Mott transition, magnetic and orbital orders in the ground state of the two-band Hubbard model using variational slave-spin mean field formalism

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We study the ground state of the Hubbard model on a square lattice with two degenerate orbitals per site and at integer fillings as a function of onsite Hubbard repulsion $U$ and Hund’s intra-atomic exchange coupling $J$. We use a variational slave-spin mean field (VSSMF) method which allows symmetry broken states to be studied within the computationally less intensive slave-spin mean field formalism, thus making the method more powerful to study strongly correlated electron physics. The results show that at half-filling, the ground state at smaller $U$ is a Slater antiferromagnet (AF) with substantial local charge fluctuations. As $U$ is increased, the AF state develops a Heisenberg behavior, finally undergoing a first order transition to a Mott insulating AF state at a critical interaction $U_c$ which is of the order of the bandwidth. Introducing the Hund’s coupling $J$ correlates the system more and reduces $U_c$ drastically. At quarter-filling with one electron per site, the ground state at smaller $U$ is paramagnetic metallic. At finite Hund’s coupling $J$, as interaction is increased above a lower critical value $U_{c,1}$, it goes to a fully spin polarized ferromagnetic state coexisting with an antiferro-orbital order. The system eventually becomes Mott insulating at a higher critical value $U_{c,2}$. The results as a function of $U$ and $J$ are thoroughly discussed.

I. INTRODUCTION

The Hubbard model has been used to describe various strongly correlated electron phenomena observed in several $d$ and $f$-electron materials. Particularly, it has been extensively studied in the context of Mott metal-insulator transition (MIT) which is obtained in transition metal oxides by varying pressure, temperature or chemical composition. MIT within the Hubbard model has been studied using various methods such as dynamical mean field theory (DMFT) etc. Gutzwiller variational theory, slave-boson mean field (SBMFT) etc. The picture of MIT in the one-band Hubbard model that emerges from these studies is that at zero temperature, the frustrated model at half-filling undergoes a continuous Mott transition from a paramagnetic (PM) metallic to a paramagnetic Mott insulating state driven by electron-electron interactions. At finite temperatures below a critical value, the transition is first order in nature. The mechanism of MIT as supported by DMFT is that it occurs via shifting of spectral weight from the Fermi level to preformed Hubbard sub-bands as the onsite Coulomb repulsion $U$ is increased, a scenario containing features of both the Brinkmann-Rice and the Mott-Hubbard mechanisms. For the non-frustrated model on a bipartite lattice, antiferromagnetic (AF) long range order sets in at low temperatures due to perfect Fermi surface nesting, and it preempts a Mott transition as the Néel temperature is higher than the MIT temperature range. The AF state becomes band insulating because of the doubling of the unit cell. The detailed nature of MIT depends on degrees of AF correlations and frustration present. Qualitatively similar features of Mott transition were also obtained for the multi-band Hubbard model at integer fillings.

The original motivation behind introducing the Hubbard model was to describe itinerant ferromagnetism in metals. However, the one-band model turned out to be inadequate for the purpose. Ferromagnetism in the one-band Hubbard model is found under extreme circumstances such as Nagaoka ferromagnetism in the limit of infinite interaction strength in the presence of a single hole or ferromagnetism in special lattice geometries, or lattices with flat band dispersions etc. Alternatively, it is also shown to occur for lattices with frustration where the density of states is asymmetric with the spectral weight shifted to the lower energy band edge. In multi-band systems with degenerate orbitals, the Hund’s exchange coupling $J$ which favors intra-atomic ferromagnetic alignment comes into play and its role in stabilizing ferromagnetism has also been explored. Since the interactions in the Hubbard model are purely local, the effects of the kinetic energy of the electrons and hence the lattice structure also comes into question. Several studies have explored these issues in the past within the multi-band Hubbard model. However the multi-band problem is theoretically much harder and in most of the studies, the spin-flip and pair hopping processes in the intra-atomic exchange term are often dropped, and also the model is studied in the limit of infinite lattice dimensions. Nevertheless, for the two-band Hubbard model with one electron per site, an effective Hamiltonian in the strong coupling was shown to describe a ferromagnetic (FM) order coexisting with a staggered orbital order the ground state. DMFT studies of the two-band Hubbard model in the limit of infinite lattice dimensions found metallic ferromagnetism for large $J$ and at band fillings with more than one electron per site (i.e. $N > 1$), where it can be explained by the double exchange mechanism. At quarter-filling ($N = 1$), FM order was found to coexist with a staggered orbital order but in the insulating phase. SBMFT calculations found FM order in the two-band Hubbard model for large $J$ where the FM phase preempts the Mott transition. As opposed to an infinite lattice, studies on square lattice using variational Monte Carlo based on Jastrow type wave functions also support the above results and in addition, it finds that when FM phase occurs at quarter-filling along with orbital order, it is always in the fully polarized state.

