Mott insulating phases and magnetism of fermions in a double-well optical lattice

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(Dated: March 4, 2022)

We theoretically investigate, using non-perturbative strong correlation techniques, Mott insulating phases and magnetic ordering of two-component fermions in a two-dimensional double-well optical lattice. At filling of two fermions per site, there are two types of Mott insulators, one of which is characterized by spin-1 antiferromagnetism below the Neel temperature. The super-exchange interaction in this system is induced by the interplay between the inter-band interaction and the spin degree of freedom. A great advantage of the double-well optical lattice is that the magnetic quantum phase diagram and the Neel temperature can be easily controlled by tuning the orbital energy splitting of the two-level system. Particularly, the Neel temperature can be one order of magnitude larger than that in standard optical lattices, facilitating the experimental search for magnetic ordering in optical lattice systems.

PACS numbers: 05.30.Fk, 67.85.-d, 71.27.+a, 03.75.-b

Introduction.- There are currently worldwide efforts in studying collective properties of cold atoms either in a single trap or in an optical lattice [1]. A central goal of these studies is to explore novel many-body quantum phases in both bosonic and fermionic systems. While both bosonic and fermionic Mott insulators have been realized in laboratories [2–5], the experimental search for magnetism in optical lattices is currently on-going. Most of these studies have been focusing on the single-band physics. For example, it is known that two-component fermions in the lowest band can be used to study spin-1/2 antiferromagnetism [6].

A question naturally arises: Is it possible to realize multi-band magnetic systems using cold atoms in optical lattices? Theoretical studies suggest, for example, exploring excited bands in optical lattices for searching novel magnetism [7, 8], partly because of the enhanced tunnel coupling in excited bands [9, 10]. While there are currently experimental efforts along this direction to populate atoms in excited bands [11, 12], whether one can overcome the finite-life time problem of atoms in excited bands still remains unclear.

On the other hand, there is a crucial practical issue on the energy and time scales of atoms in optical lattices. Ordinary optical lattices are characterized by extremely small energy scales, which also lead to slow relaxation of lattice systems to equilibrium. For example, the tunneling of the lowest band is about a few nano-Kelvin which corresponds to a time scale of a few tens of milliseconds. The energy scale associated with the super-exchange interaction $t^2/U$ is even smaller since $U \gg t$ typically. As a result, the Neel temperature of antiferromagnetism in ordinary optical lattices is far too low for experimental observation. Meanwhile, it is also challenging for the system to reach equilibrium because of the long relaxation time. A scheme to enhance the relevant energy scales is therefore very desirable, particularly in the context of the experimental study of many-body magnetism in optical lattice systems.

In this Rapid Communication, we theoretically study quantum magnetism of fermions in a double-well optical lattice. Instead of the usual spin-1/2 magnetic ordering in an ordinary optical lattice, the double-well effectively produces a spin-1 system. The associated magnetism is induced by the inter-band interaction between the lowest two bands, and is a ground state property. Moreover, the characteristic energy scale for observing magnetism can be enhanced by one order of magnitude compared with the spin-1/2 magnetism in ordinary optical lattices. As a result, the magnetism may be much easier to achieve and observe experimentally in the double-well optical lattice.

A double-well optical lattice contains two potential wells, which are separated by a barrier, on each lattice site. Its unique advantage is that the band gap between the lowest two bands is tunable [13, 14]. When these two bands are very close to each other, interesting quantum many-body phenomena, which are completely absent in ordinary optical lattices, emerge [14, 15]. We will see that the interplay between the orbital degree of freedom and the fermionic spin lies at the heart of the new physics reported here. Theoretically it is however challenging to study fermions with spin degrees of freedom in the presence of multiple bands. We employ the dynamical mean-field theory (DMFT) method [16], and study both the Mott insulating phases and magnetic properties of fermions in a double-well lattice. We show that at filling of two fermions per site, the Mott insulator developed in the system can be either the triplet $(n_s, n_p) = (1, 1)$ states or the admixture $u(2,0) - v(0,2)$. For the former case, antiferromagnetic order emerges in the spin-1 channel, which should be experimentally observable.

Model.- We consider the Hamiltonian containing a tight-binding-band part and an on-site interaction part, characterizing the two lowest bands (labeled by $s$ and $p$ respectively) in a symmetric double-well lattice, $H = H_{\text{band}} + H_{\text{int}}$. In the real space, the band part can be
FIG. 1: (Color online) (a) Profile of the double-well potential (the green line) along the x-direction. The s (red lines) and p (blue lines) orbitals are schematically shown. The hopping integrals and energies for s(p) orbitals, $t_{sx}(t_{px})$ and $\varepsilon_s(\varepsilon_p)$, are indicated. Note that the potential is not double-welled along the y-direction (not shown), where the hopping integrals are $t_{sy}$ and $t_{py}$ correspondingly. (b) $(n_s, n_p) = (1, 1)$ eigenstates in atomic limit, including triplet states with energy $E_T$ and a singlet state with energy $E_S$. (c) Linear combinations of (2, 0) and (0, 2) states as eigenstates for the Hamiltonian in atomic limit, whose energies are denoted by $E_{\pm}$. See the text for details.

