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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-hard-core bosons with weak, local interspecies repulsion. We find realistic conditions under which such a phase, defined here as the coexistence of quasisuperfluidity and quasi-charge-density-wave order, can be produced and observed in finite ultracold atom systems in a harmonic trap. Our analysis is based on Luttinger liquid theory supported by 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 [1] due to its seemingly paradoxical nature. Numerous studies of SS phases [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 Vycor glass [4,5]. 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 and 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: ultracold atoms in optical lattices. Since the demonstration of the SF–Mott-insulator transition in three dimensions (3D) [6], the technology of cooling and trapping atoms has supported studies of numerous quantum many-body phenomena, such as the BEC-BCS crossover [7], noise correlations [8], the Berezinsky-Kosterlitz-Thouless transition [9], the Tonks-Girardeau gas [10,11], transport and collisional properties of 1D gases [12], and the Mott transition in 1D [13] and 2D [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, ultracold 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-hard-core bosons with weakly repulsive interspecies 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 interspecies 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 [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 antipair 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; and 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:

$$H = -t\sum_{\langle ij\rangle,a} b^\dagger_{a,i}b_{a,j} + \frac{U}{2}\sum_{i,a} n_{a,i}(n_{a,i}-1) + U_{12}\sum_i n_{1,i}n_{2,i} + \sum_j \Omega j^2(n_{1,j}+n_{2,j}). \quad (1)$$

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 Ω 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 a lattice [16]; however, since present quasihomogeneous ultracold atomic systems are generically closer to weak coupling, the presence of a lattice is advantageous to experimental realization of supersolidity.

The basic concept of LL theory is to express the bosonic operators $b_{a,i}$ through a bosonization identity, such as Haldane's construction [17,18]:

$$b_{1,2}(x) = [n + \Pi_{1,2}(x)]^{1/2} \sum_m e^{2mi\Theta_{1,2}(x)} e^{i\Phi_{1,2}(x)}, \qquad (2)$$

where we switched to a continuum model, $b_{a,i} \to b_a(x)$. n is the average density of the two species; $\Pi_{1,2}(x)$ are the low-k parts (i.e., $k \ll 1/n$) of the density fluctuations; and the fields $\Theta_{1,2}(x)$ are given by $\Theta_{1,2}(x) = \pi n x + \theta_{1,2}(x)$, with $\theta_{1,2}(x) = \pi \int^x dy \Pi_{1,2}(y)$. $\Phi_{1,2}$ are the phase fields, the conjugate fields of the density fluctuations $\Pi_{1,2}(x)$.

In terms of these fields, the action of the two coupled bosonic SFs is given by [18,20]

$$S = \int d^2 r \Bigg[\sum_{j=1,2} \frac{1}{2\pi K} [(\partial_\tau \theta_j)^2 + (\partial_x \theta_j)^2] + \frac{U_{12}}{\pi^2} \nabla \theta_1 \nabla \theta_2 + \frac{2 g_\sigma}{(2\pi\alpha)^2} \cos(2\theta_1 - 2\theta_2) \Bigg]. \qquad (3)$$

The two SFs are characterized by a LL parameter K and a velocity v, which is contained in $\mathbf{r} = (v\tau, x)$. The LL parameter K is a measure of the intraspecies interaction; in the near-hard-core regime, we use [19]

$$K \approx 1 + \frac{8t}{U} \frac{\sin \pi n}{\pi}. \qquad (4)$$

Similarly, v can be related to the parameters of the underlying Hubbard model by $v \approx v_F(1 - 8tn \cos \pi n / U)$, where v_F is the "Fermi velocity" of an identical system of fermions, $v_F = 2t \sin \pi n$. The density-density interaction between the two SFs creates both the term containing $\nabla\theta_1 \nabla\theta_2$, as well as the backscattering term [3,20], containing $\cos(2\theta_1 - 2\theta_2)$, which describes short-range interspecies repulsion.

