Cross effect of Coulomb correlation and hybridization in the occurrence of ferromagnetism in two shifted band transition metals

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Abstract

In this work we discuss the occurrence of ferromagnetism in transition-like metals. The metal is represented by two hybridized (V) and shifted (ς) bands one of which includes Hubbard correlation whereas the other is uncorrelated. The starting point is to transform the original Hamiltonian into an effective one. Only one site retains the full correlation (U) while in the others the correlations are represented by an effective field, the self-energy (single-site approximation). This field is self-consistently determined by imposing the translational invariance of the problem. Thereby one gets an exchange split quasi-particle density of states and then an electron-spin polarization for some values of the parameters (U, V, α, ς), α being the ratio of the effective masses of the two bands and of the occupation number n.

Key words: Ferromagnetic metal; Correlation; Single-site approximation;
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1. The model

In recent years the study of magnetism in itinerant ferromagnets such as Fe, Co, Ni has been the subject of a great deal of efforts by several approaches. Examples are the dynamical mean field theory (DMFT) [1] and the modified alloy analogy (MAA) [2]. In a previous work [3] we have developed a two band model, consisting of a Hubbard like narrow band (band a) with intrasite Coulomb interaction U, hybridized with another band, which is broad and uncorrelated (band b), through the hybridization coupling V_{ab}. The two bands had the same center (symmetric regime). Now we treat a more general situation, with a shift between the centers of the two bands.

We review briefly the method [3]: The initial Hamiltonian we adopt is then

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij}^a \tilde{a}_{i\sigma}^a \tilde{a}_{j\sigma}^a + \sum_{i,j,\sigma} t_{ij}^b \tilde{b}_{i\sigma}^b \tilde{b}_{j\sigma}^b + \sum_{i} U n_{i\uparrow}^a n_{i\downarrow}^a + \sum_{i,j,\sigma} (V_{ab} \tilde{b}_{i\sigma}^b \tilde{a}_{j\sigma}^a + \text{h.c.}) \right)$$

where $n_{i\sigma}^a = a_{i\sigma}^a a_{i\sigma}^a$; $\sigma$ denotes spin. $t_{ij}$ denotes the tunneling amplitudes between neighboring sites $i$ and $j$, in each band. As in Roth's approach [4], we reduce the presence of the correlation to only one site (the origin, say), while in the others acts an effective spin and energy dependent but site independent field, the self-energy $\Sigma_{\sigma}$. This field is self-consistently determined by imposing the vanishing of the scattering T matrix associated to the origin. We thus arrive at the effective Hamiltonian

$$\mathcal{H}_{eff} = \sum_{i,j,\sigma} t_{ij}^a a_{i\sigma}^a a_{j\sigma} + \sum_{i,j,\sigma} t_{ij}^b b_{i\sigma}^b b_{j\sigma} + \sum_{i,\sigma} n_{i\sigma}^a \Sigma_{\sigma} + U n_{0\uparrow}^a n_{0\downarrow}^a + \sum_{i,j,\sigma} (V_{ab} b_{i\sigma}^b a_{j\sigma} + \text{h.c.}) - \sum_{\sigma} n_{0\sigma}^a \Sigma_{\sigma},$$

