A superfluid-droplet crystal and a free-space supersolid in a dipole-blockaded gas

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(Dated: May 17, 2010)

A novel supersolid phase is predicted for an ensemble of Rydberg atoms in the dipole-blockade regime, interacting via a repulsive dipolar potential “softened” at short distances. Using exact numerical techniques, we study the low temperature phase diagram of this system, and observe an intriguing phase consisting of a crystal of mesoscopic superfluid droplets. At low temperature, phase coherence throughout the whole system, and the ensuing bulk superfluidity, are established through tunnelling of identical particles between neighbouring droplets.

PACS numbers: 67.80.K-, 32.80.Rm, 67.85.Hj, 67.85.Jk, 67.85.-d, 02.70.Ss

The search for novel phases of matter drives much of the current research in condensed matter physics. Of particular interest are phases simultaneously displaying different types of order. A chief example, of great current interest, is the so-called supersolid, namely a phase featuring crystalline order, and also capable of sustaining dissipation-less flow. Attempts to observe experimentally a supersolid phase of matter, primarily in a crystal of solid helium, have spanned four decades since early theoretical predictions [1]. The most credible claim of such an observation to date [2] [3], has been subjected to in-depth scrutiny over the past few years, and it seems fair to state that agreement is lacking at the present time, as to whether experimental findings indeed signal a supersolid phenomenon [4].

A new, fascinating avenue to the observation of supersolid and other phases of matter not yet observed (or even thought of), is now opened by advances in cold atom physics, providing not only remarkably clean and controlled experimental systems, but also allowing one to “fashion” artificial inter-particle potentials, not arising in any known condensed matter system. This allows one to address a key theoretical question, namely which two-body interaction potential(s), if any, can lead to the occurrence of a supersolid phase. While this is well established for bosons in an optical lattice, it remains an open question how to realize this, and other novel, exotic phases, in free space.

In this Letter, we show that interaction potentials which combine a long-distance repulsion with a short-distance cutoff, will lead to the appearance of a novel self-assembled crystalline phase of mesoscopic superfluid droplets in a system of bosons. Furthermore, such a crystal can turn supersolid in the $T \to 0$ limit, as tunneling of particles across neighbouring droplets takes place, and superfluid phase coherence is established across the whole system, as individual separate Bose condensates (droplets) organize into a single, global condensate. Thus supersolidity, as arising in this system, is of a fundamentally different kind with respect to the one, defect-induced, originally envisioned by Andreev and Lifshitz [1]. Specifically, we consider the following two-body potential:

$$v(r) = \begin{cases} 
\frac{D}{a^3} & \text{if } r \leq a \\
\frac{D}{r^3} & \text{if } r > a 
\end{cases},$$

where $D$ being the characteristic strength of the interaction. This interaction potential can be realized with cold Rydberg atoms in the dipole-blockade regime [3], where $D$ and $a$ are parameters which can be controlled with external fields [6] [7], as shown below.

Our system of interest comprises $N$ identical bosons of mass $m$, confined to two dimensions [17]. The many-body Hamiltonian is the following (in dimensionless form):

$$\mathcal{H} = -\frac{1}{2} \sum_{i=1}^{N} \nabla_{i}^{2} + \sum_{i>j} v(r_{ij})$$

where $r_{ij} = |r_{i} - r_{j}|$ is the distance between particles $i$ and $j$, and $v$ is given by Eq. (1). All lengths are expressed in terms of the characteristic length $r_{c} = mD/\hbar^{2}$, and we introduce a dimensionless cutoff $R_{c} = a/r_{c}$ for the potential [1]. The system is enclosed in a square cell of area $A$, with periodic boundary conditions. The particle density is $n = N/A$, but we shall express our results in terms of the (dimensionless) inter-particle distance $r_{s} = 1/\sqrt{mr_{c}^{2}}$. The energy scale is $\epsilon_{s} = D/r_{s}^{2} = \hbar^{2}/mr_{c}^{2}$.

