Effect of hybridization on the magnetic properties of correlated two-band metals

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The magnetic properties of transition-like metals are discussed within the single site approximation, which is a picture to take into account electron correlations. The metal is described by two hybridized bands one of which includes Coulomb correlation. The presented results indicate that ferromagnetism arises for adequate values of hybridization (V), correlation (U) and occupation number(nσ). Some similarities with Dynamical Mean-Field Theory (DMFT) are indicated.

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I. INTRODUCTION

Recently, the conventional view of the origin of ferromagnetism in metals has been under criticism. Traditional mean-field calculations favor ferromagnetism but corrections tend to reduce the range of validity of that ground state [3].

Several recent works addressed the issue of ferromagnetism in metals, going beyond the Stoner model: Vollhardt et al. furnish evidence of the stability of itinerant ferromagnetism in the one-band Hubbard model(HM) at electronic densities not too close to half-filling and large enough U.

Nolting and Borgiel use, for the one-band Hubbard model(HM), a spectral density approach(SDA), a two-pole ansatz, causes important differences in the magnetic order of the model. An improved version of the AA method(HM), a spectral density approach(SDA), two-pole ansatz, favors ferromagnetism but point out that an imaginary part in the self-energy, present in the MAA method but not in the two-pole ansatz, causes important differences in the magnetic order of the model. An improved version of the AA method which incorporates the intersite magnetic correlations seems to indicate a ferromagnetic instability for large U and n ∼ 0.6.

Schwinger and Nolting consider a two-band HM, as we do, but for d → ∞ and use both the SDA and the SDA and occupation number(nσ) method(HM) and use both the SDA and the occupation number(nσ). Some similarities with Dynamical Mean-Field Theory (DMFT) are indicated.

II. THEORETICAL MODEL: THE SELF-CONSISTENT SSA

The starting Hamiltonian in this work is

\[ \mathcal{H} = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_{i,j,\sigma} t_{ij}^b b_{i\sigma}^+ b_{j\sigma} + \sum_i U n_{i\uparrow}^{(a)} n_{i\downarrow}^{(a)} + \sum_{i,j,\sigma} (V_{ab} b_{i\sigma}^+ a_{j\sigma} + V_{ba} a_{i\sigma}^+ b_{j\sigma}) , \] (1)

where \( n_{i\sigma}^a = a_{i\sigma}^+ a_{i\sigma} \) and \( \sigma \) denotes spin. \( t_{ij} \) is the tunneling amplitude between neighboring sites i and j, in each band and \( V_{ab} \) the hybridization. In the single-site approximation one adopts the following effective Hamilto-
\[ H_{\text{eff}} = \sum_{i,j,\sigma} t_{ij}^a a_{i\sigma}^a a_{j\sigma} + \sum_{i,j,\sigma} t_{ij}^b b_{i\sigma}^a b_{j\sigma} + \sum_{i \neq 0,\sigma} n_{i\sigma}^a \Sigma^\sigma \\
+ U n_{01}^a n_{01}^a + \sum_{i,j,\sigma} (V_{ab} b_{i\sigma}^a a_{j\sigma} + V_{ba} a_{i\sigma}^a b_{j\sigma}) \]

(2)

The method then replaces a translationally invariant problem, as defined by \( [1] \), by an impurity problem where only the origin incorporates the Coulomb interaction, the other sites being acted by the local (k-independent) field \( \Sigma^\sigma \). But the effective Hamiltonian \( [2] \), describes an ‘impurity problem’ in presence of Coulomb intra-atomic term and we have to resort to some approximation.

We use the Green function method \( [11] \); after some algebra one obtains for the \( a \)-band Green function

\[ G_{kk',\sigma}^{\alpha a}(w) = \frac{\delta_{kk'}}{w - \varepsilon_k^{\alpha} - \Sigma^\sigma} + \frac{1}{w - \varepsilon_k^{\alpha} - \Sigma^\sigma T^\sigma(w, \Sigma^\sigma) - \frac{1}{w - \varepsilon_k^{\alpha} - \Sigma^\sigma}} \]

(3)

where

\[ F^\sigma(w) = \sum_k \frac{1}{w - \varepsilon_k^{\sigma} - \Sigma^\sigma(w)} \]

(7)

The self-energy \( \Sigma^\sigma \) is complex and spin dependent—thus giving a spin dependent band shift. The vanishing of the T-matrix gives a self-consistent equation for the self-energy:

\[ \Sigma^\sigma(w) = U < n_{0\sigma}^a > + \Sigma^\sigma(w)[U - \Sigma^\sigma(w)]F^\sigma(w). \]

(8)

It is important to stress that Eq. (8) results from a configuration average characteristic of a CPA approach and not from a dynamical constraint.

