Degenerate orbital effect in a three orbital periodic Anderson model

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The competition between the Ruderman-Kittel-Kasuya-Yosida effect and Kondo effect is a central subject of periodic Anderson model. By using the density matrix embedding theory, we study a three orbital periodic Anderson model, in which the effects of degenerate conduction orbitals via the local magnetic moments, number of electrons, and spin-spin correlation functions, are investigated. From the phase diagram at half filling, we find there exists two different anti-ferromagnetic phases and one paramagnetic phase. To explore the difference of the two anti-ferromagnetic phases, the topology of Fermi surface and the connection with standard periodic Anderson model are considered. The spin-spin correlation functions yield insight into the competition between Ruderman-Kittel-Kasuya-Yosida interaction and Kondo interaction. We further find there is a “scaling transformation” connects different ratio of the hybridization strength.

I. INTRODUCTION

The accessible of clean interfaces between transition metal oxides provides new opportunity for electronics [1]. The reason is most of the traditional electronic devices are fabricated with semiconductor materials, whose behaviors are more predictable since the electron-electron interactions are not that strong. Both transition metal oxides and rare earth compounds are considered as strongly correlated material. Since the transition metal oxides include elements which have partially filled d orbitals, while rare earth and Actinides compounds have partially filled f orbitals. Successful fabrications of the layered superlattices of heavy fermion material [2-4] made a step towards strongly correlated electronic devices, and triggered many interesting studies on layered f-electron systems [5-7]. However several fundamental problems are still open, in both theoretical and computational aspects.

One of the fascinating question is what occurs at the interface of normal metal and strongly correlated insulator. The answer is Kondo proximity effect by dynamical mean field theory (DMFT) [8] and Kondo screening embraces both sides of the interface by determinant quantum Monte carlo (DQMC) [9]. Two neighboring conduction electron layers and one layer of localized electron layer could describe this problem [10-12]. Meanwhile the correlated layers sandwiched between normal metallic layers and even more complex structure is another interesting problem. In order to understand more about this problem, we start with a quasi-two dimensional model. The model includes three layers, and the electrons in the correlated layer is allowed hopping to the other two conduction layers.

In the context of Periodic Anderson Model (PAM), the model we studied could be interpreted as two orthogonal conduction orbital and one localized orbital on each site. So besides the connection with layered f-electron system, our work are related with the traditional degenerate orbitals problem in the fields of heavy fermions. It was pointed out that multi-orbital effect plays an essential role in some uranium-based compounds [13], and PAM which including degenerate f orbitals has been studied by DMFT [14,15]. Moreover it was suggested that multi-orbital conduction electrons may be relevant for the heavy-fermion behavior of 3d transitional metal compounds LiV$_2$O$_4$ [16].

By employing the density matrix embedding theory (DMET) [17,18], we study a three orbital PAM in this paper. We calculate local magnetic moments, number of electrons, and spin-spin correlation functions to understand the physics in the model. In the following we will describe the model first, give a brief introduction to the method, present our results in detail, and in the end we make a summary and conclusion.

II. MODEL AND METHODS

We consider a three orbital PAM on a two dimensional square lattice, the Hamiltonian is the following

$$H = -t \sum_{<ij>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c) - t \sum_{<ij>,\sigma} (d_{i\sigma}^\dagger d_{j\sigma} + h.c) + V_1 \sum_{i\sigma} (c_{i\sigma}^\dagger f_{i\sigma} + h.c) + V_2 \sum_{i\sigma} (d_{i\sigma}^\dagger f_{i\sigma} + h.c) + E_f \sum_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c_{i\sigma}^\dagger (c_{i\sigma})$ and $d_{i\sigma}^\dagger (d_{i\sigma})$ are the creation (annihilation) operators of the two conduction orbitals on site $i$ with spin $\sigma$, and $f_{i\sigma}^\dagger (f_{i\sigma})$ is the creation (annihilation) operators of localized orbital. $t$ is the hopping integral between neighboring conduction orbitals, $E_f$ is the on-site energy of the localized orbital ($f$ state), which defines the relative position of $f$ state with respect to the Fermi energy of the conduction orbital ($c$ state) . $V_1 (V_2)$ is the hybridization strength between $c (d)$ and $f$ states on the same site, and $U$ is the on-site Coulomb repulsion of the $f$ states.

