Stabilization of d-Band Ferromagnetism by Hybridization with Uncorrelated Bands

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We investigate the influence of s-d or p-d hybridization to d-band ferromagnetism to estimate the importance of hybridization for the magnetic properties of transition metals. To focus our attention to the interplay between hybridization and correlation we investigate a simple model system consisting of two non-degenerated hybridized bands, one strongly correlated, the other one quasi-free. To solve this extended Hubbard model, we apply simple approximations, namely SDA and MAA, that, concerning ferromagnetism in the single-band model, are known to give qualitatively satisfactory results. This approach allows us to discuss the underlying mechanism, by which d-band ferromagnetism is influenced by the hybridization on the basis of analytical expressions. The latter clearly display the order and the functional dependencies of the important effects. It is found, that spin-dependent inter-band particle fluctuations cause a spin-dependent band shift and a spin-dependent band broadening of the Hubbard bands. The shift stabilizes, the broadening tends to destabilize ferromagnetism. Stabilization requires relatively high band distances and small hybridization matrix elements. Super-exchange and RKKY coupling are of minor importance.

I. INTRODUCTION

The issue of magnetism in band-ferromagnets like Fe, Co and Ni is far from being settled. Magnetism in these materials is due to correlations within itinerant electron bands. The simplest model that comprises this aspects is the single-band Hubbard model. Although it was introduced to gain a first qualitative understanding of band-ferromagnetism, it took almost 30 years to answer the question whether it is a generic model for ferromagnetism at all. About ten years ago a Dynamical Mean Field Theory (DMFT) was developed, which allows a consistent (mean field) description of the whole parameter range of the single-band Hubbard model. DMFT-based calculations confirmed the existence of ferromagnetism for a wide parameter range. Today there is a general consensus that the single-band Hubbard model exhibits ferromagnetism. There is also consensus, however, that this model oversimplifies the situation in band-ferromagnets, for instance by restricting the correlations to the on-site elements. But an even more drastic simplification is the restriction to a single non-degenerated electron band. The fivefold degeneracy of the d-electrons certainly influences the magnetic properties of the system. Consequently, a lot of effort is being done by transferring certain treatments, once developed for the single-band model, to multi-band models. Let us mention Gutzwiller approximation or various treatments within the DMFT-framework.

Besides the degeneracy of the d-electrons, the single-band model also neglects weakly correlated s- and p-bands, although they are located around the Fermi energy in 3d transition-metals. The interplay between correlated and uncorrelated electrons is known to give rise to a variety of phenomena such as the Kondo effect or heavy fermions and is the central point of widely used models like the Anderson model. In the case of the periodic Anderson model (PAM), correlations in combination with the hybridization to an uncorrelated band can cause ferromagnetism as shown rigorously for the one-dimensional case at quarter filling. This indicates that uncorrelated bands may influence the magnetic phase diagram of the Hubbard model, too, and this is most likely if the band distance is smaller than the on-site Coulomb energy (charge transfer regime). Recent experiments indeed seem to indicate that ferromagnetism can be stabilized if additional p-orbitals are doped into a RECo2-system(RE = Ho, Er). The aim of this paper is to decide, whether the neglect of s- and p-bands is justified when modeling band-ferromagnets like Fe, Co, or Ni. The influence of the hybridization of d-electrons with these orbitals shall be investigated systematically.

