Stable dilute supersolid of two-dimensional dipolar bosons

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We consider two-dimensional bosonic dipoles oriented perpendicularly to the plane. On top of the usual two-body contact and long-range dipolar interactions we add a contact three-body repulsion as expected, in particular, for dipoles in the bilayer geometry with tunneling. We show that this model allows for stable continuous space supersolid states in the dilute regime and calculate the zero-temperature phase diagram. The three-body repulsion is crucial for stabilizing the system and, combined with the two-body attraction, can lead to self-trapped supersolid droplets.

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Recent advances in the field of cold polar molecules and magnetic atoms interacting via long-range dipole-dipole forces make it realistic to create novel many-body quantum states in these systems. For polar molecules, ultracold chemical reactions observed at JILA and leading to a rapid decay of the system can be suppressed by tightly confining the molecules to a (quasi)two-dimensional (2D) geometry, orienting the dipoles perpendicularly to the plane of their translational motion, and thus inducing a strong intermolecular repulsion. Therefore, 2D geometries are intensively discussed in the context of ultracold dipolar gases, together with possible experiments with non-reactive molecules, such as NaK and RbCs.

The studies of ultracold dipolar gases may open perspectives for the observation of supersolidity. This remarkable quantum phenomenon combines superfluidity with a crystalline order (see for review). It is still under debate as to what extent experimental results in solid helium prove the existence of this conceptually important phase. On the other hand, supersolidity is rather well understood theoretically for soft-core two-body potentials which can be realized, for example, in Rydberg-dressed atomic gases. However, such supersolids require a dense regime with at least several particles within the interaction range, which can be difficult to achieve. The same holds for supersolids discussed for 2D dipolar Bose gases near the gas-solid phase transition. It is thus an open question whether supersolids can exist in the dilute regime. If yes, this will allow for studies of non-conventional superfluid properties of supersolids and other aspects of supersolidity. Dilute 2D dipolar bosons may show the (helium-like) roton-maxon structure of the spectrum by fine-tuning the short-range part of the interaction potential and can be made unstable with respect to periodic modulations of the order parameter (roton instability). However, instead of forming a supersolid state when approaching such an instability, the gas collapses.

In this Letter we predict a stable supersolid state in this system. However, in addition to the contact two-body term $(g_2)$ and the dipole-dipole long-range tail characterized by the dipole moment $d$, we include a contact repulsive three-body term $(g_3)$ which prevents the collapse. Three-body forces are ubiquitous and arise naturally in effective field theories when one integrates out some of high-energy degrees of freedom in the system. In particular, our model can be realized for dipoles in the bilayer geometry with interlayer tunneling. Tracing out the degree of freedom associated with the layer index one obtains an effective single-layer model in which $g_2$ and $g_3$ can be independently controlled by tuning the interlayer tunneling amplitude. Here we work out the many-body phase diagram of this model and identify stable and metastable uniform and supersolid states. We argue that for $g_2 < 0$ these states can exist as dilute self-trapped droplets.

The Hamiltonian of the system reads

$$
\mathcal{H} = -\int d^2r \hat{\psi}^\dagger(r) \frac{\hbar^2 \nabla^2}{2m} \hat{\psi}(r) + \mathcal{H}_2 + \frac{g_3}{6} \int d^2r \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r) \hat{\psi}(r) \hat{\psi}(r),
$$

(1)

where $\hat{\psi}(r)$ is the bosonic field operator, $m$ is the particle mass, and the normalization volume is set equal to unity. The first term in Eq. (1) corresponds to the kinetic energy, the third one to the contact three-body repulsion $(g_3 > 0)$, and the two-body interaction Hamiltonian $\mathcal{H}_2$ at low energies can be substituted by an effective momentum-dependent (pseudo)potential (see, e.g.,

$$
\tilde{V}(\mathbf{k}, \mathbf{k'}) = \tilde{V}(|\mathbf{k} - \mathbf{k}'|) = g_2 - 2\pi d^2 |\mathbf{k} - \mathbf{k}'|,
$$

(2)

where $\mathbf{k}$ and $\mathbf{k'}$ are the incoming and outgoing relative momenta, $g_2$ is the contact term which depends on the short-range details of the two-body potential, and the momentum-dependent part corresponds to the long-
range dipolar tail. In terms of field operators we have
\begin{equation}
\mathcal{H}_2 = \frac{1}{2} \int dxd\ell \hat{\psi}(x) \hat{\psi}^\dagger(x) \sum_q \hat{V}(q)e^{iq(x-\ell)}\hat{\psi}(x)\hat{\psi}(\ell).
\end{equation}