In the non-interacting case, the Hamiltonian in the mo-
momentum space could be written as:

\[ H_0 = \sum_{\mathbf{k}, \sigma} \begin{pmatrix} c_{\mathbf{k} \sigma}^\dagger & d_{\mathbf{k} \sigma}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & 0 \\ 0 & \epsilon_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k} \sigma} \\ d_{\mathbf{k} \sigma} \end{pmatrix} \]

(2)

where \( \epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) \) is the dispersion relation of the conduction band. Diagonalizing the non-interacting Hamiltonian \( H_0 \) yields three bands:

\[ E(\mathbf{k}) = \begin{cases} \frac{1}{2} \left[ E_f + \epsilon(\mathbf{k}) + \sqrt{(E_f - \epsilon(\mathbf{k}))^2 + 4V_1^2 + 4V_2^2} \right] \\ \epsilon(\mathbf{k}) \\ \frac{1}{2} \left[ E_f + \epsilon(\mathbf{k}) - \sqrt{(E_f - \epsilon(\mathbf{k}))^2 + 4V_1^2 + 4V_2^2} \right] \end{cases} \]

(3)

We have plotted the dispersion relation in Fig. 1. As comparison the dispersion of the standard PAM is shown in the left panel. The hybridization of the conduction orbital and localized orbital results in two different bands, and produces a gap between the two bands (black and red). It is not difficult to prove that the gap is always there no matter how the parameters change. The dispersion relation of the three orbital PAM is similar. Except there is an additional band in the middle the other two bands. The additional band is shown as blue line in the right panel of Fig. 1. It can be proved that the blue band is always in the middle of the black and red bands. The shape of the black band and the red band is similar with the ordinary PAM. The dispersion of the additional band is the same as the conduction band, because it is a linear combination of the two conduction orbitals. At half filling the ordinary PAM is insulating, while the three orbital PAM is metallic.

Ever since it was developed DMET has been applied to several different area. Including standard Hubbard model, Hubbard Holestein model which contains phonon interaction, cuprates single impurity Anderson model, as well as quantum molecules. Besides ground state static properties, dynamic properties such as spectral function could be derived, and so does the non-equilibrium dynamics. for more detail of the methods please refer to the thesis, Ref.

In a DMET calculation, the lattice sites are first divided into different clusters as shown in Fig. 2. The clusters are chosen to tile the whole lattice, and they are always the unitcells of lattice in order to keep the translation invariance. The example of \( 1 \times 2 \) cluster are displayed in Fig. 2.

An auxiliary system with Hamiltonian \( h \) is then introduced:

\[ h = h_0 + v \]

(4)

where \( h_0 \) is the one body terms in \( H \), and \( v \) is the correlation potential within cluster. In the particle number conserving case (no superconducting phase) \( v \) has the form:

\[ v = \sum_C \sum_{i,j \in C} v_{ij \sigma} c_{i \sigma}^\dagger c_{j \sigma} \]

(5)

where \( C \) is one of the cluster that within dashed circles in Fig. 2. \( h \) is block diagonal since \( v \) is only within cluster, and \( v \) is a replacement of local interaction.

The one-body Hamiltonian \( h \) is simple enough to be solved. From the ground state \( |\Phi \rangle \) of \( h \), the embedding basis could be constructed. The sites in one of the cluster (the red sites in Fig. 2) are chosen as the impurity orbitals. The remaining sites (the blue sites in Fig. 2) are the environment orbitals. There are several mathematically equivalent unitary transformations after applying which the environment orbitals are linear combined into bath orbitals (magenta energy levels in Fig. 2), core orbitals (black energy levels) and virtual orbitals (grey energy levels). Core (virtual) orbitals are completely empty (full), thus only bath orbitals are entangled with impurity orbitals. The core orbitals and bath orbitals constitute active space, and the number of bath orbitals is at most the number of impurity orbitals. The impurity Hamilto-
\[ H_{\text{imp}} = P h P - \sum_{i,j \in \text{imp}} v_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i \in \text{imp}} n_{i\uparrow} n_{i\downarrow} \quad (6) \]

where \( P \) is the projection operator which projects the system to the active space. The correlation potentials on the impurity orbitals are replaced by the onsite Coulomb interaction. Since the impurity Hamiltonian \( H_{\text{imp}} \) is only within the active space, Exact diagonalization and other computational expensive methods could be used to solve the ground state \( |\Psi\rangle \) of \( H_{\text{imp}} \). In this work we use density matrix renormalization group (DMRG) \( \otimes \) to solve the impurity model \( H_{\text{imp}} \).

