = \sum_{\mu\nu} \Phi_\alpha^{\mu\nu} a_\mu^\dagger b_\nu^\dagger |0\rangle \tag{1}$$

where $\Phi_\alpha^{\mu\nu}$ is the Fock-space bound-state amplitude, $a_\mu^\dagger$ and $b_\mu^\dagger$ are the fermion creation operators, and $|0\rangle$ is the no-particle state (vacuum). The quantum number α stands for the centre of mass momentum, the internal energy, the spin and other internal degrees of freedom of the composite boson. The μ and ν stand for the space and internal quantum numbers of the constituent fermions. The sum over μ and ν is to be understood as a sum over discrete quantum numbers and an integral over continuous variables. In equation (1) the fermion creation and annihilation operators satisfy canonical anti-commutation relations and for convenience we work with normalized amplitudes $\Phi_\alpha^{\mu\nu}$, such that

$$\langle\alpha|\beta\rangle = \sum_{\mu\nu} \Phi_\alpha^{\mu\nu *} \Phi_\beta^{\mu\nu} = \delta_{\alpha,\beta}. \tag{2}$$

Using the fermion anti-commutation relations and the Fock-space amplitude normalization, one can easily show that the composite boson operators satisfy the following commutation relations:

$$[A_\alpha, A_\beta] = \left[A_\alpha^\dagger, A_\beta^\dagger\right] = 0 \tag{3}$$

$$\left[A_\alpha, A_\beta^\dagger\right] = \delta_{\alpha,\beta} - \Delta_{\alpha\beta} \tag{4}$$

where $\Delta_{\alpha\beta}$ is given by

$$\Delta_{\alpha\beta} = \sum_{\mu\nu} \Phi_\alpha^{\mu\nu *} \left(\sum_{\mu'} \Phi_\beta^{\mu'\nu} a_{\mu'}^\dagger a_\mu + \sum_{\nu'} \Phi_\beta^{\mu\nu'} b_{\nu'}^\dagger b_\nu \right). \tag{5}$$

The composite nature of the bosons is evident from the presence of $\Delta_{\alpha\beta}$, which is a sort of 'deformation' of the canonical boson algebra. The effect of this term becomes unimportant in the infinite tight binding limit, i.e., in the limit of point-like bosons.

The quon algebra is defined by the deformed commutation relation

$$A_\alpha A_\beta^\dagger - q A_\beta^\dagger A_\alpha = \delta_{\alpha,\beta} \tag{6}$$

where q is the deformation parameter of the algebra, A_α annihilates the vacuum $A_\alpha|0\rangle = 0$. Polynomials in the creation operators acting on the vacuum form a Fock-like space of vectors [8], i.e., the quonic Fock space (note that we are using the same symbols for both the composite and quon algebra annihilation/creation operators). If one writes $q = 1 - x$, the deformed commutator, equation (6), can be written as

$$\left[A_\alpha, A_\beta^\dagger\right] = \delta_{\alpha\beta} - x A_\alpha^\dagger A_\beta. \tag{7}$$

The (transition) number operator, $N_{\alpha\beta}$ has a complicated formal structure and should be viewed as a many-body quon operator. Its complete definition is given in [3] (and references therein) and we show below the first two terms of its expansion:

$$N_{\alpha\beta} = A_\alpha^\dagger A_\beta + (1-q^2)^{-1} \sum_\gamma \left(A_\gamma^\dagger A_\alpha^\dagger - q A_\alpha^\dagger A_\gamma^\dagger\right)(A_\beta A_\gamma - q A_\gamma A_\beta) + \cdots. \tag{8}$$

The important result to us is that the above operator follows the commutation relations:

$$\left[N_{\alpha\beta}, A_\alpha^\dagger\right] = A_\alpha^\dagger \delta_{\alpha\beta} \qquad [N_{\alpha\beta}, A_\alpha] = -A_\alpha \delta_{\alpha\beta}. \tag{9}$$

