Two-dimensional quantum droplets in dipolar Bose gases

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We calculate analytically the quantum and thermal fluctuations corrections of a dilute quasi-two-dimensional Bose-condensed dipolar gas. We show that these fluctuations may change their character from repulsion to attraction in the density-temperature plane owing to the striking momentum dependence of the dipole-dipole interactions. The roton instability is halted by such unconventional fluctuation corrections leading to the emergence of a droplet phase which is readily implementable with current experiments. The excitations and the coherence of such a state are discussed. At finite temperature, a stable droplet can exist only below certain critical temperature due to the strong thermal fluctuations.

One of the most fascinating phenomena recently observed in dipolar Bose-Einstein condensates (BEC) with Dy and Er atoms is the formation of self-bound droplets [1–4]. Theoretically, a wealth of studies have been spawned for highlighting the behavior of droplet states [5–14]. These so-called liquid droplets may preserve their shape even in absence of external trapping [3, 8, 9] and decay at temperature close to the transition [10].

In addition, the transition to the droplet state happens at relatively high density compared to the quasi-1D system [19]. The observed 2D self-bound dipolar droplets differ from the bound state of 2D weakly attracting bosons [25] and that of 2D Bose-Bose mixtures with contact interactions [20].

Utilizing variational and numerical means we point out that the size of the self-bound decreases exponentially with the number of particles. We find that the stability of the system requires a minimum critical number of atoms. The density and the shape of such a droplet are analyzed by solving the underlying generalized nonlocal 2D Gross-Pitaevskii equation (GPE). We argue that the LHY corrections invoke non-trivial enhancements in the excitations and the one-body correlation function of the droplet. Finally, we extend our study to finite temperatures and predict effects of thermal fluctuations, condensed fraction inside the droplet and the structure factor.

We consider a dilute Bose-condensed gas of dipolar bosons tightly confined in the axial direction z by an external potential \( U(r) = m\omega^2z^2/2 \) and assume that in the \( x, y \) plane the translational motion of atoms is free. The dipole moments \( d \) are oriented perpendicularly to the \( x, y \) plane. In the ultracold limit \( kr_s \ll 1 \), where \( r_s = md^2/\hbar^2 \) is a characteristic range of the DDI, the momentum representation of the two-body interaction potential \( V(r - r') \) is given as [21]

\[
V(k) = g(1 - C|k|),
\]

where \( C = 2\pi d^2/g \), \( g = g_{3D}/\sqrt{2\pi l_0} \) is the 2D contact interaction coupling constant with \( l_0 = \sqrt{\hbar/m\omega} \), and \( g_{3D} = 4\pi\hbar^2a/n \) with \( a \) being the s-wave scattering length \( (a > 0 \) throughout the paper). The Bogoliubov excitation energy is given as \( \varepsilon_k = \sqrt{E_k^2 + 2\mu_0E_k(1 - Ck)} \) [21], where \( E_k = \hbar^2k^2/2m \) and \( \mu_0 = ng \) is the zeroth order chemical potential with \( n \) being the gas density.

Small momenta the excitations are sound waves, \( \varepsilon_k = \sqrt{ng/mk} \). For \( C \) varies as \( (\sqrt{3}/3) \leq C \leq \xi \), where

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\( \xi \) is the healing length, the excitation spectrum exhibits a roton-maxon structure \(^{21}\). For \( C > \xi \), the uniform Bose gas becomes dynamically unstable.

At zero temperature, the LHY corrections to the equation of state (EoS) can be written \(^{10,21}\)

\[
\frac{\delta \mu}{E_0} = \frac{1}{2} \int V(k) \left[ \frac{E_k}{\varepsilon_k} - 1 \right] \frac{dk}{(2\pi)^2}.
\]

(2)

This integral is divergent at large momenta due to the dipolar term \(-gCk\). The main contribution to \( \delta \mu \) comes from \( k \) close to \( 1/r_s \). Using a cutoff regularization method outlined in our recent work \(^{21}\), we obtain

\[
\frac{\delta \mu}{E_0} = \left( 2a/l_0 \right)^2 n r_s^2 \left[ 1 - 2b(nr_s^2)^{1/2} - 3b^2 nr_s^2 \right] + 2b^2 nr_s^2 \ln \left[ \frac{1}{2(1-b\sqrt{nr_s^2})} \right],
\]

(3)

where \( E_0 = \hbar^2/m r_s^2 \) and \( b = \sqrt{2\pi n^2 l_0/a} \). In absence of the DDI, Eq. (3) excellently agrees with the usual short-range 2D Bose gas EoS (see e.g. \(^{26,27}\)). When the roton minimum is close to zero i.e. \( C = \xi \), one has \( \delta \mu/E_0 \approx (4a/l_0)^2 n r_s^2 \ln \left[ 1/\sqrt{b^2 nr_s^2(1-b^2 nr_s^2)} \right] \). The quantum corrections \(^{23}\) are important to halt the dipolar instability. They can also substantially impact the collective excitations and the thermodynamics of the system.