The correlation potential is updated through the 1 particle reduced density matrix (1-PDM) \( \rho^f \) of the impurity model ground state \( |\Psi\rangle \). Our goal is to minimize the difference between \( |\Psi\rangle \) and \( |\Phi\rangle \). This is accomplished by first downfolding \( |\Phi\rangle \) to the active space, and the corresponding 1-PDM is \( \rho^0 \). Then minimizing the difference of \( \rho^f \) and \( \rho^0 \).

\[
\min_{v} f(v) = \sqrt{\sum_{ij} |\rho^f_{ij} - \rho^0_{ij}(v)|^2} \quad (7)
\]

When optimizing \( f(v) \) the ground state \( |\Phi\rangle \) of the impurity model is fixed, so \( \rho^f \) is also fixed. The optimal \( v \) is used to update \( |\Phi\rangle \), the embedding basis, the impurity model \( H_{\text{imp}} \), as well as \( |\Psi\rangle \) and \( \rho^f \). Thus the self-consistent loop is formed.

In summary the DMET calculations proceed the following steps:

1. An initial guess of the correlation potential \( v_0 \) is chosen.
2. Solve the auxiliary lattice Hamiltonian to obtain the lattice wave function \( |\Phi\rangle \).
3. Embedding basis is constructed from the lattice wave function \( |\Phi\rangle \).
4. Transform to the embedding basis, and add the interaction to get impurity model \( H_{\text{imp}} \).
5. Using DMRG impurity solver to compute the ground state \( |\Psi\rangle \) of the impurity model, and calculate the corresponding 1-PDM \( \rho^f \).
6. Update the correlation potential \( v \) to minimize the difference of \( \rho^f \) and \( \rho^0 \).
7. Go back to step (2) until the correlation potential \( v \) converges.

The local observables such as local magnetic moment and the number of electrons are extracted directly from 1-PDM of \( |\Phi\rangle \). Other observables such as ground state energy and spin-spin correlation are calculated from 2-PDM of \( |\Phi\rangle \).

### III. RESULTS

We have run the DMET calculations of the three orbital PAM on a two dimensional square lattice. The lattice size in our calculation is \( 200 \times 200 \). We mainly focus on the physics at half filling, and in our simulation \( t = 1, U = 8 \).

#### A. Order parameter and phase diagram

First we focus on the symmetric case when \( V_1 = V_2 = V \). The ground state phase diagram at half filling is shown in Fig. 4, and it’s symmetric with respect to \( E_f = -\frac{U}{2} \). If \( E_f = -\frac{U}{2} \) the fermi energy of the conduction bands is zero which is just in the middle of the two energy levels of the \( f \) orbital say \(-\frac{U}{2} \) and \( \frac{U}{2} \). Away from the axis of \( E_f = -\frac{U}{2} \), considering the particle-hole symmetry, all the physical quantities map to each other. From Fig. 4, we could see there are para-magnetic phase and two different anti-ferromagnetic phases (AF1 and AF2). The magnetic transition is shown as black line in Fig. 4, from AF1 phase the magnetic transition is continuous, while from AF2 phase it’s first order. In Fig. 5 the continuous magnetic transition is the dashed black line, and the first order magnetic transition is the solid black line. The phase transition between the two magnetic order is of first order, and displayed as red solid line in Fig. 4. It is a Lifshitz transition which accompanies by the reconstruction of Fermi surface. We will discuss this in more detail later. Inside the AF2 phase, there’s a Kondo region, located within the blue dashed line in Fig. 4. In the Kondo region the occupation number of electrons on \( f \) orbital \( n_f \) is 1, and so are the \( n_c \) and \( \bar{n}_d \). It’s worth to mention that the term “Kondo region” doesn’t mean Kondo effect takes place, we just follow the nomimation in literature.