The slave-rotor mean field (SRMF) theory was introduced to overcome some of the limitations of DMFT and yet as a computationally inexpensive method, and was used to study Mott transition in the multi-orbital Hubbard model in great...
details. However, by construction SRMF theory is unable to take into account magnetic order as it introduces a single spin variable corresponding to all the orbital degrees of freedom in a lattice site. In contrast the slave-spin mean-field (SSMF) theory introduces an auxiliary slave variable for each of the spin-orbital indices in a site. Thus in principle, it is capable of giving a symmetry broken solution where the mean field parameters depend upon the orbital and spin indices. However, it turns out not true and as elaborated by Georgescu et al, the SSMF scheme does not break any symmetry and always gives a paramagnetic solution. To get around the problem, they introduced an approach based on total energy which is essentially a variational approach where one considers a symmetry broken variational wave function in the slave-particle representation and optimizes the energy with respect to the parameters. The method which we term here as the variational slave-spin mean field (VSSMF) method is described in the following in detail.

In this work, we revisit the ground state phase diagram of the two-band Hubbard model as a function of Hubbard repulsion $U$ and Hund’s exchange coupling $J$ using the VSSMF method. We show that at half-filling, the ground state evolves from a Slater antiferromagnetic state with local charge fluctuations at smaller $U$ to an antiferromagnetic Mott insulating state with complete charge localization at large $U$ via a first order transition. At quarter-filling, the ground state remains paramagnetic metallic at smaller $U$. At larger $U$ and in presence of Hund’s coupling $J$, ferromagnetic order sets in with full spin polarization coexisting with an antiferro-orbital order. The system eventually becomes Mott insulating as $U$ is increased further. The rest of the paper is organized as follows. In Sec. II, we describe the model and in Sec. III, we describe the variational slave-spin mean-field method. The results are described in Sec. IV and the final conclusion in Sec. V.

II. MODEL

We consider the following two-band Hubbard model on a square lattice,

$$
\mathcal{H} = -t \sum_{\langle i, j \rangle \sigma} \left( c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.} \right) + U \sum_{i} n_{i \uparrow} n_{i \downarrow} + U' \sum_{i \neq j} n_{i \uparrow} n_{j \downarrow} + (U - J) \sum_{i \sigma, \sigma'} n_{i \sigma} n_{i \sigma'} - J \sum_{i \neq j} c_{i \sigma}^\dagger c_{i \sigma} c_{j \sigma'}^\dagger c_{j \sigma'} + J \sum_{i \neq j} c_{i \sigma}^\dagger c_{i \sigma'}^\dagger c_{j \sigma'} c_{j \sigma}
$$

(1)

where $c_{i \sigma}^\dagger$ creates an electron at site $i$, orbital $m (= 1, 2)$ with spin $\sigma$, and $n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma}$. The first term describes diagonal hopping of electrons between nearest neighbor sites. The rest of the terms describe various interactions as follows. The first three terms represent the Coulomb repulsion of electrons in the same orbital, in different orbitals with opposite spins, and in different orbitals with the same spin. The last two terms are the spin-flip and pair hopping terms, respectively. $U$ is intra-orbital interaction strength and $J$ is Hund’s exchange coupling which favors atomic states with maximum total spin and orbital angular momenta. We take $U' = U - 2J$ in which case the Hamiltonian becomes rotationally invariant with respect to both spin and orbital degrees of freedom. The above form of the Hamiltonian is relevant to $d$-orbital systems with cubic crystal field in which the five fold degenerate $d$ orbitals splits into a three fold degenerate $e_g$ orbitals and two fold degenerate $e_u$ orbitals. Also in several transition metal oxides has layered structure where interlayer couplings can be neglected and it is sufficient to consider a two dimensional lattice.

III. VARIATIONAL SLAVE-SPIN MEAN FIELD METHOD

In the slave-spin formalism, the physical electron states are mapped to a fermionic quasiparticle states coupled to an auxiliary spin-$1/2$ degree of freedom. That is, for each site $i$ and spin-orbital index $\alpha = m\sigma$, the electron states are written as

$$
|n_{i \alpha} = 0\rangle \Rightarrow |n_{i \alpha}^f = 0, S_{i \alpha}^z = -1/2\rangle
$$

