Creating a supersolid in one-dimensional Bose mixtures

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We identify a one-dimensional supersolid phase in a binary mixture of near-hardcore bosons with weak, local interspecies repulsion. We find realistic conditions under which such a phase, defined here as the coexistence of quasi-superfluidity and quasi-charge density wave order, can be produced and observed in finite ultra-cold atom systems in a harmonic trap. Our analysis is based on Luttinger liquid theory supported with numerical calculations using the time-evolving block decimation method. Clear experimental signatures of these two orders can be found, respectively, in time-of-flight interference patterns, and the structure factor \( S(k) \) derived from density correlations.

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The supersolid (SS) phase, defined as a many-body state that simultaneously shows superfluid (SF) and charge density wave (CDW), i.e. crystalline, order, has been an intriguing notion since its first proposal \cite{1}, due to its seemingly paradoxical nature. Numerous studies of SS phases \cite{2,3} have recently been reported, motivated by fundamental theoretical interest in a system that exhibits competing orders, and by recent experimental reports of observations of supersolidity of \(^4\)He in yucor glass \cite{4,6}. This \(^4\)He system exemplifies the complexity of studying strongly correlated systems in a solid-state context: it combines strong disorder due to the porous medium, strong interactions between atoms and of atoms with surfaces. Under such circumstances it is difficult to demonstrate the existence of a SS phase, which involves a subtle competition of fluctuations.

In this paper we show that supersolidity can be studied with clarity in another physical system: ultra-cold atoms in optical lattices. Since the demonstration of the SF-Mott insulator transition in 3D \cite{12}, the technology of cooling and trapping atoms has supported studies of numerous quantum many-body phenomena, such as BCS-BEC crossover \cite{3}, noise correlations \cite{3}, the Berezinsky-Kosterlitz-Thouless transition \cite{5}, the Tonks-Girardeau gas \cite{10,11}, transport and collisional properties of one-dimensional (1D) gases \cite{11}, and the Mott transition in 1D \cite{13} and 2D \cite{14}. Appealing features of this technology, from the perspective of many-body theory, are that it creates well defined and tunable systems, and that the set of measurable quantities differs from those in solid-state systems. Thus, ultra-cold atom systems can give interesting and unusual insights into many-body states.

The objective of this paper is to propose a realistic setup of how to create and detect a supersolid with current technology. Specifically, a binary mixture of near-hardcore bosons with weakly repulsive inter-species contact interactions in a 1D potential displays both CDW and SF quasi-long range order (QLRO). Such mixtures have an inherent tendency to undergo phase separation, which can be avoided if the inter-species interactions are sufficiently weak.

We study the SS phase with analytical and numerical techniques, and present a concrete proposal for its realization in current experimental systems. First we use a Luttinger liquid (LL) approach to derive the phase diagram of the homogeneous, infinite system, with a renormalization group (RG) calculation. We then address the question of realizing such a phase under realistic conditions, for a finite system of \( \sim 10^2 \) lattice sites in a harmonic trap. Using a number-conserving time-evolving block decimation (TEBD) method \cite{15} we numerically determine, with a well-controlled error, the ground state of the system from which we extract various correlation functions. We first identify the SS phase, through signatures in the pair and anti-pair correlations. Other correlations contain information that is accessible to direct experimental observation, and we discuss possible experimental signatures of the SS phase, i.e. the coexistence of SF and CDW order; the SF order is manifest in the single-particle correlation function, which can be determined from time-of-flight (TOF) interference patterns; the CDW order is seen in density-density correlations, which is reflected in a measurable structure factor.

We consider a mixture of two species of bosonic atoms with short-range interparticle interactions, confined in a 1D optical lattice and an additional harmonic potential. Contemporary experimental realizations of such systems are usually well approximated by a Hubbard model:

\[
H = -t \sum_{<ij>,a} b^\dagger_{a,i} b_{a,j} + \frac{U}{2} \sum_{i,a} n_{a,i} (n_{a,i} - 1) + U_{12} \sum_{i} n_{1,i} n_{2,i} + \Omega j^2 (n_{1,j} + n_{2,j}).
\] (1)

Here \( t \) is the hopping energy; \( b_{a,i} \) is a boson field operator, with \( a = 1, 2 \) a species index and \( i \) a lattice site index; \( U \) (\( U_{12} \)) is the intra- (inter-)species on-site interaction energy; \( n_{a,i} = b^\dagger_{a,i} b_{a,i} \); and \( \Omega \) represents the strength of the harmonic trap, which is centered on the site \( j = 0 \).

We now derive the phase diagram of this system from...
LL theory. We consider two 1D bosonic SFs, with densities equal to each other, but incommensurate to the optical lattice. In particular we exclude half- and unit-filling, which would destroy the SF order, by choosing the density and the global trap in such a way that even at the trap center the density of each species stays below 0.5. The essential function of the optical lattice is to provide a sufficiently large ratio of $U/t$, as in [10]. We emphasize that the supersolid phase also exists in the absence of $U/t$, as in [10]. We change variables to the symmetric and antisymmetric combinations $\phi_{s,a} = \frac{1}{\sqrt{2}}(\phi_1 \pm \phi_2)$ and $\theta_{s,a} = \frac{1}{\sqrt{2}}(\theta_1 \pm \theta_2)$, and diagonalize the quadratic part of the action which gives the following parameters for the two sectors:

$$K_{s,a} = (1/K^2 \pm U_{12}/v \pi K)^{-1/2}$$

which to lowest order gives $K_{s,a} \approx K \mp U_{12} K^2/2\pi v$. The effective velocities are $\nu_{s,a} = \sqrt{v^2 \pm U_{12} K v/\pi}$. Phase separation (collapse) is reached when $\nu_{a(n)}$ becomes imaginary. The anti-symmetric sector contains the nonlinear backscattering term. To study its effect, we use an RG approach; the flow equations for which are given by [20]:

$$\frac{dg_{s,a}}{dl} = (2 - 2K_s)g_s; \quad \frac{dK_s}{dl} = -\frac{g_s^2}{2\pi^2} K_s^3$$

