

Phase diagram of an anisotropic bosonic t - J model

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We have studied by quantum Monte Carlo simulations the low temperature phase diagram of a mixture of isotopic, hard core bosons, described by the t - J_z - J_\perp model, with $J_\perp = \alpha J_z$. The coexistence of superfluid hole-rich and insulating, antiferromagnetically ordered hole-free phases is observed at sufficiently low hole density for any $\alpha < 1$. A two-component checkerboard supersolid phase is not observed. The experimental relevance and possible broader implications of these findings are discussed.

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Impressive scientific and technological advances in trapping cold atoms in optical lattices¹⁻⁴ (OLs) render it now feasible to create in the laboratory remarkably close experimental realizations of model many-body systems long thought of as of mostly academic interest. An example is the isotopic two-component Bose mixture, providing a rich playground for many-body physics due to the various phases that it is expected to display, including a number of physically distinct superfluid phases.^{5,6} The ongoing experimental investigation of this system justifies the theoretical exploration of its phase diagram not only to help in the interpretation of experimental data but also for the more general purpose of guiding the search for novel phases of strongly correlated quantum many-body systems.

In this work, we model a mixture of two different species of hard core bosons of equal masses via the two-dimensional boson t - J_z - J_\perp model:⁷

$$\hat{H} = -t \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{b}_i^\dagger \hat{b}_j + \text{H.c.}) - \frac{1}{2} [J_z (\hat{n}_i \hat{m}_j + \hat{m}_i \hat{n}_j) + J_\perp (\hat{a}_i^\dagger \hat{b}_j^\dagger \hat{a}_j \hat{b}_i + \text{H.c.})]. \quad (1)$$

A square lattice of $N=L \times L$ sites is assumed, with periodic boundary conditions. Two species (A and B) of bosons of equal masses are defined, for which \hat{a}_i^\dagger , \hat{b}_i^\dagger are creation operators, whereas $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$, $\hat{m}_i = \hat{b}_i^\dagger \hat{b}_i$ are number operators. The sum in Eq. (1) runs over all pairs of nearest-neighbor sites.

Hamiltonian (1) is defined in the subspace in which no double occupation of sites is possible. The parameters of the model, namely, t , J_z , and J_\perp , are all non-negative; henceforth, we shall take t to be our energy scale and set it equal to 1. We set $J_z = J$ and $J_\perp = \alpha J$, α expressing the anisotropy between the “antiferromagnetic” coupling J , represented by the second term in Eq. (1), and the “ferromagnetic” exchange coupling J_\perp , represented by the last term in Eq. (1). In this work, we focus on the parameter region in which both α and J are less than 1. The hole density is defined as $h \equiv 1 - (N_A + N_B)/N$, where N_A (N_B) is the number of particles of species A (B). All throughout, we assume $N_A = N_B \leq N/2$,

i.e., the system has no net “magnetization.” The isotropic version of Eq. (1) (i.e., with $\alpha=1$) can be derived from the two-component isotopic Bose-Hubbard model in the limit of large on-site repulsion and small hole concentration;⁷⁻⁹ in an optical lattice, anisotropy could arise from additional longer-ranged (e.g., dipolar) interactions among particles. At exactly half-filling (i.e., no holes), Eq. (1) can also be cast in the spin language; for example, it is isomorphic to a spin-1 antiferromagnetic Heisenberg model with uniaxial single-ion anisotropy, possibly relevant to some magnetic systems.¹⁰

The fermion counterpart of Eq. (1) with $\alpha=1$ is known as the t - J model¹¹⁻¹³ and has been the subject of a wealth of theoretical work because of its posited connection to high-temperature superconductivity (HTS). In spite of an enormous effort now spanning almost two decades, the phase diagram of the t - J model remains relatively poorly understood. Basic questions, such as the presence of a superconducting ground state, are yet largely unanswered essentially due to the lack of a sufficiently robust theoretical method for strongly correlated fermions. On the other hand, the case of Bose statistics [Eq. (1)] can be studied by quantum Monte Carlo simulations, yielding essentially exact numerical results. For this reason, some studies have used Eq. (1) as a starting point to investigate physical effects such as stripe formation, also believed to be relevant to HTS.¹⁴

In this work, we study the low-temperature phase diagram of \hat{H} as a function of the hole density h for $\alpha \leq 1$ and different values of J . Specifically, we consider the physically realistic region $J < 1$ for which the isotropic version of Eq. (1) displays no phase separation, as shown in Refs. 7 and 8. Of particular interest is the effect of anisotropy on the phase diagram of Eq. (1), chiefly with regard to phase separation, superfluidity, and the possible presence of a two-component checkerboard supersolid phase. We use the worm algorithm (WA) in the lattice path-integral representation¹⁵ to compute thermal expectation values of physical operators; the calculation requires a relatively straightforward extension of the WA to allow for the simulation of physical processes associated with the exchange term of Eq. (1).