Now we discuss how the phase diagram is determined. We have calculated the local magnetic moments and the number of electrons, and they are shown in Fig. 4. The definitions of those physical quantities are:

\[
\begin{align*}
m^\alpha_i &= \langle n^\alpha_{i\uparrow} - n^\alpha_{i\downarrow} \rangle \\
n^\alpha_i &= \langle n^\alpha_{i\uparrow} + n^\alpha_{i\downarrow} \rangle
\end{align*}
\quad (8)
\]

Here \( n^\alpha_{i\sigma} \) is the number of spin \( \sigma \) electrons of \( \alpha \) orbitals on site \( i \). As we mentioned before that \( m^f_i \) and \( n^f_i \) are symmetric with respect to \( E_f = -\frac{U}{2} \), since the particle-hole symmetry. In order to display more details we only plotted the data when \( E_f > -\frac{U}{2} \). At half filling \( n^f_i + n^d_i + n^f_i = 3.0 \), considering \( n^c_i = n^d_i \) in the symmetric case, so only \( n^f_i \) is plotted.

At small value of \( V \), there are mainly five regions: (1) Maximally occupied \( f \) states where \( n_f = 2 \), when \( E_f < E_c^{(0)} - U \); (2) First mixed valence region where \( 1 < n_f < 2 \), when \( E_c^{(0)} - U < E_f < E_c^{(1)} - U \); (3) Kondo
region where \( n_f = 1 \), when \( E_c^{(1)} - U < E_f < E_c^{(1)} \); (4) Second mixed valence region where \( 0 < n_f < 1 \), when \( E_c^{(1)} < E_f < E_c^{(2)} \); (5) Empty \( f \) states where \( n_f = 0 \), when \( E_f > E_c^{(2)} \). The \( E_c^{(0)} \) (\( E_c^{(2)} \)) is the lowest (highest) energy level of the conduction band, and \( E_f \) is the fermi energy of the conduction band. In Fig. (a) only the Kondo region \((-8 < E_f < 0)\) and second mixed valence region \((0 < E_f < 4)\) are shown. As the hybridization strength \( V \) increases the two mixed valence regions expands, at the same time the other three regions shrinks. The Kondo region becomes smaller and smaller as \( V \) increases, and from \( V \approx 1.20 \) it becomes a point (only the symmetric point \( E_f = -4 \) belongs to the Kondo region). At the symmetric point \( E_f = -4 \), \( n_f = 1 \) no matter how the hybridization strength \( V \) changes.

The anti-ferromagnetic long range order is formed in the Kondo region when the value of \( V \) is small. If \( V \) is fixed, and \( E_f \) goes away from the symmetric axis, the magnetic transition to a para-magnetic phase takes place in the mixed valence region. It’s obvious in Fig. 3 that there exists a finite step in both local magnetic moment and number of electrons when \( V = 0.5 \) and \( V = 1.0 \) (the red and blue line in Fig. 3). This is due to the occurrence of Lifshitz transition. Even though it has been several studies of Lifshitz transition on PAM, it happens at half filling is still unusual.

In order to understand how the Lifshitz transition occurs, we plotted the band structure of the two anti-ferromagnetic phases in Fig. 4. As we mentioned in the previous section, in a DMET calculation, the correlation potential is self-consistently determined. Adding a converged correlation potential to the non-interacting part of the Hamiltonian, and diagonalizing the auxiliary Hamiltonian, the band structure could be derived. The presence of anti-ferromagnetic order makes the unit-cell twice than before, so the first Brillouin zone of the reciprocal lattice becomes half of the non-magnetic case. The bigger square in the upper right panel of Fig. 4 is the first Brillouin zone (\( \Gamma \) point is in the center) in the PM phase, and the grey shaded smaller square is the first Brillouin zone in the presence of anti-ferromagnetic order. The lower right panel is a quarter of the upper panel with all the high symmetry point marked. From the upper panel we know the Brillouin zone is folded along two neighboring \( X \) point. The band structure repeat itself along the dashed line in the lower panel. So there are six bands in the band dispersion figures of the two AF phases. The left upper panel belongs to the AF1 phase, and at half filling it has a hole type Fermi surface around \( \Gamma \) point. While the left lower panel belongs to the AF2 phase, and at half filling it has a electron type Fermi surface around \( \Gamma \) point. The Fermi surface topology of PM phase is the same as AF1 phase, the phase transition between these two phases is continuous. However the AF2 phase has a different Fermi surface topology, the transitions to the other two phases are first order.
B. Spin correlations and Kondo singlet

