Theory of quantum antiferromagnetism of fermions in an optical lattice with a half-filled *p* band

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We study Fermi gases in a three-dimensional cubic optical lattice with five fermions per site, i.e., the *s* band is completely filled and the *p* band with threefold degeneracy is half filled. We show that for repulsive interaction between fermions, the system will exhibit spin-3/2 antiferromagnetic order at low temperature. This conclusion is obtained both in strong interaction regime by strong coupling expansion and in weak interaction regime by the Hartree–Fock mean-field theory with analysis of the Fermi surface nesting. We also show that in the strongly correlated regime the Néel temperature for *p* band antiferromagnetism is 2 to 3 orders of magnitudes higher than that of *s* band, which is much more promising to be attained in cold atom experiments.

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I. INTRODUCTION

Studying the strong correlations in lattice Fermi gases has now become an emerging forefront of cold atom physics mainly because of the flexibility of varying interactions and controlling filling number to access various quantum phases. One major effort pursued in many laboratories now is to use ultracold Fermi gases to simulate the Hubbard model, which exhibits various metallic, insulating, and superconducting phases with different magnetic behaviors.[1] Despite of huge efforts extending over several decades, there are still lots of controversial issues on this model, which hopefully cold atom experiments can shed light on.

The most solid conclusion of the Hubbard model is drawn for a half-filled cubic lattice, which says a spin-1/2 antiferromagnetic (AF) order exists for all range of repulsive interaction. For weak interaction, the AF order arises from the nesting geometry of the Fermi surface while for strong interaction, it is caused by the superexchange interaction.[2–5] Observing this AF order in cold atom experiments, especially in strong interaction regime, is considered as a hallmark of seeing the strong correlations in the lattice Fermi gases and the starting point for more ambitious goals along this direction.

On the other hand, in optical lattices, physics can be much richer than the single-band Hubbard model. When there are more than two fermions at one lattice site, fermions will start to occupy the excited bands like the *p* band. Unlike in condensed matter systems, there is no Jahn–Teller effect in optical lattices, so the threefold orbital degeneracy of the *p* band is well maintained.

Recently, there are increasing theoretical and experimental interests in studying the bosons in the *p* band, where a host of intriguing quantum phenomena due to orbital degeneracy has been pointed out.[6–10] We expect the physics of *p* band fermions will be easier for experimental study because the Pauli exclusion principle prevents the decay into the lower band. Thanks to the orbital degeneracy, *p* band Fermi gases are expected to exhibit more diverse phases compared to single-band Hubbard model. Nevertheless, the first step towards revealing these exciting phases is to understand the unfrustrated spin order at half filling. Here, we consider a three-dimensional cubic lattice whose three degenerate *p* bands are half filled by three fermions per site. (The *s* band is already completely filled by another two fermions and does not need to be worried about.)

With the complexity in *p* band model, even for half filling, there are issues that are not clear; for instance, (i) whether the *p* band Fermi surface still has some nesting properties, which give rise to a magnetic instability in weak interaction regime; (ii) with multiple hopping channels in different orbitals and multiple choices of intermediate states, whether superexchange processes can still yield a simple Heisenberg-type model as in the *s* band situation; and (iii) as there are various types of orders due to orbital degrees of freedom, whether the strong and weak interaction regimes share the same order or there is quantum phase transition in between. These questions will be answered in this work. The main results of this paper can be summarized as follows:

(I) In strong interaction regime, at each isolated site, the ground state of three fermions in *p* orbitals are spin-3/2 states with fourfold degeneracy due to the Hund's rule. The coupling between two neighboring spins is caused by virtual hopping of fermions, which gives rise to an isotropic spin-3/2 Heisenberg model,

$$\mathbf{H}_J = J_{\mathrm{ex}} \sum_{\langle ij \rangle} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j \right), \tag{1}$$

where $\vec{S}_i$ is an on-site spin-3/2 operator. $J_{\mathrm{ex}} > 0$, which means the ground state of this system has spin-3/2 antiferromagnetic order.

