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Sign-Alternating Interaction Mediated by Strongly-Correlated Lattice Bosons

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We reveal a generic mechanism of generating sign-alternating inter-site interactions mediated by strongly correlated lattice bosons. The ground state phase diagram of the two-component hard-core Bose-Hubbard model on a square lattice at half-integer filling factor for each component, obtained by worm algorithm Monte Carlo simulations, is strongly modified by these interactions and features the solid+superfluid phase for strong anisotropy between the hopping amplitudes. The new phase is a direct consequence of the effective nearest-neighbor repulsion between "heavy" atoms mediated by the "light" superfluid component. Due to their sign-alternating character, mediated interactions lead to a rich variety of yet to be discovered quantum phases.

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The first proposal for studying models of strongly correlated systems with cold atoms in optical lattices was put forward a decade ago [1]. Since then, control over lattice geometry and interaction strength has increased dramatically, opening up new directions in the study of quantum phases of cold gases. (For reviews, see [2, 3].) Thanks to refinements in experimental and theoretical tools, it is now possible to look at exotic quantum states which arise in bosonic systems with pseudospin degrees of freedom or multiple species. In the realm of two-component systems, one goal is to realize models of quantum magnetism by using hyperfine states of an atom [4]. By controlling superexchange interactions of particles confined in an optical lattice, it is possible to switch between different ground states [5]. Another important development is experimental realization of heteronuclear bosonic mixtures of $^{87}\mathrm{Rb} - {}^{41}\mathrm{K}$ in a three-dimensional optical lattice [6]. Moreover, Ref. [7] reports results for fine control over interspecies scattering length, including the zero-crossing point. These achievements indicate that two-component systems in optical lattices with tunable interspecies interaction via Feshbach resonances are within the reach of current experiments. The two-component 2D bosonic system is also in the focus of Optical Lattice Emulator project supported by DARPA and aimed at the development, within the next few years, of experimental tools of accurately mapping phase diagrams of lattice systems by emulating them with ultracold atoms in optical lattices.

Experimental studies of lattice solids—states with broken translation symmetry—are intriguing and fundamentally important, especially in 2D. For the prominent example, we refer to the problem of deconfined criticality proposed for the solid-to-superfluid quantum phase transition in 2D. The matter of interdisciplinary interest here is to validate the idea of a (hidden) duality between the superfluid and solid orders leading to a conceptually new criticality [8]. Lattice solids also offer the possibility of having a supersolid phase featuring both broken translation symmetry and the ability to support a superflow, e.g. in a single-species square-lattice bosonic system with soft-core on-site interactions *and* appropriately strong nearest-neighbor interactions [13].

Solid phases in the single-species bosonic system require going beyond the on-site interaction. The standard Bose-Hubbard model [1] supports only two phases: a superfluid (SF) and a Mott insulator (MI); the latter is not a solid because it lacks the broken translation symmetry. A considerable theoretical effort has been made to understand how inter-site interactions can be generated in atomic gases. One proposal is to use cold polar molecules [14] featuring long range dipole-dipole interactions (see also review [14], and references therein). In Refs. [16], the authors suggest a technique for tuning the shape of long-range interactions between polar molecules by applying static and microwave fields. Another, experimentally more challenging, proposal is to excite atoms to higher bands in an optical lattice [17].

Within this framework, the two-component bosonic system with purely on-site interactions is a reasonable alternative route to obtain exotic single-species systems (at present, it is hard to reach low temperatures with lattice fermions). At a commensurate filling and strong enough interaction, opening a gap in the net-charge sector, the two-component mixture becomes equivalent to a single-component system with nearest-neighbor interactions, describing the iso-spin sector [9, 10, 11, 12]. The checker-board (CB) solid phase arising in this case is equivalent to the Néel antiferromagnet [9, 10, 12]. The CB-SF quantum phase transition (with respect to the original components, the SF state is a super-counter-fluid (SCF) [10], or, equivalently, planar ferromagnet in iso-spin terminology [10, 12]) is known to be of the first order. Unfortunately, the supersolid phase is not predicted in this parameter regime. There have been extensive theoretical studies of quantum phases in two-component systems [10, 11, 12, 18, 19], but, to the best of our knowledge, all studies overlooked the possibility of having various solids in the *absence* of the net-charge localization. Namely, they missed a generic mechanism of inducing inter-site sign-alternating interactions by strongly-correlated *bosonic* environment (cf. [20]), analogous to the RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction mediated by fermions [21].

