Demixing in symmetric supersolid mixtures

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The droplet crystal phase of a symmetric binary mixture of Rydberg-blockaded dipolar Bose gases is studied by computer simulation. At high temperature each droplet comprises on average equal numbers of particles of either component, but the two components demix below the supersolid transition temperature, \textit{i.e.}, droplets mostly consist of particles of one component. Droplets consisting of the same component will also favor clustering. Demixing is driven by quantum tunnelling of particles across droplets over the system, and does not take place in a non-superfluid crystal. This effect should be easily detectable in a cold gas experiment.

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The separation at low temperature of the individual components of a mixture (demixing) is a topic of long standing interest in physics and chemistry. It typically occurs due to differences in interactions, but quantum-mechanical effects, either related to mass differences (zero-point motion) or to quantum statistics, can play an important role. One of the most interesting examples of binary mixture whose phase diagram is significantly affected by quantum statistics, is that of a mixture of the two isotopes of helium, which historically had a profound influence on refrigerating.\textsuperscript{1}

In recent years, renewed interest in quantal binary mixtures has been motivated by experimental advances in cold atom physics, allowing for the controlled study of the phase diagram of multicomponent systems, notably mixtures of Bose-Einstein condensates (BECs). The potential advantage that ultracold gases offer, compared to ordinary condensed matter systems, is that demixing can be observed on considerably shorter time scales and directly in real space with individual particle resolution.\textsuperscript{2} The first experimental realization of a two-component Bose mixture, consisting of two hyperfine states of Rb, was reported in 1997 by Pethick and Smith.\textsuperscript{3} Successively, a mixture of different atomic species (K and Rb) was also stabilized.\textsuperscript{4}

Early work on bosonic mixtures predicted phase separation at exactly zero temperature for isotopes of different masses or concentrations.\textsuperscript{5,6} The focus of more recent theoretical work has been on identifying the conditions under which demixing occurs in binary BEC mixtures with repulsive interactions.\textsuperscript{7,11,12} The systems we are looking at in this work have a SU(2)-symmetric Hamiltonian

$$H = \int dr \psi_{\sigma}^\dagger(r) H_0 \psi_{\sigma}(r)$$

$$+ \frac{1}{2} \int dr \int dr' V(r - r') \psi_{\sigma}^\dagger(r) \psi_{\sigma'}^\dagger(r') \psi_{\sigma'}(r') \psi_{\sigma}(r),$$

where $H_0$ is the kinetic energy (it may contain also an external one-body potential), $V(r - r')$ the two-body interaction term, $\psi_{\sigma}$ the Bose field operators for components $\sigma = 1, 2$ and the summation is performed over repeated Greek indices. The dispersion for both species is identical. Separation of species 1 and 2 is usually characterized in terms of a parameter $\Delta = U_{12} - U_{11}^2$, defined in terms of the relative intraspecies ($U_{11}, U_{22}$) and interspecies ($U_{12}$) characteristic interaction strengths. When $\Delta < 0$, \textit{i.e.}, unlike particles repel more strongly, separation of the two components occurs, whereas for $\Delta \geq 0$ they remain mixed.\textsuperscript{7,10} However, in trapped bosonic mixtures, it was recently shown that the effective attraction between identical Bose particles leads to demixing at low finite temperatures, even in purely repulsive (dipolar) Bose mixtures that are SU(2) symmetric (\textit{i.e.}, a stricter condition than $\Delta = 0$).

Recent studies of demixing arising from quantum-mechanical effects have focused primarily on the gas or liquid phases, although a solid $^3\text{He} - ^4\text{He}$ mixture, extensively studied experimentally and theoretically in the past, remains arguably the most important example of low temperature isotopic separation. In that case, all interactions are very nearly identical, and effects of quantum statistics are negligible at the temperature at which onset of phase separation is observed. Separation is driven by single-particle tunnelling, and can be ascribed to the mass difference between the two isotopes, resulting in different equilibrium densities. Cold gases seem the ideal playground in which fundamental questions about demixing in the solid phase can be addressed experimentally, with a high degree of control. The observable selection of ground states has been suggested for isotopic SU(2) symmetric BECs,\textsuperscript{20} when lowering the temperature below the superfluid transition. Potentially interesting is the study of demixing in solid phases not occurring in ordinary condensed matter.\textsuperscript{19}
In this Letter, we predict low-temperature demixing in a SU(2) symmetric two-component supersolid Bose mixture. The crystalline phase considered here features a multiply-occupied unit cell (essentially a “droplet” or cluster of particles), and turns supersolid at sufficiently low temperature through the tunnelling of particles between adjacent (locally superfluid) droplets. It arises at low temperature in the presence of a specific pair-wise interaction, featuring a soft repulsive core at short distances \[20, 23\]. This type of interaction can be artificially fashioned by means of a mechanism known as the Rydberg Blockade \[24\]. The excitation spectrum of the one-component system was recently shown to display two distinct modes in the supersolid phase \[25\].