The Green function \( G_{kk',\sigma}^{\alpha a} \) then becomes

\[ G_{kk',\sigma}^{\alpha a}(w) = \frac{1}{w - \varepsilon_k^{\alpha} - \Sigma^\sigma(w)} \]

(9)

while \( G_{kk',\sigma}^{bb} \) is

\[ G_{kk',\sigma}^{bb}(w) = G_k^b(w) + V^2G_k^a(w)G_{kk',\sigma}^{aa}(w)G_{kk',\sigma}^{bb}(w) \]

(10)

with

\[ G_k^a(w) = \frac{1}{w - \varepsilon_k^a}, \]

(11)

the Green function of the bare \( b \) band.

In this expression

\[ \tilde{\varepsilon}_k^\alpha = \epsilon_k^\alpha + \frac{V_{ab}^2(k)}{w - \varepsilon_k^b}, \]

(4)

is the recursion relation of the \( a \) band including hybridization and

\[ \epsilon_k^\sigma = \frac{t_a (\cos(k_x a) + \cos(k_y a) + \cos(k_z a))}{A} \]

(5)

is the respective recursion relation of the bare band. In this paper we use \( t_a = 1 \) and \( A = 3 \), in arbitrary energy units. All energy magnitudes are taken in units of \( t_a \), making them dimensionless. The bare \( a \) band width is then \( W = 2 \). For simplicity we use \( \epsilon_k^b = \alpha \epsilon_k^a + \epsilon_s \) (homothetic bands), for the bare \( b \) band. \( \epsilon_s \) is the shift between the center of the bands. From now on we take \( k_1 a \rightarrow k_i, i = x, y, z \) and \( V_{ab} = V_{ba} \equiv V = \text{constant independent of } k_i \). The scattering \( T^\sigma \)-matrix in Eq.(3) is given by

\[ T^\sigma(w, \Sigma^\sigma) = \frac{U < n_{0\sigma}^a > + \Sigma^\sigma(w)[U - \Sigma^\sigma(w)]F^\sigma(w)}{[1 - (U - \Sigma^\sigma(w))F^\sigma(w)](1 + \Sigma^\sigma(w)F^\sigma(w))}. \]

(6)

The procedure presented here has some similarity to the one used in the Dynamical Mean-Field Theory (DMFT) \( [13] \) in the following sense: here the original lattice model with correlation in every site is replaced by an effective one, where the correlation is present only at the origin (‘the impurity’) but at the same dimension \( d = 3 \).

### III. NUMERICAL RESULTS AND CONCLUSIONS

In the numerical calculations one chooses the total number of electrons per site as being about \( n = 2.2 \), a little more than half-filling. We start with \( \langle n_{sp}^\uparrow \rangle = 0.52 \) and \( \langle n_{sp}^\downarrow \rangle = 0.45 \) in eq.(8), searching for a ferromagnetic solution in a less than half filled \( a \)-band. The dynamics generated by \( V \) and \( U \), then, redistributes the \( a \) and the \( b \) band electrons, mixing the up and down states eventually producing a magnetization. In ref.\( [1] \), however, the density of the correlated band, rather than \( n \), is kept fixed. For comparison, in figs \( [11] \) and \( [12] \), we took \( n = 2.2, \alpha = 1.5 \) and \( \epsilon_s = 1.0 \) while in fig \( [13] \), \( \alpha = 2.5, n = 2.0 \) and \( \epsilon_s = 1.0 \).

We found that, for a certain range of parameters \( U \) and \( V \), a ferromagnetic state (FS) develops. We then investigate the effect of \( V \) in this state, for a given \( U \) in the weak \( (U < W) \), in the intermediate \( (U \sim W) \) and in the strong coupling \( (U > W) \) limits. In fig \( [11] \) we...
FIG. 1: (Color online) Magnetization $m = < n^a_\uparrow > - < n^a_\downarrow >$ of the correlated a-band versus $V$ in a regime $U/W < 1$, namely, $U = 1$.

FIG. 2: (Color online) Magnetization $m = < n^a_\uparrow > - < n^a_\downarrow >$ of the correlated a-band versus $V$ in a regime $U/W \sim 1$, namely $U = 2$.

In the intermediate limit, e.g., $U = 2$, $U/W \sim 1$, as shown in fig(2), ferromagnetism is also observed; again increasing $V$ the metal tends to a non-magnetic state.

In fig(3) we exhibit the magnetization for a typical strong coupling situation, namely, $U = 5$. We notice that the decrease of the magnetization with $V$ is now slower than for smaller $U$.

We have shown that the present method is computationally feasible, producing reliable and physically sensible results compatible with the existing literature on this important subject, opening new insights concerning the possible $U/W$ regimes. Further work, for $T > 0$, and extending the model to include a two sublattice system in order to describe possible antiferromagnetic states, is in progress.

FIG. 3: (Color online) Magnetization $m = < n^a_\uparrow > - < n^a_\downarrow >$ of the correlated a-band versus $V$ in a regime $U/W > 1$, namely $U = 5$.

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