written as

$$H_{\text{band}} = \sum_{r\sigma} \left[ (\varepsilon_s - \mu)s_{s,r}^\dagger s_{s,r} + (\varepsilon_p - \mu)p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r} \right]$$

$$+ \sum_{r\sigma} \left( -t_{sx}s_{s,r}^\dagger s_{s,r+x} - t_{sy}s_{s,r}^\dagger s_{s,r+y} + t_{px}p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r+x} + t_{py}p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r+y} + h.c. \right),$$

where $s_{s,r}^\dagger(p_{\alpha,\sigma,r}^\dagger)$ creates a fermion with spin $\sigma$ on the s(p) orbital of site $r$, $\varepsilon_s$ and $\varepsilon_p$ are the energies for s and p orbitals, and $\mu$ is the chemical potential. The hopping amplitude for s and p orbitals may differ in x and y directions, thus we label them by $t_{sx}, t_{sy}, t_{px}, t_{py}$ respectively.

The interacting part of the Hamiltonian can be written as

$$H_{\text{int}} = \sum_{r} \left[ U_s n_{s\uparrow,r} n_{s\downarrow,r} + U_p n_{p\uparrow,r} n_{p\downarrow,r} \right.$$

$$+ U_{sp}(n_{s\uparrow,r} n_{p\downarrow,r} + n_{s\downarrow,r} n_{p\uparrow,r})$$

$$- U_{sp} \left( s_{s\uparrow,r}^\dagger p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r} s_{s\downarrow,r} + h.c. \right) \right],$$

where $n_{\alpha,\sigma,r} = c_{\alpha,\sigma,r}^\dagger c_{\alpha,\sigma,r} \ (\alpha = s,p)$ is the number operator for orbital $\alpha$ at site $r$, $U_s = \frac{4\pi a_s^2}{\hbar^2 m - \int d^3 x W_s^2(x)}$ denotes the intra-band interaction, while $U_{sp} = \frac{4\pi a_{sp}^2}{\hbar^2 m - \int d^3 x W_s^2(x) W_p^2(x)}$ denotes the inter-band interaction, where $a_s$ is the scattering length, $M$ is the mass of the fermion, and $W_\alpha(x)$ is the Wannier wave function for each band. The inter-orbital terms in Eq. (2) characterized by $U_{sp}$ are referred as density-density, spin-exchange and pair-hopping interaction. This model is essentially the rotationally invariant Slater-Kanamori interaction widely studied in transitional metal oxides [17]. The main difference here is that the spin-exchange and pair-hopping are as strong as the inter-orbital density-density interaction. An important parameter which controls the multi-band physics is the energy level splitting between the two levels, defined as $\Delta \equiv \varepsilon_s - \varepsilon_p$. When $\Delta$ is small or intermediate, interactions between the two orbitals give rise to interesting phenomena, as we discuss below. When $\Delta$ becomes very large the physics reduces to that of the single-band model. The Hamiltonian in Eq. (2) has been previously considered for fermions at resonance in an ordinary optical lattice in one-dimension [18]. In our case, the reduced band gap makes the realization of a two-band system more practical in current experiments. Moreover, higher dimensionality of our system gives distinct physical phenomena not accessible in one dimension.

We start from the atomic limit, where the tunneling terms are absent. We are interested in the states at filling of two fermions per site, the schematics of which are shown in Fig. 1(b) and 1(c). When there is one fermion in each orbital, they form triplets which is denoted as $(n_s, n_p) = (1, 1)$, namely, $p_{\alpha,\sigma,r}^\dagger |0\rangle$, $\frac{1}{\sqrt{2}} \left( p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r}^\dagger \right) |0\rangle$, and $p_{\alpha,\sigma,r}^\dagger |0\rangle$, with degenerate energy $E_T = 2(\varepsilon_s - \mu) + \Delta$. The singlet state $|\frac{1}{\sqrt{2}} (p_{\alpha,\sigma,r}^\dagger p_{\alpha,\sigma,r}^\dagger) |0\rangle$ has a higher energy $E_S = 2(\varepsilon_s - \mu) + \Delta + 2U_{sp}$. $E_S > E_T$ simply because two fermions interact with each other by s-wave short-range interaction. In the spirit of the Hubbard model, atoms with different spins repel with each other and atoms with the same spin do not interact. On the other hand, the two fermions can also form admixtures $u(2,0) \pm v(0,2)$, as shown in Fig. 1(c), due to the pair-hopping interaction. The eigenenergies are $E_{\pm} = 2(\varepsilon_s - \mu) - \Delta + \frac{U_s + U_p}{2} \pm \sqrt{\left( \Delta + \frac{U_s - U_p}{2} \right)^2 + U_{sp}^2}$. By controlling $\Delta$ in the double-well lattice, $E_{\pm}$ can be made either smaller or larger than $E_T$. Throughout the paper we fix parameters $U_s = 12t$, $U_p = 14t$, $U_{sp} = 12t$, and vary $\Delta$ and the temperature $T$. Straightforward algebra reveals that at the critical value $\Delta_c = 4t, E_+ = E_- = E_T$. For latter use we note that the hopping integrals are chosen as $t_{sx} = t_{sy} = t_{py} = t, t_{px} = 2t$. The large $t_{px}$ stems from the fact that p bands are spatially more extended along the x-direction. However, our solution to the lattice model as well as the physics therein does not depend on this particular set of parameters in any important way.