(2)

$$
|n_{i \alpha} = 1\rangle \Rightarrow |n_{i \alpha}^f = 1, S_{i \alpha}^z = +1/2\rangle
$$

where $n_{i \alpha} = c_{i \alpha}^\dagger c_{i \alpha}$ is the number operator for electrons and $n_{i \alpha}^f = f_{i \alpha}^\dagger f_{i \alpha}$ is that for the fermionic quasiparticles (spinons). $S_{i \alpha}^z$ is the auxiliary spin-$1/2$ degree of freedom coupled to the spin-orbital. The mapping enlarges the local Hilbert space introducing unphysical states $|n_{i \alpha}^f = 0, S_{i \alpha}^z = +1/2\rangle$ and $|n_{i \alpha}^f = 1, S_{i \alpha}^z = -1/2\rangle$. These are in principle eliminated by enforcing the constraint,

$$
|n_{i \alpha}^f = S_{i \alpha}^z + \frac{1}{2}
$$

(3)

The electron operators are decomposed accordingly as $c_{i \alpha} = f_{i \alpha} O_{i \alpha}$ and $c_{i \alpha}^\dagger = f_{i \alpha}^\dagger O_{i \alpha}$. Several representations for $O_{i \alpha}$ are possible which act in the physical Hilbert space identically but give different solutions when the constraint is enforced approximately. In the $Z_2$ representation, which we use here,

$$
O_{i \alpha} = S_{i \alpha}^z + g_{i \alpha} S_{i \alpha}^z
$$

(4)

The gauge factors $g_{i \alpha}$s are fixed by requiring that in the non-interacting limit, the solution matches with that of the corresponding original Hamiltonian. In this new representation, the kinetic energy term becomes,

$$
\mathcal{H}_k = -t \sum_{\langle i, j \rangle} \left( O_{i \alpha}^\dagger O_{j \alpha} f_{i \alpha}^\dagger f_{j \alpha} + \text{h.c.} \right) - \mu \sum_{i \alpha} n_{i \alpha}^f - \sum_{i \alpha} \mu_{i \alpha} \left[ n_{i \alpha}^f - (S_{i \alpha}^z + \frac{1}{2}) \right]
$$

(5)

where we have introduced a chemical potential term to control the particle number. The last term which is zero because of the constraint, is introduced to enforce the constraints at the
mean field level as mentioned later, with the factors $h_{i\alpha}$'s acting as Lagrange multipliers. The density-density terms in the interaction part of the Hamiltonian can be written entirely in terms of the spin variables. Since $n_{i\alpha} = n_{i\alpha}^f = S_{i\alpha} - \frac{1}{2}$ by the constraint, we can write

$$n_{i\alpha} n_{i\alpha}' = S_{i\alpha} S_{i\alpha}' + \frac{1}{2} (S_{i\alpha} + S_{i\alpha}') + \frac{1}{4}$$ (6)

The spin-flip and the pair hopping terms cannot be represented entirely in terms of the slave-spin operators. In most of the studies, these two terms are dropped as their contribution is small. However, these can be represented approximately by replacing $c_{i\alpha}^+$ with $S_{i\alpha}^-$ which reproduces the energy spectrum in the atomic limit. Here we use this approximate mapping for these two terms. Dropping the constants, the interaction part of the Hamiltonian becomes,

$$\mathcal{H}_i^S = U \sum_{i} S_{i\alpha}^+ S_{i\alpha}^- + U' \sum_{i \neq j} S_{i\alpha}^+ S_{j\alpha}^- + (U' - J) \sum_{i \neq j} S_{i\alpha}^+ S_{j\alpha}^- + J \sum_{i \neq j} S_{i\alpha}^+ S_{j\alpha}^- S_{i\alpha}^-$$ (7)

where we have defined $S_{i\alpha} S_{i\alpha}' = S_{i\alpha}^2 + (S_{i\alpha} + S_{i\alpha}')/2$. The full Hamiltonian in the slave-spin representation becomes,

$$\mathcal{H} = -t \sum_{\langle i,j \rangle \alpha} \left( O_{i\alpha} f_{i\alpha} f_{j\alpha} + h.c. \right) - \mu \sum_{i\alpha} n_{i\alpha}$$

$$\quad - \sum_{i\alpha} \left[ n_{i\alpha} - \left( S_{i\alpha}^z + \frac{1}{2} \right) \right] + \mathcal{H}_i^S$$ (8)

We take the ground state to be $|\Psi\rangle = |\Psi_f\rangle |\Psi_S\rangle$. The first component belongs to the spin sector and is the ground state of the following spin Hamiltonian,

$$\mathcal{H}_f = \langle \Psi_S | \mathcal{H} | \Psi_S \rangle = -t \sum_{\langle i,j \rangle \alpha} \left( B_{i\alpha,ja} f_{i\alpha} f_{j\alpha} + h.c. \right)$$

$$\quad - \sum_{i\alpha} \left[ (\mu + h_{i\alpha}) n_{i\alpha} \right]$$ (9)