In the absence of holes (i.e., $h=0$), Hamiltonian (1) does not differentiate between Bose and Fermi statistics; for $\alpha < 1$, the system features a transition (at finite temperature

T_N) to an antiferromagnetically ordered state, in which a particle of type $A(B)$ is preferentially surrounded by particles of type $B(A)$.¹⁶ At $\alpha=1$, it is $T_N=0$, but the ground state is still ordered.¹⁷ For $\alpha>1$, the system is superfluid (SF) below the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature T_{BKT} but with no net flow of matter as the flow of one component is exactly compensated by the counterflow of the other.¹⁸

The presence of mobile holes is generally expected to result in a reduction of the antiferromagnetic order as holes scramble it with their motion, as well as to give rise to a SF phase of holes at low temperature; of interest is the possible existence of a *supersolid* phase, in which both types of orders may coexist in a single homogeneous phase.

The occurrence of checkerboard or antiferromagnetic order can be ascertained by numerical simulations of the staggered density order parameter $\chi(h)=\sqrt{S(\pi,\pi)}$, where $S(\mathbf{q})=\langle\hat{\rho}_{\mathbf{q}}\hat{\rho}_{-\mathbf{q}}\rangle$, with

$$\hat{\rho}_{\mathbf{q}} = \frac{1}{N} \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i} (\hat{n}_i - \hat{m}_i), \quad (2)$$

and where \mathbf{r}_i is the position of the i th lattice site, and $\langle\cdots\rangle$ stands for thermal expectation value. The SF density $\rho_s(h)$ of the fluid of holes is computed using the usual “winding number” estimator.

We discuss the isotropic ($\alpha=1$) case first. As shown in Refs. 7 and 8, the system features a homogeneous ground state for any hole concentration for $J\lesssim 1.5$. The AF order that exists in the undoped system at $T=0$ is suppressed by an arbitrarily small hole concentration. The underlying mechanism is simple: holes break the $SU(2)$ symmetry of the undoped state in favor of the XY plane. We have explicitly verified this conclusion by performing finite-size scaling analysis of $\chi(h)$. This physical result is analogous to that observed for a system of lattice hard core bosons with a nearest-neighbor repulsive interaction potential of strength $V=2t$, for which doping away from half-filling destroys the checkerboard order.²⁰ This points to a significant difference between model (1) with Fermi and Bose statistics. In the case of the fermion t - J model, the AF is reduced but not completely eliminated by hole doping²¹ since the $SU(2)$ spin symmetry is preserved.

The ensuing, uniform hole gas is SF at $T=0$ and features a BKT transition to a normal fluid (NF) at finite temperature. The transition temperature T_c can be obtained using the well known renormalization flow and the universal jump of the superfluid density ρ_s at T_c .²² Results for the case $J=0.4$ are shown in Fig. 1.

A richer phase diagram occurs in the anisotropic ($\alpha<1$ case). The ground state energy per hole is defined as^{23,24}

$$e(h) = \frac{E(h) - E(0)}{Nh}, \quad (3)$$

where $E(h)$ is the total energy of the system in the presence of Nh holes. A minimum of $e(h)$ at a finite hole density h_{cr} signals the separation of the system into two phases at

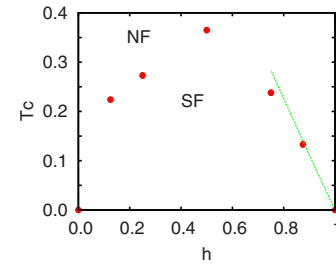


FIG. 1. (Color online) Superfluid transition temperature of the uniform hole gas in model (1) with $\alpha=1$ (i.e., isotropic) as a function of hole density h . The filled circles show numerical estimates of T_c (in units of t) determined as explained in the text. The dotted line at high h is the theoretical behavior predicted by the theory of the dilute Bose gas (Ref. 19). Here, $J=0.4$.

$h < h_{cr}$, one with no holes and the other with hole density h_{cr} .

Figure 2 shows $e(h)$ as a function of hole density and for different values of the anisotropy parameter α . The value of J is 0.4. Our numerical results show a minimum for $e(h)$ at a finite hole concentration $h_{cr}(\alpha)$ for any $\alpha<1$; that is, the system separates into hole-rich and hole-free phases for hole doping below $h_{cr}(\alpha)$ [with $h_{cr}(\alpha)\rightarrow 0$ as $\alpha\rightarrow 1$].

The hole-free phase features AF order (and obviously no hole-based superfluidity), whereas the hole-rich phase is SF but not antiferromagnetically ordered. The occurrence of PS in the anisotropic model can be understood based on the “string” picture.²⁵ In the anisotropic model, a hole leaves behind in its motion a string of bosons of either species displaced by one lattice site. Thus, separation of the system in hole-rich and hole-free phases becomes energetically advantageous at low hole density as a way to limit the damage caused by the holes to the antiferromagnetic order. In the $\alpha\rightarrow 1$ limit, however, quantum fluctuations associated with the J_{\perp} term of Eq. (1) “mend” the damage due the hole motion, restoring local order.²⁶ These considerations are clearly independent of quantum statistics, i.e., they ought to apply to the fermion models as well.