We also define [5]:

$$[N] = \frac{1-q^N}{1-q}. \tag{10}$$

The similarity between equations (7) and (4) becomes evident if we follow the approach of [9]. There, the amplitudes in equation (5), written in momentum space, are approximated by a rectangular distribution over a certain region of space, for which the deformation term acquires the form

$$\Delta_{\alpha\alpha} = k N_F \tag{11}$$

where k is a constant and N_F is the operator for the total number of fermions in the system in the state α. In the quon algebra, the deformation term is $x A_\alpha^\dagger A_\alpha = x[N_{\alpha\alpha}]$, which is a relation obeyed by any q-deformed algebra [5]. In the general case, the product of fermion operators $a_{\mu'}^\dagger a_\mu$ and $b_\mu^\dagger b_{\nu'}$ weighted by the Φ in equation (5) is effectively modelled by the term $x A_\alpha^\dagger A_\beta$ in equation (7).

Since we wish to describe a system of 'identical' composite bosons, we impose that the state vectors of a many-body composite particle system are invariant by the permutation of the particle indices. So we assume that the physical subspace which is adequate for the description of a bosonic composite system is composed only of totally symmetric states, which means that we have to project out from the basis of states only totally symmetric states.

It is possible to show that the most general symmetric basis state for a system of N quons can be written as [4]

$$|n_\alpha n_\beta n_\gamma \ldots ; S\rangle = \sqrt{\frac{n_\alpha ! n_\beta ! n_\gamma ! \ldots}{N![N]!}} \widehat{S}_N \left(A_\alpha^\dagger\right)^{n_\alpha} \left(A_\beta^\dagger\right)^{n_\beta} \left(A_\gamma^\dagger\right)^{n_\gamma} \ldots |0\rangle \tag{12}$$

where $\widehat{S}_N$ is an operator that generates all possible combinations that are symmetric under the permutation of any of the creation operators, i.e.,

$$\widehat{S}_{\mathrm{N}} \left(A_\alpha^\dagger\right)^{n_\alpha} \left(A_\beta^\dagger\right)^{n_\beta} \left(A_\gamma^\dagger\right)^{n_\gamma} \ldots |0\rangle \equiv \frac{1}{n_\alpha ! n_\beta ! n_\gamma ! \ldots} \sum_{P_{\mathrm{N}}} A_1^\dagger A_2^\dagger \ldots A_{n_\alpha}^\dagger A_{n_\alpha+1}^\dagger \ldots A_{n_\alpha+n_\beta+1}^\dagger \ldots A_N^\dagger |0\rangle \tag{13}$$

where $n_\alpha + n_\beta + n_\gamma + \cdots = N$ and the summation runs over all the $N!$ permutations, P_{N}, in the indices $1, 2, \ldots, N$. We order these indices such that $1, 2, \ldots, n_\alpha$ correspond to the α-state, $n_\alpha + 1, n_\alpha + 2, \ldots, n_\alpha + n_\beta$ to the β-state and so on. The factorials in the denominator account for repeated terms in the summation and [5, 10] $[N]! = [N][N-1]\ldots[2][1]$ with $[0]!=1$. Another important result that we are going to use next is the following [4]:

$$A_\alpha |n_\alpha n_\beta n_\gamma \ldots ; S\rangle = \sqrt{\frac{[N]}{N}} \sqrt{n_\alpha} |n_\alpha - 1, n_\beta n_\gamma \ldots .; S\rangle. \tag{14}$$

Using now equation (14) twice, it is easy to show that

$$A_\alpha A_\beta |n_\alpha n_\beta n_\gamma \ldots ; S\rangle = A_\beta A_\alpha |n_\alpha n_\beta n_\gamma \ldots ; S\rangle. \tag{15}$$

Taking the Hermitian conjugate of the above equation we conclude that the commutation relations of equation (3) are now valid also for quons if we restrict ourselves to the physical subspace, i.e., the one built only from the symmetric subspace. In this way, the analogy between a composite particle and a quon is complete (in the weak sense).

