Magnetism of Cold Fermionic Atoms on p-Band of an Optical Lattice

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We carry out \textit{ab initio} study of ground state phase diagram of spin-1/2 cold fermionic atoms within two-fold degenerate p-band of an anisotropic optical lattice. Using the Gutzwiller variational approach, we show that a robust FM phase exists for a vast range of band fillings and interacting strengths. The ground state crosses over from spin density wave state to spin-1 Neel state at half filling. Additional harmonic trap will induce spatial separation of various phases. We also discuss several relevant observable consequences and detection methods. Experimental test of the results reported here may shed some light on the long-standing issue of itinerant ferromagnetism.

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\textbf{Introduction:} Recently, research of ultracold atomic gases have simulated a new wave of studying the many-body problems. One can create periodic potentials to confine the ultracold atoms by intersecting laser beams. Because of the experimental controllability of atom number, dimensionality, geometry as well as interaction strength \textit{etc}., the optical lattice provides an ideal playground for investigating many body problems. Specifically, the experimental realization of a Mott-insulator phase transition in the optical lattice \cite{1} \cite{2} brings us to the forefront of the strongly correlated systems. More recently, the experimental progress makes it possible to put fermions into the optical lattices and control the interaction between them \cite{3} \cite{4}. These advances open a new channel to investigate numerous phenomena that play important roles in the condensed matter physics, such as quantum magnetism \cite{5} \cite{6} \cite{7}, high-temperature superconductivity \cite{8} and physic associated with band degeneracy \cite{9} \cite{10}.

Itinerant ferromagnetism in transition metals is another controversial issue in condensed matter physics. Despite long history dating back to Stoner \cite{12}, a fully understanding of its mechanism is still lacking \cite{13}. However, a consensus is reached that the appearance of robust ferromagnetism is not a generic feature of the single band Hubbard model in a cubic lattice. \textit{Non-bipartite} lattice structures may stabilize FM order, degenerate bands and the Hund’ rule coupling may also help. Testing various scenarios using the ultra-cold fermionic atoms in optical lattice may shed light on this issue. The highly tunable and neatness of cold atom experiments also permit calculations with no adjustable parameters, the phase diagram and experimental signatures could be determined through the following first principle parameters: the depth of the optical lattice $V$ for each directions and the s-wave scattering length $a_s$.

In this paper, we first perform band structure calculations to identify a parameter region of $V$ and $a_s$ where fermionic atoms on an optical lattice could be effectively described by a two-band Hubbard model. Band calculation also provides effective coupling strengths of the model. We then obtain zero temperature phase diagram as function of the coupling strength and the density of fermionic atoms by applying Gutzwiller variational approach. Finally, we consider the effect of external harmonic trap within the local spin density approximation (LSDA), which is shown to induce concentric shell structures of different phases. In particular, a robust ferromagnetic shell composed of spin polarized fermions emerges.

\textbf{The model and the band structure calculations:} Six counter-propagating lasers generate potential of the form $V(r) = V_x \sin^2(k_L x) + V_y \sin^2(k_L y) + V_z \sin^2(k_L z)$. Atoms trapped by this potential form a simple cubic lattice with
lattice spacing $a = \frac{\hbar}{E_\text{c}}$. Fig. 1 shows the band structures of the optical lattices with $V_x = V_y = 16E_R$, $V_z = 36E_R$, where $E_R = k_F^2/2m$ is the recoil energy. The degenerate $p_x$ and $p_y$-band are well separated from the low lying $s$-band, $p_z$-band are pushed up by the large $V_z$. Assuming the $s$-band is fully occupied, as long as the band gaps are much larger than the interaction scales within each band, we can focus on the degenerate $p_x$ and $p_y$ bands. Authors of [4] assume that atoms mainly interact in the p-wave channel thus could be effectively treat as spinless fermions and they studied effects of different lattice structures. In the present study, we focus on cubic lattice and consider the s-wave pseudo-potential $V(r - r') = \frac{4\pi\hbar^2}{M} \delta(r - r')$, which makes the problem more relevant to condensed matter system where spin 1/2 fermions plays the main role. Neglect all interaction terms except the largest on-site one, we introduce an effective two-band Hubbard model on cubic lattices:

$$H = H_{\text{kin}} + H_{\text{int}}$$

$$H_{\text{kin}} = \sum_{k,\alpha,\sigma} \varepsilon_{k\alpha} \hat{c}_{k\alpha\sigma}^\dagger \hat{c}_{k\alpha\sigma} + h.c.$$  

$$H_{\text{int}} = U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow} \hat{n}_{i\alpha\downarrow} + U' \sum_{i\sigma} \hat{n}_{i\sigma\uparrow} \hat{n}_{i\sigma\downarrow}$$

$$+ J \sum_{i\alpha} (\hat{c}_{i\alpha \uparrow}^\dagger \hat{c}_{i\alpha \downarrow} \hat{c}_{i\alpha \downarrow}^\dagger \hat{c}_{i\alpha \uparrow} + \hat{c}_{i\alpha \downarrow}^\dagger \hat{c}_{i\alpha \uparrow} \hat{c}_{i\alpha \uparrow}^\dagger \hat{c}_{i\alpha \downarrow})(1)$$

With

$$U = \frac{4\pi\hbar^2a_s}{M} \int d\mathbf{r} w_\sigma(\mathbf{r})^4$$

$$U' = J = \frac{4\pi\hbar^2}{M} \int d\mathbf{r} w_\sigma(\mathbf{r})^2 w_\sigma(\mathbf{r})^2$$

(2)

where $\alpha = x, y$ is the band index, $\sigma = \uparrow, \downarrow$ denote spins, $\varepsilon_{k\alpha}$ is energy dispersion for each band. $a_s$ is the s-wave scattering length which could be tuned by Feshbach resonance technique over a large scope of magnitude. We only consider repulsive interaction ($a_s > 0$) in this study. Parameter $U$ describes the on-site Coulomb repulsive interaction between atoms reside in the same orbital, while $U'$ describes the repulsive interaction for two atoms in different orbitals. $J$ controls the strength of Hund’s rule coupling between different orbitals. In the present system only transverse part of the Hund’s rule coupling survives, i.e. the spin flip and pair hopping processes. The absence of the density-density interaction for atoms with the same spins is due to the short range $\delta$ type pseudo-potential. This fact can also be understood as a fully canceling between the longitudinal part of the Hund’s rule coupling and corresponding terms in the inter-orbital density-density interactions. All of the interaction parameters are expressed as overlaps of maximally localized Wannier functions [15].

Both the band dispersions $\varepsilon_{k\alpha}$ and the coupling constants in Eq. 2 are determined by experimentally controllable parameters $V$ and $a_s$. Due to the anisotropic nature of the p-orbitals, the system shows dimension reduction behavior: the PDOS has Van Hove singularity near the band edge resembling of 1D character. This feature is also included by the tight binding model with an anisotropic hopping amplitude along different directions [16]. At half filling, the Fermi surface has nesting property with the nesting vector $(\pi, \pi, \pi)$ [17]. In contrast to the isotropic case (s-band), here the singularity in PDOS and Fermi surface nesting occur at separable energy scales and lead to remarkable consequence: instability towards to different magnetic orders dominates at different fillings. For the given lattice depth $V_x = V_y = 16E_R$, $V_z = 36E_R$, our calculation shows the bandwidth $W$ of the two-fold degenerate $p$-band is 0.45$E_R$, while band gaps separated $p_x$, $p_y$-bands with $s$ and $p_z$-bands are 6.79$E_R$ and 4.10$E_R$ (Fig 1(b)). Overlap of Wannier functions gives $U/E_R = 8.63k_La_s$ and $U' = J = 0.299U$, while the interaction scale within $s$-band is 13.1$(k_La_s)E_R$. Not exceeding the band gaps pose 0.0755$\alpha$ as the upper limit for $a_s$. Within this restriction, one could still tune the system from weak to strong coupling ($U \sim 9W$) region by Feshbach resonance technique.