(II) In weak interaction regime, the Fermi surface of a half-filled *p* band exhibits a perfect nesting symmetry with the nesting momentum $\vec{\pi} = (\pi, \pi, \pi)$. The mean-field analysis shows that this nesting will induce antiferromagnetic order at low temperature and the order parameter coincides with the $S = 3/2$ spin order in strong interaction regime. We also show that this order should be the only order parameter.

Based on (I) and (II), we anticipate that despite the complexity with *p* band orbital degeneracy, the half-filled *p* band

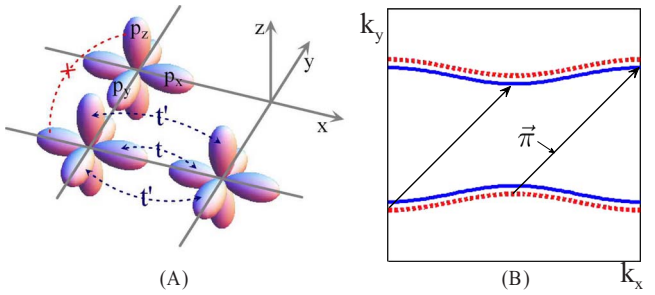

FIG. 1. (Color online) (a) Schematic of fermion hopping in p band. For a fermion in p_x orbital in i site, its hopping amplitude to $i+\hat{x}$ site is t, to $i+\hat{y}$ site and $i+\hat{z}$ site is $t'(t' \ll t)$, and it cannot hop to p_y (or p_z) orbital of its neighboring site. (b) Illustration of the p band Fermi surface nesting at half filling. The red line and blue line are the Fermi surfaces in k_x-k_y plane for $k_z=\pi/3$ and $k_z=-2\pi/3$, respectively. These two Fermi surfaces parallel with the nesting momentum $\vec{\pi}=(\pi,\pi,\pi)$ (the solid black arrow).

Hubbard model exhibits only the spin-3/2 antiferromagnetic order for all range of interaction strength and the system undergoes a crossover from weak to strong interaction, a situation similar to the half-filled single-band Hubbard model.

In the experiments of cold atoms in optical lattices, the major difficulty in achieving the AF order in strongly correlated regime comes from the fact that the Néel temperature is very low due to the ultrasmall energy scale of superexchange interaction. In this work, we show that in strong interaction regime, the Néel temperature for p band AF can reach a few nano-Kelvin, which is 2 to 3 orders of magnitude higher than that of s band. Because of this, we suggest to study the p band Fermi gas as a more realistic and promising route to reveal strongly correlated physics in optical lattices.

II. MODEL

The model for Fermi gases in optical lattices contains a nearest-neighbor hopping $\mathbf{H}_t$ and an on-site interaction $\mathbf{H}_U$. The hopping term $\mathbf{H}_t$ can be written as

$$\mathbf{H}_t = \sum_{i,s}^{\alpha,\beta=x,y,z} T_{\beta}^{p_\alpha} c_{i,p_\alpha,s}^{\dagger} c_{i+\hat{\beta},p_\alpha,s} + \text{H.c.} \tag{2}$$

Since an optical lattice is a separable potential in three dimensions $[V_0(\sin^2 Kx+\sin^2 Ky+\sin^2 Kz)]$, the hopping term conserves the orbital index due to the orthogonality of Wannier wave functions and the hopping amplitude is anisotropic $T_{\beta}^{p_\alpha}=t\delta_{\alpha\beta}-t'(1-\delta_{\alpha\beta})$ with $t,t'>0$. Moreover, there is also no next-nearest-neighbor hopping.[4] Figure 1(a) is a schematic of hoppings in the p band. t is much larger than t', for instance, for an optical lattice with the depth $V_0=11E_R$ $[E_R=\hbar^2K^2/(2m)$ is the photon recoil energy], $t\approx 20t'$. For ultracold neutral gases, the interaction is dominated by short-range s-wave repulsion $V(\mathbf{r}_{12})=(4\pi\hbar^2a_s/m)\delta(\mathbf{r}_1-\mathbf{r}_2)$, which takes place between unlike spins only.[3] The on-site interaction $\mathbf{H}_U$ then has the form,