The low-temperature phase diagram of such a system has been explored by means of first principles numerical simulations, based on the Continuous-space Worm Algorithm [8] [9]. It is important to note at the outset that, while the numerical results presented here were obtained with the two-body potential [1], the main physical conclusions do not depend on its detailed form. Indeed, we have observed the same physical behaviour with potentials featuring a smoother merge of short- and long-range behaviours, as well as a different long-range tail than Eq. (1) – we come back to this point below.

Numerical results shown here pertain to simulations with a number of particles $N$ varying between 50 and
400, in order to carry out extrapolation of the results to the thermodynamic limit. Our ground state estimates are obtained as extrapolations of results at finite temperature. Details of the simulations are standard, as the use of the potential (1) entails no particular technical difficulty.

In the limit \( R_c \ll r_s \), the truncation of the dipolar potential at short distances does not play an important role, and the low temperature phase diagram of (2) is that of purely dipolar bosons in two dimensions, investigated previously by several authors [10, 11]. It is known that for \( r_s \approx r_s^c = 0.06 \) the ground state of the system is a triangular crystal, whereas for \( r_s \approx r_s^c = 0.08 \) it is a uniform superfluid (in the intermediate density range a more complex scenario is predicted [12]). As we show below, a very different physics sets in when \( R_c \gtrsim r_s \), in the density ranges which correspond to either the crystalline or superfluid phase in the purely dipolar system.

Fig. 1 shows typical configurations (i.e., particle world lines) produced by Monte Carlo simulations of a system of bosons interacting via the potential (1), at a nominal density corresponding to \( r_s = 0.14 \), at different temperatures spanning three orders of magnitude. The value of the cutoff \( R_c \) in this case is 0.3. At the highest temperature, a simple classical gas phase is observed, as shown by the pair correlation function \( g(r) \), shown in Fig. 1(a), which is just a constant (note that \( g(r) \) does not vanish at the origin, owing to the flattening off of the potential at short distance). As \( T \) is decreased, an intriguing effect takes place, namely particles bunch into mesoscopic droplets, in turn forming a regular (triangular) crystal. This is shown qualitatively in the snapshots in Fig. 1 but also confirmed quantitatively by the structure of the \( g(r) \) as well (Fig. 2(a)), which displays pronounced, broad maxima, as well as well-defined dips, where the function approaches zero. We henceforth refer to this phase as the droplet-crystal phase.

The formation of such droplets is a purely classical effect, that depends on the flattening off of the repulsive inter-particle potential below the cutoff distance. In fact, a simple estimate of the number \( N_d \) of particles per droplet, can be obtained by considering a triangular lattice of point-like dipoles, each one of strength \( \propto N_d \) (as it comprises \( N_d \) particles), and by minimizing with respect to \( N_d \) the potential energy per particle, for a fixed density. The result is

\[
N_d = \gamma \left( \frac{R_c}{r_s} \right)^2
\]

where \( \gamma \approx 2.79 \). Eq. (3) furnishes a fairly accurate estimate of \( N_d \) for the (wide) range of values of the parameters \( r_s \) and \( R_c \) explored here. For instance, using the parameters of Fig. 1 we find from (3) \( N_d \approx 13 \), which agrees quite well with our simulation result. It is worth noting that a similar sort of pattern formation, due to competing interactions, has been previously established for classical colloidal systems [13, 14].

In the \( T \to 0 \) limit, long exchanges of identical particles can take place, as a result of particles tunneling from one droplet to an adjacent one. Long exchanges of particles can result in a finite superfluid response throughout
the whole system \cite{18}, and indeed for \( R_c \geq r_s^L \) we observe such a bulk superfluid signal, in a range of values of \( r_s \) in the vicinity of \( R_c/2 \). Because superfluidity arises in concomitance with the droplet-crystal structure, the denomination supersolid seems appropriate. At \( T=0 \), such a phase is sandwiched between an insulating droplet crystal at high density (i.e., lower \( r_s \) and a homogeneous superfluid phase at lower density. For \( R_c \leq r_s^C \), only two insulating phases are observed, namely the insulating droplet crystal at high density and the crystal of single particles, already detected in Refs. \cite{10,11}, as well as a superfluid phase at lower density. All of this is summarized in the schematic phase diagram shown in Fig. 3.