Demixing in the two-component system is a consequence of the same physical mechanism that underlies the supersolid transition in the single-component system. In the normal solid phase, at temperatures where quantum statistical effects are negligible, unit cells feature on average the same numbers of particles of either species. At lower temperatures, but where the system is still insulating, unit cells comprise prevalently particles of one of the two species due to exchanges within each droplet. Further, below the supersolid transition, macroscopic separation (demixing) of the two components is also predicted, i.e., clusters containing particles of a given type are surrounded by clusters of the same type of particles. This effect should be observable experimentally, for example using a bosonic system where the bosons have an internal degree of freedom.

Our model consists of a two-component mixture, with particles confined to moving in two dimensions and with only pair-wise interactions. Let 1 and 2 be the two components, both obeying Bose statistics, and \(N_1\) and \(N_2\) the corresponding numbers of particles. We are interested here in the type of soft-core repulsive potentials which are known to underlie the supersolid phase described above \[23\], and for definiteness we take the same expression considered in Ref. \[21\], namely

\[
V(r) = \begin{cases} 
\frac{C}{a^2} & \text{if } r \leq a \\
\frac{C}{r^2} & \text{if } r > a
\end{cases},
\]

with \(a\) being the interaction cutoff. Henceforth, all lengths are expressed in terms of the characteristic unit \(r_o = mc^2/\hbar^2\), and we also introduce the energy scale \(\epsilon_o = C/r_o^3 = \hbar^2/mc^2\). It is important to state up front that the main physical results discussed here do not depend on the detailed form of the potential for \(r > a\), but only on the existence of a soft repulsive core. The Hamiltonian is symmetric with respect to an interchange of the component labels 1 and 2. Thus, any phase separation must arise exclusively as a result of Bose statistics.

With the two-body interaction \(2\), we have investigated the finite temperature equilibrium properties of the system using Quantum Monte Carlo simulations based on the continuous-space Worm algorithm \[30, 31\] in the grand canonical ensemble. This methodology yields results that are numerically exact to within a statistical error, which may be made arbitrarily small by sampling from a sufficient number of configurations of the system. We consider a system with a Rydberg blockade interaction cutoff \(a/r_o = 0.27\), contained in a square simulation cell with periodic boundary conditions in both directions; we adjust the chemical potential so that the mean inter-particle separation is \(r_s = 0.15\) (equivalent to an average density \(\rho r_s^2 = 45\)). For this choice of parameters, the one-component system displays a low temperature supersolid phase \[21\].

In our grand canonical simulations, we can directly observe the phenomenon of phase separation, which manifests itself as spontaneous symmetry breaking between the populations of species 1 and 2. That is, at equilibrium either species will have a greater population, although the total population of both species is fixed by the chemical potential. This effect is shown clearly in Fig. 1 which plots the number of particles of each species as a function of simulation time at three temperatures. Obviously, because our simulated system only comprises around 170 particles, the system will typically be observed to switch between two different configurations, in which either species dominates. At \(T = 20\epsilon_o\) [Fig. 1(a)] the populations of each species fluctuates around the same mean value. For \(T = 10\epsilon_o\) [Fig. 1(b)] we observe longer periods of population imbalance, whereas at the lowest temperature \(T = 5\epsilon_o\) [Fig. 1(c)] we observe a species 1-rich phase over the entire duration of the simulation, indicative of phase separation \[32\]. For comparison we have also plotted the populations for each species obeying Boltzmann statistics (i.e., where exchanges are not permitted) at the lowest temperature. In this case we find, as expected, that \(N_1 \approx N_2\). Thus, demixing in the symmetric mixture is a direct result of Bose statistics \[27\]. We also fail to see demixing if the simulation is carried out for values of the model parameters \(r_s\) or \(a\) such that the droplet crystal phase of the single-component Bose system is not supersolid \[21\].