TABLE I. Eigenstates and eigenenergies of three fermions at an isolated site. In these three tables, we define that, for example, $|d\uparrow 0\rangle$ means p_x is double occupied, p_y is occupied by a spin-$\uparrow$ fermion, and p_z is empty.

$E=0(S=3/2)$	$E=3W(S=1/2)$	$E\geq U$
$\|\uparrow\uparrow\uparrow\rangle$	$(\|\uparrow\uparrow\downarrow\rangle-\|\uparrow\downarrow\uparrow\rangle)/\sqrt{2}$	Double
$\|\downarrow\downarrow\downarrow\rangle$	$(\|\downarrow\uparrow\uparrow\rangle-\|\uparrow\downarrow\uparrow\rangle)/\sqrt{2}$	Occupied
$(\|\downarrow\uparrow\uparrow\rangle+\|\uparrow\downarrow\uparrow\rangle+\|\uparrow\uparrow\downarrow\rangle)/\sqrt{3}$	$(\|\downarrow\downarrow\uparrow\rangle-\|\downarrow\uparrow\downarrow\rangle)/\sqrt{2}$	States
$(\|\downarrow\downarrow\uparrow\rangle+\|\uparrow\downarrow\downarrow\rangle+\|\downarrow\uparrow\downarrow\rangle)/\sqrt{3}$	$(\|\uparrow\downarrow\downarrow\rangle-\|\downarrow\uparrow\downarrow\rangle)/\sqrt{2}$	

$$\mathbf{H}_U = \sum_i \{U\sum_\alpha n_{i,p_\alpha,\uparrow}n_{i,p_\alpha,\downarrow} + W\sum_{\alpha\neq\beta}(n_{i,p_\alpha,\uparrow}n_{i,p_\beta,\downarrow} + c_{i,p_\alpha,\uparrow}^{\dagger}c_{i,p_\beta,\downarrow}^{\dagger}c_{i,p_\alpha,\downarrow}c_{i,p_\beta,\uparrow} + c_{i,p_\alpha,\uparrow}^{\dagger}c_{i,p_\alpha,\downarrow}^{\dagger}c_{i,p_\beta,\downarrow}c_{i,p_\beta,\uparrow})\}, \tag{3}$$

$$U = \frac{4\pi\hbar^2 a_s}{m}\int d^3\mathbf{r}|w_{p_\alpha}(\mathbf{r})|^4, \tag{4}$$

$$W = \frac{4\pi\hbar^2 a_s}{m}\int d^3\mathbf{r}|w_{p_\alpha}(\mathbf{r})|^2|w_{p_\beta}(\mathbf{r})|^2, \tag{5}$$

where w_{p_α} is the p_α-orbital Wannier wave function. There are totally four terms due to s-wave interaction. The first term is the interaction within the same orbital, the second term is the interaction between unlike orbitals, the third term represents the spin exchange between unlike orbitals, and the fourth term represents two fermions hopping processes from one orbital to another. Usually, U is three times larger than W.

III. STRONG INTERACTION REGIME

When the on-site interaction is dominative, we shall first ignore the hopping term and calculate all the eigenstates of an isolated site. The results for three, four, and two fermions per site are summarized in Tables I–III, respectively. As one can see from Table I, the low-energy Hilbert space is constituted by four spin-3/2 states. Because these spin states are symmetric superpositions of three atoms, their spatial wave functions have to be antisymmetric and the interactions are completely quenched. In this limit, the system is a spin-3/2 Mott insulator.[11]

The coupling of spins between neighboring sites can be obtained by taking the hopping term as the second-order per-

TABLE II. Eigenstates and eigenenergies of four fermions at an isolated site.