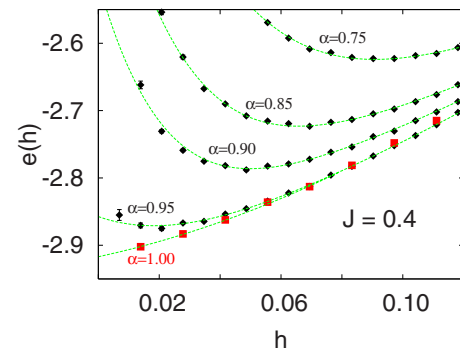


FIG. 2. (Color online) Ground state energy per hole $e(h)$ [defined in Eq. (3)] for Hamiltonian (1) as a function of the hole density h for different values of the anisotropy parameter α (diamonds). The boxes show estimates of $e(h)$ for the isotropic ($\alpha=1$) case. The dotted lines are polynomial fits to the data. Numerical calculations were carried out on a 12×12 lattice. Here, the temperature $T=0.025t$ and $J=0.4$.



FIG. 3. (Color) Snapshot of an instantaneous (β -averaged) configuration of the system of a 64^2 -site lattice. Color coding is as follows: sites that are drawn in red (blue) are occupied by a particle of type A; the greater the probability, the bigger the size of the circle; sites that are drawn in black are occupied by holes and both types of particles with similar probability; the smaller the circle, the more likely for the site to be empty. Here, $J=0.4$, $J_{\perp}=0.3$, and $h=0.0586$ at $T=0.025t$.

The separation of the two phases can be visually observed by examining configurations generated at low T by our algorithm on lattices of sufficiently large size, e.g., $N=4096$ sites (see Fig. 3). We have consistently observed this effect for $J < 1$ and for as little as 1% anisotropy. Based on this numerical evidence, we argue that PS will occur in the $T \rightarrow 0$ limit at sufficiently low hole concentration for *arbitrarily weak* anisotropy.

At finite temperature, entropy favors mixing of the two phases and the occurrence of a homogeneous phase. Because both SF and AF transition temperatures are finite, an obvious question is whether a homogeneous phase featuring both types of order, namely, a “two-component checkerboard supersolid” (i.e., a superfluid gas of holes inside a checkerboard quantum antiferromagnet formed by the two components), may exist at finite temperature.

Our simulations have not yielded any evidence of such a checkerboard supersolid phase. On raising the temperature, the system evolves into either a nonsuperfluid antiferromagnet (NF) or into a SF with no antiferromagnetic order. We find that the region where all transition lines come close to each other is extremely hard to study since all standard finite scaling techniques fail. In Fig. 4, we sketch the simplest phase diagram consistent with our data, also the one which we find most plausible; in this scenario, NF-SF and NF-AF lines meet the coexistence dome at one point, close to its maximum. However, at this time, we cannot exclude other scenarios. For example, the AF line may feature a tricritical point, and the BKT transition may be terminated at the first-order AFM line. The possible crossing of the second order

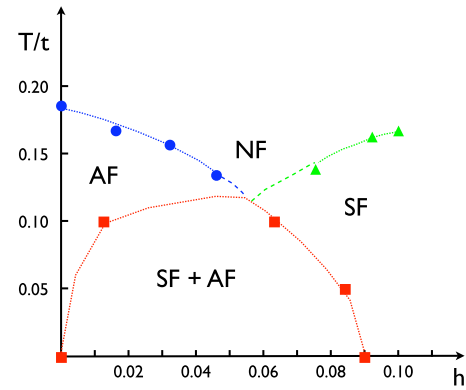


FIG. 4. (Color online) Computed phase diagram of the boson t - J_z - J_{\perp} model on the square lattice. The horizontal axis shows hole concentration and the vertical the temperature. The figure shows actual Monte Carlo data obtained for $J_{\perp}=0.75$, $J_z=0.3$, but the same schematic phase diagram is obtained for all values of the model parameters considered here. The circles represent the normal-to-antiferromagnetic transition, the triangles show the normal to superfluid, whereas the boxes show the boundary of the region in which the coexistence of superfluid and antiferromagnetic phases is observed. The dashed lines are only meant as a guide to the eye. Statistical errors are comparable to the sizes of the symbols.

AF and BKT lines, giving rise to a small region of existence of a two-component checkerboard supersolid sitting over the phase separation dome, has been thoroughly investigated but not observed in any of our simulations.

There are obviously interesting similarities between the phase diagram schematically represented in Fig. 4 and the basic phase diagram of HTS. In the case of the model investigated here, anisotropy is crucial in stabilizing the AF phase, which disappears upon doping in the fully isotropic model, as shown above. Anisotropy might also play a role in shaping the phase diagram of the fermion counterpart of Eq. (1), deemed relevant to HTS, as assuming a stronger AF coupling in the z direction may be physically justified by considerations of interplane exchange coupling.²⁷ As mentioned above, however, in the case of Fermi statistics, AF order is not completely destroyed by the injection of mobile holes.

The interesting interplay of phases shown in the phase diagram of Fig. 4 suggests that an experimental system described by Eq. (1) may be worth investigating in OLS.

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