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Supersolid Droplet Crystal in a Dipole-Blockaded Gas

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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 neighboring droplets.

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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 dissipationless 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 interparticle 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 in free space (i.e., not on a lattice).

In a recent article [5], Henkel *et al.* have proposed, based on a mean-field treatment, that a Bose condensate of particles interacting through an effective potential which flattens off at short distance, might support a density modulation. In this Letter, we show by first principle numerical simulations that interaction potentials which combine a long-distance repulsion with a short-distance cutoff, lead in fact 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 $T \rightarrow 0$ limit, as tunneling of particles across neighboring 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. Specifically, we consider the following two-body potential:

$$v(r) = \begin{cases} D/a^3 & \text{if } r \leq a \\ D/r^3 & \text{if } r > a \end{cases} \quad (1)$$

D being the characteristic strength of the interaction. This kind of interaction potential can be realized with cold dipole-blockaded Rydberg atoms [6–10]. The parameters D and a above can be controlled with external fields [5,11] (we come back to this point below).

Our system of interest comprises N identical bosons of mass m , confined to two dimensions [12]. The many-body Hamiltonian is the following (in dimensionless form):

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

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ 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 $r_0 = mD/\hbar^2$, and we introduce a dimensionless cutoff $R_c = a/r_0$ 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) interparticle distance $r_s = 1/\sqrt{nr_0^2}$. The energy scale is $\epsilon_0 = D/r_0^3 = \hbar^2/mr_0^2$.

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 [13,14]. 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 Eq. (2) is that of purely dipolar bosons in two dimensions, investigated previously by several authors [15,16]. It is known that for $r_s \lesssim r_s^C = 0.06$ the ground state of the system is a triangular crystal, whereas for $r_s \gtrsim r_s^L = 0.08$ it is a uniform superfluid (in the intermediate density range a more complex scenario is predicted [17]). 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.

Figure 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 3 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. 2(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 minima, 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

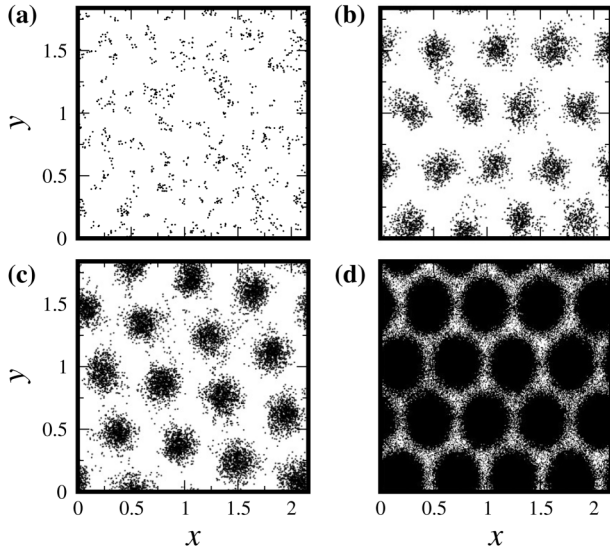


FIG. 1. Snapshots of a system of bosons interacting via potential (1), at the four different temperatures 200 (a), 20 (b), 1.0 (c) and 0.1 (d), expressed in units of ϵ_0 . Points shown are taken along individual particle world lines. The nominal value of r_s in this case is 0.14, whereas the cutoff of the potential (1) is $R_c = 0.3$.

interparticle 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 pointlike 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

$$N_d = \gamma \left(\frac{R_c}{r_s} \right)^2 \quad (3)$$

where $\gamma \approx 2.79$. Equation (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 Eq. (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 [18,19].