The magnetic physics of the PAM can be characterized by the spin-spin correlations. We study the spacial spin-spin correlation functions, and the definitions are:

\[ C_{fi}(r = 0) = \langle m_i^f \cdot m_i^c \rangle = \langle (n_{i\uparrow}^f - n_{i\uparrow}^c)(n_{i\downarrow}^f - n_{i\downarrow}^c) \rangle \]
\[ C_{ff}(r = 1) = \langle m_i^f \cdot m_j^f \rangle = \langle (n_{i\uparrow}^f - n_{i\downarrow}^f)(n_{j\uparrow}^f - n_{j\downarrow}^f) \rangle \]

Here \( C_{fi}(r = 0) \) measures the magnetic correlations between the localized orbital \( f \) and conduction orbital \( c \) on the same site. While \( C_{ff}(r = 1) \) measures the correlations of localized orbital \( f \) between neighboring sites. To explore the magnetic property the hybridization \( V \) is fixed first. The results are displayed in the left panel of Fig. 6. Starting from the symmetric point at \( E_f = -4 \) the system evolves from AF2 phase to PM phase directly when \( V = 1.0 \). In the AF2 phase the correlation function \( C_{fi}(r = 0) \) is almost constant, and it drops to zero gradually in the PM phase. Moreover there’s a kink at the magnetic transition point. While the behavior of \( C_{ff}(r = 1) \) is rather similar to the local magnetic moment. Its absolute value decreases slowly in the AF2 phase, and after a finite step, it approaches to zero gradually. Apart from the discontinuous of \( n^f \) and \( m^f \), the step here is another evidence that the transition from AF2 phase to PM phase is first order. Meanwhile the absolute value of \( C_{fi}(r = 0) \) is smaller when \( V = 0.3 \) and \( V = 0.5 \). The reason is the hybridization strength \( V \) increases the anti-ferromagnetic spin-spin interaction between \( f \) and \( c \) orbitals. The system undergoes all the three phases when \( V = 0.3 \) and \( V = 0.5 \). The absolute value of \( C_{fi}(r = 0) \) increases slightly in the AF2 phase. It mainly decreases in the AF1 phase, and of course becomes to zero eventually in the PM phase. However the minimum point of the \( C_{fi}(r = 0) \) curve is not the Lifshitz transition point. Unlike the order parameter there’s no sudden change when entering in a new phase.

Next we check the results in the right panel of Fig. 6. They are calculated by fixing \( E_f \) and varying \( V \) continuously. Different colors in the figures represent different value of \( E_f \). If the value of \( V \) is small, \( E_f = -4 \), \( E_f = 0.5 \) and \( E_f = 6 \) correspond to the Kondo region, the second mixed valence region and empty \( f \) states. The behavior of \( C_{ff}(r = 1) \) is easy to interpret. When \( E_f = 6 \) the anti-ferromagnetic long range order never shows up, so it keeps to zero at all value of \( V \). For the other two value of \( E_f \), the long range order is present at small value of \( V \), so there’s anti-ferromagnetic correlations between neighboring \( f \) orbitals. As \( V \) increases, it becomes to zero gradually. However the \( C_{fi}(r = 0) \) curves are more interesting. Although there’s no anti-ferromagnetic long range order when \( E_f = 6 \), the anti-ferromagnetic correlation between \( f \) and \( c \) orbitals increases monotonously as \( V \) increases. While the situation when \( E_f = 0.5 \) and \( E_f = -4 \) is different. If the long range order presents, the absolute value of \( C_{fi}(r = 0) \) increases rapidly. And in the PM phase it increases slightly and then decreases very slowly. At large value of \( V \), regardless of the value of \( E_f \), the value of \( C_{fi}(r = 0) \) approaches \( -1/4 \) (dashed line in Fig. 6b)). This suggests that the paramagnetic phase at large value of \( V \) is different from the phase when \( E_f \) is far away from the symmetric point.