In order to give a physical meaning for the deformation parameter x (or q), in [7], a system consisting of N composite bosons in a large box of volume V at zero temperature has been treated. The closest analogue of the ideal gas ground state is the N quons state:

$$|N\rangle = \frac{1}{\sqrt{[N]!}} \left(A_0^\dagger\right)^N |0\rangle. \tag{16}$$

One can show that the expectation value of $A_0^\dagger A_0$ in the state $|N\rangle$ is then

$$N_0 = \langle N | A_0^\dagger A_0 | N \rangle = [N] \tag{17}$$

where $[N]$ is defined in equation (10). So, there is a depletion on the amount of condensed bosons due to Pauli principle effects among the composite bosons. As said before, in [7] an estimation for the deformation parameter x is made for a free ideal gas in terms of macroscopic parameters of the system. Other recent calculations to estimate the effects of the internal structure of the boson were done in [2, 11].

3. The Gross–Pitaeviskii equation for composite bosons

We now use the quon algebra formalism in the BEC. We consider a system of N composite bosons interacting in a spherical harmonic oscillator trap. We assume that the effective

Hamiltonian describing such a system is given by [1]

$$\begin{aligned} H &= T + V + V_{\text{trap}} \\ &= \sum_{\alpha,\beta} \langle \alpha|T|\beta\rangle A_\alpha^\dagger A_\beta + \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta|V|\gamma\delta\rangle A_\alpha^\dagger A_\beta^\dagger A_\gamma A_\delta + \sum_{\alpha,\beta} \langle \alpha|V_{\text{trap}}|\beta\rangle N_{\alpha\beta} \end{aligned} \tag{18}$$

where T, V_{trap} and V correspond to the kinetic energy, trap harmonic oscillator potential and the interaction among the composite bosons, respectively. Note that for the kinetic and interaction terms we preserve the usual one- and two-body character of the corresponding operators, but we write the trap potential in terms of the number operator. Also, as usual in the Gross–Pitaevskii dynamics, we take

$$T(\vec{x}) = -\frac{\hbar^2}{2m}\triangle_{\vec{x}} \qquad V(\vec{x},\vec{y}) = g\delta(\vec{x}-\vec{y}) \tag{19}$$

where g is a constant. To obtain the equation describing the condensate of composite bosons we follow the usual Hartree–Fock approach [12]. So we assume for the ground-state trial function a completely symmetric product wavefunction:

$$|\psi, S\rangle = \frac{\left(A_0^\dagger\right)^N}{\sqrt{[N]!}}|0\rangle. \tag{20}$$

We then impose the variational principle

$$\langle \psi, S|H|\delta\psi, S\rangle = 0 \tag{21}$$

where the arbitrary variational symmetrized state has the form

$$|\delta\psi, S\rangle = \hat{S}A_\mu^\dagger A_0|\psi, S\rangle \qquad (\mu \neq 0) \tag{22}$$

and the symbol $\hat{S}$ is a symmetrizer operator as defined in section 2. Equation (21) is equivalent to the expression

$$\langle \psi, S|\sum_{\alpha\beta}\left(\langle \alpha|T|\beta\rangle A_\alpha^\dagger A_\beta + \frac{1}{2}\sum_{\gamma\delta}\langle \alpha\beta|V|\gamma\delta\rangle A_\alpha^\dagger A_\beta^\dagger A_\gamma A_\delta + \langle \alpha|V^{\text{trap}}|\beta\rangle N_{\alpha\beta}\right)|\delta\psi, S\rangle = 0. \tag{23}$$