In the $T \rightarrow 0$ 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

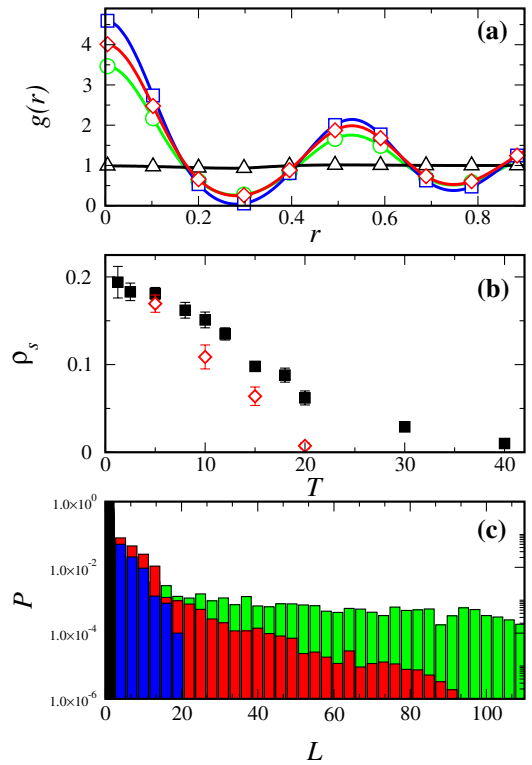


FIG. 2 (color online). Results shown are for $r_s = 0.14$ and $R_c = 0.3$. Temperature is in units of ϵ_0 . (a) Pair correlation function $g(r)$ at a temperature $T = 200$ (triangles), 20 (squares), 1.0 (diamonds) and 0.1 (circles). The simulated system comprises $N = 200$ particles. (b) Superfluid density vs T for systems with $N = 100$ (square), and 200 (diamond) particles. (c) Frequency of occurrence of permutation cycles of length L at the same four temperatures reported in panel (a). Longer permutation cycles occur at lower temperature.

result in a finite superfluid response throughout the whole system, and indeed for $R_c \gtrsim r_s^L$ we observe such a bulk superfluid signal, in a range of values of r_s in the vicinity of $R_c/2$. A typical result is shown in Fig. 2(b)[20]. Because superfluidity arises in concomitance with the droplet-crystal structure, the denomination *supersolid* seems appropriate.

In order to establish that droplets are individually superfluid, one may consider the statistics of permutation cycles. Figure 2(c) 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. At low temperature they involve almost all the particles in the system; however, even at a higher temperature [e.g., $T = 20$ in Fig. 2(c)] 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. That droplets should be superfluid at low T is not surprising, given that particles in a droplet are essentially noninteracting, 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.

At $T = 0$, the supersolid 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 $R_c \lesssim r_s^C$, only two insulating phases are observed, namely, the insulating droplet crystal at high density and the crystal of single particles, already detected in Refs. [15,16], 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 behavior in this system originates from tunnelling of particles between droplets which are themselves individually superfluid, so that 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.

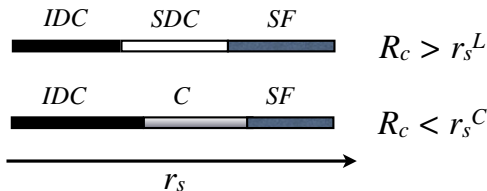


FIG. 3 (color online). Schematic ground state phase diagram of Eq. (2) as a function of r_s . The superfluid droplet crystal (SDC) is sandwiched between an insulating droplet crystal (IDC) and a superfluid (SF). For $R_c \lesssim r_s^C$, an IDC phase, a single-particle crystal (C) phase and a superfluid phase are observed. The widths of the SDC and C regions depend on the value of R_c .

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), confined by an external potential. 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.

Figure 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 calculations.

Here too, droplets with a well-defined average number of particles form, and organize themselves on a triangular lattice. Correspondingly, the momentum distribution, which is directly observable experimentally by time-of-flight measurements [21], develops a sharp central peak, with additional structure on its sides. The secondary peaks correspond to oscillations in the one-body density matrix, in turn reflecting particle tunnelling to adjacent droplets. They are therefore connected to the appearance of the supersolid phase, as explained above.

