Stability of quasi-two-dimensional Bose-Einstein condensates with dominant dipole-dipole interactions

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We consider quasi-two-dimensional atomic/molecular Bose-Einstein condensates with both contact and dipole-dipole interactions. It is shown that, as a consequence of the dimensional reduction, and within mean-field theory, the condensates do not develop unstable excitation spectra, even when the dipole-dipole interaction completely dominates the contact interaction.

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Dilute Bose-Einstein condensates with long-range interactions offer promising opportunities to explore the potentially strong correlations induced by the interaction, which go beyond the comparatively weak correlations induced by the local contact interaction pseudopotential conventionally sufficient to describe most atomic condensates. The recent realization of a concrete physical system in which atomic magnetic dipoles play a significant role [1], is a first experimental step towards the exploration of dipolar condensate physics [2, 3, 4, 5, 6]. To investigate dipole-dominated physics, greater potential than by magnetic dipoles is offered by heteronuclear molecules with an electric dipole moment [7, 8], due to the fact that the electric dipole interaction strength is generally dependent on the value of the contact interaction coupling strength [9]. For the statements made in the present paper, the actual ratio \( g_{3D}/g_d \) and the absolute value of the (unscreened) \( g_d \) will be relevant.

\[
i \frac{\partial}{\partial t} \Psi(r, t) = \left\{ \begin{array}{l}
-\frac{\nabla^2}{2} + \frac{1}{2} \omega_z^2 z^2 + g_{3D}|\Psi(r, t)|^2 \\
+ \int d^3 r' V_{dd}(r - r')|\Psi(r', t)|^2 
\end{array} \right\} \Psi(r, t).
\]

The trapping in the plane is assumed to be negligible as compared with the strong confinement, of harmonic trapping frequency \( \omega_z \), in the \( z \) direction. The term in the second line contains the dipole-dipole interaction of the atoms/molecules, with all dipoles oriented by an applied field along the strongly confining \( z \) direction:

\[
V_{dd}(r) = \frac{3g_d}{4\pi} \frac{1 - 3z^2/|r|^2}{|r|^3}.
\]

The dipole coupling reads \( g_d = \mu_0 a_s^2/3 \) for magnetic and \( g_d = d_e^2/3\epsilon_0 \) for electric dipoles. In the units which we employ, the \( g_d \) are having dimensions of length like the 3D contact interaction \( g_{3D} = 4\pi a_s \), for which the length scale is set by the \( s \)-wave scattering length \( a_s \). We note that the value of the contact interaction coupling strength generally depends on the value of \( g_d \) (in an effective-dimension dependent manner), because the long-range dipole-dipole interaction affects the short-range scattering processes [8]. For the statements made in the present paper, the actual ratio \( g_{3D}/g_d \) and the absolute value of the (unscreened) \( g_d \) will be relevant.
For a quasi-2D Bose-Einstein condensate, the motion of the atoms/molecules is by definition restricted to zero point oscillations in a harmonic oscillator potential. We then take as a general ansatz for the density

$$\rho(r) = |\Psi(r)|^2 = \frac{1}{\sqrt{\pi d_z^2}} \exp \left[ -\frac{z^2}{d_z^2} \right] n(x, y), \quad (3)$$

where the density in the plane, $n(x, y)$, is normalized to the total number of particles $N$. We treat $d_z$ as a parameter minimizing the Gross-Pitaevski energy functional. Assuming homogeneous density in the plane, the equation determining $d_z$ reads $\alpha = d_z^{-4} + (g_{3D} + 2g_d)nN d_z^{-3}/\sqrt{2\pi}$. If the right-hand side is dominated by the first (kinetic energy) term, $d_z$ equals the harmonic oscillator length $1/\sqrt{\alpha}$. The state is quasi-2D, and the above Gaussian gives the density profile exactly. Defining a parameter $\alpha \equiv \omega_z d_z^2$, we have $\alpha = 1$ if the system is quasi-2D and $\alpha \gg 1$ deep into the 3D regime, where $\alpha$ becomes an interaction dependent.

