Phase separation in the bosonic Hubbard model with ring exchange

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We show that soft core bosons in two dimensions with a ring exchange term exhibit a tendency for phase separation. This observation suggests that the thermodynamic stability of normal Bose liquid phases driven by ring exchange should be carefully examined.

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Interest in ring exchange interactions in quantum many-body systems has a long history, both theoretically and experimentally. Recently, the ring exchange interaction has been invoked in an effort to understand various aspects of high temperature superconductivity. While the Heisenberg model alone provides a rather accurate picture of magnetic excitations in the parent compounds of the cuprate superconductors, estimates of the magnitude of the ring exchange term are as high as one quarter of the exchange coupling and it therefore has been of interest to understand how this term might modify magnetic properties. Ring exchange interactions have also been suggested as a likely candidate to reconcile the properties of the underdoped pseudogap regime. The basic picture is that the ring exchange interaction can give rise to a new normal “Bose metal” phase at zero temperature in which there are no broken symmetries associated with superfluidity or charge density wave phases, and in which the compressibility is also finite.

With these motivations partly in mind, Sandvik et al. studied the phase diagram of the two-dimensional spin-1/2 XY model with spin exchange interaction on a square lattice,

\[ H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{\langle ijkl \rangle} P_{ijkl} \]  

(1)

where

\[ B_{ij} = S_i^+ S_j^- + S_i^- S_j^+ = 2(S_i^x S_j^x + S_i^y S_j^y), \]

\[ P_{ijkl} = S_i^x S_j^x S_k^x S_l^x + S_i^y S_j^y S_k^y S_l^y \]  

(2)

and \( \langle ij \rangle \) denotes nearest neighbours and \( \langle ijkl \rangle \) are sites at the corners of a plaquette. As is well known, for \( K = 0 \) this model is exactly equivalent to the hard core bosonic Hubbard model, at half filling, with no interactions apart from the constraint on site occupations, and it has only a superfluid phase. Sandvik et al. studied the phase diagram as a function of \( K \) using the Stochastic Series Expansion algorithm. They found that as \( K \) increases, the superfluid density, \( \rho_s \), decreases up to a critical value, \( K_c \), where a phase transition takes place, and \( \rho_s \) goes to zero with long range order appearing in the momentum expansion algorithm. They found that as \( K \) increases, \( \rho_s \) decreases up to a critical value, \( K_c \), where a phase transition takes place, and \( \rho_s \) goes to zero with long range order appearing in the momentum expansion algorithm.

\[ \Phi = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + U \sum_i n_i(n_i - 1) \]  

(3)

\[ + K \sum_{\langle ijkl \rangle} (a_i^\dagger a_j^\dagger a_k a_l + a_i^\dagger a_j a_k^\dagger a_l^\dagger) \]

where the destruction and creation operators satisfy \( [a_i, a_j^\dagger] = \delta_{ij} \), \( n_i = a_i^\dagger a_i \) is the number operator at site \( i \) and \( U \) is the onsite interaction strength. For our quantum Monte Carlo (QMC) simulations we used the World Line algorithm with four-site decoupling. We verified our code for \( K = 0 \) by comparing with existing results for hard and soft core bosons with and without nearest and next near neighbor interactions. For the \( K \neq 0 \) case, we compared with the hard core results of

Before discussing results for the full many-body system, it is interesting to study the behaviour of two bosons, since the formation of a bound state is closely related to the issue of phase separation. Ring exchange, like an attractive potential, favors proximity of two bosons, since the action of such a term is nonzero only when the two bosons live on the same plaquette. In Fig. 1 we show the average separation \( \langle |\Phi_0| |\Phi_0|^2 \rangle \) of two bosons, normalized to the number of sites \( L^2 \) on an \( L \times L \) lattice. As \( K \) increases, there is a crossover at \( K/t \approx 3 \) from a regime where the boson separation grows linearly with system size, so that the normalized separation is size independent, to one in which the boson separation does not
FIG. 1: Average ground state separation $\langle \Phi_0 | r^2 | \Phi_0 \rangle$ of two bosons, normalized to the system size, as a function of the magnitude of the ring exchange energy scale $K$. Here the hopping $t = 1$ and the soft-core repulsion $U = 12$. At small $K$, the normalized separation is independent of lattice size, indicating that the two bosons are spread independently throughout the lattice. At larger $K$ the bosons prefer smaller separation to optimize the ring exchange energy, indicating the formation of a bound state.