Gutzwiller variation results: For this complex two-band Hubbard model we adopt a generalized version of the Gutzwiller variational approach [18, 19, 20, 21, 22]. Historically, the variational approach has been successfully used to treat strong correlated systems such as normal $^3$He [23] and Mott transition [24]. Generalization of it is used to investigate physics associate with band degeneracy, such as orbital selective Mott transi-
tion and transition metal ferromagnetism. The variational wave function is \( |\Phi_G > = P_G |0 > \), where \( |0 > \) is uncorrelated state which could be fermi liquid, spin density wave or superconductivity ground state. And \( P_G = \prod \lambda_{i,G} m_{i,G} \) are projection operator onto atomic configurations, \( \lambda_{i,G} \) are corresponding variational parameters. Under Gutzwiller approximation (GA) one can evaluate expected values of operators over the projected wave function. By minimizing the total energy one gets the ground state configurations, from which one can identify various orders e.g., charge density wave order, orbital order, FM and AF order etc. GA neglects spatial correlations and is only exact in infinite dimension, this approximation has also been proven to be equivalent to the saddle point of Kotliar-Ruckenstein slave boson functional treatment. Since it is non-perturbative in nature, the variational approach treats the Fermi liquid as well as the Mott localized state on equal footing and hence gives a coherent description of the intermediate coupling strength, connecting the weak coupling mean field to the strong coupling perturbation results. And the result of the present method is superior to Hartree-Fock mean field that often overestimates the tendency towards the ordered phases.

Disregard any long range order, at commensurate filling a reasonable large on-site repulsive interaction would localize fermions and drive the system into the paramagnetic Mott insulator phase. The transition (Brinkman-Rice transition) could be described naturally within Gutzwiller variational approach via quasi-particle spectral function. It could also be interpreted as the renormalization factor of kinetic energy, the height of Fermi step or inverse of mass enhancement factor. As \( Z \) approaches to zero, fermions becomes more and more localized and finally transforms into the Mott insulator phase. However in the present case the large Hund’s rule coupling \( J = U' \) has dramatic effect on the paramagnetic Mott transition: there is no Brinkman-Rice transition at quarter filling, see Fig 2(a). The on-site interaction Hamiltonian Eq 1 has doubly occupied spin-triplet as its lowest energy states, which are degenerate with the empty and singly occupied states. Charge fluctuation through this channel is allowed at quarter filling thus the system does not become localized when \( U \) increases. At half filling this kind of fluctuation is blocked by the large on-site intra-orbital repulsive interaction \( U \) and the Brinkman-Rice transition manifests itself as shown in Fig 2(a). However because of the huge spin entropy of the paramagnetic Mott state, it would not act as the ground state at zero temperature. When the system cools down the degeneracy will be lifted and various magnetic/orbital orders develop depending on the residual interactions between the spin/orbital degrees of freedom.

Next we discuss the magnetic order of the p-band fermions. As the previous section indicated, the band structure (Fermi surface nesting and the Van Hove singularity) favors AF and FM order at different energy scales, and the on-site Hund’s rule coupling may help stabilizing them. Thus, it is possible that these two phases may exist even for weak or intermediately coupling strength. And it is interesting to observe the coexistence of them in the optical lattices with an external harmonic trap.

