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 ^{23}Na, ^{39}K, and ^{87}Rb, which have hyperfine spin $F = 1$, without freezing F_z. 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,

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

in one dimension. The boson creation (destruction) operators $a^\dagger_{i\sigma}(a_{i\sigma})$ have site i and spin σ 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 $\hat{n}_i \equiv \sum_\sigma \hat{n}_{i\sigma} = \sum_\sigma a^\dagger_{i\sigma} a_{i\sigma}$ counts the total boson density on site i. The on-site repulsion is given by U_0. The spin operator $\vec{F}_i = \sum_{\sigma,\sigma'} a^\dagger_{i\sigma} \vec{F}_{\sigma\sigma'} a_{i\sigma'}$, with $\vec{F}_{\sigma\sigma'}$ 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, $\mu(N) = E(N+1) - E(N)$ 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 $n_i = 1$ on each site has $\mathcal{E}_M(1) = 0$. In the Mott-2 state with $n_i = 2$, the energy is $\mathcal{E}_M(2) = U_0 - 2U_2$, if the bosons form a singlet, $F = 0$, and is $\mathcal{E}_{M2} = U_0 + U_2$ 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 nth to the $(n+1)$th Mott lobe is $\mu(n \to n+1) = \mathcal{E}_{n+1} - \mathcal{E}_n$.

For $U_2 > 0$, the energy of Mott lobes at odd filling, n_o, is $\mathcal{E}_M(n_o) = U_0 n_o(n_o - 1)/2 + U_2(1 - n_o)$ and at even filling, n_e, $\mathcal{E}_M(n_e) = U_0 n_e(n_e - 1)/2 - n_e U_2$. So, the boundaries of the lobes, going from low to high filling, are $\mu[n_e \to (n_e + 1)] = n_e U_0$ and $\mu[n_o \to (n_o + 1)] = n_o U_0 - 2U_2$. 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 $U_0 = 2U_2$.

For $U_2 < 0$, the ground state is ferromagnetic [maximal F: $F^2 = n(n+1)$] which gives for all Mott lobes $\mathcal{E}_M(n) = n(n-1)(U_0 + U_2)/2$. Consequently, the boundary of the nth and $(n+1)$th Mott lobes $\mu(n \to n+1) = n(U_0 + U_2)$. 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 $U_2 > 0$, 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 $U_2 < 0$, 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 $U_2 < 0$ 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_2 [13].

For $U_2 > 0$ (e.g., ^{23}Na), which favors low total spin states, Fig. 1 shows the total number density $\rho = N/L$ against μ 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 ρ vs μ 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 BHM, first order transitions are exposed by the appearance of negative compressibility [14], $\kappa = \partial\rho/\partial\mu$, which is absent here. The transition into the second Mott lobe is expected to be first order and driven by the formation of bound pairs of bosons in singlet states. Therefore, in the canonical ensemble, we expect that near this transition there will be phase coexistence between singlets arranged in a Mott region and superfluid.

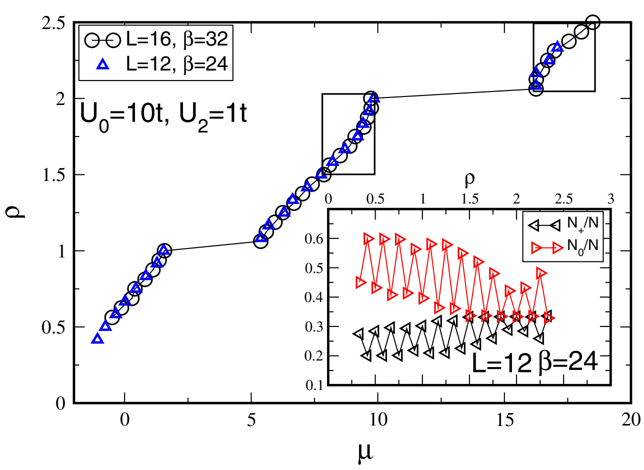

FIG. 1 (color online). $\rho(\mu)$ exhibits Mott plateaux: gapped, insulating phases at commensurate fillings. Inset: N_+/N and N_0/N vs $\rho = N/L$. Singlets form where N_+/N and N_0/N are equal (see text).