Similarly, the second component is the ground state of the slave-spin Hamiltonian,

$$\mathcal{H}_S = \langle \Psi_f | \mathcal{H} | \Psi_f \rangle = -t \sum_{\langle i,j \rangle \alpha} \left( \chi_{i\alpha,ja} O_{i\alpha} f_{j\alpha} + h.c. \right)$$

$$\quad + \sum_{i\alpha} h_{i\alpha} \left( S_{i\alpha}^z + \frac{1}{2} \right) + \mathcal{H}_i^S$$ (10)

Thus we get two coupled Hamiltonians which need to be solved self-consistently. The mean field parameters are given by,

$$\chi_{i\alpha,ja} = \langle \Psi_f | f_{i\alpha} f_{ja} | \Psi_f \rangle, \quad B_{i\alpha,ja} = \langle \Psi_S | O_{i\alpha} f_{ja} | \Psi_S \rangle$$ (11)

The Lagrange multipliers $h_{i\alpha}$'s are adjusted so as to satisfy the constraint on the average,

$$\langle \Psi_f | n_{i\alpha} | \Psi_f \rangle = \langle \Psi_S | S_{i\alpha}^z | \Psi_S \rangle + \frac{1}{2}$$ (12)

The spinon Hamiltonian is a non-interacting one and can be solved readily. The slave-spin Hamiltonian is fully interacting and we solve it using mean field. In the single site approximation, we mean field decouple the terms connecting the $i$-th site (cluster) to the other sites (bath) as,

$$O_{i\alpha}^j O_{ja} \approx O_{i\alpha}^j \Phi_{\alpha} \quad j \in \text{bath}$$ (13)

where $\Phi_{\alpha} = (O_{ja})$ is the order parameter which is assumed independent of the site index due to translational symmetry. The quasiparticle (QP) weight which plays a crucial role in the theory, is defined as $Z_{\alpha} = |\Phi_{\alpha}|^2$. It denotes the degree of charge fluctuation in the system and gives a measure of effective mass enhancement due to correlations, $m^* = m/Z_{\alpha}$. $Z_{\alpha}$ is unity in the non-interacting limit. As $U$ is increased, $Z_{\alpha}$ drops indicating a correlated metallic state. Mott transition is indicated by the vanishing of $Z_{\alpha}$ at a critical interaction $U_c$.

In this single site approximation, $B_{i\alpha,ja} = Z_{\alpha}$. Therefore the spinon and slave-spin Hamiltonians become,

$$\mathcal{H}_f = -t \sum_{\langle i,j \rangle \alpha} Z_{\alpha} \left( f_{i\alpha} f_{ja} + h.c. \right) - \sum_{i\alpha} \left( (\mu + h_{i\alpha}) n_{i\alpha} \right)$$ (14)

$$\mathcal{H}_S^{\text{site}} = \sum_{\alpha} \left( \eta_{\alpha} O_{i\alpha}^j + h.c. \right) + \sum_{\alpha} h_{i\alpha} \left( S_{i\alpha}^z + \frac{1}{2} \right) + \mathcal{H}_i^S$$ (15)

where $\eta_{\alpha} = -i \Phi_{\alpha} \sum_{\alpha} Z_{\alpha}$, with the sum being over the neighboring sites of $i$. The gauge factors in Eq. (4) are obtained by requiring $Z_{\alpha} = 1$ in the limit $U = J = 0$ which gives $\xi_{\alpha} = \frac{1}{\sqrt{\eta_{\alpha}(\eta_{\alpha} - 1)}}$,

$$n_{\alpha}^{0} = \langle \Psi_f | n_{i\alpha} | \Psi_f \rangle$$ (16)

where $|\Psi_f\rangle$ is the spinon ground state obtained by putting $U = J = 0$ in the slave-spin Hamiltonian. The non-interacting solution yield the Lagrange multipliers given by,

$$h_{i\alpha}^{0} = \frac{\mu}{\eta_{\alpha}} (1 - n_{\alpha}^{0}) (1 + g_{\alpha})^2, \quad c_{\alpha} = \eta_{\alpha}/\Phi_{\alpha}$$ (17)

If non-zero, it introduces an extra chemical potential to the spinon Hamiltonian even in the non-interacting limit which is not desirable. To nullify the effect, one needs to shift the chemical potential to $\mu - h_{i\alpha}^{0}$ in Eq. (14). With all the ingredients in place, Eq. (14) and (15) are solved self-consistently to find all the mean field parameters and the quasiparticle weight $Z_{\alpha}$. Though in principle, these parameters depend upon the index $\alpha$ and can give rise to spin-resolved solutions, in practice the obtained solutions always turn out to be non-magnetic. This is at first disappointing given that the whole formalism is based on introducing an auxiliary variable for each spin-orbital. However, symmetry broken solutions can be obtained by introducing an external field and minimizing the total energy as described below.