We now calculate the total dipole-dipole energy given that the density profile in $z$-direction is prescribed by the above Gaussian. In accordance with Eq. (1), the Gross-Pitaevskii energy functional, yields the Gaussian in the plane, the equation determining $d_z$ takes the form $\pi d_z^2/\sqrt{(2\pi)} = \exp[-4k_d^{-2}d_z^2] n(k_x, k_y)$. Integrating over the $k_z$ direction, the effective dipole-dipole energy is then given by a two-dimensional integral in $(k_x, k_y)$ space

$$H_{dd} = \frac{g_d}{2} \frac{1}{(2\pi)^2} \int d^2k \tilde{n}(k_x, k_y) \tilde{\rho}(-k_x, -k_y) \times \left\{ \frac{2}{\sqrt{2\pi d_z}} + \frac{3}{2} \exp \left[ -\frac{k_d^2}{2} \right] k \text{Erfc} \left( \sqrt{\frac{k_d}{2}} \right) \right\}, \quad (5)$$

where the complementary error function Erfc $(z) = 1 - \text{erf}(z) = 1 - (2/\sqrt{\pi}) \int_0^z \exp(-t^2)dt$ and $k = (k_x^2 + k_y^2)^{1/2}$; $\tilde{n}(k_x, k_y)$ is the Fourier transform of the 2D density. Employing the same procedure of integrating out the Gaussian in the $z$ direction, for the contact interaction part in the Gross-Pitaevskii energy functional, yields the well-known result for the 2D effective coupling $g_{2D} = 2\sqrt{2\pi a_s/d_z}$ (valid in the limit that the 3D s-wave scattering length $a_s \ll d_z$ [12]).

From the relation (4) for the dipole-dipole contribution in the interaction energy, it follows that the Fourier transform of the total, contact plus dipole, interaction potential assumes the form

$$\tilde{V}_{tot}^{2D}(\zeta) = \frac{A}{\rho(0)\sqrt{\pi d_z^2}} \left\{ 1 - \frac{3R \zeta}{2} w \left( \frac{\zeta}{\sqrt{2}} \right) \right\} \quad (6)$$

where we made use of the $w$ function, related to Erfc$(z)$ by $w(z) = \exp[z^2] \text{Erfc}(z)$ [13]. The dimensionless wavevector $\zeta = k d_z$, and the two dimensionless parameters occurring in $\tilde{V}_{tot}^{2D}(\zeta)$, using the central 3D density $\rho(0)$, are defined to be

$$A = \frac{\rho(0)\sqrt{\pi d_3^2 g_d}}{R}, \quad R = \frac{\sqrt{\pi/2}}{1 + g_{3D}/2g_d}. \quad (7)$$

The value of the parameter $R$ ranges from $R = 0$ if $g_{3D}/g_d \rightarrow 0$, to $R = \sqrt{\pi/2}$ for $g_{3D}/g_d \rightarrow \infty$. The second term in the curly brackets in Eq. (6) rapidly decreases as a function of $\zeta$ and approaches a constant, which is due to the fact that $w(z/\sqrt{2}) \rightarrow \sqrt{2\pi} \zeta^{-1}$ for $\zeta \to \infty$, cf. the plot of $\tilde{V}_{tot}^{2D}(\zeta)$ in Fig. 1. For small $\zeta$, the quasi-2D Fourier transform behaves like $\tilde{V}_{tot}^{2D}(\zeta) \approx \frac{A}{\rho(0)\sqrt{\pi d_z^2}} \left\{ 1 - \frac{3R \zeta}{2} + \frac{3R \zeta}{2\sqrt{\pi} \zeta^2} + O(\zeta^3) \right\}$. Observe that $\tilde{V}_{tot}^{2D}(\zeta)$ possesses a well-defined value at the origin $\zeta = k = 0$, as opposed to the 3D Fourier transform of the dipole-dipole interaction potential.