In this Letter, we reveal and quantify the mechanism of the mediated sign-alternating interactions, and discuss it in the context of the ground state phase diagram for *hard-core* bosons with repulsive interspecies interaction at half filling for each component:

$$H = -\sum_{<ij>} \left(t_{\rm a} a_i^\dagger a_j + t_{\rm b} b_i^\dagger b_j \right) + U \sum_i n_i^{(\rm a)} n_i^{(\rm b)} \ , \quad (1)$$

where, $a_i^\dagger (a_i)$ and $b_i^\dagger (b_i)$ are bosonic creation (annihilation) operators, $t_{\rm a}$ and $t_{\rm b}$ are hopping matrix elements between the nearest neighbor sites for two species of bosons (A and B) on a simple square lattice with $N = L \times L$ sites, and $n_i^{(\rm a)} = a_i^\dagger a_i$, $n_i^{(\rm b)} = b_i^\dagger b_i$. This model can be implemented experimentally [7] and is considered to be the simplest one with purely contact interactions and yet highly nontrivial phase diagram.

Model (1) was studied previously using a combination of variational and mean field theories [12] which, in general, can not guarantee the accuracy of results. With Monte Carlo (MC) simulations by Worm Algorithm [22], we obtain the first precise data for the ground state phase diagram. For weak anisotropy between $t_{\rm a}$ and $t_{\rm b}$ and large U, our results confirm the basic phases and transitions between them proposed in Ref. [12]. We, however, find strong quantitative differences (up to 50% to 100%) in the location of transition lines. For large anisotropy and moderate-to-weak interactions we find a completely new structure of the phase diagram. It is shaped by the effective Hamiltonian obtained for the "heavy" (small hopping) component after the "light" component is integrated out. The resulting nearest-neighbor and longer-range interactions (similar to the effective potential between the ions in solids mediated by electrons) stabilize the checker-board (CB) solid phase of heavy atoms for sufficiently strong anisotropy between $t_{\rm b}$ and $t_{\rm a}$. A surprising result of the present study is that effective mediated interactions are oscillating from strong on-site attraction to much weaker nearest neighbor repulsion and back to a tiny attractive tail. In a broad perspective, this type of mediated interactions will result in interesting solid, and guaranteed supersolid [13] orders in related models. Moreover, for soft-core bosons, one can look for phases and phase transitions which involve multi-particle bound states and order parameters ("multi-mers").

Before we discuss our findings in more detail let us review the key phases and limiting cases of model (1). In the strong coupling limit, $U \gg t_{\rm a}, t_{\rm b}$, it can be mapped (within the second-order perturbation theory) onto the spin-1/2 Hamiltonian (see e.g. [9, 10, 12]) $H_{XXZ} = \sum_{<ij>} [-J_{xy}(\sigma_j^x \sigma_i^x + \sigma_j^y \sigma_i^y) + J_z \sigma_j^z \sigma_i^z]$ with positive $J_{xy}, J_z \sim t^2/U$. The latter features two possible ground states: (i) an antiferromagnetic state with z-Néel order for $J_z > J_{xy}$, and (i) an XY-ferromagnetic state for $J_{xy} > J_z$. In bosonic language, the z-Néel state corresponds to the CB solid order for both A- and B-particles (we will abbreviate it as 2CB). It is characterized by non-zero structure factor $S_{\rm a,b}(\mathbf{k}) = N^{-1} \sum_{\mathbf{r}} \exp[i\mathbf{kr}] \langle n_0^{(\rm a,b)} n_{\mathbf{r}}^{(\rm a,b)} \rangle$. The XY-state is representing the SCF phase featuring an order parameter $\langle a^\dagger b \rangle$. Both 2CB and SCF have to be regarded as Mott insulators as far as the total number of particles is concerned, i.e. there exist a finite gap to dope the system. Thus only counter-propagating A- and B-currents with the zero net particle flux posses superfluid properties in the SCF state. Under the mapping one finds that $J_z > J_{xy}$ everywhere except at $t_{\rm a} = t_{\rm b}$ when the spin Hamiltonian becomes SU(2)-symmetric. Thus higher-order symmetry-breaking terms are necessary to decide which phase, 2CB or SCF, survives. Ref. [12] provided a variational argument showing that SCF is stabilized in the vicinity of the $t_{\rm a} = t_{\rm b}$ line, and our data unambiguously confirm the validity of this conclusion.