### A. Variational formalism

In the variational formalism, we introduce symmetry breaking fields $b_{i\alpha}$ to the spinon Hamiltonian and write

$$\mathcal{H}_f^\text{var} = -t \sum_{\langle i,j \rangle \alpha} Z_{\alpha} \left( f_{i\alpha} f_{ja} + h.c. \right) - \sum_{i\alpha} \left( (\mu + h_{i\alpha}) n_{i\alpha} \right)$$

$$\quad + \sum_{i\alpha} h_{i\alpha} n_{i\alpha}$$ (18)

The quantities $\{b_{i\alpha}\}$ constitute the variational parameters. Let $|\Psi_{\text{var}}\rangle$ be the ground state of $\mathcal{H}_f^\text{var}$. With this, we take the following as the variational wave function of the slave-spin Hamiltonian defined in Eq. (8),

$$|\Psi_{\text{var}}(\{b_{i\alpha}\})\rangle = |\Psi_f(\{b_{i\alpha}\})\rangle |\Psi_S(\{b_{i\alpha}\})\rangle$$ (19)
Assuming that the wave function is normalized, the variational energy is obtained as

\[
E_{\text{var}}(\{n_{\alpha}\}) = \langle \Psi_{\text{var}} | \mathcal{H} | \Psi_{\text{var}} \rangle \\
= -t \sum_{\langle \alpha, \beta \rangle} \left[ \langle O^\dagger_{\alpha} O_{\beta} f^\dagger_{\alpha} f_{\beta} + h.c. \rangle \right] - \sum_{\alpha} (\mu + h\alpha) \langle n^\dagger_{\alpha} \rangle \\
+ \sum_{\alpha} h\alpha \left( \langle S^z_{\alpha} + \frac{1}{2} \rangle \right) + \langle \mathcal{H}_{\text{int}} \rangle
\]  

(20)

In the single site approximation, the above expression for the energy becomes,

\[
E_{\text{var}} = \sum_{\alpha} e_{\alpha} - \sum_{\alpha} (\mu + h\alpha) \langle n^\dagger_{\alpha} \rangle + \sum_{\alpha} h\alpha \left( \langle S^z_{\alpha} + \frac{1}{2} \rangle \right) + \langle \mathcal{H}_{\text{int}} \rangle
\]  

(21)

where \( e_{\alpha} = -t \sum_{\beta} Z_{\alpha,\beta} \xi_{\alpha,\beta} \) and the sum is over the the nearest neighbor sites of \( \alpha \). In the above the averages are calculated with respect to the variational states. The variational wave function \( |\Psi_{\text{var}}(\{n_{\alpha}\})\rangle \) is determined by setting the external fields as in Eq. (18) and solving \( \mathcal{H}_{\text{var}} \) and \( \mathcal{H}_{\text{int}} \) self-consistently. The variational energy is minimized with respect to the external fields and the optimal solution determines the variational ground state.

### IV. RESULTS

We discuss the results of our calculations for the ground state of the two-band Hubbard model at two integer fillings, e.g. at \( N = 2 \) (half-filling) and \( N = 1 \) (quarter-filling). In the variational calculations, at half-filling, we consider a single external field corresponding to a two-sublattice antiferromagnetic order given by \( b_{\text{int}} = (-1)^m \eta(\sigma) b_{\text{AF}} \), where the \( \eta(\sigma) \) is + (−) for \( \sigma = \uparrow (\downarrow) \). At quarter-filling, we simultaneously apply two fields. One corresponds to ferromagnetic order, \( b_{\text{int}} = -\eta(\sigma) b_{\text{FM}} \) and the other corresponds to an antiferromagnetic orbital order, \( b_{\text{int}} = (-1)^{m+1} b_{\text{o}} \) where \( m = 1, 2 \) and \( i \) is the site index. In the followings, the energy values mentioned are energy per site in units of \( t \).