The nature of the transitions is revealed by the evolution of the spin populations in the system as ρ increases. Since the singlet wave function is $|0,0\rangle = \sqrt{2/3}|1,1\rangle|1,-1\rangle - \sqrt{1/3}|1,0\rangle|1,0\rangle$, this state has $\rho_+ = \rho_0 = \rho_-$. We plot in Fig. 1 (inset) the population fractions, N_0/N and $N_-/N = N_+/N$ vs the total density. As ρ increases, N_+/N and N_0/N oscillate: For even N, singlet bound states of two particles try to form drawing N_+/N and N_0/N closer together. However, singlets form fully, making $N_+ = N_0$, only close to the second Mott lobe, $\rho = 2$, where we clearly see $N_+/N = N_0/N$ for a range of even values of N. When N is odd, singlets cannot form and the spin populations are much farther from that given by the singlet wave function. In the thermodynamic limit and fixed N, one expects true phase separation into $\rho = 2$ singlet MI regions and $\rho < 2$ SF regions. For a finite system, phase separation commences for (even) fillings where we first have $N_+/N = N_0/N$, i.e., $1.5 \leq \rho < 2$ and similar behavior for $\rho > 2$. Another interesting feature in the inset of Fig. 1 is that the difference between N_+/N and N_0/N, for even N, decreases linearly as the density approaches the transition at $\rho = 1.5$. No such behavior is seen as the first Mott lobe is entered from below or above $\rho = 1$: The transition is continuous as predicted for odd lobes.

The boxes in Fig. 1 show the values of ρ corresponding to phase coexistence rather than to one stable thermodynamic phase. It is, therefore, clear that the canonical calculation of the phase boundaries, i.e., simply adding a particle to, or removing it from, the MI, is not applicable in the presence of a first order transition.

Figure 1 reveals the SF-MI transition at fixed, sufficiently large U_0 when ρ is varied. In Fig. 2 we show the transition when the density is fixed, $\rho = 2$, and U_0 is the control parameter with $U_2/U_0 = 0.1$ (main figure) and 0.01 (inset). Singlet formation is clearly shown by $\langle F^2\rangle \to 0$, as t/U_0 decreases and the second MI is entered [15]. The superfluid density, $\rho_s = L\langle W^2\rangle/2t\beta$, where W is the winding number, is a topological quantity and truly characterizes the SF-MI phase transition which is continuous in this case. As L is increased from 10 to 16 and 20, the vanishing of ρ_s gets sharper. We find that the critical value of t/U_0 for the $\rho = 2$ lobe is somewhat less than that reported in DMRG [11], indicated by the dashed line. We believe this is because with DMRG the phase boundaries were obtained using finite differences of the energy with small doping above and below commensurate filling. As discussed above, this is not appropriate for a first order transition.

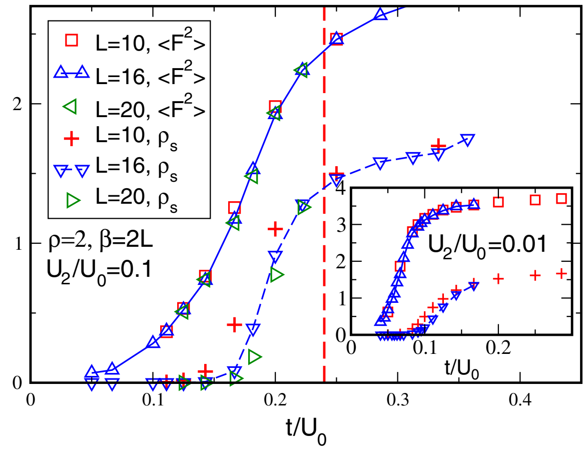

FIG. 2 (color online). The square of the local moment, $\langle F^2 \rangle$, and the superfluid density, ρ_s, vs t/U_0 for $\rho = 2$. In the Mott lobe, $\langle F^2 \rangle \to 0$ signaling singlet formation and $\rho_s \to 0$ indicating an insulator. The dashed line indicates the critical t/U_0 from Rizzi *et al.* [11]. Inset: Same but with $U_2/U_0 = 0.01$.

For $2dU_2/U_0 < 0.1$ and $d = 2$ and 3, the mean field [16,17] predicts that, when $t/U_0^{c1} \sim \sqrt{U_2/4dU_0}$ is in the MI, then Mott lobes of even order are comprised of two phases: (a) the singlet phase for $t/U_0 \le t/U_0^{c1}$ and (b) a nematic phase for $t/U_0^{c1} \le t/U_0 \le t/U_0^c$, where t/U_0^c is the tip of the Mott lobe. Inside the lobe, the nematic-to-singlet transition is predicted to be first order, which raises the following question: Are the singlet-to-SF and the nematic-to-SF transitions of the same order? Figure 2 shows that the SF-MI transition, $\rho_s \to 0$, occurs at larger t/U_0 than singlet formation, $\langle F^2 \rangle \to 0$, both for $U_2/U_0 = 0.1$ and 0.01. The passage of $\langle F^2 \rangle$ to zero gets sharper for smaller U_2/U_0 but remains continuous, not exhibiting any signs of a first order transition. We have verified this for $U_2/U_0 = 0.1$, 0.05, 0.01, and 0.005. Furthermore, the insensitivity of $\langle F^2 \rangle$ to finite size effects indicates that it does not undergo a continuous phase transition. We have also verified that for the second Mott lobe, the SF-MI transition is first order regardless of whether t/U_0 is less than or greater than t/U_0^{c1}. We conclude that while $\rho_s \to 0$ is a continuous critical transition, $\langle F^2 \rangle \to 0$ is a *crossover*, not a phase transition. This, of course, does not preclude the possibility of a first order transition for $d = 2$ and 3.