$\mathcal{H}_{eff}$ still includes the difficulty of dealing with the Coulomb intra-atomic term at the origin. We use the Green function method [5]; the equations of motion for the corresponding Green functions $G_{i\uparrow}(w) = \langle \langle c_{i\sigma} d_{j\sigma}^+ \rangle > w$, where $c, d = a, b$, are...
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Green function, whose equation of motion, after the neglecting of the broadening correction[9] reduces to
\[ wG_{ij,\sigma}^{\alpha\alpha}(w) = \delta_{ij} + \sum_{l} t_{il}^{\alpha} G_{ij,\sigma}^{\alpha\alpha}(w) + \Sigma^{\alpha\alpha}_{ij,\sigma}(w) + \sum_{l} V_{ab}(R_{i} - R_{l}) G_{ij,\sigma}^{\alpha\alpha}(w) \]
where \( G_{ij,\sigma}^{\alpha\alpha}(w) = \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} = \Gamma_{ij,\sigma}^{\alpha\alpha}(w) \) is a higher order Green function, whose equation of motion, after neglecting the broadening correction, reduces to
\[ w\Gamma_{ij,\sigma}^{\alpha\alpha}(w) = \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} = \sum_{l} t_{il}^{\alpha} \Gamma_{ij,\sigma}^{\alpha\alpha}(w) + \Sigma^{\alpha\alpha}_{ij,\sigma}(w) + \sum_{l} V_{ab}(R_{i} - R_{l}) \Gamma_{ij,\sigma}^{\alpha\alpha}(w) \]
\[ + \delta_{ij}(U - \Sigma^{\alpha\alpha}_{ij,\sigma})(G_{ij,\sigma}^{\alpha\alpha}(w)) \]
The resonance broadening occurs, in the terminology of the alloy analogy (AA), when the opposite spin direction are not kept frozen. Some remarks are in order about Eq.(4). The scattering correction is already included; in the Hubbard terminology[10] of an AA of up and down spins, this correction would correspond to disorder scattering and produces a damping of the quasi-particles. Secondly, the hybridization generates a new function \( \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} \) and its equation of motion, again after neglecting the broadening correction, reduces to
\[ w \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} = \sum_{l} t_{il}^{\alpha} \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} + V_{ab}(R_{i} - R_{l}) \Gamma_{ij,\sigma}^{\alpha\alpha}(w) \]
At this point we have an effective impurity problem; the
direction of the impurity spin is not fixed.

We solve explicitly the problem defined by Eq.(3),
Eq.(4) and Eq.(5), obtaining, after imposing \( T = 0 \), the following Green function for the \( a \) band:
\[ G_{kk',\sigma}^{\alpha\sigma}(w) = \frac{\delta_{kk'}}{w - \epsilon_{k}^{\alpha} - \Sigma^{\alpha\sigma}(w)} \]
In this equation
\[ \epsilon_{k}^{\alpha} = \epsilon_{k}^{\alpha} + \frac{|V_{ab}|^{2}(k)}{w - \epsilon_{k}^{\alpha}} \]
is the recursion relation of the \( a \) band modified by the
hybridization \( V \) and \( \epsilon_{k}^{\alpha} \) and \( \epsilon_{k}^{\beta} \) denote the bare bands, with
\[ \epsilon_{k}^{\alpha} = \frac{t_{a}(\cos(k_{x}a) + \cos(k_{y}a) + \cos(k_{z}a))}{A} \]
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 adopt homothetic bands
\[ \epsilon_{k}^{\alpha} = \epsilon_{s} + \alpha \epsilon_{k}^{a} \]
\( \epsilon_{s} \) is the center of the \( b \) band; as the \( a \) band is centered at the origin, this parameter represents a shift in the bands. \( \alpha \) is a phenomenological parameter describing the ratio of the effective masses of the \( a \) and the \( b \) electrons. From now on we take \( k_{a} \rightarrow k_{i}, i = x, y, z \) and \( V_{ab} = V_{ba} \equiv V \) = real and constant independent of \( k_{i} \).

The vanishing of the T-matrix gives further a self-consistent equation for the self-energy:
\[ \Sigma^{\alpha\sigma} = U \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} + (U - \Sigma^{\alpha\sigma}) F^{\sigma}(w, \Sigma^{\sigma}) \Sigma^{\alpha\sigma}, \]
with
\[ F^{\sigma}(w, \Sigma^{\sigma}) = N^{-1} \sum_{k} G_{kk,\sigma}^{\alpha\sigma} \]

2. Numerical Results

We perform the self-consistency in both \( \Sigma^{\alpha} \) and in
\( \langle< n_{0\sigma} a_{\sigma}^{+} >_{\sigma} \rangle_{w} \), for each total occupation \( n = \langle< n_{a} > \rangle_{w} < \langle< n_{b} > \rangle_{w} \).
The total number of electrons per site, is fixed at \( n = 1.6 \) (but see below), a little less than half-filling. We want now to exhibit the combined effect of \( U, V, \alpha, n, \) and \( \epsilon_{s} \) at \( T = 0K \).