The hybridization between conduction and localized orbitals is responsible for the creation of the Kondo singlet, and in the mean field level the hybridization parameters are introduced to qualify the formation of Kondo singlet. In order to characterize the Kondo screening, a hybridization parameter \( V_u \) is defined as:

\[ V_u = \frac{1}{2}(V_a + V_b) \]

Here \( V_a \) and \( V_b \) are hybridization parameters defined on the two sublattices A and B: 

\[ V_a = \langle c_{iA\uparrow}^\dagger f_{iA\uparrow} \rangle = \langle c_{iB\uparrow}^\dagger f_{iB\uparrow} \rangle \]
\[ V_b = \langle c_{iA\downarrow}^\dagger f_{iA\downarrow} \rangle = \langle c_{iB\downarrow}^\dagger f_{iB\downarrow} \rangle \]
varies with different parameters, the results are shown in Fig. 3. Since the Kondo coupling $J$ between the localized moment and conduction electrons is proportional to the square of hybridization strength $V$, it’s more and more likely to form Kondo singlet as $V$ increases. The three different curves in the left panel of Fig. 3 are accord with the fact that Kondo effect dominates more as $V$ increases. In both the AF1 phase and AF2 phase the hybridization parameter $V_{u}$ increases as $E_{f}$ increases. This indicates the competition between the Kondo effect and RKKY effect, as the RKKY effect becomes weak as $E_{f}$ is away from the symmetric point. However in the PM phase $V_{u}$ decreases as $E_{f}$ goes away from the symmetric point. This is due to the number of electrons in $f$ orbitals are descending as $E_{f}$ increases. Near the magnetic transition point $V_{u}$ reaches its maximum. If AF1 phase is present, the maximum is located in the AF1 phase, otherwise the maximum is in the PM phase.

By fixing $E_{f}$ the hybridization parameter $V_{u}$ increases as $V$ increases monotonously. At large value of $V$, the hybridization parameter $V_{u}$ approaches 0.5. In both the AF1 phase ($E_{f} = 0.5, V < 0.285$) and AF2 phase ($E_{f} = -4, V < 1.325$) the hybridization parameter $V_{u}$ increases rapidly. After entering into the PM phase, the slope of $V_{u} - V$ becomes smaller and smaller. When the hybridization strength $V$ is large enough $V_{u}$ approaches $1/3 \approx 0.3333$, that is plotted as dashed line in Fig. 3(b).

C. Non-symmetric case $V_1 \neq V_2$

We further consider the non-symmetric case when $V_1 \neq V_2$. The hybridization strength $V_1 = V$ and $V_2 = \gamma V_1$, and in the following simulations only $V$ is varied continuously. The data with different hybridization ratio $\gamma$ are all connected with each other through a “scaling transformation”, transformed after which all the data collapse just like the finite size scaling.

The scaling transformation of local magnetic moment is:

$$
\begin{align*}
& m^{c}(V, \gamma V) = \frac{2}{1 + \gamma^2} \tilde{m}^{c} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right) \\
& m^{d}(V, \gamma V) = \frac{2 \gamma^2}{1 + \gamma^2} \tilde{m}^{c} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right) \\
& m^{f}(V, \gamma V) = \tilde{m}^{f} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right)
\end{align*}
$$

(12)

Here $\tilde{m}^{\alpha}$ is the local magnetic moment on orbital $\alpha$ in the case of $V_1 = V_2 = V_0$, and the value of the hybridization strength $V_0$ is $\sqrt{\frac{1 + \gamma^2}{2} V}$. After the transformation $m^{c}$ and $m^{f}$ are displayed in Fig. 3(a)(c), and the insets are the original data from simulation. Different ratio of the hybridization strength are displayed with different color. $\gamma = 1, \gamma = 1.5, \gamma = 2$, and $\gamma = 3$ is black, green, red, and blue in Fig. 3.

In Fig. 3, $m^{d}$ is connected with $m^{c}$ through $\gamma \rightarrow 1/\gamma$, so only $m^{c}$ is displayed.