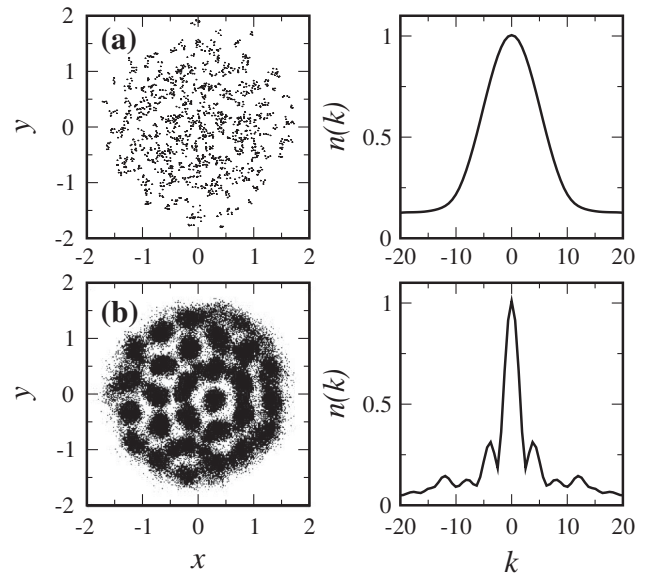


FIG. 4. Left panels: Monte Carlo snapshots of a system of $N = 400$ particles, interacting via the potential (1), confined in a harmonic trap of strength $\Gamma = 500\epsilon_0$, at the two temperatures $T = 100 \epsilon_0$ (a) and $T = 0.5 \epsilon_0$ (b). Right panels: corresponding momentum distributions, all normalized to unity for comparison purposes. The value of R_c in this case is 0.3. The development of secondary peaks at low temperature signals the occurrence of a supersolid phase.

Summarizing, accurate numerical simulations of a system of dipolar particles interacting via a potential softened at short distance, reveal the existence of a low-temperature crystalline phase of superfluid droplets. This phase turns superfluid (supersolid) at $T \rightarrow 0$ through a mechanism of tunnelling of particles between adjacent droplets. At higher density this tunnelling is suppressed and an insulating droplet crystal occurs, a phase which has not previously been predicted. The interaction that underlies such intriguing, until now unobserved physical behavior, can be realized with dipolar atoms in the dipole-blockade regime.

A comment is in order, concerning the dependence of the results on the particular form of potential utilized here, namely, Eq. (1) with its abrupt, sharp cutoff at $r = a$. First off, the superfluid 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 van der Waals-like potentials [i.e., $v(r) \sim r^{-6}$]. Second, we have obtained qualitatively similar results with different model potentials, featuring a more realistic “flat” region at short distances, as well as a smoother merge of long- and short-range behaviors. For example, we considered the potential $V(r) = D/(a^3 + r^3)$, which is naturally realized in a cold gas of alkali atoms by weakly dressing the ground state $|g\rangle$ of each atom with an excited Rydberg state $|r\rangle$ with a large dipole moment d , in the kDebye range [11].

While several dressing schemes are possible [5,22], here we consider $|r\rangle$ as the lowest-energy state of a Rydberg manifold with principal quantum number n for an atom in the presence of a homogeneous electric field $F < F_{IT}$ in the linear Stark regime, with $F_{IT} \propto 1/n^4$ the Inglis-Teller limit. For a laser with (effective) Rabi frequency Ω and red detuning $|\Delta| \gg \Omega$, the dressed ground state reads $|\tilde{g}\rangle \sim |g\rangle - (\Omega/2\Delta)|r\rangle$, and thus $D \propto (\Omega/\Delta)^4 d^2$, with $d \propto n^2$, while the cutoff $a \simeq (d^2/\hbar|\Delta|\epsilon_0)^{1/3}$ arises because of the Rydberg-blockade mechanism [6]. Spontaneous emission rates γ_r from $|r\rangle$ are strongly reduced to values of at most $\gamma \simeq (\Omega/\Delta)^2 \gamma_r$. Observability of the phases above benefits from large values of ϵ_0 , and, in particular, of the ratio $\epsilon_0/(h\gamma) = [\Omega^2/(4\pi|\Delta|\gamma_r)]R_C^3$, favoring comparatively small values of r_0 [23]. For example, for ^{87}Rb atoms in an electric field $F = 25$ kV/m, with $n = 20$, $\Omega/2\pi = 50$ MHz and $|\Delta|/2\pi = 3$ GHz, we obtain $d = 1450$ Debye, $a \simeq 400$ nm, $r_0 \simeq 210$ nm, $\epsilon_0/(h\gamma) \simeq 90$, and $\epsilon_0/k_B \simeq 120$ nK. Collective many-body effects in the Rydberg-blockade regime [22] 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.

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