In fig 1 we plot magnetization versus V. It is clear that small values of \( V \) help stabilize the ferromagnetic order but larger ones tend to inhibit it [2]. This is because hybridization, apart from changing the occupations of the \( a \) and \( b \) bands, together with the \( \epsilon_{s} \) increases (small \( V \)) and decreases (large \( V \)) the a-density of states at the Fermi level.

In fig 2 the magnetization is plot versus \( \epsilon_{s} \). We see that
the shift then tends to favor ferromagnetism.

In fig 3 we plot the charge transference \( a - b \) or vice-versa as function of \( \epsilon_{s} \) and it is seen that from \( \epsilon_{s} \approx 0.8 \) on, this transference increases the number of \( a \) electrons thus tending to favor ferromagnetism.

\[ \text{Fig. 1. Magnetization versus hybridization V for } U = 3, \alpha = 1.5, n = 1.6 \text{ and } \epsilon_{s} = 1.0. \text{ Small values of hybridization tend to favor ferromagnetism.} \]

In fig 4 one exhibits the dependence of the magnetization on the ratio of the effective masses between the correlated and the uncorrelated bands. We argue that the increasing of \( \alpha \) is proportional to a decreasing of the effective
Fig. 2. Magnetization versus band shift for $U = 3, V = 0.4, \alpha = 1.5$ and $n = 1.6$. Larger values of the band shift tend to favor ferromagnetism.

Fig. 3. Charge transference versus band shift for $U = 3, V = 0.4, \alpha = 1.5$ and $n = 1.6$.

Fig. 4. Magnetization versus $\alpha$, the band width relation for $U = 3, V = 0.4, n = 1.6$ and $\epsilon_s = 1.0$. Small values of hybridization tend to favor ferromagnetism.

Fig. 5. Magnetization versus total occupation $n$ for $U = 3, V = 0.4, \alpha = 1.5$ and $\epsilon_s = 1.0$.

In fig (4) we present the density of states (DOS) of the $a$-band for $U = 3, V = 0.4$ and $\epsilon_s = 1.0$. The Fermi level is at $E_F = 0.443$ and a magnetization of 0.174 arises. The combined effect of hybridization and the band shift produces a band broadening. The DOS here obtained exhibits a bimodal structure characterizing a Hubbard strongly correlated regime.

In fig (5) we show the density of state (DOS) of the uncorrelated $b$ band, for the same set of parameters, namely $U = 3, V = 0.4, \alpha = 1.5$ and $\epsilon_s = 1.0$. We verify that the renormalized band remains almost unchanged when compared with the bare one. In fact, hybridization affects this band, enlarging it, but no noticeable $b$ magnetic moment arises. Moreover, it does not present a bimodal structure.

For the sake of completeness we display in fig (6) a situation involving the weak correlation regime, $U/W << 1$. Now
3. Final comments

The traditional view of the origin of ferromagnetism in metals has been under intense scrutiny recently [1][2][8][9]. Conventional mean-field calculations favor ferromagnetism but corrections tend to reduce the range of validity of that ground state [9]. In this paper, using the single site approximation, we obtain ferromagnetic solution for a set of parameters (e.g. $U/W = 1.5$, $V/W = 0.2$, $\epsilon_s = 1.0$ and $\alpha = 1.5$).

As a continuation of this systematic study, the generation of the phase diagram [10] for the model is in progress.

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