The LHY may instead enhance the density of 2D bright solitons for \( \epsilon_{dd} = r_s/a > 1 \)^{28}\. For \( 0.1 < nr_s^2 < 0.87 \), the effective LHY attraction furnishes an extra term \( \propto -n^2 - n^2 \ln(1-n) \) arresting the dipolar instability, results in the formation of a stable self-bound droplet. This droplet phase has a universal peak density at \( nr_s^2 \approx 0.87 \) where the energy reaches its minimal value (see the inset of Fig.1). For \( nr_s^2 > 0.87 \), \( \delta \mu \) grows logarithmically and thus, the system undergoes an instability as the complexity increases.

To gain more insights into these quantum ensembles, we solve the generalized GPE in which \( \delta \mu \to \delta \mu(r) \):

\[
i\hbar \Phi(r,t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + g n + \bar{\mu}(r) \right] \Phi(r,t),
\]

(4)

where \( \bar{\mu}(r) = \delta \mu(r) + \int dr' d^2n(r')/|r^3 - r'^3| \). The wavefunction must satisfy the normalization condition \( 2\pi \int dr |\Phi|^2 = N \). In 3D geometry, Eq.(4) has been intensively used to describe the static and the dynamics of the droplet \(^3\,7\,11\) and already validated by quantum Monte Carlo simulations \(^\ddagger\). In the model \(^\ddagger\) the effect of higher-momentum modes is just a local density-dependent term and the depletion is assumed to be small. The numerical simulation of \(^\ddagger\) was performed using the split-step Fourier transform method. The results are shown in Fig2 for parameters relevant to \(^{164}\)Dy atoms. We observe that a stable droplet is formed due the competition between mean-field energy and LHY corrections (see Fig.2a). Increasing more the interaction, the droplet develops a central peak with some small structures around its edge due to the roton instability induced by the DDI as is seen in Fig2b.

\[ \text{FIG. 1. The LHY corrections to the EoS from Eq. (3) as a function of } n r_s^2 \text{ for } a/l_0 = 0.025. \text{ The inset shows the energy shift due to the LHY corrections } (\delta E = \int \delta \mu dn). \text{ These parameters are sufficient to reach the roton regime.} \]

\[ \text{FIG. 2. Density profile of Dy droplet for } aN/l_0 = 25 \text{ and } \epsilon_{dd} = 1.4 \, (a) \epsilon_{dd} = 1.6 \, (b). \]

In order to estimate the size \( \sigma \) of the bound state, we minimize the energy functional evolving (4) with respect to \( \sigma \). The energy can be calculated using a Gaussian trial wavefunction \( \Phi(r) = \sqrt{1/\pi \sigma^2} \exp(-r^2/2\sigma^2) \). Assuming that the radial width is much larger than the oscillator length which is required for the quasi-2D approximation, we then find the optimal size of the droplet is \( \sigma \approx B \exp(\pi^2 l_0^2/4a^2 N) \), where \( B = \exp[a(\epsilon_{dd} - 1/4)/(\sqrt{2\pi} l_0)] \). This shows that the size of the droplet decreases exponentially with the number of particles.
The critical number of particles above which the self-bound droplet is stable reads
\[ N_{\text{cr}} = \frac{540\pi^2}{163 - 270\gamma + 15\ln(4\sqrt{2\pi}a/l_0)} \]  
(5)
where \( \gamma = a^2/l^2(1 - 4\pi\sqrt{2\pi}\epsilon_d l_0/a) \). For \( N > N_{\text{cr}} \), the droplet contracts to infinitesimal size. For instance, using the parameters of Fig 4b for Dy atoms, we find that a stable droplet is emerged at \( N_{\text{cr}} \lesssim 270 \) atoms which is in agreement with our numerical simulation.

The collective excitations of the self-bound droplet can be determined within the realm of the phase-density representation which provides an extension of the usual Bogoliubov-de-Gennes theory [29]. Writing the field operator in the form \( \hat{\psi} = \sqrt{n}\hat{e}e^{i\phi} \), where \( \hat{\phi} \) and \( \hat{n} \) are the phase and density operators, which obey the commutation relation \( [\hat{n}(\mathbf{r}), \hat{\phi}(\mathbf{r}')] = i\delta(\mathbf{r} - \mathbf{r}') \). Expanding the density and the phase in the basis of the excitations: \( \hat{n}(\mathbf{r}) = \sqrt{n}(\mathbf{r}) \sum_k \sqrt{E_k}/E_k \hat{b}_k + \text{H.C.} \) and \( \hat{\phi}(\mathbf{r}) = [i/2\sqrt{n}(\mathbf{r})] \sum_k \sqrt{E_k}/E_k \hat{a}_k \hat{b}_k - \text{H.C.} \) (see e.g. [20, 27, 30]). As is seen in Fig 3a, the spectrum \( E_k \) exhibits a roton-maxon structure. The position and the energy of the roton are changed owing to the LHY corrections.