However the formula of the transformation is bit more complex for $n^{c}$ and $n^{d}$:

$$
\begin{align*}
& n^{c}(V, \gamma V) = \frac{2}{1 + \gamma^2} \tilde{n}^{c} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right) + \frac{\gamma^2 - 1}{\gamma^2 + 1} n^{g}(V, \gamma V) \\
& n^{d}(V, \gamma V) = \frac{2 \gamma^2}{1 + \gamma^2} \tilde{n}^{c} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right) - \frac{\gamma^2 - 1}{\gamma^2 + 1} n^{g}(V, \gamma V) \\
& n^{f}(V, \gamma V) = \tilde{n}^{f} \left( \sqrt{\frac{1 + \gamma^2}{2} V} \right)
\end{align*}
$$

(13)

As in Fig. 3(b)(d), after the transformation all the data collapse, exotic just like the finite size scaling. Since $n^{c} + n^{d} + n^{f}$ is 3.0 and $n^{d}$ is connected with $n^{c}$ through $\gamma \rightarrow 1/\gamma$, we only show the results of $n^{c}$ and $n^{d}$.

We will explain the physical meaning of $n^{g}$ soon, before this let’s have a look at the spin-spin correlation functions. Although the correlation functions are four fermionic operators, the scaling transformations still exist. The transformations are:

$$
\begin{align*}
& C_{fc}(r = 0) = \langle m^{f}_{1} \cdot m^{c}_{1} \rangle = \tilde{C}_{fc}(r = 0) = \frac{2}{1 + \gamma^2} \langle \tilde{m}^{f}_{1} \cdot \tilde{m}^{c}_{1} \rangle \\
& C_{fc}(r = 1) = \langle m^{f}_{1} \cdot m^{c}_{2} \rangle = \tilde{C}_{fc}(r = 1) = \frac{2}{1 + \gamma^2} \langle \tilde{m}^{f}_{1} \cdot \tilde{m}^{c}_{2} \rangle \\
& C_{fd}(r = 1) = \langle m^{f}_{1} \cdot m^{d}_{2} \rangle = \tilde{C}_{fd}(r = 1) = \frac{2 \gamma^2}{1 + \gamma^2} \langle \tilde{m}^{f}_{1} \cdot \tilde{d}^{2}_{2} \rangle \\
& C_{ff}(r = 1) = \langle m^{f}_{1} \cdot m^{f}_{2} \rangle = \tilde{C}_{ff}(r = 1) = \langle \tilde{m}^{f}_{1} \cdot \tilde{m}^{f}_{2} \rangle
\end{align*}
$$

(14)

The notations are same as previously, and the results are displayed in Fig. 3. We don’t bother the readers with all the data, but the equation in Eq. 12-14 are all correct. Why the scaling transformations hold for so many different physical quantities?

After the scaling transformation all the data with different ratio of hybridization strength collapse. Now we
A number of theoretical and numerical work has examined the physics at the interface of Mott insulator and metal. Inhomogeneous DMFT predicts fragile fermi liquid appears in finite layers of Mott insulator sandwiched between metallic leads. In this paper, by introducing a three orbital periodic Anderson model, we have studied one insulator layer sandwiched between two metallic layers with DMET.

The model we studied is a periodic Anderson model with degenerate conduction orbitals. We start with the symmetric case, when the two conduction orbitals has equal hybridization strength with the localized orbital. We found there are three different phases at half filling. When the hybridization strength $V$ is week, the RKKY effect dominates, and the ground state is in anti-ferromagnetic phase. As $V$ increases the Kondo effect becomes important, and para-magnetic phase appears. In the region when $V$ is small, there exists two different anti-ferromagnetic phases.

The phase transition between the two AF phases is the Lifshitz transition, which is accompanied by the Fermi surface reconstruction. From the band structure we discussed the topology of the Fermi surface. We further studied the non-symmetric case, and found the equivalence of the model to another model. In the picture of the other model, the mechanism of the Lifshitz transition is more clear. We also studied the spin-spin correlation functions carefully. When $V$ is small, even though the Kondo effect is not that strong, as $E_f$ is away from the symmetric point, the Kondo effect becomes more important at first, then disappears as expected. However the quantization of the Kondo screening is not well defined, otherwise it will be interesting to unearth it deeply.

Our work on the three orbital PAM is a first step in the applications of DMET to superlattice $f$ electron models. The model we studied here is too simple to describe real experiments. Our results indicates the physics of the quasi-two dimensional model is different from the standard model. In order to study more complex and realistic system, developing more powerful impurity solvers, with high precision and low computational cost will be significant. We only restricted ourselves at half filling. There will be more exotic and fascinating phenomena far away from half filling, such as complex magnetic order and unconventional superconductivity.

**IV. CONCLUSIONS**

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