It is important to stress that supersolid behaviour in this system does not originate from highly mobile point defects, such as vacancies or interstitials. Rather, tunnelling of particles between droplets which are themselves individually superfluid occurs, and the individual superfluid droplets connect to form a bulk superfluid. This is reminiscent of the phase-locking mechanism in a (self-assembled) array of Josephson junctions.

In order to establish that droplets are individually superfluid, one may consider the statistics of permutation cycles. Fig. 2(b) shows the frequency of occurrence of exchange cycles involving a varying number \( L \) of particles (1 \( \leq L \leq N \)), at three different temperatures, at the physical conditions of Fig. 1. As one can see, as the temperature is lowered exchange cycles involving growing numbers of particles occur, involving almost all particles \( N \) at the lowest temperature; however, even at a higher temperature (e.g., \( T=20 \) in Fig. 2) one observes exchanges comprising a number of particles up to \( \sim N_d \), i.e., particles inside an individual droplet. This is evidence that droplets are individually Bose condensed and superfluid, even though the system as a whole does not display superfluidity. This is observed to be the case at low \( T \), for all values of \( R_c \) and \( r_s \) for which droplets form. That droplets should always be superfluid at low \( T \) is not surprising, given that particles in a droplet are essentially non-interacting, due to the flatness of the potential at short distance. However, that droplets are themselves superfluid does not imply that a bulk supersolid phase will always occur in the \( T \rightarrow 0 \) limit, as discussed above.

The results discussed so far pertain to numerical simulation of the system described by Eq. (2) in its bulk phase. However, in any experiment aimed at probing the physics of such a system, the assembly of particles must necessarily be finite (a few thousand particles is a typical number for current experiments with cold dipolar atoms), held together by an external potential, due to the purely repulsive nature of the interaction. In order to enable a direct comparison with possible future experiments, we have performed simulations of the same system spatially confined in-plane by a harmonic trap, i.e., the term \( \Gamma \sum_i r_i^2 \) is added to Eq. (2), \( \Gamma \equiv m \omega^2/2 \) being the strength of the trap.

Fig. 4 shows typical many-particle configurations of a trapped system comprising \( N=400 \) particles, at two different temperatures. Also shown are the associated momentum distributions \( n(k) \), which are obtained by Fourier transforming of the spherically and translationally averaged one-body density matrix, computed by Monte Carlo. The momentum distributions are all nor-
many-body effects in the Rydberg-blockade regime \[16\] and achieves a relatively high $\Omega / F$ number, allowing to Rydberg states with large principal quantum number $n$, for example, $n = 45$ and experimentally reasonable $\Omega / 2\pi \times 10$MHz and $\Delta / 2\pi = 180$MHz, one obtains $a \approx 500$nm and $\gamma \approx (\Omega / \Delta)^2 \gamma_R = 0.1$s. Collective many-body effects in the Rydberg-blockade regime \[10\] not described by Eq. \[2\] should be negligible provided $(R_c / r_s)^2 \ll (2\Delta / \Omega)^2$, which is readily satisfied for parameters as in Fig. \[1\].

It is worth noting that the droplet crystal phase does not crucially depend on the dipolar form of the interaction at long distances. Indeed, it is also observed in our simulations for an interaction of the type discussed in Ref. \[17\], namely $v(r) \sim 1/r^6$. All of this suggests that this phase should be observable experimentally, using cold atoms, under relatively broad conditions.

This work was supported in part by the Natural Science and Engineering Research Council of Canada under research grant 121210893, and by the Alberta Informatics Circle of Research Excellence (iCore), IQOQI, the FWF, MURI, U Md. PFC/JQI, EOARD, NAME-QUAM.

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\[17\] A system of cold dipolar atoms or molecules can be confined to two dimensions using a tight (magnetic or optical) trap along $z$.
\[18\] We compute the superfluid fraction through the usual \textit{winding number} estimator for the bulk system.