Magnetic and Superfluid Transitions in the One-Dimensional Spin-1 Boson Hubbard Model

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Recent progress in experiments on trapped ultracold atoms has made it possible to study the interplay between magnetism and superfluid-insulator transitions in the boson Hubbard model. We report on quantum Monte Carlo simulations of the spin-1 boson Hubbard model in the ground state. For antiferromagnetic interactions favoring singlets, we present exact numerical evidence that the superfluid-insulator transition is first (second) order for even (odd) Mott lobes. Inside even lobes, we search for nematic-to-singlet first order transitions. In the ferromagnetic case where transitions are all continuous, we map the phase diagram and show the superfluid to be ferromagnetic. We compare the quantum Monte Carlo phase diagram with a third order perturbation calculation.

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The single band fermion Hubbard model offers one of the most fundamental descriptions of the physics of strongly correlated electrons in the solid state. The spinful nature of the fermions is central to the wide range of phenomena it displays, such as interplay between its magnetic and transport properties [1]. Such complex interplay is absent in the superfluid to Mott insulator transition [2–5] in the spin-0 boson Hubbard model (BHM). However, purely optical traps [6] can now confine alkali atoms 23Na, 39K, and 87Rb, which have hyperfine spin $F = 1$, without freezing $F_c$. The nature of the superfluid-Mott insulator (SF-MI) transition is modified by the spin fluctuations which are now allowed. Initial theoretical work employed continuum, effective low-energy Hamiltonians and determined the magnetic properties and excitations of the superfluid phases [7].

To capture the SF-MI transition, we study the spin-1 bosonic Hubbard Hamiltonian,

$$
H = -t \sum_{\langle ij \rangle, \sigma} (a_{i\sigma}^\dagger a_{j\sigma} + \text{H.c.}) + \frac{U_0}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{U_2}{2} \sum_i (\hat{F}_i^2 - 2 \hat{n}_i),
$$

in one dimension. The boson creation (destruction) operators $a_{i\sigma}^\dagger (a_{i\sigma})$ have site $i$ and spin $\sigma$ indices, $\sigma = 1, 0, -1$. The first term describes near neighbor, $\langle ij \rangle$, jumps, and $t = 1$ sets the energy scale. The number operator $\hat{n}_i \equiv \sum_{\sigma} \hat{n}_{i\sigma}$ counts the total boson density on site $i$. The on-site repulsion is given by $U_0$. The spin operator $\hat{F}_i = \sum_{\sigma, \sigma'} a_{i\sigma}^\dagger \hat{\sigma}_{\sigma\sigma'} a_{i\sigma'}$, with $\hat{\sigma}_{\sigma\sigma'}$ the standard spin-1 matrices, contains further contact interactions and also interconversion terms between the spin species. We treat the system in the canonical ensemble where the total particle number is fixed and the chemical potential is calculated, $\mu(C) = E(N + 1) - E(N)$ where $E(N)$ is the ground state energy with $N$ particles. This holds only when each energy used is that of a single thermodynamic phase and not that of a mixture of coexisting phases as happens with first order transitions. It is therefore incorrect to determine first order phase boundaries with the naive use of this method. Here, there is the added subtlety that the three species are interconvertible. These issues will be addressed in more detail below.

Important aspects of the spin-1 BHM are revealed by analysing the no-hopping limit, $t/U_0 = 0$. The Mott-1 state with $n_1 = 1$ on each site has $E_M(1) = 0$. In the Mott-2 state with $n_1 = 2$, the energy is $E_M(2) = U_0 - 2U_2$, if the bosons form a singlet, $F = 0$, and is $E_M = U_0 + U_2$ if $F = 2$. Thus $U_2 > 0$ favors singlet phases while $U_2 < 0$ favors (on-site) ferromagnetism. This applies to all higher lobes as well. In the canonical ensemble, the chemical potential at which the system goes from the $n$th to the $(n + 1)$th Mott lobe is $\mu(n \rightarrow n + 1) = E_{n+1} - E_n$.

For $U_2 > 0$, the energy of Mott lobes at odd filling, $n_e$, is $E_M(n_e) = U_0 n_e (n_e - 1)/2 + U_2 (1 - n_e)$ and at even filling, $n_e$, $E_M(n_e) = U_0 n_e (n_e - 1)/2 - n_e U_2$. So the boundaries of the lobes, going from low to high filling, are $\mu(n_e \rightarrow (n_e + 1)) = n_e U_0$ and $\mu(n_e \rightarrow (n_e + 1)) = n_e U_0 - 2U_2$. This fixes the “bases” of the Mott lobes in the $(t/U_0, \mu/U_0)$ ground state phase diagram. For $U_2 > 0$ the even Mott lobes grow at the expense of the odd ones, which disappear entirely for $U_2 = 2U_0$.

For $U_2 < 0$, the ground state is ferromagnetic [maximal $F$, $F^2 = n(n + 1)$] which gives for all Mott lobes $E_M(n) = n(n + 1)/2$. Consequently, the boundary of the $n$th and $(n + 1)$th Mott lobes $\mu(n \rightarrow n + 1) = n(U_0 + U_2)$. The bases of both the odd and even Mott lobes shrink with increasing $|U_2|$, in contrast to the $U_2 > 0$ case where the even Mott lobes expand.

Mean-field treatments of this model capture the SF-MI transition as $t$ is turned on, and they have been performed...
both at zero and finite temperature [8–10]. Even when \( U_2 = 0 \), the spin degeneracy alters the nature of the transition. For \( U_3 > 0 \), the order of the phase transition depends on whether the Mott lobe is even or odd. These mean-field calculations assume a nonzero order parameter \( \langle a_{i\sigma} \rangle \), which cannot be appropriate in \( d = 1 \) or in \( d = 2 \) at finite \( T \). Therefore it is important to verify these predictions for the qualitative aspects of the phase diagram, especially in low dimension. A quantitative determination of the phase boundaries requires numerical treatments. Indeed, density matrix renormalization group (DMRG) [11] and quantum Monte Carlo (QMC) [12] results for \( U_2 > 0 \) and \( d = 1 \) reported the critical coupling strength and showed that the odd Mott lobes are characterized by a dimerized phase that breaks translation symmetry.