To make the concept of phase separation more rigorous we define the demixing parameter:

\[
D = \langle(N_1 - N_2)^2\rangle/\langle(N_1 + N_2)^2\rangle,
\]

which is related to the expectation value of the square of the isospin \(S_z\) operator of the underlying SU(2) algebra. By construction, when \(D = 1\) the system is fully demixed whereas \(D = 0\) corresponds to a mixed state.

Fig. 2(a) shows \(D\) as a function of temperature. In order to assess that phase separation \((D > 0)\) is concomitant with supersolidity, we show in Fig. 2(b) the superfluid fraction of component 1, denoted \(f_s\), calculated using the winding number estimator. For clarity we omit the superfluid fraction for component 2 noting that this quantity is equal for both components to within statis-
FIG. 1. (Color online) Number of particles per species \( N_\alpha \) \((\alpha = 1, 2)\) as a function of simulation time at temperatures (a) \( T = 20\epsilon_0 \), (b) \( T = 10\epsilon_0 \) and (c) \( T = 5\epsilon_0 \) (all temperatures are in units of \( \epsilon_0 \)). Phase equilibrium requires that the chemical potentials for both species be equal, with \( \mu_1 = \mu_2 \), chosen so the total number of particles is \( N \approx 170 \). Note the blue curve corresponds to species \( \alpha = 1 \), the red to \( \alpha = 2 \) whereas the dotted curves represent the equivalent simulation but in the case of Boltzmann statistics.

There are in fact three characteristic scales that determine the phase diagram of the symmetric two component system: the thermal de Broglie wavelength \( \lambda_{dB} = (2\pi\hbar^2/mk_BT)^{1/2} \), the mean interparticle separation \( r_s = 1/\sqrt{\rho} \), and the Rydberg blockade interaction cutoff \( a \). When the interaction cutoff exceeds the interparticle separation \((a > r_s)\), we expect the system to aggregate into droplets purely through classical potential energy considerations. Moreover, as the temperature of the system is lowered, so that the de Broglie wavelength becomes comparable to (and larger than) the interparticle separation, quantum statistical effects become important. In particular, the world line configurations of the system can involve permutation cycles of more than one particle (of a given bosonic species), this being a manifestation of the exchange symmetry of identical bosons (and being the same mechanism responsible for both superfluidity and Bose-Einstein condensation). There are two regimes for which quantum statistical effects prevail. First, when the de Broglie wavelength is less than or of the order of the interaction cutoff, there exists demixing only within individual droplets. Second, when the de Broglie wavelength is comparable to or larger than the interaction cutoff, permutation cycles can involve particles in adjacent droplets and droplets that are farther away. It is in this situation that phase separation emerges as well as long range order, so the system becomes supersolid.

The mechanism that leads to demixing can equally be observed in lattice models. The lattice two-component Bose-Hubbard model (2CBHM), obtained by setting \( V(r-r') = U\delta(r-r') \) in Eq. 1 and performing a tight binding analysis to the lowest Wannier band in the presence of an external lattice potential, has clear parallels with the free-space supersolid system considered here since each multiply-occupied lattice site acts like a single droplet in the supersolid system. With equal values of the
nearest-neighbor hopping and the on-site inter- and intra-species repulsion, and with a density that is sufficiently high, the same type of phase separation is observed. Each of the two components breaks a $U(1)$ symmetry, and the ground state wavefunction is a superposition of the phase separated condensates, leading to spatial demixing. For unit density and strong interactions however, the phase diagram features a phase with counterflow in which only one $U(1)$ symmetry is broken. The existence of such a phase was previously shown in [28] for hard-core bosons. In case of $SU(2)$ symmetric interactions and a phase with counterflow, no superposition takes place. Finally, we remark that the difference in ground state wavefunction between a Boltzmann and a Bose system vanishes according to Feynman’s theorem [29]. Remixing is hence expected at exactly $T = 0$ in our system as well.

In summary, we have shown that a symmetric 2-component bosonic crystal with equal inter- and intra-species Rydberg-blockaded interactions exhibits phase separation, as is evident from a spontaneous symmetry breaking of the particle number for each species, concomitantly with its transition to a supersolid phase at low temperature. Controlling such mixtures during a cooling process and the detection of the demixing are within reach of current technology.

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\[ \text{FIG. 2. (Color online) (a) Demixing parameter } D \text{ as a function of temperature. (b) Corresponding superfluid fraction } f_s \text{ for component } a. \text{ Parameters are } r_s/r_0 = 0.15 \text{ and } a/r_0 = 0.27. \text{ Where error bars are absent, statistical errors are smaller than the point size.} \]
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