From equations (14) and (9), one obtains the matrix elements

$$\begin{aligned} &\langle \psi, S|A_\alpha^\dagger A_\beta|\delta\psi, S\rangle = \frac{[N]}{N}\sqrt{N}\delta_{\alpha 0}\delta_{\beta\mu} \\ &\langle \psi, S|N_{\alpha\beta}|\delta\psi, S\rangle = \sqrt{N}\delta_{\alpha 0}\delta_{\beta\mu} \\ &\langle \psi, S|A_\alpha^\dagger A_\beta^\dagger A_\gamma A_\delta|\delta\psi, S\rangle = \frac{[N]}{N}\frac{[N-1]}{N-1}\sqrt{N}(N-1)(\delta_{\alpha 0}\delta_{\beta 0}\delta_{\gamma\mu}\delta_{\delta 0} + \delta_{\alpha 0}\delta_{\beta 0}\delta_{\gamma 0}\delta_{\delta\mu}). \end{aligned}$$

Using these expressions in equation (23), one obtains

$$\frac{[N]}{N}T_{0\mu} + V_{0\mu}^{\text{trap}} + \frac{[N][N-1]}{N}V_{000\mu} = 0. \tag{24}$$

Therefore, the variational principle leads in coordinate space to the equation

$$\left[-\frac{\hbar^2}{2m}\triangle_{\vec{x}} + \frac{N}{[N]}V^{\text{trap}}(\vec{x}) + g[N-1]|\phi(\vec{x})|^2\right]\phi(\vec{x}) = \epsilon\phi(\vec{x}). \tag{25}$$

This equation may be interpreted as a generalization of the Gross–Pitaevskii equation to quons and, as mentioned previously, will be denoted as qGP. The interaction constant can be written as $g = 4\pi\hbar^2 a/m$, where a is the s-wave scattering length for the two-atom collision.

4. The solution of the quon Gross–Pitaeviskii equation and applications

Many authors have recently presented different methods to solve the usual GP equation. Here, we follow a variational approach, in which we expand the ground-state wavefunction in a three-dimensional harmonic oscillator basis with angular momentum $l = 0$. Good convergence has been achieved within the method and we were able to reproduce to very good accuracy results obtained in the literature with other methods when we go to the limit $q = 1$.

As an application, we consider the case of a repulsive interaction. In this case, the number of atoms in the trap can reach large numbers (N up to $\sim 10^7$), which can raise the question of validity for the use of the GP equation for such high densities. On the other hand, some recent experimental techniques [13] provide a way to increase by orders of magnitude the atomic scattering length a. In a recent calculation [14], effects that go beyond the usual GP (or mean field) solution were also considered and shown to lead to a systematic, small increase in the chemical potential of the condensate. In our formalism we may obtain the same behaviour by preserving the original GP dynamics but relaxing the condition that the particles are true bosons. To see how this happens, we now rewrite equation (25) in a slightly different form

$$\left[H_{\mathrm{osc}} + \left(\frac{N}{[N]} - 1\right) V^{\mathrm{trap}}(\vec{x}) + g[N-1]|\phi(\vec{x})|^2\right]\phi(\vec{x}) = \epsilon\phi(\vec{x}) \tag{26}$$

where H_{osc} is the usual three-dimensional harmonic oscillator Hamiltonian. Based on our discussion in section 2, one may interpret the number of condensed atoms as $N_0 = [N]$. We then conclude that only the term proportional to $N/[N] - 1$ differs from the usual GP equation. However, for q close enough to 1, this term is small ($\ll 1$) even for large values of N, and therefore one may treat this term as a perturbation to the non-deformed solution. At this point it is worthwhile to note that this term will always increase the energy of the condensate by a small amount. Of course, the increase will depend on the value of q (or x) used. In order to make a phenomenological estimation of the effect of this perturbation we relate the depletion of the condensate to the calculation presented in section 3 of [1]. There, the depletion is given by

$$\frac{N - N_0}{N_0} = \frac{5\sqrt{\pi}}{8}\sqrt{a^3 n(0)} \tag{27}$$

where $n(0)$ is the central ($r = 0$) density of the condensate. Taking $N_0 = [N]$ and expanding in powers of x, we obtain to lowest order

$$x \cong \frac{10\sqrt{\pi}}{8N}\sqrt{a^3 n(0)}. \tag{28}$$

Note that a dependence of the deformation parameter on the number of atoms (or on the density) appears very naturally here. As discussed in [7], an N-independent deformation parameter x is physically reasonable only for very low-density systems. In the present situation of a repulsive interaction, the number of atoms in the trap can be very large and our above prescription seems to be more adequate.