For \( U_3 < 0 \), the nature of the SF-MI transition does not depend on the order of the Mott lobe while for \( U_2 > 0 \) it is predicted to be continuous (discontinuous) into odd (even) lobes. Consequently, it suffices to study the first two Mott lobes for both \( U_2 > 0 \) and \( U_3 < 0 \) to demonstrate the behavior for all lobes. Furthermore, in what follows we will focus on the case \( |U_2/U_0| = 0.1 \) in order to compare our results for \( U_2 > 0 \) with Rizzi et al. [11].

Here, we will use an exact QMC approach, the stochastic Green function algorithm with directed update, to study the spin-1 BHM in \( d = 1 \) for both positive and negative \( U_3 \) [13].

For \( U_2 > 0 \) (e.g., \( ^{23}\text{Na} \)), which favors low total spin states, Fig. 1 shows the total number density \( \rho = N/L \) against \( \mu \) for \( U_0 = 10t \) and \( U_2 = t \). It displays clearly the first two incompressible MI phases. In agreement with the \( t/U_0 = 0 \) analysis, \( U_2 \) causes an expansion of the second Mott lobe, \( \rho = 2 \), at the expense of the first, \( \rho = 1 \). Our Mott gaps agree with DMRG results [11] to within symbol size. However, the \( \rho \) vs \( \mu \) curve in Fig. 1 does not betray any evidence of the different natures of the phase transitions into the first and second Mott lobes. For a spin-0

![FIG. 1 (color online). \( \rho(\mu) \) exhibits Mott plateaux: gapped, insulating phases at commensurate fillings. Inset: \( N_+/N \) and \( N_0/N \) vs \( \rho = N/L \). Singlets form where \( N_+ \) and \( N_0 \) are equal (see text).](image-url)
sensitivity of the possibility of a first order transition for a phase transition. This, of course, does not preclude the insulator. The dashed line indicates the critical point of an insulator. The passage of the tip of the Mott lobe. Inside the lobe, the nematic-to-SF transitions of the same order? Figure 2 shows the singlet phase for $t/U_0 = 1$ and $d < 2$, but with $U_2/U_0 = 0.01$.

As discussed above, $U_2 < 0$ favors “local ferromagnetism,” namely, high spin states on each of the individual lattice sites. As with the fermion Hubbard model, the kinetic energy gives rise to second order splitting, which lifts the degeneracy between commensurate filling strong coupling states with different intersite spin arrangements. We can therefore ask whether the local moments order from site to site: Do the Mott and superfluid phases exhibit global ferromagnetism [10]? To this end, we measure the magnetic structure factor:

$$S_{\sigma\sigma}(q) = \sum_F e^{iq\cdot F} \langle F_{\sigma,\sigma} \rangle$$

where $\sigma = x$ or $z$. Figure 4 shows $S_{xx}(q)$ in the superfluid phase at half filling [18]. The peak at $q = 0$ grows linearly with lattice size, indicating the superfluid phase does indeed possess long range ferromagnetic order. We find that the MI phase is also ferromagnetic.

To determine the phase diagram, we scan the density as in Fig. 3 for many values of $U_0$ with $U_2/U_0$ constant.
show a similar level of agreement with the QMC results.

Early in the evaluation of the phase boundaries of the spin-0 BHM it was observed that a perturbation calculation [4] agreed remarkably well with QMC results [3]. We now generalize the spin-0 perturbation theory to spin-1 and show a similar level of agreement with the QMC results. If we assume the system always to be perfectly magnetized, then $n$ bosons on a site will yield the largest possible spin, $F^2 = n(n+1)$. Consequently, the interaction term in the Hamiltonian, Eq. (1), reduces to $(U_0 - U_2)\sum_i F_i^z F_i^z$, giving a Hamiltonian identical to the spin-0 BHM but with the interaction shifted to $(U_0 - U_2)/2$. One can then repeat the perturbation expansion to third order in $(U_0 - U_2)$ to determine the phase diagram [4]. The result is shown as the dashed line in Fig. 5 and is seen to be in excellent agreement with QMC calculations. The agreement further suggests that the finite lattice effects in the phase diagram are small. Such a perturbation calculation is not possible for the $U_0 > 0$ case since $F^2$ depends on the phase, SF vs MI, and on the order of the MI lobe. (The dipolar) interactions between spinful bosonic atoms confined to a single trap have been shown to give rise to fascinating “spin textures” [19]. An additional optical lattice causes a further enhancement of interactions, and opens the prospect for the observation of the rich behavior associated with Mott and magnetic transitions and comparisons with analogous properties of strongly correlated solids [16,17]. Here, we have quantified these phenomena in the one-dimensional spin-1 BHM with exact QMC methods. We have shown that, for $U_2 > 0$, the MI phase is characterized by singlet formation clearly seen for even Mott lobes where $(F^2) \rightarrow 0$ as $U_0$ increases. We also showed that the transition into odd lobes is continuous while that into even lobes is discontinuous (first order). We emphasized that the naive canonical determination of the phase boundaries is not appropriate for a first order transition. For $U_2 < 0$, we showed that all MI-SF transitions are continuous and that both the SF and MI phases are ferromagnetic. The phase diagram in the $(\mu/U_0, t/U_0)$ plane obtained by QMC calculations can be described very accurately using third order perturbation theory.

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