The onset of supersolidity is frequently associated with the presence of a low-lying roton minimum in the excitation spectrum \cite{19,32,33}. In our case the standard Bogoliubov approach applied to a uniform Bose condensate of density \( n \) gives the excitation spectrum
\begin{equation}
\epsilon(k) = \sqrt{(\hbar^2 k^2/m)(g_2n + g_3n^2 - 2\pi n d^2k + \hbar^2 k^2/4m)},
\end{equation}
where we certainly assume that \((g_2 + g_3n) > 0\). The validity conditions for the mean-field approximation read
\begin{equation}
m^2 \ll 1; \quad m(g_2 + g_3n)/\hbar^2 \ll 1,
\end{equation}
where \( r_s = md^2/\hbar^2 \) is a characteristic range of the dipole-dipole interaction. The structure of the spectrum is characterized by a dimensionless parameter \( \beta \) given by
\begin{equation}
\beta = \gamma/(1 + g_2/2g_3n); \quad \gamma = 4\pi^2h^2r_s^2/mg_3.
\end{equation}
For small \( \beta \), i.e., at low densities or for small dipole moments, \( \epsilon(k) \) is a monotonic function of \( k \). However, it shows a roton-maxon structure (local maximum and minimum at finite momenta) for \( \beta \) in the interval \( 8/9 < \beta < 1 \), and at \( \beta = 1 \) the roton minimum touches zero. In a narrow vicinity of this point the density fluctuations become large and the Bogoliubov approach fails.

By minimizing Eq. (8) with respect to \( k \) we obtain
\begin{equation}
\mathcal{E}(k = k_m) = g_2n^2C_0 + g_3n^3(\mathcal{T}_\theta - 2\gamma \sin^2\theta \mathcal{D}_\theta),
\end{equation}
where \( k_m = 4\pi nr_sD_\theta \). In the dilute limit of Eq. (7) the number of particles per unit modulation volume is given by \( n(2\pi/k_m)^2 \sim 1/nr_s^4 \gg 1 \), which justifies the mean-field approach.

Equation (9) can be expanded in powers of \( \theta \). The zero-order term \( \mathcal{E}(\theta = 0) = g_2n^2/2 + g_3n^3/6 \) gives the energy density of the uniform state. The expansion contains terms \( \propto \theta^3 \), which is a consequence of the fact that the vectors \( \mathbf{k}_1, \mathbf{k}_2, \) and \( \mathbf{k}_3 \), form a closed triangle (“triad”, \( \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0 \)) \cite{15}. According to the Ginzburg-Landau theory \cite{34,35}, the US-SSS transition is then expected to be first-order, so that \( \theta \) jumps from 0 to a finite value. Note that the lattice structure in Eq. (7) substantially changes when going from \( \theta > 0 \) (triangular lattice) to \( \theta < 0 \) (hexagonal lattice), and there can be first-order transitions between SSS\(_{\theta>0}\) and SSS\(_{\theta<0}\).

First-order transitions are convenient to analyse in the grand-canonical picture. In order to calculate the phase diagram we minimize the grand potential \( \Omega = \mathcal{E} - \mu n \) with respect to \( \theta \) and \( n \) for a given chemical potential \( \mu \) and interaction parameters \( g_2, g_3 \) and \( d \).

First, let us consider \( g_2 = 0 \). In this case the energy functional \( \mathcal{E} \) only contains terms \( \propto n^3 \), and the phase di-
and we find that for intervalibility of the system is given by continuous across the transition. The inverse compressibility, and other thermodynamic quantities are due to the fact that the density dependence of \( g \) out [see Eq. (9) with \( \beta = 0 \)]. The phase diagram can be presented in the parameter space \((\mu, \gamma)\) and the phases are characterized by \( \theta \in [-\pi/2, \pi/2] \) and \( \tilde{n} \).

In Fig. 1 we show the phase diagram for \( g_2 > 0 \). In this case finite-density states exist only for positive \( \tilde{\mu} \). They are globally stable only for \( \gamma < \gamma_c \) (below the horizontal red solid line). Above this critical value the grand potential \( \tilde{\Omega} \) decreases with density faster than linearly and the global minimization procedure leads to \( n = \infty \) (collapse) irrespective of \( \tilde{\mu} \). One can easily see that in the high-density regime \( \tilde{\Omega} \) is dominated by the term \((T_0 - 2\gamma \sin^2 \theta D_0^2)\tilde{n}^3\), whereas the two-body contact interaction, i.e., the term containing \( C_0 \), becomes irrelevant. We thus obtain the same stability condition as in the case of \( g_2 = 0 \).

In the region \( \gamma < \gamma_c \) we find stable US and SSS phases separated by a first-order transition line (the black solid line in Fig. 1). The transition is characterized by a jump of \( \theta \) from 0 to a finite positive value and is accompanied by a discontinuity in the density. Below this line, the ground state is a uniform condensate \( (\theta = 0) \) with \( \tilde{n} = \sqrt{1 + 2\tilde{\mu} - 1} \). For large \( \tilde{\mu} \) the density is also large and the critical value of \( \gamma \) approaches \( \gamma_0 \), i.e, the \( g_2 = 0 \) value \( \beta = 0 \). The US-SSS transition line and the collapse line cross each other at \( \tilde{\mu} = 4.528 \), and a globally stable SSS can only exist at higher chemical potentials. Above the collapse line, \( \gamma > \gamma_c \), the US and SSS continue to exist as metastable local minima of \( \tilde{\Omega} \).