Fig. 2(b) shows the development of the stagger magnetization with increase of \( U \) near half filling (\( n = 2 \)). Due to the Fermi surface nesting, an arbitrary small \( U \) drives the instability of the two-sublattice antiferromagnetism at exact half filling. At weak coupling it follows the spin density wave mean field prediction, the stagger magnetization increases as \( t e^{-t/U} \). Approaching the strong coupling limit the stagger magnetization comes to its saturation value 2. In this limit, the large repulsive interaction quenches the charge degree of freedom while the on-site Hund’s rule coupling locks the local spins to form spin-1 moments. Virtual hopping process leads to the antiferromagnetic coupling of these local moments and the original fermions model reduces to a spin-1 antiferromagnetic Heisenberg model. This high spin AF order is more stable against the quantum fluctuations. The present method also gives a coherent description of the weak to strong crossover region, where the stagger magnetization shows non-monotonic behavior for \( n = 1.8 \) as shown in Fig 2(b). The condensation energy of AF order is roughly \( W^2/U \), which is 10 times larger than the s-band, see Fig 1(b)(c). Due to the large energy gain of the antiferromagnetic order, we anticipate the transition temperature to be two orders higher than that of the s-band case at the strong coupling limit. At intermediate coupling strength the transition temperature may attain its maximum value, which is accessible in current cold atomic experiments.

Upon doping, the AF order is destroyed by movement...
of holes and the system has featureless PM ground state. But at even lower fillings where the Van Hove singularity plays a role the system has FM ground state. Actually for the present depth of optical lattice, the singularity in DOS plays the main role and the Hund’s rule coupling further stabilizes the tendency and enlarges the region of FM order in the phase diagram. It is possible to tune the optical lattice to change the relative weight of contribution of singularity in DOS and the Hund’s rule coupling, and this will shed light on the long controversial issue of competition of the external potential and cohesive energy of the ordered phase gives fine structures of spin density profiles. Regions where spin density around 1 are more likely to enter into AF phase, as long as the energy gain from AF phase exceeds correspondingly energy loss from density redistribution. Plateaus formed by AF (or PM Mott Insulator) phase was also reported in previous Quantum Monte Carlo [28] and Dynamical Mean Field theory [29] study on single band inhomogeneous cold fermionic atom systems. For regions with average filling less than 0.5 or larger than 1.5 there are tendency towards ferromagnetic order. But due to the conservation of total spins, FM region will consist of two domains of half-shell shape with opposite spin polarization, see Fig. 4(a), similar structure is anticipated in 30 concerns Nagaoka ferromagnetism. To sum up, p-band cold fermionic atoms will form shell structures with an external trap potential, for different radii the system crosses the $U - n$ phase diagram and shows an band insulator, PM, FM and AF phases Fig. 4(b).

**Experimental signatures:** Population of higher bands have been detected by time of flight (TOF) images [31]. Noise correlation [32] from TOF images may also detect spin order through spin-spin correlation functions. Specifically, AF phase opens a charge transfer gap which could be detected by Raman spectroscopy [33], while the doubling of unit cell might be detected by spin selective Bragg spectroscopy [34]. Spatial distribution of spin densities in harmonic trap reported in this paper could be detected by spatially microwave transition and spin-changing collisions techniques, which measure the integrated density profiles along chosen directions [35].

![FIG. 4: (a). Side view of spin density profile in a harmonic trap with different total number of atoms, two spin state are 50 : 50 mixture. The frequency of the external trap is $\Omega = 0.005E_R$. (b). Top view of various phases. Dark Blue region denotes antiferromagnetic phases, Black region denotes band insulator and shallow blue/red for two kinds of polarized fermions (ferromagnetic phase). Only density of atoms on the p-band are shown in the figure, s-band spin densities provides a homogeneous background near the center of the trap.](image-url)
Summary: Combining the band structure calculations and the Gutzwiller variational approach, we perform a first principle calculation of the zero temperature phase diagram of spin-1/2 cold fermionic atoms on the two-fold degenerate p-band in an optical lattice. We show that the system has robust ferromagnetic and antiferromagnetic ground state at different fillings. We have traced back the physical picture to the single particle feature included anisotropy of orbital orientations and Fermi surface nesting as well as correlated effects such as Hund’s rule coupling. We also discuss the inhomogeneous spatial distribution induced by an external harmonic potential.

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