Dipolar Bose gas with three-body interactions at finite temperature

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Received 12 May 2017, revised 12 November 2017
Accepted for publication 20 November 2017
Published 29 December 2017

Abstract
We investigate effects of three-body contact interactions on a trapped dipolar Bose gas at finite temperature using the Hartree–Fock–Bogoliubov approximation. We analyze numerically the behavior of the transition temperature and the condensed fraction. Effects of the three-body interactions, anomalous pair correlations and temperature on the collective modes are discussed.

Keywords: Bose–Einstein condensate, three-body interactions, dipole–dipole interactions, HFB theory

(Some figures may appear in colour only in the online journal)

1. Introduction

Recently, Bose–Einstein condensates (BEC) with dipole–dipole interactions (DDI) have received considerable attention both experimentally and theoretically [1–4]. Dipolar quantum gases, in stark contrast to dilute gases of isotropic interparticle interactions, offer fascinating prospects of exploring ultracold gases and novel many-body quantum phases with atomic interactions that are long-range and spatially anisotropic. Major efforts have been directed towards the ground states properties and elementary excitations of such dipolar systems at both zero and finite temperatures [5–17].

Three-body interactions (TBI) are ubiquitous and play an important role in a wide variety of interesting physical phenomena, and yield a new physics and many surprises not encountered in systems dominated by the two-body interactions. Recently, many experimental and theoretical techniques have been proposed to observe and realize the TBI in ultracold Bose gas [18–22]. For instance, inelastic three-body processes, including observations of Efimov quantum states and atom loss from recombination have been also reported in [23–27]. Few-body forces induce also nonconventional many-body effects such as quantum Hall problems [28] and the transition from weak to strong-pairing Abelian phase [29, 30]. In 2002, Bulgac [31] predicted that both weakly interacting Bose and Fermi gases with attractive two-body and large repulsive TBI may form droplets. Dasgupta [32] showed that if the two-body interactions were attractive, the presence of the TBI leads to a nonreversible BCS-BEC crossover. Furthermore, many proposals dealing with effects of effective TBI in ultracold bosonic atoms in an optical lattice or a superlattice are reported in [33–36]. Moreover, it has been found that the TBI in dilute Bose gases may give rise to considerably modify the collective excitations at both zero and finite temperatures [37–39], the transition temperature, the condensed depletion and the stability of a BEC in one (1D) and two (2D)-dimensional trapping geometries [40, 41].

However, little attention has been paid to effects of TBI on dipolar BECs. For instance, it has been argued that the TBI play a crucial role in the stabilization of the supersolid state in 2D dipolar bosons [42] and in the quantum droplet state of 3D BEC with strong DDI [43–47].

Our main aim here is to study effects of the TBI on weakly interacting dipolar Bose gases in a pancake trap at finite temperature. To this end, we employ the full Hartree–Fock–Bogoliubov (HFB) approximation. This approach which takes into account the pair anomalous correlations has been extensively utilized to describe the properties of both homogeneous and inhomogeneous Bose condensed gases with contact interactions [48]. We will show in particular how the interplay between the DDI, the TBI and the temperature can enhance the density profiles, the condensed fraction and the collective modes of the system.

The rest of the paper is organized as follows. In section 2, we introduce the full HFB formalism for dipolar BECs with TBI. We discuss also the issues encountered in our model and present the resolution of these problems. Section 3 is devoted...
to presenting and discussing our numerical results. Our conclusions are drawn in section 4.

2. Three-body model for dipolar bosons

Consider a dipolar BEC with contact repulsive two-body interactions and TBI confined in a pancake-shaped trap with the dipole moments of the particles oriented perpendicular to the plane. It is straightforward to check that the condensate wavefunction \( \Phi(r) = \langle \hat{\psi}(r) \rangle \), with \( \hat{\psi}(r) \) being the Bose field operator, satisfies the generalized Gross–Pitaevskii (GP) equation [47]

\[
\frac{i\hbar}{\partial t} \hat{\psi}(r, t) = \{-\hbar^2/2m\} \Delta + U(r) \hat{\psi}(r, t) + \frac{\hbar^2}{2} \hat{n}(r, t) \hat{\psi}(r, t) + \hat{n}(r, t) \Phi^2(r, t) \hat{\psi}(r, t)
\]