The one-body density matrix which plays a key evidence for droplet quantum coherence, is defined as \( g_1(\mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(0) \rangle \). We see from Fig 3b that the one-body correlation function is tending to its asymptotic value at \( t \to \infty \) signaling the existence of the long-range order allowing formation of a droplet in quasi-2D geometry at zero temperature. This confirms the scenario foreseen above whereby the combined effect of the quantum fluctuations and the rotonization leads to a supersolid droplet. Close to the roton region, \( g_1(\mathbf{r}) \) exhibits pronounced oscillations when \( r \) is approaching to zero. These oscillations are most likely signature of the destruction of the long-range order, unlocking the possibility of the formation of a novel state of matter consisting of a supersolid droplet. This exotic state could be well described within either lattice or a stripe models [22].

Now we turn to the last part of our study, where we deal with the behavior of the droplet at finite temperature. In uniform Bose gas, at any nonzero temperature, thermal fluctuations distort the condensate [31, 32]. However, according to Berezinskii-Kosterlitz-Thouless (BKT) [33, 34], quasicondensate takes place at low temperature, characterized by a power-law decay of the one-body spatial correlation function [20, 27]. In such a quasicondensate, the phase coherence governs only regime of a size smaller than the size of the condensate, marked by the coherence length [26]. For a distance smaller than the coherence length, one can work with the true BEC theory [26, 35].

The correction to the chemical potential due to thermal fluctuations reads
\[ \delta \mu_{\text{th}} = \int V(\mathbf{k}) \frac{E_k}{\varepsilon_k} \left[ \exp(\varepsilon_k/T) - 1 \right]^{-1} \frac{dk}{(2\pi)^2} \]  
(6)
where
\[ \Xi = n_{\text{sat}} \left( \frac{T}{T_0} \right)^3 \]
\[ \Xi = n_{\text{sat}} \left( \frac{T}{T_0} \right)^4 \]
In contrast to the zero temperature case, integral (6) is convergent. At low \( T \), the main contribution to (6) comes from the phonon branch. This yields
\[ \frac{\delta \mu_{\text{th}}}{E_0} = \frac{l_0}{2a} \left[ \frac{\zeta(3)}{2} (nr_0^2)^{-2} \left( \frac{T}{E_0} \right)^3 - b \frac{120\pi^2}{120\pi^2 (nr_0^2)^{-5/2}} \left( \frac{T}{E_0} \right)^4 \right] \]
where \( \zeta(3) \) is the Riemann Zeta function. The leading term in Eq. (7) arises from the short-range interactions while the subleading term accounts for the DDI. The most striking feature of the thermal fluctuations (7) which introduce a new extra term \( \propto -n^{-5/2}T^4 \), is that they change their nature from repulsive at lower \( T \) to attractive interactions at higher \( T \). Notice that at \( T > gn \), the leading term for the chemical potential is the same as that for the ideal gas.
numerical method. Figure 4a depicts that beyond a certain critical temperature \((T \simeq 3.2E_0)\) for \(Na/l_0 = 30\), the droplet evaporates into an expanding gas owing to the strong thermal fluctuations. The condensed fraction and the critical temperature are reducing by increasing the interaction parameter \(Na/l_0\).

At finite temperature, the coherence of the droplet appears in the static structure factor \(S(k)\) which is related to the pair correlation function and defined as \(S(k) = (\varepsilon_k/\varepsilon_0)\coth(\varepsilon_k/2T)\). As one can see in Fig 4b, as the temperature is increased, \(S(k)\) develops a peak in the region of small momenta indicating that the droplet starts to disappear. This means that in quasi-2D systems, the thermal fluctuations become strong enough to destroy the off-diagonal long-range order and hence preventing the occurrence of a droplet phase at temperatures \(T \gtrsim E_0\). At large momenta, \(S(k)\) is tending to unity.

In conclusion, we predicted the formation of a self-bound droplet in quasi-2D dipolar Bose gas. We derived analytical formulas which allow to analyze in detail effects of LHY quantum and thermal fluctuations. The competition between such LHY corrections which present intriguing density dependence and the DDI instability leads to the emergence of a quantum droplet in the roton region. We found that the excitations and the one-body density matrix of this novel phase exhibit remarkable behavior. At finite temperature, we revealed that the droplet state can survive only below certain critical temperature \((T_c = \alpha E_0)\), where \(\alpha\) is some constant depending on the interaction which should be smaller than the BKT transition temperature. The BKT transition and the vortices that accompany it could be analyzed by means of Kibble-Zurek mechanism. One can expect, on the other hand, that the unusual density dependence of the quantum corrections persists also in the presence of three-body correlations \([10, 37, 38]\). The insights obtained in the present study may offer a fresh view of the supersolid droplet. Further investigations both experimental and Monte carlo simulation are required in the future in order to fully understand the confidentiality of the droplet state in 2D configuration.

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