$E=U+2W(S=1)$	$E=U+4W(S=0)$
$\|d\uparrow\uparrow\rangle$, $\|\uparrow d\uparrow\rangle$, $\|\uparrow\uparrow d\rangle$, $\|d\downarrow\downarrow\rangle$,	$(\|d\uparrow\downarrow\rangle-\|d\downarrow\uparrow\rangle)/\sqrt{2}$
$\|\downarrow d\downarrow\rangle$, $\|\downarrow\downarrow d\rangle$, $(\|d\uparrow\downarrow\rangle+\|d\downarrow\uparrow\rangle)/\sqrt{2}$	$(\|\uparrow d\downarrow\rangle-\|\downarrow d\uparrow\rangle)/\sqrt{2}$
$(\|\uparrow d\downarrow\rangle+\|\downarrow d\uparrow\rangle)/\sqrt{2}$	$(\|\uparrow\downarrow d\rangle-\|\downarrow\uparrow d\rangle)/\sqrt{2}$
$(\|\uparrow\downarrow d\rangle+\|\downarrow\uparrow d\rangle)/\sqrt{2}$	

TABLE III. Eigenstates and eigenenergies of two fermions at an isolated site.

$E=0(S=1)$	$E=2W(S=0)$	$E\geq U-W$
$\|0\uparrow\uparrow\rangle$, $\|\uparrow 0\uparrow\rangle$, $\|\uparrow\uparrow 0\rangle$,	$(\|0\uparrow\downarrow\rangle-\|0\downarrow\uparrow\rangle)/\sqrt{2}$	Double
$\|0\downarrow\downarrow\rangle$, $\|\downarrow 0\downarrow\rangle$, $\|\downarrow\downarrow 0\rangle$	$(\|\uparrow 0\downarrow\rangle-\|\downarrow 0\uparrow\rangle)/\sqrt{2}$	Occupied
$(\|0\uparrow\downarrow\rangle+\|0\downarrow\uparrow\rangle)/\sqrt{2}$	$(\|\uparrow\downarrow 0\rangle-\|\downarrow\uparrow 0\rangle)/\sqrt{2}$	States
$(\|\uparrow 0\downarrow\rangle+\|\downarrow 0\uparrow\rangle)/\sqrt{2}$		
$(\|\uparrow\downarrow 0\rangle+\|\downarrow\uparrow 0\rangle)/\sqrt{2}$		

turbation with the Brillioun–Wigner approximation,[2]

$$\mathbf{H}_J=-\sum_e P_G\mathbf{H}_t P_e\frac{1}{\mathbf{H}_U}P_e\mathbf{H}_t P_G, \tag{6}$$

where P_e means the projection into excited Hilbert space and P_G means the projection into $S=3/2$ Hilbert space. To proceed, we make the following observations: (i) The virtual hopping processes only take place within the same orbital, otherwise, the final state will have double occupancy, which should be projected out. For instance, if a p_x fermion hops from i site to j site, it must be followed by a p_x fermion hops from j site to i site. (ii) By using Tables I–III, one can show that only one type of excited states can be connected to the unperturbed ground states via hopping, which is the lowest energy states of four fermions ($S=1$ and $E=U+2W$) in one site and the lowest energy states of two fermions ($S=1$ and $E=0$) in its neighborhood.[12] So, the intermediate states always has energy $U+2W$.