This set of flow equations has two qualitatively different fixed points: Either $g_s$ diverges, driving a pairing transition, which in turn renormalizes $K_s$ to zero, or $g_s$ is renormalized to zero. In the latter case the Gaussian fixed point is restored with a finite effective value $K^*_s$. Therefore the correlation functions are again algebraic, containing this effective parameter. It is this second scenario that we are interested in, not the actual phase transition itself.
To determine the phase diagram we consider the correlation functions of these order parameters: single-particle SF, described by $O_{SF} = b_a$, CDW order, corresponding to the $2k_F$-component of the density operator $O_{CDW} = n_a$, and paired SF, $O_{PSF} = b_1 b_2$, which appears on the attractive side. The form of these correlation functions is $\langle O(x)O(0) \rangle \sim |x|^{a-2}$, except for the single-particle SF in the paired regime, where it decays exponentially. An order parameter $O(x)$ has QLRO, if its correlation function is algebraic, and $a > 0$. This implies that the corresponding susceptibility is divergent, indicating an instability towards ordering $|x|^{a-2}$. The scaling exponent of $O_{SF}$ is $\alpha_{SF} = 2 - 1/4K - 1/4K_a$, the one of $O_{CDW}$ is $\alpha_{CDW} = 2 - K_a - K_a$, and PSF has $\alpha_{PSF} = 2 - 1/K_a$. We also consider the anti-pair operator $b_1 b_2$, which has a scaling exponent of $2 - 1/K_a$. We use the latter two correlation functions in the numerical fitting procedure. In Fig. 1 we see the resulting phase diagram. For attractive interactions we see the formation of a paired phase, in which two regimes of quasi-order are found: in the entire paired regime, PSF is the dominant QLRO, whereas for part of that regime we find CDW as a subdominant order. The latter can be considered a SS of pairs, whereas single-particle SF is destroyed. On the repulsive side we find the SS phase that we look for in this paper. Using the flow invariant $g_2^2 - 4\pi^2(K_a + 1)^2$, and Eq. 4, we determine the nearly linear SS phase boundary for small repulsive interactions to be: $U_{12}/v \geq 32\ell \sin \pi n/\ell/U$.

Having given the phase diagram of the infinite, homogeneous system, we now address the question of how supersolidity can be found in actual cold atom systems. For this, we use a TEBD method to obtain the ground state of the system. We choose a small value for $t/U$, to reach the near-hardcore regime, and a positive $U_{12}$ of the order of $t$, to avoid phase separation. We choose the atom number and the global trap parameter, such that the density is smaller than 0.5 throughout the system. In Fig. 2 we show the densities of the two species for the case $t/U = 0.005$, $U_{12}/U = 0.04$, $\Omega = 10^{-5}U$, and a particle number of 17 of each atom species, on a lattice of 90 sites, as an illustration of the ground state. One can clearly see the density modulation of each species, whose wavelength is determined by the density, not the lattice.

A central question when studying ‘phases’ in finite-size, non-homogeneous systems, is whether a given state can be reasonably related to a phase of the associated system in the thermodynamic limit. We address this question by numerically fitting the correlation functions of the pair and the anti-pair operator in the bulk of the system with power-law functions. We find a very good fit, and we depict the scaling exponents extracted from the numerical data in Fig. 3 as a function of the interaction $U_{12}$.

Having established that the state of the system is indeed a supersolid, we now turn to the crucial question of how this phase can be detected in experiment. We propose two measurements that would address this question: 1) a TOF interference measurement to determine the single-particle correlation function, which is the defining quantity of SF QLRO, and 2) a measurement of the structure factor to determine the density correlation function, which is the defining quantity of CDW QLRO.

**TOF measurement.** We assume that when the optical lattice is turned off, the atoms expand freely, that is $b_a(x,t) = \sum_j w(x - r_j) b_{a,j}$, where $w(x,t) = \sqrt{d/\sqrt{2\pi \Delta(t)^2}} \exp(-x^2/4\Delta(t)^2)$, with $\Delta(t)^2 = d^2 + ith/2m$, $a$ the lattice constant, $d$ the width of the initial state, assumed Gaussian, $t$ the expansion time, and $m$ the atomic mass. We calculate the density $n(x) = \langle b_d^\dagger(x,t) b(x,t) \rangle$, which contains the single particle correlation function of the original system, which we show in
be created and probed in present ultracold atom experiments: in particular, with only local interatomic interactions. Using LL theory, we identified the generic phase diagram of this system for incommensurate filling; with TEBD simulations we found a concrete example of a finite, realistic system, including a global trap, which shows both SF and CDW QLRO. Two well-established measurement techniques, the TOF signal and the structure factor, provide clear experimental signatures of the two orders present in this remarkable state of matter.

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