Quantum antagonism of ferromagnetic order

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We study the interplay of superfluidity, glassy and magnetic orders of hardcore bosons with random frustrating interactions. In the classical limit, this model reduces to a $\pm J$ Edwards-Anderson Ising model with concentration $p$ of the ferromagnetic bonds, which hosts a glassy-ferromagnetic transition at a critical concentration $p^c_1 \sim 0.77$ on a 3D cubic lattice. Our quantum Monte Carlo simulation results using the worm algorithm show that quantum fluctuations stabilize the coexistence of superfluidity and glassy order ("superglass"), and shift the (super)glassy-ferromagnetic transition to $p_c > p^c_1$. In contrast, antiferromagnetic order coexists with superfluidity to form a supersolid, and the transition to the glassy phase occurs at a higher $p$.

\textbf{Introduction—} Spin glasses are frustrated magnetic systems with quenched disorder, hosting glassy phases with extremely slow dynamics\textsuperscript{[1]}. Traditionally, the simplest model that exhibits spin glass (SG) behavior is the $\pm J$ Ising model, or Edwards-Anderson (EA) model\textsuperscript{[2]}, in which Ising spins interact via randomly distributed nearest-neighbor (NN) ferromagnetic (FM) and antiferromagnetic (AFM) bonds with probability $p$ and $1-p$ respectively. This model has been studied extensively with Monte Carlo simulations and exhibits a finite temperature glass transition in 3D $[3,4]$. It is shown that this model has a second order transition from a SG to a FM (AFM) phase at a critical concentration $p^c_2 \sim 0.77$ $(1-p^c_2 \sim 0.23)$ as one increases (decreases) the fraction of FM bonds, and there exists reentrance of the spin glass phase in the temperature-disorder phase diagram\textsuperscript{[5,7]}. One natural question to ask is how the transition can be changed by quantum fluctuations\textsuperscript{[8,10]}. In particular, understanding the behavior of granular superfluidity in a frozen amorphous structure may give us hints on the microscopic mechanism of the formation of supersolids (SS)\textsuperscript{[11]}.

The observation of supersolidity in solid Helium 4 (He\textsuperscript{4})\textsuperscript{[11]} has spurred immense interests on the connection between superfluidity and disorder in bosonic systems. Strong experimental evidences suggest that disorder may play a role in how the supersolid forms\textsuperscript{[12,13]}. A recent experiment observed ultraslow dynamics in solid He\textsuperscript{4}\textsuperscript{[14]}, suggesting a glassy type of supersolid, or a “superglass” (SuG)\textsuperscript{[9,10,15,16]}. Quantum Monte Carlo (QMC) studies on the extended hardcore Bose-Hubbard model with random frustrating interactions on a 3D cubic lattice indicate that glassiness can coexist with superfluidity, and quantum fluctuations and random frustration are both crucial in stabilizing the supglass state\textsuperscript{[9]}.

While the phase transitions into superfluidity or magnetic/glassy states have been studied in some detail, the nature of the various transitions into a SS/SuG are yet unknown. In this Letter, we study the extended hardcore Bose-Hubbard model with random frustrating interactions model, in order to characterize transitions by tuning the amount of disorder present in the interactions, which is potentially relevant to the behavior noted in He\textsuperscript{4}. We demonstrate that the presence of quantum exchange terms greatly increases the temperature dependence of the SuG-FM transition by pushing the low temperature phase boundary to a higher critical concentration than $p^c_1$. The SuG-SS phase boundary is also drawn to a higher critical concentration, and an asymmetry for SuG-SS and SuG-FM transitions arises.

\textbf{Model—} The Hamiltonian for hardcore boson with a random NN interaction is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} V_{ij} \langle n_i - 1/2 \rangle \langle n_j - 1/2 \rangle - t \sum_{\langle i,j \rangle} \langle b_i^\dagger b_j + b_i b_j^\dagger \rangle,$$

where $\langle i, j \rangle$ indicates the NN lattice sites. $n_i$ is the number operator for hard-core bosons at lattice site $i$, $t$ is the hopping parameter and $V_{ij}$ are interactions with a bimodal distribution given as

$$p(V_{ij}) = p \delta(V_{ij} - V) + (1-p) \delta(V_{ij} + V).$$

This model can be readily mapped into the standard XXZ model:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_x S_i^x S_j^z - \frac{1}{2} J_{xy} \sum_{\langle i,j \rangle} (S_i^- S_j^+ + S_i^+ S_j^-),$$

where $J_{xy} = 2t$ and $J_x = V_{ij}$. This model reduces to the classical EA model if $J_{xy} = 0$.

There exist both diagonal and off-diagonal long-range orders in this model. Possible diagonal long-range orders are FM, AFM and SG, with corresponding order parameters: magnetization (FM), staggered magnetization (AFM), and the Edwards-Anderson order parameter (SG). The EA order parameter is defined as

$$q_{EA} = \frac{1}{N} \left[ \sum_i \langle (n_i - 1/2)^2 \rangle \right]_av,$$

where $\langle \cdots \rangle$ denotes a thermal average and $[\cdots]_{av}$ an average over disorder realizations. As the EA order parameter will also capture FM and AFM ordering, one must look for a...
non-zero $q_{\text{EA}}$ while the other order parameters remain zero in order to identify an SG phase.