In order to perform numerical calculations, one needs $n(0)$, which can be taken from the $x = 0$ solution of the GP equation and the value for N, which in turns depends on x. However, for our purposes here we may evaluate the order of magnitude of x making $N = N_0$ in equation (28). Also, we use $a/b_t = 5 \times 10^{-2}$, which is consistent with recent experimental conditions as explained in [13] and with b_t being the trap oscillator length. In table 1 we present our numerical results for the chemical potential ϵ in units of the trap oscillator energy spacing $\hbar\omega_t$, for different N_0 values. Note that, although our initial conditions are different from the ones chosen for the calculations in [14], the results are qualitatively equivalent, in the sense that we get always a bigger value for the chemical potential, as compared to the usual GP

Table 1. Chemical potential ϵ—in units of $\hbar\omega_t$—of the condensate for four values of the number of atoms N_0, using the usual GP formalism and the qGP equation. The values of x used in each case are also shown and were obtained as explained in the text.

N_0	$\epsilon_{\rm GP}$	$\epsilon_{\rm qGP}$	x
1×10^3	7.31	7.47	1.0×10^{-4}
1×10^4	17.84	18.32	1.3×10^{-5}
1×10^5	44.59	46.69	2.0×10^{-6}
1×10^6	111.94	131.16	5.1×10^{-7}

solution. Also, although the value of x decreases about one order of magnitude as N increases by about the same factor, the correction on the energy increases with N through the factor $N/[N] = N/N_0$, once the compositeness of the constituent boson should be a cumulative effect. This feature is self-contained in the parametrization given by equation (28), which stresses the fact that the deformation depends on N and also on the relative volume of the boson with respect to the volume of the system.

5. Conclusions

We have considered in this work the quon algebra to describe in an effective and phenomenological way the departure from purely bosonic behaviour of a system of composite bosons. The formalism was developed previously and relies on the projection of the whole quonic space onto the symmetric subspace. The main idea is to preserve the bosonic behaviour and leave to the deformation parameter the description of possible deviations. As a specific application we have considered the derivation of the Gross–Pitaeviskii equation within the quon algebra, which can be done in a straightforward way using our formalism. The interpretation of the modified Gross–Pitaeviskii equation obtained is consistent with our initial qualitative considerations.

For a numerical calculation we have obtained the chemical potential for the case of a repulsive force between trapped atoms. This is a more favourable situation to test our model, since recently it became experimentally feasible to create condensates with a much larger number of atoms as compared to the attractive case. Using a phenomenological estimation for the deformation parameter, for which a density dependence arises very naturally, we are able to calculate the correction in the chemical potential.

Natural extensions of the present work would include the investigation of the effect of the q-deformation on other observables of the BE condensates, as for example the well-known collapse for attractive forces [15]. Also, there are many other interesting systems for which the quon algebra could be useful to describe deviations from purely bosonic behaviour of many-body systems of composite bosons. One example, as stated in section 1, is the case of excitons [2]. Work in these directions is underway.

Finally, we would like to mention that the formal relation between composite particles and the quon algebra deserves a more profound investigation. As stated in section 2, their relationship here is based on heuristic and approximated expressions. A possible way to establish a formal equivalence could start with a mapping from the fermionic to the q-deformed quonic space. In this respect, some work has already been done [16], though not yet directly applied to the problem addressed in the present paper.

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