Because of (i) and (ii), $\mathbf{H}_J$ on the link between i and $i+\hat{x}$ site reads

$$\sum_{p_\alpha}\frac{2|T_x^{p_\alpha}|^2}{U+2W}P_G\left(\sum_{ss'}c^\dagger_{i,p_\alpha,s}c_{i,p_\alpha,s'}c^\dagger_{i+\hat{x},p_\alpha,s'}c_{i+\hat{x},p_\alpha,s}\right)P_G.$$

Note that

$$c^\dagger_{i,p_\alpha,s}c_{i,p_\alpha,s'}=\frac{1}{3}\left(\sum_{p_\beta}c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}+\sum_{p_\beta}\Xi^{s,s'}_{i,p_\alpha,p_\beta}\right),$$

where

$$\Xi^{s,s'}_{i,p_\alpha,p_\beta}=c^\dagger_{i,p_\alpha,s}c_{i,p_\alpha,s'}-c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}, \tag{7}$$

and with the help of Table I, one can show that

$$P_G\Xi^{s,s'}_{i,p_\alpha,p_\beta}P_G=0, \tag{8}$$

$$P_G\sum_{p_\beta}c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}P_G=\sum_{p_\beta}c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}. \tag{9}$$

Then, H_J on this link can be written as

$$\sum_{p_\alpha}\frac{2|T_x^{p_\alpha}|^2}{9(U+2W)}\sum_{ss'}\sum_{p_\beta}c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}\sum_{p_\beta}c^\dagger_{i,p_\beta,s}c_{i,p_\beta,s'}$$
$$=\frac{1}{2}J_{\rm ex}\sum_{p_\alpha,p_\beta}\sum_{s,s'}(c^\dagger_{i,p_\alpha,s}c_{i,p_\alpha,s'})(c^\dagger_{i+\hat{x},p_\beta,s'}c_{i+\hat{x},p_\beta,s}),$$

where

$$J_{\rm ex}=4(t^2+2t'^2)/(9U+18W). \tag{10}$$

We now introduce $\vec{S}_i$ as

$$\vec{S}_i=\frac{1}{2}\sum_{p_\alpha}\sum_{ss'}c^\dagger_{i,p_\alpha,s}\vec{\sigma}_{ss'}c_{i,p_\alpha,s'}, \tag{11}$$

and $\vec{\sigma}$ are the Pauli matrices. Restricted in the low-energy Hilbert space, $\vec{S}_i$ acts as $S=3/2$ spin operator. Hence, we have shown the first main result that in the strong interaction regime, the superexchange processes induce an isotropic spin-3/2 Heisenberg model,

$$\mathbf{H}_J=J_{\rm ex}\sum_{\langle ij\rangle}\left(\vec{S}_i\vec{S}_j-\frac{1}{4}n_in_j\right), \tag{12}$$

which describes the low-energy spin dynamics of p band Mott insulator. $J_{\rm ex}>0$. Below Néel temperature, it will give rise to an antiferromangetic long range order of $\langle S_i^+\rangle=(-1)^i|\langle S_i^+\rangle|\neq 0$.

IV. WEAK INTERACTION REGIME

In this regime, we use the usual Hartree–Fock mean-field theory, for which the Hamiltonian is rewritten into momentum space. The hopping term can be written as

$$\mathbf{H}_t=\sum_{\mathbf{k},\alpha}\epsilon^{p_\alpha}_{\mathbf{k}}c^\dagger_{p_\alpha,\mathbf{k}}c_{p_\alpha,\mathbf{k}}, \tag{13}$$

where

$$\epsilon^{p_\alpha}_{\mathbf{k}}=2t\cos k_\alpha-2t'\sum_{\beta\neq\alpha}\cos k_\beta-\mu. \tag{14}$$

For half filling, $\mu=0$, and the Fermi surface for one of the p bands is plotted in Fig. 1(b).