To determine the phase transition point, we look at the Binder cumulants \cite{17} for the order parameter, which should cross at the transition point for different system sizes. The Binder cumulants of the magnetization $m = \frac{1}{N} \sum_i S_i^z$, and staggered magnetization $m_s = \frac{1}{N} \sum_i (-1)^i S_i^z$ are

$$g_m = \frac{1}{2} \left( 3 - \frac{\langle m^4 \rangle_{\text{av}}}{\langle m^2 \rangle_{\text{av}}^2} \right); \quad g_{sm} = \frac{1}{2} \left( 3 - \frac{\langle m_s^4 \rangle_{\text{av}}}{\langle m_s^2 \rangle_{\text{av}}^2} \right)$$

(5)

which approaches one in the FM/AFM phase and goes to zero otherwise. We measure the superfluid density through winding number fluctuations \cite{18},

$$\rho_s = \frac{1}{3 NT} \sum_{k=x,y,z} \sum_{k=x,y,z} \langle W_k^2 \rangle_{\text{av}},$$

(6)

where $W_k$ is the winding number along the $k$ direction. In our simulation, we identify the SS phase by the coexistence of AFM and SF orders, and the SuG phase by the coexistence of SG and SF orders.

\textbf{Method—} We use the worm algorithm QMC \cite{19} to solve this model and simulate many different realizations of the disorder—sets of interactions $V_{ij}$ for a given parameter set. In the following, we choose $V/t = 4$ such that the superglass phase exists at $p = 0.5$\cite{31}. The average over these realizations gives us an estimate of the thermodynamic limits of our observables. Each realization is simulated independently and equilibrium is determined by reaching measurements that stabilize within our error bars. Typically, for the hardest cases this requires on the order of $10^7$ Monte Carlo steps, where one Monte Carlo step is defined as $N_{\text{sites}}$ completed worm loop updates. Equilibration times vary across phases: worm update loops tend to be long while in SF phases, and under increasing ferromagnetic order the worms have a low probability of hopping producing short loops. After equilibration, the final measurements are taken for $\sim 1/5$ of the required equilibration steps. Since most of the measurement error arises from the disorder average, it is inefficient to spend large amounts of computer time getting better statistics on each individual sample.

\textbf{Results—} The classical 3D EA model undergoes a $T = 0$ SG-FM transition at $p_c^2 \sim 0.770$, with very little temperature dependence at finite $T$. Also, the classical phase diagram is symmetric about $p = 0.5$ if one identifies the ferromagnetic with the antiferromagnetic regime. Figure 1 summarizes our QMC results in a temperature-disorder ($T$-$p$) phase diagram. The SuG-FM transition appears to be strongly temperature dependent, deviating from the classical behavior. Likely this is due to the encroaching superfluid order and subsequent competition. Meanwhile, the AFM state allows for superfluidity, creating a region of supersolidity within the arm of the superfluid transition line, which may be why the AFM state is more stable in the quantum model. Furthermore, the SuG-SS line pushes deeper into the SG phase, suggesting interesting correlation between the AFM and SF orders.

\textbf{The results for our analysis of the magnetic ordering are presented in Fig. 1.} For an even mix of bonds $p = 0.5$, the transition to superfluidity occurs near $\beta_c \sim 1$. Given that we expect the superfluidity to be killed off by ferromagnetism, it is reasonable to guess that $\beta_c$ should increase as $p$ increases. Thus, for our data in the vicinity of $p_c$ at $\beta = 1$, we don’t expect much interference from quantum mechanical effects. Data at $\beta = 1.5, 2$ (not shown) are similar, though with finite-size effects (FSE) starting to increase in magnitude.

At $\beta = 3$ in Fig. 1(a), it is also clear there would not be a transition for $p < 0.80$. This is markedly different from the classical results. The classical transition line $p_{c1}$ as a function of $\beta$ is only weakly temperature dependent, shifting less than a percent between the multicritical point and zero