At weak inter-species interaction, $U \ll t_{\rm a}, t_{\rm b}$, we expect that the ground state is that of two miscible strongly interacting (due to hard-core intra-component repulsion) superfluids (2SF). Finally, for $t_{\rm b} \ll U \leq t_{\rm a}$ we should have a phase where B-particles form the CB solid if effective interactions mediated by the superfluid A-component are repulsive and short-ranged (we abbreviate it as CB+SF).

Our simulation method is based on the lattice path integral representation and Worm Algorithm [22]. The original version was generalized to deal with two-component systems following ideas introduced for classical j-current models [23]. The simulation configuration space now includes the possibility of having two types of disconnected worldlines (worms) representing off-diagonal correlation functions (Green's functions). In order to allow efficient sampling of the SCF phase (any paired phases for that matter) it is necessary to enlarge the configuration space and consider worldline trajectories with two worms propagating simultaneously. The results for the phase diagram are summarized in Fig. 1. To detect the SCF phase we have calculated the stiffness of the *relative* superfluid flow from the standard winding number formula [24] $\rho_{\rm SCF} = \beta^{-1} \langle (W_{\rm a} - W_{\rm b})^2 \rangle$, where $W_{\rm a(b)}$ are winding numbers of worldlines $A(B)$, and β is the inverse temperature. In SCF the sum of winding numbers is zero in the thermodynamic limit. We confirm the SCF ground state for $t_{\rm a} \sim t_{\rm b}$ and sufficiently strong interactions. It survives at arbitrary large U along the diagonal $t_{\rm a} = t_{\rm b}$, directly demonstrating that higher order terms in the effective spin-1/2 Hamiltonian break the SU(2) symmetry in favor of the XY-order. To locate the weakly first-order superfluid-solid 2CB-SCF line (circles in Fig. 1) we have used the flowgram method which works well for both first and second order transitions, and is particularly helpful for telling the former from the latter (see Ref. [25] for details).

Though the 2CB-SCF transition is expected to be first-order, one may not exclude the possibility of the interme-