When the hopping terms are switched on, we employ the single-site DFT [16] to solve the strongly-correlated interacting lattice fermion problem. The key approxima-
Magnetic order.- When the $(1,1)$ states dominate the on-site Fock states for small $\Delta$, the interacting Hamiltonian can be mapped to a spin-1 Heisenberg model, which can be written as

$$H_{\text{eff}} = \sum_r (J_x S_r \cdot S_{r+x} + J_y S_r \cdot S_{r+y}) ,$$

where

$$J_x = \frac{2t^2_{sx}}{U_s + U_{sp}} + \frac{2t^2_{sx}}{U_p + U_{sp}}, \quad J_y = \frac{2t^2_{sy}}{U_s + U_{sp}} + \frac{2t^2_{sy}}{U_p + U_{sp}} ,$$

$S_r = A^\dagger \Sigma A$ is a spin-1 operator, $\Sigma$ is spin-1 Pauli matrices, and $A = (\Psi_0^\dagger, \Psi_0^\dagger \Psi_1^\dagger)^T$ are creation operators for triplet states $p^\dagger s^\dagger_0 [0]$, $\frac{1}{\sqrt{2}} (p^\dagger s^\dagger_0 + p^\dagger s^\dagger_1) [0]$, and $p^\dagger s^\dagger_1 [0]$. Physically, the spin-exchange terms in Eq. (3) come from the exchange of fermions with different spins between the nearest-neighbor sites in either of the two orbitals. Both orbitals contribute to the spin-exchange terms in the effective Hamiltonian.

In the one-dimensional case, Eq. (3) has previously been derived in Ref. [19]. For that case, it has been known that the one-dimensional spin-1 chain does not have any magnetic order, rather the Haldane phase. Nevertheless, a two-dimensional spin-1 system can develop antiferromagnetic ground states[20–22]. Therefore, one expects to see antiferromagnetic spin ordering in a double-well optical lattice when the gap $\Delta$ is small and the temperature is low[23].

To characterize the magnetization, we define $m = |n_{s\uparrow} - n_{s\downarrow} + n_{p\uparrow} - n_{p\downarrow}|$ and solve the full Hamiltonian $H = H_{\text{band}} + H_{\text{int}}$. The results for $m$ as a function of the temperature for different $\Delta$ are shown in Fig. 3(b). Clearly, the magnetization arises below the Neel temperature (denoted by $T_{\text{Neel}}$), and saturates to its maximum value as the temperature approaches zero. For $\Delta = 0$, the antiferromagnetic ordering is most pronounced: it has the highest Neel temperature $T_{\text{Neel}} \approx 0.37t$. However, this must be interpreted with caution because experimentally it is very difficult to tune the two bands overlap with each other while keeping the tight-binding model valid. We therefore focus on the cases with nonzero $\Delta$. As $\Delta$ is increased, the magnetization drops faster as $T$ increases, and the Neel temperature decreases. For a relatively large $\Delta = 4.5t$, $T_{\text{Neel}} \approx 0.21t$. Note that this
value of $\Delta$ is already above the critical value $\Delta_c = 4t$ in the atomic limit where $u(2,0) - v(0,2)$ is the ground state. This indicates that many-body effects, such as the correlation between nearest-neighbor sites, enhance the threshold of $\Delta_c$ for a finite $m$ to emerge.

To give a broader picture, we show in Fig. 3(b) a color plot of the magnetization on a plane, of which the axes are the energy level splitting $\Delta$ and the temperature $T$. The blue dashed line, separating colored and white regimes, indicates the Neel temperature, above which no magnetic order, while for low $T$ the magnetization reaches the maximum value, indicated as dark colors. The Neel temperature is shown as blue dashed lines separating colored and white regimes. Note that the $y$-axis does not start from zero: it starts from the lowest temperature $T = 0.05t$ reached in the DMFT calculation.

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Neel temperature can be one order of magnitude larger than that of the one-band system in ordinary optical lattices, thus perhaps enabling the direct experimental observation of the elusive Neel antiferromagnetism in cold atomic systems. Our work should facilitate the search of magnetic order in optical lattice systems.

Acknowledgements: We thank M. Cheng and A. J. Millis for discussions. This work is supported by JQI-NSF-PFC, ARO-DARPA-OLE, JQI-ARO-MURI, and JQI-AFOSR-MURI. The impurity solver in the DMFT procedure is based on a code primarily developed by P. Werner, and uses the ALPS library[24].

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