where \( U(r) = -\hbar^2/2m \Delta + U(r) \) is the single particle Hamiltonian, \( m \) is the particle mass, \( U(r) = m \omega_x^2 (x^2 + \lambda^2 z^2)/2 \), \( \omega_x \) is the trapping frequencies in the axial and radial directions. The two-body coupling constant is defined by \( g_2 = 4\pi\hbar^2a/m \) with \( a \) being the s-wave scattering length which can be adjusted using a magnetic Feshbach resonance. The three-body coupling constant \( g_3 \) is in general a complex number with \( \text{Im}(g_3) \) describing the three-body recombination loss and \( \text{Re}(g_3) \) accounting for the three-body scattering parameter. In the present paper, we do not consider the three-body recombination terms i.e. \( \text{Im}(g_3) = 0 \), so the system is stable which is consistent with recent experiments [26, 43]. The DDI potential is \( V_{DDI}(r) = C_{DDI}(1 - 3 \cos^2 \theta)/(4\pi r^4) \), where \( C_{DDI} = M_0 M^2/(2d^2/\epsilon_0) \) is the magnetic (electric) dipolar interaction strength, and \( \theta \) is the angle between the relative position of the particles and the direction of the dipole. The condensed, noncondensed and anomalous densities are defined, respectively as \( n_c(r) = |\Phi(r)|^2, \hat{n}(r) = \langle \hat{\psi}^\dagger(r) \hat{\psi}(r) \rangle \) and \( \hat{n}(r) = \langle \hat{\psi}^\dagger(r) \hat{\psi}(r) \hat{\psi}(r) \rangle \). The total density is given by \( n(r) = n_c(r) + \hat{n}(r) \). The terms \( \hat{n}(r, r') \) and \( \hat{n}(r, r') \) are respectively, the normal and the anomalous one-body density matrices which account for the dipole exchange interaction between the condensate and noncondensate.

Equation (1) describes the coupled dynamics of the condensed, noncondensed and anomalous components. For \( g_3 = 0 \), one recovers the generalized nonlocal finite temperature GP equation with two-body interactions. For \( \hat{n} = 0 \), equation (1) reduces to the HFB–Popov equation [10, 11, 47] which is a gapless theory. For \( \hat{n} = 0 \), it reduces to the standard GP equation that describes dipolar Bose gases only at zero temperature.

Upon linearizing equation (1) around a static solution \( \Phi_0 \), utilizing the parameterization \( \Phi(r, t) = \Phi_0(r) + \delta \Phi(r, t) \) \( e^{-i\omega t}/\hbar \), where \( \delta \Phi = \sum_k [u_k(r) e^{-i\omega t}/\hbar + v_k(r) e^{i\omega t}/\hbar] \) with \( \varepsilon_k \) being the Bogoliubov excitations energy. The quasi-particle amplitudes \( u_k(r) \) and \( v_k(r) \) satisfy the generalized nonlocal Bogoliubov–de-Gennes equations [47]:

\[
\varepsilon_k u_k(r) = \hat{\Lambda} u_k(r) + \int dr' V_d(r - r') n(r, r') u_k(r'),
\]

\[
\varepsilon_k v_k(r) = \hat{\Lambda} v_k(r) + \int dr' V_d(r - r') n(r, r') v_k(r'),
\]

where \( \hat{\Lambda} = \hbar^2/2m + 2g_2 n(r) + 3g_2 n_1(r) + 4n_2(r)n(r) + m^2(r) \Phi^2(r) + \hat{n}(r) \Phi^2(r)/2 + \int dr' V_d(r - r') n(r, r') - \mu, \hat{\Lambda} = g_3 [\Phi_0^2(r) + \hat{n}(r)] + g_3 [n_1^2(r) + 3\Phi_0^2(r)n(r) + 3\Phi_0^2(r)\hat{n}(r)], n(r, r') = \Phi_0^2(r')\Phi_0(r) + \hat{n}(r, r') \) and \( \hat{n}(r, r') = \Phi_0^2(r')\Phi_0(r) + \hat{n}(r, r') \). Equations (2) and (3) describe the collective excitations of the system. The normal and the anomalous one-body density matrices can be obtained by employing the transformation \( \hat{\psi} = \sum_k [u_k(r) \hat{b}_k + v_k(r) \hat{b}^\dagger_k] \)

\[
\hat{n}(r, r') = \sum_k [ [u_k^* (r') u_k (r) + v_k (r') v_k^* (r)] N_k (r) + v_k (r') v_k^* (r)],
\]

\[
\hat{n}(r, r') = - \sum_k [ [u_k (r') v_k^* (r) + u_k (r) v_k (r')] N_k (r) + u_k (r') v_k^* (r)],
\]

where \( N_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle = [\text{exp}(\varepsilon_k / \hbar T) - 1]^{-1} \) are occupation numbers for the excitations. The noncondensed and anomalous densities can simply be obtained by setting, respectively \( \hat{n}(r, r) = n(r, r) \) and \( \hat{m}(r, r) = \hat{m}(r, r) \) in equations (4) and (5).

From now on we assume that \( \hat{m}(r, r') = \hat{m}(r, r') \equiv 0 \) for \( r = r' \) [9, 10]. It is worth stressing that the omission of the long-range exchange term does not preclude the stability of the system [10, 12, 13, 47, 49–51].