While we do not show the associated data, plots of $\langle \Phi_0 | r^2 | \Phi_0 \rangle$ for different soft-core repulsion $U$ reveal that the average separation is insensitive to the value of $U$. This will obviously be true in the unbound regime at small $K$, since the density is so dilute. It is less clear that this should be so in the bound regime at large $K$. However, as can be seen from the data in Fig. 1, the radius of the bound state is several lattice spacings ($\langle r^2 \rangle \propto L^2$ whence $r \propto 0.3L$), so here too the effect of $U$ is expected to be relatively small.

Fig. 1 suggests that there might be a tendency for ring exchange to cause the bosons to clump together, and, in an extreme scenario, to undergo phase separation. However, at densities higher than the dilute two boson case, this effect is opposed by the repulsion $U$. The focus of this paper is to examine this competition and determine the phase diagram of the soft core case as a function of both $U$ and $K$ at half filling.

The most straightforward indication of phase separation comes from a real space image of the boson density during the course of a simulation. Fig. 2 shows the average density distribution for $L = 16$, $U = 4$ and $K = 2.5$. We see indications that the bosons undergo phase separation: At less than quarter filling (top panel) the bosons stretch out in stripe across the lattice (bottom panel).

We will now demonstrate that phase separation is characteristic of a large portion of the $K-U$ phase diagram by examining the density-density correlation function and its associated structure factor, fixing $U$ (or $K$) and scanning $K$ (or $U$). As Fig. 2 illustrates, if the bosons phase separate, they may form a structure in which a set of contiguous sites of about half the system size will have appreciable boson occupation. The other half of the lattice is essentially empty. Therefore, if one examines the structure factor of the density-density correlation function,

$$ S(k_x, k_y) = \frac{1}{L^2} \sum_r C(r)e^{-ir.k} $$

with

$$ C(r) = \frac{1}{L^2} \sum_{r'} \langle n(r')n(r+r') \rangle, $$

one should observe a peak in $S$ at small momentum, e.g. $(2\pi/L, 0)$, $(0, 2\pi/L)$ or $(2\pi/L, 2\pi/L)$ depending on the precise orientation of the clump. By looking at the sum of the density structure factor at these three smallest momentum values we are sensitive to phase separation regardless of whether it occurs in a middle of the lattice.
roughly circular shape (Fig. 2a) or in some more elongated pattern (Fig. 2b). Fig. 3 clearly shows this behaviour: For \( K < 2 \) at \( U = 4 \), \( S \) is very small at the relevant momenta. For \( K > 2 \), phase separation sets in. Data for \( 16 \times 16 \) and \( 24 \times 24 \) lattices are shown and their agreement indicates that this phase separation is not a finite lattice effect. The critical value of \( K \) grows roughly linearly with \( U \).

It is also interesting to understand the behaviour of the superfluid density \( \rho_s \). One does not necessarily expect \( \rho_s \) to vanish when phase separation occurs. In fact, as is well known, \( \rho_s \neq 0 \) for the soft-core boson Hubbard model at all fillings, including commensurate density, if \( U/t \) is sufficiently small. Similarly, here it is possible that \( \rho_s \) can survive in the dense region of the phase separated lattice\[20, 21\]. Our simulations show that when phase separation first occurs, the populated region forms a band that spans the whole system. The bosons may then delocalize along that band, maintaining an (anisotropic) superfluid density. We have found that when the bosons form such a band, the plaquette-plaquette structure factor is also anisotropic and has long range correlations along the direction of the band. As \( K \) is increased further, the populated region of the lattice takes the form of an island. In such a case, the system may not be considered a superfluid in that one cannot establish superflow across the system. However, the bosons may still be delocalized over the extent of the island\[16\]. Fig. 4 shows \( \rho_s \) versus \( K \).

By making scans like those of Fig. 3 at several values of \( U \), we construct the phase diagram which we show in Fig. 5. Above the solid line, the system undergoes phase separation.

![The average structure factor](image1.png)

**FIG. 3:** The average structure factor, \( (S(2\pi/L, 0) + S(0, 2\pi/L) + S(2\pi/L, 2\pi/L))/3 \) versus \( K/t \). We see a sharp increase in \( S \) at \( K = 2 \) for \( U/t = 4 \) and \( K \approx 4 \) for \( U/t = 8 \). The simulations were done for \( \beta = 8 \), and \( \rho = 0.5 \).