For performing mean-field decomposition, we reconstruct the interaction term $\mathbf{H}_U$ as $\mathbf{H}_U^0+\mathbf{H}_U'$, where

$$\mathbf{H}_U^0=-V_1\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\hat{\Delta}^\dagger_{\mathbf{k},\mathbf{q}}\hat{\Delta}_{\mathbf{k}',\mathbf{q}}, \tag{15}$$

$$\mathbf{H}_U'=\sum_{\mathbf{k},\mathbf{k}',q}^{\alpha\neq\beta}(-V_2\hat{\Gamma}^{\alpha\beta\dagger}_{\mathbf{k},\mathbf{q}}\hat{\Gamma}^{\alpha\beta}_{\mathbf{k}',\mathbf{q}}-2W\hat{\Sigma}^{\alpha\beta\dagger}_{\mathbf{k},\mathbf{q}}\hat{\Sigma}^{\alpha\beta}_{\mathbf{k}',\mathbf{q}}), \tag{16}$$

with $V_1=3(U+2W)$ and $V_2=2(U-W)/3$. Here, we introduce

$$\hat{\Delta}^\dagger_{\mathbf{k},\mathbf{q}}=\sum_{p_\alpha}S^{\mathbf{q}+}_{p_\alpha,p_\alpha,\mathbf{k}}/3, \tag{17}$$

and

$$\hat{\Gamma}^{\alpha\beta\dagger}_{\mathbf{k},\mathbf{q}}=(S^{\mathbf{q}+}_{p_\alpha,p_\alpha,\mathbf{k}}-S^{\mathbf{q}+}_{p_\beta,p_\beta,\mathbf{k}})/2, \tag{18}$$

$$\hat{\Sigma}^{\alpha\beta\dagger}_{\mathbf{k},\mathbf{q}} = (S^{\mathbf{q}+}_{p_\alpha,p_\beta,\mathbf{k}} + S^{\mathbf{q}+}_{p_\beta,p_\alpha,\mathbf{k}})/2, \tag{19}$$

where $S^{\mathbf{q}+}_{p_\alpha,p_\beta,\mathbf{k}} = c^\dagger_{\mathbf{k},p_\alpha,\uparrow} c_{\mathbf{k}+\mathbf{q},p_\beta,\downarrow}$ is the spin lifting operator. As illustrated in Fig. 1(b), each of three p band Fermi surfaces exhibits nesting symmetry with the nesting momentum $\vec{\pi}=(\pi,\pi,\pi)$ at half filling. It means that for each $\mathbf{k}$ at Fermi surface, $\mathbf{k}+\pi$ also locates at Fermi surface. Therefore, the maximum contribution to $\mathbf{H}_U$ comes from $\mathbf{q}=\vec{\pi}$. For this reason, we only consider $\mathbf{q}=\vec{\pi}$ component in the mean-field approximation and we introduce three order parameters, which are $\Delta = V_1 \Sigma_{\mathbf{k}} \langle \hat{\Delta}_{\mathbf{k},\pi} \rangle$, $\Gamma = V_2 \Sigma_{\mathbf{k}} \langle \hat{\Gamma}^{\alpha\beta}_{\mathbf{k},\pi} \rangle /3$, and $\Sigma = 2W \Sigma_{\mathbf{k}} \langle \hat{\Sigma}^{\alpha\beta}_{\mathbf{k},\pi} \rangle$, where Γ and Σ are independent of index α and β because of the permutation symmetry between orbitals. Note that Δ is the same spin order as in strong interaction regime, we separate the mean-field Hamiltonian into two parts as $\mathbf{H}_{\mathrm{MF}} = \mathbf{H}_0 + \mathbf{H}'$, where

$$\mathbf{H}_0 = \sum_{\mathbf{k}} \left[\sum_{p_\alpha,\sigma} \epsilon^{p_\alpha}_{\mathbf{k}} c^\dagger_{\mathbf{k},p_\alpha,\sigma} c_{\mathbf{k},p_\alpha,\sigma} + (\Delta \hat{\Delta}^\dagger_{\mathbf{k}} + \mathrm{H.c.}) \right] + \frac{\Delta^2}{V_1}$$

and

$$\mathbf{H}' = \sum_{\mathbf{k}}^{\alpha\neq\beta} [\Sigma \hat{\Sigma}^{\alpha\beta\dagger}_{\mathbf{k}} + \mathrm{H.c.}] + \frac{\Gamma^2}{V_2} + \frac{\Sigma^2}{2W}$$

Note that $\mathbf{H}'$ does not contain $\hat{\Gamma}$ terms because they all cancel out due to the permutation symmetry of three orbitals; therefore, $\Gamma = 0$.