\begin{table}[h]
\centering
\caption{Parameters of the simulations}
\begin{tabular}{|c|c|c|c|c|}
\hline
$\beta$ & $L$ & $p$ range & $\sim N_{\text{amp}}$ & $\sim N_{\text{sweep}}$ \\
\hline
1.00 & 3 & 0.70 - 0.80 & 2000 & 4000 \\
1.00 & 4 & 0.75 - 0.78 & 2000 & 16000 \\
1.00 & 5 & 0.75 - 0.78 & 800 & 128000 \\
1.00 & 6 & 0.75 - 0.78 & 150 & 256000 \\
1.00 & 4 & 0.12 - 0.28 & 1000 & 16000 \\
1.00 & 6 & 0.12 - 0.28 & 1000 & 16000 \\
1.00 & 8 & 0.12 - 0.28 & 100 & 128000 \\
2.00 & 4 & 0.20 - 0.30 & 1000 & 8000 \\
2.00 & 6 & 0.20 - 0.28 & 1000 & 8000 \\
2.00 & 8 & 0.20 - 0.28 & 500 & 128000 \\
3.00 & 3 & 0.75 - 0.85 & 2000 & 4000 \\
3.00 & 4 & 0.75 - 0.85 & 500 & 16000 \\
3.00 & 5 & 0.75 - 0.85 & 300 & 500000 \\
3.00 & 6 & 0.75 - 0.85 & 100 & 2000000 \\
\hline
\end{tabular}
\end{table}
FIG. 2. (Color online) (a) Finite size scaling of $g_m$ at $\beta = 1, 3$ to determine the SG-FM transition. Data for $\beta = 3$ are shifted vertically for clarity. $\beta = 1$ agrees with the classical model while $\beta = 3$ suggests the transition is pushed to higher $p$. (b) Data for $\rho_s$ showing the transition out of superfluidity appearing in the same vicinity.

FIG. 3. (Color online) Finite size scaling of the staggered magnetization cumulant $g_{sm}$. Data for $\beta = 2$ are shifted vertically for clarity. Results at $\beta = 1$ suggest the SuG-SS transition has been drawn into the classical SG region.

FIG. 4. A sample arrangement one might see in a state near the SuG-SS line. The hop move indicated is energetically neutral with respect to the bonds and destroys the local AFM order. However, the new state allows fewer fluctuations so is not favored with respect to entropy.

The specific mechanism behind the increased temperature dependence of the SuG-FM transition should be rooted in how superfluidity favors the spin glass phase over the ferromagnetic phase. We hypothesize that, first, as the exchange terms cause the system to destroy ferromagnetic order to allow hopping of particles, clusters of FM-ordered spins are suppressed. Second, glassy clusters more readily allow superfluid fluctuations amongst them, perhaps following lines of sites that are weakly constrained due to frustration. Finally, this results in the transition line moving to allow for a broader spin glass (thus superglass) phase.

We also looked at the behavior on the other side, $p < 0.5$, which is different due to the asymmetry of the ground state quantum fluctuations—spin exchange is forbidden out of a pure FM ground state, while possible from a pure AFM ground state. Notably, we find superfluid transitions at higher temperatures: $\beta_c(1 - p) < \beta_c(p)$. Fig. 3 shows data for the Binder cumulant using the staggered magnetization, $g_{sm}$ at $\beta = 1$ and 2. The staggered magnetization data suffer from larger FSE and subsequently require larger lattices to achieve comparable precision, restricting the current study from exploring lower temperatures.

The position of the crossing at $\beta = 1$ lies around $p_c \sim 0.25$ indicating that the SuG-SS line is noticeably shifted from classical behavior. The data at lower $T$ are less conclusive due to larger sizes being out of reach at present, but suggest an even
larger shift. Above the SF transition at $\beta = 0.7 (T = 1.43)$, the AFM-SG transition agrees with the classical transition point $p = 1 - p_c^{cl} = 0.23$. Thus, the stronger the quantum mechanical nature becomes—the deeper into the superfluid behavior we go—the stronger the AFM order appears. This is at first counterintuitive, but we can provide a simple, consistent picture for both this and the SuG-FM behavior. When an FM bond is satisfied, i.e. two neighboring sites are in the same state, this forbids hopping along that bond. Conversely, when an AFM bond is satisfied, the two sites are in an opposite state and will allow the system to gain kinetic energy through hops. As this is energetically favorable, we can consider the AFM bonds to have a larger effective bond strength. Consequently, the fraction of frustrating FM bonds it would require to destroy the AFM order should rise, and we see the present shift in phase boundary.

Speaking more generally, we can consider the change in the entropy of the system, with respect to quantum fluctuations, when moving towards higher AFM or FM order. Under pure FM order no hopping is allowed, while under pure AFM order each site has the ability to engage in virtual hopping. Using a 2D lattice as an example, Fig. 4 shows a typical local snapshot of a system with AFM order being frustrated by FM bonds. The indicated move would go against three NN bonds while satisfying three others, making the diagonal component energetically neutral, and this would turn the local AFM order into FM order. However, after this move the system is now considerably more constrained regarding the number of hoppings available. Originally, the two interior sites could be involved with seven different hop moves, but these sites now have a single move: to return back to the original state. In this way, the AFM state is favored as it allows for more gain in kinetic energy.

Summary—We have presented our QMC results of a bosonic model exhibiting a superglass phase in order to study the phase transitions achieved by directly tuning the level of disorder present. These results indicate that the addition of the exchange terms act to stabilize the classical spin glass phase against the formation of ferromagnetic clusters which impede hopping. In addition, the favoring of AFM bonds to FM bonds leads to a shift in the SuG-SS phase boundary. An interesting issue not addressed here is whether there is always a SG phase between the FM and SuG phases. Recent work\cite{21} on disordered Bose systems suggests that this may be true. Unfortunately, our current precision is not high enough to be conclusive. Future work is required to clarify this issue.

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