#### A. Half-filling

Here we discuss the results for \( N = 2 \) particles per site, that is the half-filled band. First, let us consider the paramagnetic sector. The quasiparticle weight \( Z \) in the PM sector are shown in Fig. 1 as a function of \( U/W \) where \( W \) is the non-interacting bandwidth, at various Hund’s couplings \( J/U \). It agrees well with results from previous SSMF studies. \( Z \) is unity in the non-interacting case at \( U = 0 \). It decreases with increasing \( U \) signifying a correlated metallic state for small \( U \). As \( U \) is further increased, \( Z \) vanishes continuously at a critical interaction strength \( U_c \) beyond which we get the Mott insulating state. The \( U_c \) value decreases sharply with increasing \( J \). This \( J \) dependence of \( U_c \) can be qualitatively understood as follows. The atomic Mott gap for a charge transfer between two isolated atoms with \( N = 2 \) electrons per atom is \( \Delta_{\text{Mott}} = U + J \). A condition for Mott transition is obtained by equating \( \Delta_{\text{Mott}} \) to the effective bandwidth \( W \) in presence of \( J \) which gives \( U_c \approx W(J) - J \). Thus \( U_c \) decreases with \( J \) as it correlates the system more. The decrease is not linear in \( J \) as the effective bandwidth \( W \) is also reduced by \( J \) because of its effect on the intra-atomic ferromagnetic alignment of the spins.

Now we turn to the variational calculations. We apply an external symmetry breaking field given by \( b_{\text{int}} = (-1)^m \eta(\sigma) b_{\text{AF}} \) which favors a two sub-lattice AF order with the quantity \( b_{\text{AF}} \) acting as the variational parameter. We optimize the resulting variational wave function by minimizing the energy of the original Hamiltonian with respect to \( b_{\text{AF}} \). The energy gain in the AF state is given by \( \Delta E = E_{\text{var}}(b_{\text{AF}}) - E_0 \) where \( E_0 \) is the energy of the PM state. Fig. 2 shows \( \Delta E \) as a function of \( b_{\text{AF}} \) for various \( U \) at a fixed \( J/U = 0.1 \). As the figure shows, the minimum of the energy is obtained only at

![Fig. 1. Mott transition in the two-band Hubbard model at half-filling in the paramagnetic sector and the effect of Hund’s coupling \( J \). The figure shows the QP weight \( Z \) as a function of \( U/W \) at various Hund’s couplings \( J/U \). At half-filling, \( J \) reduces the critical interaction \( U_c \) drastically.](image1.png)

![Fig. 2. Energy gain \( \Delta E = E_{\text{var}}(b_{\text{AF}}) - E_0 \) of the AF state as a function of \( b_{\text{AF}} \) for different values of \( U/J = 0.1 \) shown on the curves. \( J/U = 0.1, N = 2 \).](image2.png)
Za Slater AF insulator. There are however fairly large local charge folding of the two degenerate bands. Therefore the system becomes translational symmetry and doubles the unit cell which leads to the approaching the Heisenberg limit where the AF gap is dominated globally incompressible. The AF order parameter increases as soon as the interaction $U$ is turned on. The AF order reduces translational symmetry and doubles the unit cell which leads to the folding of the two degenerate bands. Therefore the system becomes a Slater AF insulator. There are however fairly large local charge fluctuations as the value of $Z$ shows (Fig. 4(b)), though the state is globally incompressible. The AF order parameter $m_{AF}$ increases linearly with $U$ for small $U$. This is driven by the gain in potential energy as double occupancies are reduced. However for larger $U$, it reaches a peak and starts to drop. This happens due to the system approaching the Heisenberg limit where the AF gap is dominated by the superexchange process which goes as $\sim -4t^2/U$. In fact, it was shown that the Slater and the Heisenberg limits are separated by the Mott transition where the gains in KE and PE components switch sign\cite{gabatos2013}. We do not see this in our results, likely because the single site approximation used here to solve the interacting slave-spin problem does not take into account spatial fluctuations properly. Increasing Hund’s coupling $J$ favors further localization and gives higher $m_{AF}$ driven by lower onsite energy when both the spins in the two orbitals are parallel. The QP weight $Z$ decreases with increasing $U$ and vanishes abruptly at a critical interaction strength $U_c$ where $m_{AF}$ jumps to saturation giving rise to the Néel order. Thus we get a first order transition from a Slater AF state with local charge fluctuations to an AF Mott insulating state with localized charge degree of freedom. Indeed within the single site formalism as mentioned above, the system goes to the atomic limit where the kinetic energy vanishes completely. One notable feature of the results here is that the paramagnetic sector underestimates the effect of correlation and the Mott transition occurs at much higher interaction. In the AF state, the $U_c$ values are much lower. For instance, at $J = 0$, $U_c \sim W$ in AF state whereas it is $\sim 2.5W$ in the PM state. Introducing $J$ further reduces $U_c$ by correlating the system more as mentioned before.

**B. Quarter-filling**

The case of quarter-filling with $N = 1$ particle per site is more interesting. Previous studies of the two-band Hubbard model found itinerant ferromagnetism at band fillings greater than one and for large $J$\cite{32,33,34,35}. At $N = 1$, the FM order was found to coexist with staggered orbital order but in an insulating phase\cite{33,35}. Variational Monte Carlo studies of the model on 2D lattice also find coexisting staggered orbital order with fully saturated ferromagnetism\cite{37,38,39}.