Because the three orbitals are now separable in $\mathbf{H}_0$, it can be easily diagnolized by Bogoliubov transformation,

$$\mathbf{H}_0 = \sum_{\mathbf{k},\alpha} \xi^{p_\alpha}_{\mathbf{k}} (\gamma^\dagger_{\mathbf{k},p_\alpha} \gamma_{\mathbf{k},p_\alpha} + \eta^\dagger_{\mathbf{k},p_\alpha} \eta_{\mathbf{k},p_\alpha} - 1) + \frac{\Delta^2}{V_1}, \tag{20}$$

where

$$\xi^{p_\alpha}_{\mathbf{k}} = \sqrt{(\epsilon^{p_\alpha}_{\mathbf{k}} - \epsilon^{p_\alpha}_{\mathbf{k}+\vec{\pi}})^2/4 + (\Delta/3)^2}, \tag{21}$$

and $\gamma_{\mathbf{k},p_\alpha}$ and $\eta_{\mathbf{k},p_\alpha}$ are quasiparticle operators.[13] The equation for Δ is

$$\frac{1}{V_1} = \sum_{\mathbf{k},p_\alpha} \frac{\tanh(\xi^{p_\alpha}_{\mathbf{k}} \beta/2)}{\xi^{p_\alpha}_{\mathbf{k}}}, \tag{22}$$

the solution of which yields nonzero value of Δ and the critical temperature for having nonzero Δ.

Next, we shall examine whether there will be symmetry breaking of Σ also, for which we treat $\mathbf{H}'$ as perturbation on top of $\mathbf{H}_0$ and the energy can be expanded in powers of Σ as $E_{\mathrm{MF}} = E_0(\Delta) + \chi(\Delta)\Sigma^2 + O(\Sigma^4)$. So whether there is an instability for developing finite Σ depends on the sign of χ. Straightforward calculation shows that

$$\chi(\Delta) = -\sum_{\mathbf{k},\alpha\neq\beta} \frac{|\tau^{\alpha\beta}_{\mathbf{k}}|^2}{2(\xi^{p_\alpha}_{\mathbf{k}} + \xi^{p_\beta}_{\mathbf{k}+\vec{\pi}})} + \sum_{\mathbf{k},\alpha} \frac{V_1}{2W} \frac{1}{\xi^{p_\alpha}_{\mathbf{k}}}, \tag{23}$$

where $\tau^{\alpha\beta}_{\mathbf{k}} = v_{\mathbf{k},p_\alpha} v_{\mathbf{k}+\vec{\pi},p_\beta} - u_{\mathbf{k},p_\alpha} u_{\mathbf{k}+\vec{\pi},p_\beta}$.[13] We numerically compute Eq. (23) and find that it is always positive, which indicates that there will be no symmetry breaking of Σ. Mathematically, it is because $\xi_{\mathbf{k},p_\alpha} \neq \xi_{\mathbf{k}+\vec{\pi},p_\beta}$ except for a few specific points in momentum space. In the limit of $\Delta \to 0$, the first term in the right hand side of Eq. (23) diverges only around those few points, while the second term diverges around the whole Fermi surface; hence, the second term will always be dominative and the whole summation is positive. Physically, it is because the AF instability crucially relies on the nesting of the Fermi surface and the fact that there is no nesting between two different p bands prevents interorbital spin order. Hence, we have reached the second main result that in the weak interaction regime, the only spin order at low-temperature is $\Delta = \langle \Sigma_{\mathbf{k},\alpha} c^\dagger_{\mathbf{k},p_\alpha,\uparrow} c_{\mathbf{k}+\vec{\pi},p_\alpha,\downarrow} \rangle \neq 0$ and this order coincides with that in strong interaction regime.