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:

$$K_{s/a} = (1/K^2 \pm U_{12}/v\pi K)^{-1/2}, \qquad (5)$$

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

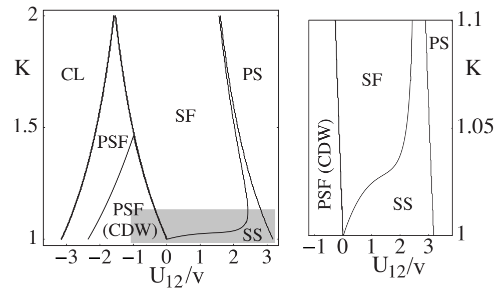

FIG. 1. Phase diagram of a Bose mixture, from LL theory, as a function of the interspecies interaction U_{12} (in units of v, see text) and the LL parameter K of the uncoupled system [Eq. (4)]; on the left the full diagram, on the right (corresponding to the shaded area) the near-hard-core, repulsive regime with the supersolid (SS) phase. For attractive interactions, in the paired regime, paired SF (PSF) is dominant, with CDW QLRO being subdominant in parts of it. Outside of that regime, SF is the dominant quasiorder, but for the repulsive, near-hard-core regime we have CDW QLRO as well, which constitutes a supersolid phase. For large repulsive interactions, the system phase separates (PS); for large attractive ones, it collapses (CL).

$$\frac{dg_\sigma}{dl} = (2 - 2K_a) g_\sigma, \qquad \frac{dK_a}{dl} = -\frac{g_\sigma^2}{2\pi^2} K_a^3. \qquad (6)$$

This set of flow equations has two qualitatively different fixed points: Either g_σ diverges, driving a pairing transition, which in turn renormalizes K_a to zero, or g_σ is renormalized to zero. In the latter case the Gaussian fixed point is restored with a finite effective value K_a^*. 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 $\langle O(x) O(0) \rangle \sim |x|^{\alpha - 2}$, 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 $\alpha > 0$. This implies that the corresponding susceptibility is divergent, indicating an instability toward ordering [20]. The scaling exponent of O_{SF} is $\alpha_{SF} = 2 - 1/4K_s - 1/4K_a$, the one of O_{CDW} is $\alpha_{CDW} = 2 - K_s - K_a$, and PSF has $\alpha_{PSF} = 2 - 1/K_s$. We also consider the antipair operator $b_1^\dagger b_2$, 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 quasiorder 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 $g_\sigma^2 - 4\pi^2 (K_a - 1)^2$ and Eq. (4), we determine the nearly linear SS phase boundary for small re-

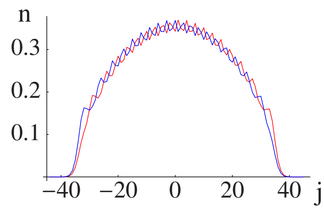

FIG. 2. (Color online) The single-atom density of species 1 (red) and 2 (blue) of a system of 90 sites, with 17 atoms of each type, with $t/U=0.005$, $U_{12}/U=0.04$, and a trap parameter $\Omega=10^{-5}U$.

pulsive interactions to be $U_{12}/v \geqslant 32t \sin \pi n/U$.

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 [15] to obtain the ground state of the system. We choose a small value for t/U to reach the near-hard-core 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, nonhomogeneous 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 antipair operators 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: (a) a TOF interference measurement to determine the single-particle correlation function, which is the defining quantity of SF QLRO, and (b) a measurement of the structure factor [21] to determine the density correlation function, which is the defining quantity of CDW QLRO.

(a) *TOF measurement*. We assume that when the optical lattice is turned off, the atoms expand freely—that is, $b_a(x,t)=\Sigma_j w(x-r_j) b_{a,j}$, where

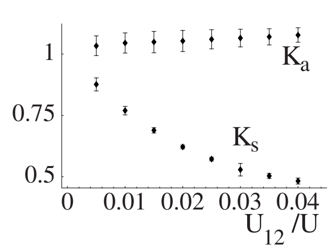

FIG. 3. LL parameters K_s and K_a, as a function of U_{12}, for the same parameters as in Fig. 2, from numerical fitting.