Whereas ^{23}Na has positive U_2, ^{87}Rb has $U_2 < 0$, leading to different behavior. We begin with ρ vs μ in Fig. 3. Unlike the $U_2 > 0$ case, the SF-MI transitions are continuous for both even and odd Mott lobes: The inset shows that the spin populations do not oscillate as for $U_2 > 0$. The population ratio, $\rho_0 = 2\rho_+$, can be understood as follows. As shown above for $t/U_0 \to 0$, maximum spin states are favored when $U_2 < 0$. So, when a site is doubly occupied, the spin-2 state is favored. But, since our study is in the $S_z^{\rm tot} = N_+ - N_- = 0$ sector, the wave function of the spin-2 state is $|2, 0\rangle = 1/\sqrt{3}|1, 1\rangle|1, -1\rangle + \sqrt{2/3}|1, 0\rangle|1, 0\rangle$ and thus $\rho_0 = 2\rho_+ = 2\rho_-$.

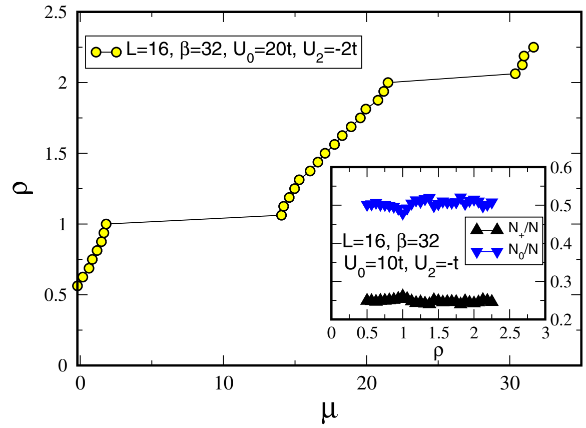

FIG. 3 (color online). The density ρ vs chemical potential μ exhibits the usual Mott plateaux at commensurate filling for $U_2 < 0$. Inset: The spin population fractions showing $\rho_0 = 2\rho_+$. They do not exhibit oscillations like in Fig. 1.

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:

$$S_{\sigma\sigma}(q) = \sum_l e^{iql} \langle F_{\sigma,j+l} F_{\sigma,j} \rangle, \tag{2}$$

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

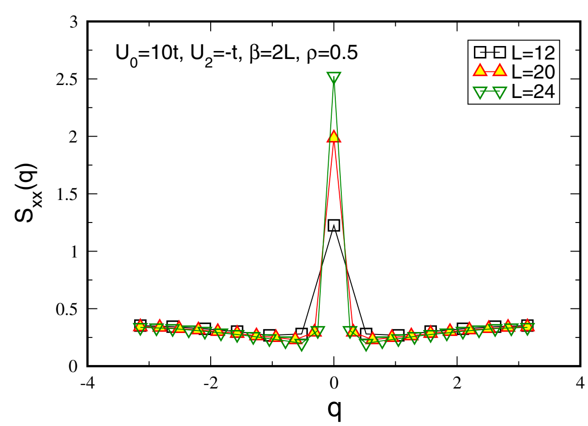

FIG. 4 (color online). The magnetic structure factor $S_{xx}(q)$ for $U_2 < 0$ and $\rho = 0.5$ exhibits a sharp $q = 0$ peak indicating ferromagnetic order.

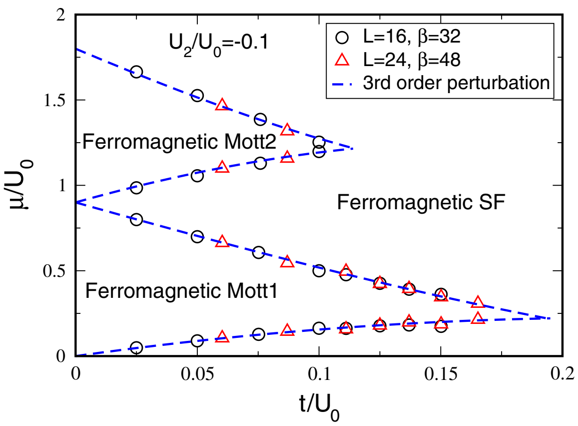

FIG. 5 (color online). Phase diagram of the spin-1 BHM for $U_2/U_0 = -0.1$.

(-0.1 in our case). The resulting phase diagram is shown in Fig. 5. Comparison of data for two lattice sizes demonstrates that finite size effects are small.

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 $(U_0 - U_2)\sum_i \hat{n}_i(\hat{n}_i - 1)/2$, 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 $t/(U_0 - U_2)$ 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 $\langle F^2 \rangle \to 0$ 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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