![Figure 1](image-url) (color online) Phase diagram for \( g_2 > 0 \).

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Also shown in Fig. 1 is the “rotonized” (blue shaded) region enclosed by the lines of constant \( \beta = 8/9 \) and \( \beta = 2/3 \), where the roton first emerges in the spectrum, and the upper one to \( \beta = 1 \), where it touches zero. One can clearly see that the US-SSS transition happens before the roton touches zero.

We have also considered other lattice structures, in particular, the stripe phase, quadratic lattice, and the state built up on many \( k \)-vectors (with equal modulus) in the \( x, y \) plane. The triangular-lattice ansatz \( (7) \) turns out to be the most energetically favorable, which is consistent with general arguments of Ref. \( ([36]) \).

The phase diagram for an attractive two-body contact interaction, \( g_2 < 0 \), is shown in Fig. 2. In contrast to the \( g_2 > 0 \) case, there is a region in which the ground state is a SSS with \( \theta < 0 \) corresponding to a hexagonal lattice symmetry. The US-SSS\( \theta < 0 \) (dashed) and SSS\( \theta > 0 \) (dotted) transitions are first-order. They cross at the tricritical point \( \tilde{\mu} = 3/2, \gamma = 2/3 \), where the grand potential \( \tilde{\Omega} = \text{const} + O(\theta^4) \), i.e., the terms \( \propto \theta^2 \) and \( \propto \theta^2 \) are absent. This is the only point in the phase diagram where the transition is second-order and occurs when the roton minimum touches zero. To the right of this point the supersolid phase with \( \theta < 0 \) disappears and the dashed line marks a weak first-order US-SSS\( \theta > 0 \) transition. As expected, this line approaches \( \theta = \gamma_0 \) at large \( \tilde{\mu} \), i.e., in the high-density limit.

Strictly speaking, nonlinearities in Eq. \( (7) \) couple the wave function Eq. \( (7) \) to plane waves with higher wave vectors (sums of integer multiples of \( k_x \)). However, for small \( \theta \) corrections to Eq. \( (7) \) are small. The leading contribution comes from plane waves with the wave vectors \( \pm 2k \) and \( k_x = k_{x+1} \). Their amplitudes are \( \propto \theta^2 \) and the corresponding contribution to the energy functional is \( \propto \theta^4 \). Thus, the tricritical point and the structure of the mean-field phase diagram around it is not an artifact of the variational approach (we have checked that the overall coefficient in front of \( \theta^2 \) in \( \tilde{\mathcal{E}} \) is positive in the vicinity of the tricritical point).

In Fig. 2 we also show the region of a uniform rotonized superfluid constructed in the same manner as in the case of \( g_2 > 0 \). We see again that the US-SSS transition happens before the roton touches zero; everywhere except the tricritical point the dashed line is inside the rotonized.
We should point out that first-order transitions involving density jumps are forbidden in 2D systems with dipolar interaction tails. The reason is that the surface tension in between two such phases can have a negative contribution which logarithmically diverges with the length of the interface and can thus overcome the positive local scale-independent contribution [38] (see also discussion in [16]). This means that the first-order transition lines that we describe here become (narrow) regions of intermediate "microemulsion" phases [38]. It is argued [16] that the observation of these phases requires exponentially large system sizes which most likely are much larger than the size of a typical ultracold sample. Nevertheless, we note that already the simplest vacuum-US interface that we predict to exist in our dilute weakly-interacting system should be a good candidate for studying these interfacial effects. However, we leave this subject for future work.

In conclusion, we have found that a dilute 2D dipolar Bose gas can reside in a variety of supersolid phases stabilized by three-body repulsion. Our results represent a starting point for the analysis of collective modes of homogeneous, trapped or self-trapped supersolids. The developed approach can also be employed in the studies of novel vortex and soliton structures, and in the search for translationally nonperiodic phases, in particular density-disordered superfluid (superglass) phases. Promising candidates for the creation of such dipolar Bose gases are (nonreactive) polar molecules in the bilayer geometry with interlayer tunneling. At 2D densities $n \sim 10^8$ cm$^{-2}$, for the dipole moment $d \sim 0.5$ D one has $r_s \sim 200$ nm and $nr_s^2 \ll 1$. Then $g_3$ can be made such [30] that $\gamma \sim 1$ and one may cover the whole range of parameters in the phase diagrams of Fig.1 and Fig.2. Finally, our results have implications for magnetic atoms such as erbium or dysprosium, which are necessarily dilute due to their small $r_s$. However, a mechanism for generating a sufficiently strong three-body repulsion in such gases has yet to be discussed.

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