From the Fourier transform of the interaction (6), we conclude that the squared Bogoliubov spectrum $\tilde{V}_{tot}^{2D}(k)$, for excitations confined to the plane, $\omega^2 = \rho(0)\sqrt{\pi d_z} \tilde{V}_{tot}^{2D}(k)$, is in units of $1/d_z^2$, given by

$$\epsilon^2(\zeta) = A \zeta^2 \left[ 1 - \frac{3R \zeta}{2} w \left( \frac{\zeta}{\sqrt{2}} \right) \right] + \frac{\zeta^4}{4}. \quad (8)$$

The main observation of the present analysis is that, as opposed to the 3D case (or, in an exacerbated manner, the quasi-1D case [14]), the Bogoliubov spectrum (8) does not necessarily become unstable if the dipole interaction coupling exceeds the contact interaction coupling. Assuming $g_{3D}/g_d \rightarrow 0$, i.e. $R \rightarrow \sqrt{\pi/2}$, the above squared
spectrum can assume negative values, and hence the excitation energies become imaginary, when $A$ exceeds the critical value $A_c = 3.446$, cf. Fig. 2 where we show a sequence of four spectra for different $A$ at constant $R = \sqrt{\pi/2}$.

The critical value of $A_c = 3.446$ corresponds to a critical dipole coupling given by $(gd)_c = 2.436/\rho(0)d_z^2$. Using numbers appropriate for atomic magnetic moments $\mu_n = N_m \mu_B$, we find that $gd = 5.4 \times 10^{-6} \mu_M M N_n^2$ ($M$ is the mass of the atoms or molecules in units of the atomic mass unit = $1.66 \times 10^{-27}$ kg). In the case of electric dipoles, with moment $d_e = N_e$ Debye, we find $gd = 6.2 \times 10^{-2} \mu_M M N_n^2$. The critical coupling $(gd)_c$ for dominant dipole-dipole interactions then translates into a critical central 3D density $\rho_c(0) = 4.5 \times 10^{16}$ cm$^{-3} N_n^{-2} \alpha^{-1} \omega_z [2\pi \times \text{kHz}]$ and $\rho_c(0) = 3.8 \times 10^{12}$ cm$^{-3} N_n^{-2} \alpha^{-1} \omega_z [2\pi \times \text{kHz}]$ in the case of magnetic and electric dipoles, respectively.

The quantity $\sqrt{\pi \rho(0)}gd/R$, a measure of the energy per particle (the chemical potential), is equal to $A/d_z^2$. For the system to be quasi-2D, we therefore need $A \ll \omega_z d_z^2 = \alpha \equiv 1$. Furthermore, the Bogoliubov spectrum in Fig. 2 does not possess any points where $d\epsilon^2/d\zeta^2 = 0$ for values $A < A_{\text{min}} = 1.249$ (when $R = \sqrt{\pi/2}$). That is, a “roton” minimum cannot develop within the regime of quasi-2D. Thus we conclude that a quasi-2D purely dipolar system of bosons is always stable, and that the instability of the condensate takes place in the crossover region to 3D. By contrast, deep inside the 3D regime, $g_{3D} \ll gd$ implies collapse of the condensate for any reasonable value of the density, and in the Thomas-Fermi limit the condensate will be unstable for any $gd$ slightly exceeding $g_{3D}$.

The critical value of $A_c(R)$, at which the gas becomes unstable, obtained by numerically finding the large momentum zeros of the Bogoliubov spectrum, exponentially increases for smaller $R$ (increasing $g_{3D}/gd$), and diverges at $R = 2\sqrt{\pi/2}$ (i.e., for $g_{3D} = gd$), where the Fourier transform $\tilde{U}_{\text{3D}}^2$ becomes positive everywhere. Comparing the critical values of $A$ thus obtained to those from a full 3D solution of the Bogoliubov-de Gennes equations, the present approach reproduces the critical $A$ sufficiently accurate in the dipole-dominated case, for which the instability takes place in the crossover regime from quasi-2D to 3D. Deep into the 3D regime, the critical value $A_c$ calculated from $U_{\text{3D}}^2$ is strongly over-estimated, mainly because it is exponentially sensitive on the exact form of the spectrum.