Before we discuss the results from VSSMF calculations, it is again worthwhile to examine the paramagnetic sector results obtained using the simple SSMF method. Fig. 5 shows the QP weight in the paramagnetic sector as a function of interaction $U$. The system undergoes a continuous transition from paramagnetic metallic to Mott insulating state at a critical interaction $U_c$ which depends upon $J$. In contrast to the half-filled case, here the effect of $J$ on $U_c$ is the opposite. This can again be understood by looking at the atomic gap which at quarter-filling is given by $\Delta_{at} = U - 3J$. Hence $U_c$ is estimated to vary as $U_c \sim W(J) + 3J$. Thus increasing $J$ at this filling decorrelates the system more and increases $U_c$ substantially. Next, we consider the possibility of symmetry broken phase using the variational approach. In the strong coupling limit and with $J > 0$, one can

![FIG. 3. Kinetic energy $(KE)$ and potential energy $(PE)$ as a function of $b_{AF}$ at $U/t = 2$, $J/U = 0.1$. The pink dot near the x-axis indicates the point of minimum total energy. Particles per site, $N = 2$.](image)

![FIG. 4. As the figure shows, the scenario in this case is strikingly different to the results in the PM sector. The system develops AF ordering as soon as the interaction $U$ is turned on. The AF order reduces translational symmetry and doubles the unit cell which leads to the folding of the two degenerate bands. Therefore the system becomes a Slater AF insulator. There are however fairly large local charge fluctuations as the value of $Z$ shows (Fig. 4(b)), though the state is globally incompressible. The AF order parameter $m_{AF}$ increases linearly with $U$ for small $U$. This is driven by the gain in potential energy as double occupancies are reduced. However for larger $U$, it reaches a peak and starts to drop. This happens due to the system approaching the Heisenberg limit where the AF gap is dominated by the superexchange process which goes as $\sim -4t^2/U$. In fact, it was shown that the Slater and the Heisenberg limits are separated by the Mott transition where the gains in KE and PE components switch sign\cite{gabatos2013}. We do not see this in our results, likely because the single site approximation used here to solve the interacting slave-spin problem does not take into account spatial fluctuations properly. Increasing Hund’s coupling $J$ favors further localization and gives higher $m_{AF}$ driven by lower onsite energy when both the spins in the two orbitals are parallel. The QP weight $Z$ decreases with increasing $U$ and vanishes abruptly at a critical interaction strength $U_c$ where $m_{AF}$ jumps to saturation giving rise to the Néel order. Thus we get a first order transition from a Slater AF state with local charge fluctuations to an AF Mott insulating state with localized charge degree of freedom. Indeed within the single site formalism as mentioned above, the system goes to the atomic limit where the kinetic energy vanishes completely. One notable feature of the results here is that the paramagnetic sector underestimates the effect of correlation and the Mott transition occurs at much higher interaction. In the AF state, the $U_c$ values are much lower. For instance, at $J = 0$, $U_c \sim W$ in AF state whereas it is $\sim 2.5W$ in the PM state. Introducing $J$ further reduces $U_c$ by correlating the system more as mentioned before.](image)

![FIG. 4. (a) AF order parameter $m_{AF}$ and (b) quasiparticle weight $Z$ as a function of $U/W$ at various $J/U$.](image)

![FIG. 5. Quasiparticle weight $Z$ as a function of $U/W$ at quarter-filling for various $J/U$.](image)
easily see that the ground state of a two-site lattice with one electron per site is a spin triplet and orbital singlet. This is shown schematically in Fig. 6. In this state, the sequence of hopping generated by the action of the low energy effective Hamiltonian creates an intermediate state of lowest energy thus making it the ground state of the system. In order to examine the situation for the extended lattice, we apply two external fields, one given by $b_{im\sigma} = -\eta(\sigma)b_{FM}$ corresponding to the spin FM order and the other by $b_{im\sigma} = (-1)^{m+i}b_{l}$ with $m = 1, 2$ being the orbital index, corresponding to the antiferromagnetic order. Thus here we have two variational parameters, $b_{FM}$ and $b_{l}$. The calculations in this case become numerically more extensive as the energy needs to be optimized with respect to two variational parameters at each point in the parameter space and each self-consistent calculation takes longer time to converge. We carried out the calculations and find that at smaller $U$, the energy minimum is obtained only at $b_{FM} = b_{l} = 0$ implying paramagnetic ground state at these values of $U$. At $J = 0$, the system continues to be paramagnetic metal as $U$ increased until MIT occurs at a higher $U$. However for non-zero $J$, as $U$ is increased above a lower critical value $U_{c1}$, the energy gets substantially lowered by simultaneous application of fields $b_{FM}$ and $b_{l}$. This is shown in Fig 7 where we plot the variational energy as a function of these two parameters for particular value of $U$ and $J$. Thus for $U > U_{c1}$ we get a ferromagnetic state coexisting with antiferro-orbital order. If we look at the magnetization per site, we find it to be fully saturated with all the spins flipped parallel. This fully spin polarized state with orbital ordering was also obtained in variational Monte Carlo studies. The orbital ordering is however not saturated as it is disrupted by charge fluctuations. We calculate the staggered orbital order parameter as, 