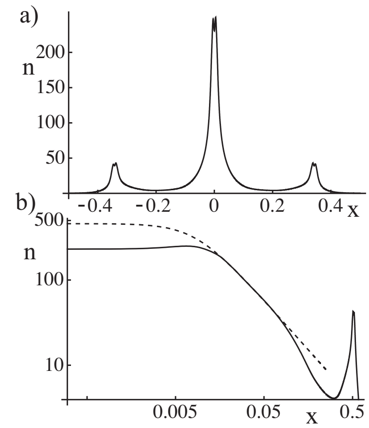

FIG. 4. Interference pattern of the atomic mixture, with the parameters of Fig. 2, when interpreted as ^{87}Rb, released from an optical lattice with lattice constant $a=400$ nm, localized states with a length scale $d=60$ nm, after an expansion time $t=30$ ms. This could be realized with an optical lattice potential of $18E_R$ in the longitudinal and $30E_R$ in the transversal directions, E_R being the recoil energy. In (a) we see the 1D density n of the full pattern (in units mm^{-1}), as a function of the spatial coordinate x (in mm). In (b) we fit the central interference peak with a power law. The good numerical fit indicates the presence of single-particle quasisuperfluidity.

$$w(x,t) = \sqrt{d/\sqrt{2\pi}\Delta(t)^2}\, \exp[-x^2/4\Delta(t)^2],$$

with $\Delta(t)^2=d^2+it\hbar/2m$, 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 $n(x)=\langle b^\dagger(x,t)b(x,t)\rangle$, which contains the single-particle correlation function of the original system, which we show in Fig. 4. Figure 4(a) shows the full interference pattern, and Fig. 4(b) the central peak with a fit with a power-law function $c(x^2+a^2)^{\alpha/2-1}$, shown on a log-log scale. The good agreement with power-law scaling indicates the presence of SF QLRO.

(b) *Structure factor*. We assume, as an example, an *in situ* measurement of the same system described before. The real-space structure factor is related to the density-density correlation function of the lattice system by

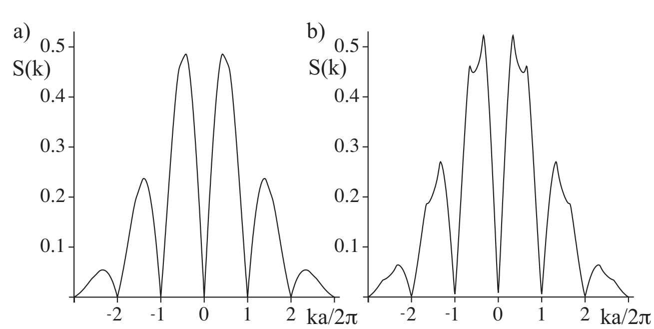

FIG. 5. Structure factor of the atomic mixture, with the same parameters as in Fig. 4, in $1/\mu$m, as a function of k in units of $2\pi/a$. (a) corresponds to very weak interactions $U_{12}/U=0.0025$ and shows no particular structure beyond a SF signature; (b) corresponds to $U_{12}/U=0.04$. We see additional peaks, which indicate CDW QLRO at a momentum that is consistent with the density at the center of the trap.

$$S(k) \approx \int \frac{dx_1 dx_2}{L} e^{-ikx_{12}}(\langle n_{x_1} n_{x_2}\rangle - \langle n_{x_1}\rangle\langle n_{x_2}\rangle), \qquad (7)$$

with $x_{12}=x_1-x_2$, and the real-space correlation function defined as

$$\langle n_{x_1} n_{x_2}\rangle = \sum_{i_1,i_2} |w(x_1 - r_{i_1})|^2 |w(x_2 - r_{i_2})|^2 \langle n_{i_1} n_{i_2}\rangle.$$

$\langle n_{x_1}\rangle\langle n_{x_2}\rangle$ is similarly defined. Figure 5 shows $S(k)$ for $U_{12}/U=0.04$ and a nearly noninteracting example $U_{12}/U=0.0025$. The envelope of the function is given by the inverse width of the Wannier state; the periodic shape comes about because we map a lattice quantity onto real space. We clearly see the onset of a peaked structure at momenta that are consistent with the density at the trap center. These peaks are related to algebraic cusps in the static structure factor, when the CDW regime is reached, $S(2k_F+q) \sim |q|^{1-\alpha_{CDW}}$. A measurement of the dynamic structure factor would lead to an even more striking result, since these cusps would translate into algebraic divergencies. We also note that a measurement of the lattice density *in situ* [22] could depict a profile as in Fig. 2 and that repeated measurements and a correlation analysis as in [8], but without expansion, could give the real-space density correlation function directly.

In conclusion, we have presented a proposal of how a supersolid phase of binary bosonic mixtures in 1D can 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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