At nonzero temperature, 2D Bose-Einstein condensates do not exist in the homogeneous case, while trapping in the plane enables the existence of a condensate also at finite $T$. On the other hand, in the presently discussed $T = 0$ case, it is a well-established fact that even without trapping, Bose-Einstein condensation occurs in two spatial dimensions, see, e.g., [19]. We next turn to a discussion of the zero temperature value of the number density of excitations above the condensate, the so-called quantum depletion.

To this end, we use a mode expansion for the annihilation operators $\hat{\chi}_k$ of the original bosons in terms of the Bogoliubov quasiparticle operators $\hat{a}_k, \hat{a}_k^\dagger$:

$$\hat{\chi}_k = \sqrt{\frac{k^2}{2 \epsilon_k}} \left[ \left( \frac{1}{2} + \frac{\epsilon_k}{k^2} \right) \hat{a}_k + \left( \frac{1}{2} - \frac{\epsilon_k}{k^2} \right) \hat{a}_k^\dagger \right]. \tag{9}$$

The above form of the Bogoliubov transformation results, after inversion, in the usual phonon quasiparticle operators at low momenta, and gives $\hat{\chi}_k = \hat{a}_k$ at $k \to \infty$, i.e., the quasiparticles and the bare bosons become, as required, identical at large momenta.

The quantum depletion density at zero temperature is calculated by evaluating the expectation of $\hat{\chi}^\dagger \hat{\chi}$ in the quasiparticle vacuum defined by $\hat{a}_k |\text{vac}\rangle = 0$:

$$\langle \hat{\chi}^\dagger \hat{\chi} \rangle = \frac{1}{2 \pi d_z^2} \int_0^\infty d\zeta \frac{\zeta^3}{2\epsilon(\zeta)} \left( \frac{1}{2} - \frac{\epsilon(\zeta)}{\zeta^2} \right)^2. \tag{10}$$

The instability generally happens because in-plane excitations become of imaginary frequency, above the calculated critical value of $A = A_c$, the in-plane excitations have vanishing energy, and the quantum depletion diverges. Using the in-plane momentum integral above to calculate the depletion, with the effective dispersion relation, assumes that the corrections due to the neglected out-of-plane Bogoliubov excitations, characterized by transverse quantum numbers, are small. This is justified because the dominant contribution to quantum depletion is, for a dilute Bose gas, from large momentum excitations with (approximately) vanishing energy. Out-of-plane excitations have large energies at the relevant in-plane momenta of order $1/d_z$; they thus do not contribute significantly to the depletion. In Fig. we show the result for the quantum depletion in the case of dipole-interaction dominated condensates, for which we can expect the in-plane spectrum to be sufficiently accurate.
up to \( A \simeq A_c \). At the critical value \( A = A_c(\sqrt{\pi/2}) \simeq 3.4 \) (dotted vertical line in Fig. 3), the condensate depletion diverges, and the mean-field condensate will yield to a new quantum phase.

In conclusion, we have shown that dipolar quasi-2D Bose-Einstein condensates are extremely stable systems as compared to their 3D counterparts. This offers the potential of approaching, starting from the mean-field physics of condensates, a strongly correlated regime of dilute atomic/molecular gases with long-range interactions. A conceivable experimental procedure is to start from a quasi-2D dipolar condensate, and, by decreasing \( \omega_z \), to enter the crossover regime to 3D, where the quantum depletion of the condensate sets in are rather small, even for \( \omega_m \), the condensate depletion still remains small. On the other hand, it is evident from the second line of Eq. (11), that for electric dipoles the densities at which strong depletion of the condensate sets in are rather small, even for strongly increased axial trapping.

Among further lines of research offered by the stability potential of quasi-2D dipolar condensates are the phenomena expected when they are set in rotation. When both contact and dipole interaction are present, various of these phenomena have been explored in [21]: quantum Hall states of purely dipolar Fermi gases were studied in [22]. The interplay of quasi-two-dimensionality and rotation may generally yield interesting new physics [23]. It will, furthermore, be of interest to determine the change in the system’s stability region when the dipoles are no longer locked in one direction, and thus to investigate the influence of spin waves on the stability of dipolar quantum gases of bosons.

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