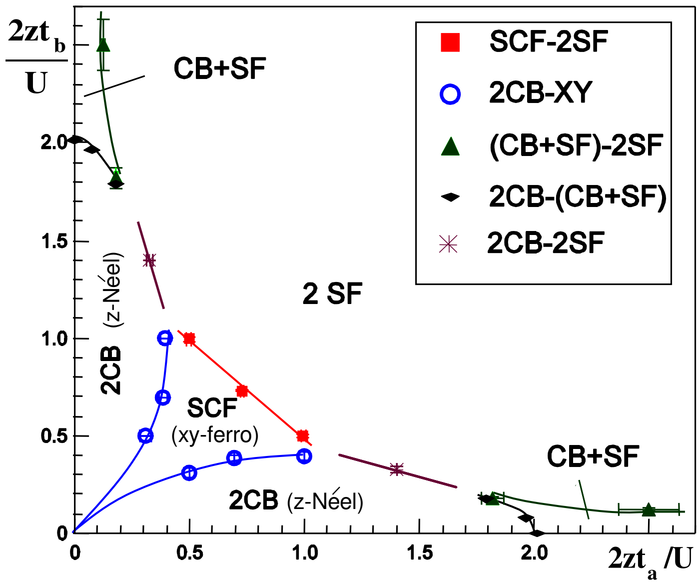

FIG. 1: (Color online). Phase diagram of model (1) on a square lattice at half-integer filling factor for each component. The observed transition lines are 2CB-SCF (first-order), SCF-2SF (second-order), 2CB-2SF (first-order), 2CB-CB+SF (second-order), and CB+SF-2SF (first-order). Lines are used to guide an eye.

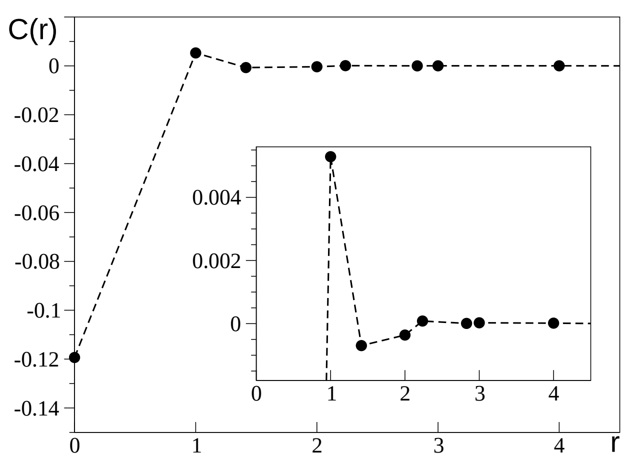

FIG. 2: The $C(r)$ function in a system of light hard-core bosons at half-integer filling; the distance r is measured in units of lattice spacing. The calculation was done for the $L \times L = 10 \times 10$ system at low temperature. The nearest neighbor repulsion is clearly visible, though the overall strength of the effective coupling is very small. Error bars are smaller than symbol size.

diate supersolid phase. We did search for evidence of the state featuring both the SCF and CB orders but did not find any. On the contrary, we observed phase coexistence which brings us to the conclusion that the 2CB-SCF line remains un-split.

The continuous SCF-2SF transition (squares in Fig. 1), is expected to be in the $(d+1)$-dimensional U(1) universality class characteristic of the MI-SF quantum phase transition [23] . As the system crosses into the 2SF phase, it develops single-component order parameters $\langle a \rangle \neq 0$ and $\langle b \rangle \neq 0$ along with the non-zero superfluid stiffness in the total winding number channel, $\rho_{2SF} = \beta^{-1}\langle (W_{\rm a} + W_{\rm b})^2 \rangle$. To locate the transition line precisely we have employed standard finite size scaling arguments and extracted the critical point from the intersection of $\rho_{2SF}(U/t_{\rm a,b})L$ curves calculated for different system sizes L at $\beta \propto L$.

The SCF phase disappears for $U/t_{\rm a,b} \lesssim 8$. In this parameter region, the system undergoes the first-order 2CB-2SF transition (stars in Fig. 1) up to $U/t_{\rm a,b} \simeq 4$ where the 2CB phase disappears.

Not too surprisingly for the 2D case, the mean-field and variational treatments turn out to rather inaccurate quantitatively: The actual transition lines are 50% to 100% away from the predicted ones. For comparison, in Fig. 1 we have used the same units as in Ref. [12] ($z = 4$ is the coordination number on the square lattice). Even for strong inter-species interaction $U/t_{\rm a,b} \sim 16$ we do not find good quantitative agreement.