$$\alpha_{l} = \frac{1}{2} \sum (\sigma) (n_{im} - n_{ib})$$

where $n_{im}$ ($n_{ib}$) is the electron number in orbital $m \leq 1$ ($m = 2$) of a site "i". The magnetization per site, $m_{FM}$ and $\alpha_{l}$ are shown in Fig. 8. As $U$ is increased further, the system becomes Mott insulating via a first order transition at a higher critical interaction $U_{c2}$. In the Mott state, the charge degree of freedom gets frozen and the antiferro-orbital order becomes complete. The values of $Z_{\sigma}$ are shown in Fig. 9 as a function of $U$ at various $J/U$. In the paramagnetic state $Z_{\uparrow} = Z_{\downarrow}$ and it decreases with increasing $U$.

In the case of finite Hund’s coupling $J$, $Z_{\uparrow}$ drops to zero at $U = U_{c1}$ as the down spin carrier density vanishes at the transition. The QP weight for up-spin, $Z_{\uparrow}$ shows a jump at the transition driven by a gain in the kinetic energy by the superexchange process as mentioned before. $Z_{\downarrow}$ eventually drops to zero at the higher critical interaction $U_{c2}$. Thus in this orbitally degenerate system, the Hund’s exchange coupling which favors intra-atomic spin alignment in isolated atoms also brings about ferromagnetic order in the band limit.

V. CONCLUSION

We have revisited the ground state of the orbitally degenerate two-band Hubbard model on a square lattice using variational slave-spin mean field theory. The ordinary slave-spin mean field theory which is a numerically less intensive technique to study correlated electron systems, gives solutions where no symmetry is broken. This work extends the method to study symmetry broken phases thus making it more powerful. Using the method, we find that at half-filling, the ground state of the model at smaller $U$ is a Slater antiferromagnetic insulator with sizeable local charge fluctuations. As $U$ is increased, the system goes to a Mott insulating state with Néel antiferromagnetic order via a first order transition. The critical interaction $U_{c}$ for

![Fig. 6](image_url)

**Fig. 6.** The spin triplet and orbital singlet state of a two-site lattice with one electron per site. The kinetic exchange process shown schematically gives energy $\sim -4t^{2}/(U - 3J)$ which is the lowest.

![Fig. 7](image_url)

**Fig. 7.** Energy $E_{\text{var}}$ versus $b_{l}$ for different values of $b_{FM}$ shown on the curves. $U/t = 6$ and $J/U = 0.1$. Particles per site, $N = 1$.

![Fig. 8](image_url)

**Fig. 8.** Magnetic and orbital order parameters $m_{FM}$ and $\alpha_{l}$, respectively as a function of $U/W$ at $J/U = 0.3$.

![Fig. 9](image_url)

**Fig. 9.** Quasiparticle weight $Z_{\sigma}$ versus $U/W$ for different $J/U$. In the case of finite Hund’s coupling $J$, $Z_{\uparrow}$ drops to zero at $U = U_{c1}$ as the down spin carrier density vanishes at the transition. The QP weight for up-spin, $Z_{\uparrow}$ shows a jump at the transition driven by a gain in the kinetic energy by the superexchange process as mentioned before. $Z_{\downarrow}$ eventually drops to zero at the higher critical interaction $U_{c2}$. Thus in this orbitally degenerate system, the Hund’s exchange coupling which favors intra-atomic spin alignment in isolated atoms also brings about ferromagnetic order in the band limit.
the Mott transition is much smaller compared to the corresponding
value in the paramagnetic sector. Increasing Hund’s coupling \( J \) cor-
relates the system more and reduces \( U_c \). At quarter-filling, the ground
state is paramagnetic metallic at smaller \( U \). When Hund’s coupling
is present, the system goes to a fully spin-polarized ferromagnetic

state with a coexisting antiferro-orbital order as \( U \) is increased above
a critical value \( U_c \). The spinon band structure becomes gapped due
to the staggered orbital ordering, but local charge fluctuation per-
sists. As \( U \) is increased further, a first order transition takes place
at a critical interaction \( U_{c2} \) where charge fluctuation vanishes com-
pletely giving rise to a Mott insulating state.

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