As is well known, the full HFB theory sustains some hindrances notably the appearance of an unphysical gap in the excitations spectrum and the divergence of the anomalous density. In fact, this violation of the conservation laws in the HFB theory is due to the inclusion of the anomalous density which in general leads to a double counting of the interaction effects. The common way to circumvent this problem is to neglect \( \hat{m} \) in the above equations, which restores the symmetry and hence leads to a gapless theory, but this is nothing else than the Popov approximation. To go consistently beyond the Popov theory, one should renormalize the coupling constant taking into account many-body corrections for
scattering between the condensed atoms on the one hand and the condensed and thermal atoms on the other. Following the procedure outlined in \cite{52–56} we obtain
\[
g_{3}|\phi|^2\phi + g_{2}m\bar{\phi}^\ast + \frac{3}{2}g_{3}n_{c}\bar{m}\bar{\phi}^\ast
= g_{2}\left[1 + \frac{\bar{m}(1 + 3g_{3}n_{c}/g_{2})}{\bar{\phi}^2}\right]|\phi|^2\phi
= g_{df}|\phi|^2\phi. \tag{6}
\]
This spatially dependent effective interaction, \(g_{df}\) is somehow equivalent to the many-body \(T\)-matrix \cite{48}. A detailed derivation of \(g_{df}\), including the term \(g_{3}\), will be given elsewhere. It is easy to check that if one substitutes (6) in the HFB equations, we therefore, reinstate the gaplessness of the spectrum and the convergence of the anomalous density.

3. Numerical results

For numerical purposes, it is useful to set equations (1)–(6) into a dimensionless form. We introduce the following dimensionless parameters: the relative strength \(\epsilon_{dd} = C_{dd}/3g_{2}\) (\(\epsilon_{dd} = 0.16\) for Cr atoms) which describes the interplay between the DDI and short-range interactions, and \(\tilde{g}_{3} = g_{3}n_{c}/g_{2}\) describes the ratio between the two-body interactions and TBI. Throughout the paper, we express lengths and energies in terms of the transverse harmonic oscillator length \(l_{0} = \sqrt{\hbar/m\omega_{r}}\) and the trap energy \(\hbar\omega_{r}\), respectively.

Figure 1 shows that the noncondensed and the anomalous densities increase with the TBI which leads to reduce the condensed density. A careful observation of the same figure reveals that \(\tilde{\mu}\) is larger than \(\bar{\mu}\) at low temperature which is in fact natural since the anomalous density itself arises and grows with interactions \cite{57, 58}. When the temperature approaches the transition, \(\tilde{\mu}\) vanishes similarly to the case of a BEC with a pure contact interaction \cite{57, 58}.

In figure 2 we compare our prediction for the condensed fraction \(N_{c}/N\) with the HFB–Popov theoretical treatment and the noninteracting gas. As is clearly seen, our results diverge from those of the previous approximations due to the effects of the TBI. This means that both the condensed fraction and the transition temperature decrease with increasing the TBI. For instance, for temperatures of order half the critical temperature, the condensate fraction is shifted by 10% due to the TBI and the DDI. In absence of the TBI, the resulting condensate fraction is reduced by 5%. The critical temperature is changed only by 0.3% as is seen in the same figure. Note that the HFB–Popov theory without the TBI states that \(T_{c}\) is almost unchanged \cite{10}, while the analytical formula of \cite{59, 60} predicts a very small reduction of 0.51% in the critical temperature.

Before leaving this section, let us unveil the role of the TBI on the collective excitations. According to figure 3 we can observe that our results deviate from the HFB–Popov (which have also been found in \cite{10}) at \(T \gtrsim 0.72T_{c}\) for \(m = 0\) and 2 excitations. The reason of such a downward shift which enlarges as the temperature approaches \(T_{c}\), is the inclusion of both anomalous pair correlations and TBI. A similar behavior holds in the case of BEC with short-range interactions (see e.g. \cite{48}). Figure 3 depicts also that both the full HFB and the HFB–Popov produce a small shift from 1 for the Kohn mode \(\epsilon_{l}/\hbar\omega_{r} = 1\) at temperatures \(T \gtrsim 0.8T_{c}\). One possibility to fix this problem might be the inclusion of the dynamics of the noncondensed and the anomalous components. A suitable formalism to explore such a dynamics is the time-dependent HFB theory \cite{54–58, 61–63}.

4. Conclusion

In conclusion, we have deeply investigated the properties of a dipolar Bose gas confined by a cylindrically symmetric harmonic trapping potential in the presence of TBI at finite temperature. The numerical simulation of the full HFB model emphasized that the condensed fraction and the transition temperature are reduced by the TBI. Effects of TBI and temperature on the collective modes of the system are notably...
highlighted. We found that the full HFB approach in the presence of the TBI reproduces the HFB–Popov results of [10] only at low temperature while both approaches diverge each other when the temperature is approaching to $T_c$.

The same behavior could persist in the case of a density-oscillating ground state known as a biconcave state predicted in [9]. For a dipolar BEC in a cigar-shaped trap, one can expect a small enhancement in the condensed fraction and the $T_c$-shift due to the competition between the effectively attractive DDIs which lead to increase $N_c/N$ at any temperature, hence increasing also $T_c$, and the repulsive TBI which tend to decrease both $N_c/N$ and $T_c$. The collective frequencies might be also slightly shifted owing to the same reason.

Acknowledgments

We are grateful to Dmitry Petrov and Axel Pelster for the careful reading of the manuscript and helpful comments.

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