We now turn to the most interesting, for purposes of this Letter, region of the phase diagram with strong anisotropy between hopping amplitudes. In this regime one of the components is much heavier (let it be component B) than the other. As the hopping amplitude $t_{\rm a}$ increases, the light component undergoes a second-order MI-SF transition in $(d+1)$-dimensional U(1) universality class (diamonds in Fig. 1). [Since translation invariance is broken by the CB order of B-particles, the filling factor of A-particles is unity per unit cell.] Beyond this transition, the superfluid A-bosons provide an effective interaction for B-bosons which for sufficiently small $t_{\rm b}$ stabilizes the CB order in the heavy component. Though formally CB+SF breaks both translation and gauge symmetries it can not be called a supersolid because the density wave in the A-component is induced from "outside" by an insulating heavy phase (this is reminiscent of conventional solid-state superconductors). However, in cold atomic systems with A and B particles referring to different hyperfine states of the same atom we have an experimental "knob" to render the CB+SF phase a genuine supersolid by inducing an arbitrary small hybridizing interaction $g(a^\dagger b + H.c.)$.

To describe the CB+SF phase semi-quantitatively let us look at the limit $t_{\rm b} \ll U \ll t_{\rm a}$. Within the lowest-order perturbation theory in U an effective mediated interaction between heavy atoms is pairwise and of the order of $U^2/zt_{\rm a}$. Since the superfluid liquid of hard-core A-particles is strongly correlated, the actual strength and form of $V_{ij}^{\rm eff}$ has to be computed numerically. We determine it from the exact (at $U/t_{\rm a} \to 0$) relation $V^{\rm eff}(r) = (U^2/t_{\rm a})\, C(r)$, where

$$C(r) = \lim_{U/t_{\rm a} \to 0} \frac{n(r) - 1/2}{U/t_{\rm a}}$$

is the scaled density profile in response to the heavy atom at the origin, and r is the dimensionless distance between the B-atoms. Since $C(r)$ is expected to decay exponentially fast with r [26], the simulated system can be relatively small. The result is shown in Fig. 2. It turns out that $V^{\rm eff}(r)$ is more than an order of magnitude smaller then a naive estimate U^2/zt_a. Moreover, it is sign-alternating, with strong on-site attraction, much weaker nearest-neighbor repulsion, and nearly negligible attractive tail for longer range interactions. For the hard-core model studied here, the dominant interaction is the nearest-neighbor one, $V^{\rm eff}(1) \approx 5.4 \times 10^{-3}\ U^2/t_{\rm a}$, explaining the origin of the CB phase of heavy atoms.

On the basis of $V^{\rm eff}(1)$, the melting first-order (CB+SF)-2SF transition is predicted to occur along the $t_{\rm b} \approx V^{\rm eff}(1)/2$, or $4z^2 t_{\rm b} t_{\rm a}/U^2 \approx 0.17$, line, i.e. the CB+SF phase survives close to the vertical and horizontal axis in Fig. 1 all the way to $t_{\rm a,b}/U \to \infty$. The above asymptotic estimate is less than a factor of two smaller than the data points in Fig. 1, even though U is still relatively large.

In conclusion, we have presented accurate results, based on path integral Monte Carlo, for the phase diagram of the two component hard core Bose-Hubbard model on a square lattice and half-integer filling factor for each component. The system can be realized experimentally with heteronuclear bosonic mixtures in optical lattices with tunable interspecies interactions. We reveal the existence of an additional CB+SF state which radically changed the topology of the phase diagram. The CB+SF phase, which exists for strong anisotropy between the hopping amplitudes and weak enough interaction, is a direct consequence of effective interactions mediated by the light, strongly correlated superfluid component. Mediated interactions are sign-alternating, and lead to exciting possibilities of realizing new quantum phases in the two-species bosonic systems.

Many questions remain open. Finite temperature properties and melting of the z-Néel/xy-ferromagnet phases are of interest in the study of quantum magnetism. Studies of soft core bosons are of special interest because they admit the possibility of forming "multi-mers" due to strong mediated on-site attraction. One may also study supersolid phases on square and triangular lattices, not to mention the need for dealing with more realistic systems, i.e. including effects of parabolic confinement and finite number of particles as in experimental setups.

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