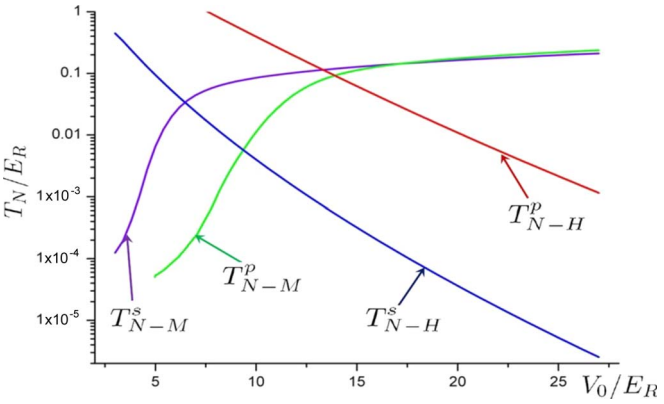

FIG. 2. (Color online) Néel temperature T_N as a function of optical lattice depth V_0. Four curves are p band T_N from Heisenberg model T^p_{N-H} and from mean-field theory T^p_{N-M} and s band T_N from Heisenberg model T^s_{N-H} and from mean-field theory T^s_{N-M}. For parameters, we use ^{40}K in optical lattices as an example (Ref. 14). The lattice spacing $\lambda = 1064$ nm, $K = \pi/\lambda$, and $a_s = 15$ nm. The energy units is taken as E_R, which corresponds to 0.21 μK.

V. NÉEL TEMPERATURE

Here, we first calculate the Wannier functions in an optical lattice potential and use them to deduce the parameters t, t', U, and W in our model. Then, we calculate the Néel temperature T_{N-H}, which is $1.276 J_{\mathrm{ex}} S(S+1)$,[4] given by Heisenberg model of Eq. (12) and also calculate T_{N-M} given by mean-field theory by solving Eq. (22) for the onset of nonzero Δ. We display our calculation of these two T_N for both half-filled p band and s band in Fig. 2. T_{N-H} decreases as the lattice height increases, while T_{N-M} increases as the lattice height increases.

For small V_0, where $T_{N-M} \ll T_{N-H}$, the AF order is caused by mean-field effect while for large V_0, where $T_{N-H} \ll T_{N-M}$, the AF order is driven by superexchange processes and the system is in strongly correlated regime. The regime where T_{N-M} and T_{N-H} cross is the crossover regime from weak to strong interactions, where both two methods will fail and more advanced numerical technique such as dynamical mean-field theory (DMFT) and quantum Monte Carlo (QMC) is required in order to give accurate Néel temperature.[5] We will leave this for further investigation. However, the key point is that the s-band T_{N-H} is already of the order of 0.1 nK when the lattice height enters the

strongly correlated regime of great experimental interests, and it decreases to below 10^{-2} nK rapidly as V_0 increases, while the p band T_{N-H} remains on the order of 1 nK even when V_0 increases to $\sim 20E_R$. It is simply because the Wannier wave function in p band is much more extended, its hopping amplitude t is one to two orders larger than that of s band, which consequently leads to much larger J_{ex}.

In addition to higher Néel temperature, the spin-3/2 of p band AF state could have a better signal-to-noise radio than s-band spin-1/2 AF. All these provide great advantage for experimental study of quantum AF and its related phenomena due to superexchange. Besides, we leave the effect of trapping potential to future investigation which may introduce shell structure in density profile and the finite size effect into the problem. We hope that this work will open up a new route for studying strongly correlated Fermi gases in optical lattices and be the basis for future efforts along this direction.

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