![The superfluid density](image2.png)

**FIG. 4:** The superfluid density as a function of \( K \) for \( U = 8 \). \( \rho_s \) remains finite in the phase separated region, indicating that the bosons are delocalized across the clump of occupied sites. Inset: The hard core limit for which, instead, \( \rho_s \to 0 \).

![The phase diagram](image3.png)

**FIG. 5:** The phase diagram of the half-filled Bose Hubbard model in the \( U - K \) plane. Below the solid line, the system is superfluid while above the line it phase separates. See text.
The data shown in Fig. 2 are not a snapshot of a single configuration, but an average over a whole simulation run. In principle for extremely long simulations, the puddle of occupied sites will gradually move around the whole lattice and give a uniform density, $\rho_i = \frac{1}{2}$ on every site $i$. In practice, such motion of the large collection of bosons is extremely slow.

Finally, let us comment on the implications of our work for the phase diagram of the spin-1/2 quantum Heisenberg model with a ring exchange term. The kinetic energy term in the hard-core boson Hubbard model maps onto $J \sum (S_i^x S_j^x + S_i^y S_j^y)$ with exchange constant $J = 2t$. At the value $\bar{U} = 4t$ in our soft core model, double occupancy is already very rare at half-filling, and hence we are almost in the hard-core limit. The value of the ring exchange energy scale required to drive phase separation for this $U$ is $K \approx 2t$, or in other words, $K \approx J$. To replicate the near-neighbor coupling of the $z$ components of spin in the Heisenberg model we must include a near-neighbor repulsion in the bose-Hubbard model, a term which clearly would suppress phase separation. Thus we expect ring exchange to have the potential to drive phase separation in the Heisenberg model only for $K$ considerably greater than $J$.

Note added: After the completion of this work a preprint by Melko, Sandvik and Scalapino (cond-mat/0311080) appeared where the phase diagram of the doped hardcore system with ring exchange was determined.

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[1] D.J. Thouless, Proc. Phys.Soc. London B86, 893 (1965).
[2] E. Manousakis, Rev. Mod. Phys. 63, 1 (1991).
[3] R. Coldea et al., Phys. Rev. Lett. 86, 5377 (2001).
[4] A.A. Katanin and A.P. Kampf, Phys. Rev. B66, 100403(R) (2002).
[5] E. Muller-Hartmann and A. Reischl, Eur. Phys. J. B127, 173 (2002).
[6] M. Roger and J.M. Delrieu, Phys. Rev. B39, 2299 (1989).
[7] Y. Honda et al., Phys. Rev. B47, 1329 (1993).
[8] J. Lorenzana et al., Phys. Rev. Lett. 83, 5122 (1999).
[9] M. Matsuda et al., Phys. Rev. B62, 8903 (2000).
[10] A. Paramekanti et al., Phys. Rev. B66, 054526 (2002).
[11] A. W. Sandvik et al., Phys. Rev. Lett. 89, 247201 (2002)
[12] A. W. Sandvik and J. Kurkijarvi, Phys. Rev. B43, 5950 (1991).
[13] The data shown in Fig. 2 are not a snapshot of a single configuration, but an average over a whole simulation run. In principle for extremely long simulations, the puddle of occupied sites will gradually move around the whole lattice and give a uniform density, $\rho_i = \frac{1}{2}$ on every site $i$. In practice, such motion of the large collection of bosons is extremely slow.
[14] When $U$ is reasonably large and all sites are either empty or singly occupied, the structure factor at $S(k = (0,0))$ is just the density.
[15] Reference [11] found that the plaquette stripe order extends at least up to $K/J \approx 12$ and perhaps up to $K/J = 16$. See [12] for more detail.
[16] There are interesting analogies between this sort of ‘local’ superfluidity and the behaviour of bosons in a confining potential. See, e.g. M. Greiner et al., Nature 415, 39 (2002).
[17] E. Loh et al., Phys. Rev. B31, 4712 (1985).
[18] G.G. Batrouni and R.T. Scalettar, Phys. Rev. Lett. 84, 1599 (2000).
[19] F. Hebert, et al., Phys. Rev. B65, 014513 (2002).
[20] M.P.A. Fisher et al., Phys. Rev. B40, 546 (1989).
[21] G.G. Batrouni et al., Phys. Rev. Lett. 65, 1765 (1990).