The paper is organized as follows. In the next section a suitable Hamiltonian is formulated and we try to give a qualitative overview of the interplay between the two different kinds of electrons. In section II we will apply certain approximations to the Hamiltonian. Thereby we will try to get as much insight as possible into the mechanisms, by which the d-band magnetism is altered. While the above mentioned DMFT-based treatments give certainly reliable values for magnetic properties, it is challenging to give a direct physical meaning to auxiliary quantities used in this theory (e.g. the energy- and spin-dependent hybridization function). For these reasons we will formulate the much simpler Hubbard-I decoupling (Hu-I), the spectral density approcimation (SDA) and the modified alloy analogy (MAA) for the described multi-band model. These theories are conceptually restricted to high energy excitations in the strong coupling regime. This is, however, the interesting case concerning band-ferromagnetism. For the single-band model in the limit of infinite spatial dimensions the theories are thoroughly tested against numerical exact results available in this limit. It is found that the SDA as well as the MAA systematically overestimate magnetic quantities such as the Curie temperature but turn out to give a qualitative satisfying description of band-ferromagnetism. For our
purpose the main advantage of these theories is the possibility for analytical estimations. In section IV the main results concerning the p-band influence on ferromagnetism are shown. Within the SDA we will derive analytical expressions for the quasiparticle band structure in the strong coupling limit. This allows a vivid physical interpretation of the mechanism by which the properties of the correlated subsystem are influenced by uncorrelated bands. We will see that the main impact is due to spin dependent inter-band fluctuations, which may enhance or reduce the spin asymmetry of the interacting density of states. Finally we discuss alternative mechanisms that involve the new states, like superexchange and RKKY-coupling.

II. GENERAL CONSIDERATIONS

We want to study the influence of weakly correlated bands to d-band ferromagnetism within the following extension of the single-band Hubbard model:

\[ H = \sum_{ijkl} (T_{ij}^d - \mu) d_{ij \sigma}^d d_{kl \sigma}^d + \frac{U}{2} \sum_{i} n_{i \sigma}^d n_{i \bar{\sigma}}^d \]

\[ + \sum_{ijkl} (T_{ij}^p - \mu) p_{i \sigma}^+ p_{j \sigma}^+ + V \sum_{i} (d_{i \sigma}^+ p_{i \sigma} + p_{i \sigma}^+ d_{i \sigma}) (1) \]

This Hamiltonian is similar to those used e.g. in reference 4 and reduces to the periodic Anderson model (PAM) in the limit \( T_{ij}^d \to 0 \) for \( i \neq j \). The weakly correlated electrons are described by a quasi-free "p-band", with the hopping integrals \( T_{ij}^p \), while the single-band Hubbard model describes the d-system. \( T_{ij}^d \) are the hopping integrals within the d-band and \( U \) is the local Coulomb interaction. The bands are coupled by a hybridization \( V \). The hopping integrals are the Fourier transformed Bloch energies and \( \mu \) denotes the chemical potential. The free band structure \( \epsilon_k^d \) shall be the result of a tight-binding approximation. The relative position of the bands is characterized by two parameters: The difference of the free centers of gravity \( \Delta T_0 \) and the ratio of the free band widths \( \alpha \):

\[ \Delta T_0 = T_0^p - T_0^d \quad \alpha = \frac{W_0^p}{W_0^d}. \]

\[ T_0^p,d = T_0^{p,d} \]

are the centers of gravity of the free bands. To achieve a realistic description of transition metals we choose \( \alpha > 1 \) and \( \Delta T_0 > 0 \). As a consequence of the tight binding approximation the dispersions are connected via

\[ \epsilon_k^p = T_0^p + \alpha \cdot (\epsilon_k^d - T_0^d) \]

Let us now discuss the possible influences of the p-band on the d-system within this model. First of all, there is a rather trivial particle number effect. Magnetism depends sensitively on the d-particle density. If now the new band is added while the total particle number in the system stays fixed, the electron density within the correlated subsystem is changed. The same holds if the parameters \( V \) or \( \Delta T_0 \) are tuned. We do not want to address these effects here. Note, that our intention is not to describe effects resulting from an experimental tuning of the hybridization strength, e.g. by applying pressure. Rather we want to decide if the neglect of the s-p-d hybridization is a good approximation for many body model calculations. In this context it is assumed that even when the s- and p-electrons are neglected the correct d-particle number per site is used. This generally non-integer number is already the result of the hybridization to other bands. Thus we will regard this case (where the change of the d-particle number due to the hybridization is already considered) and the case of an explicitly treated hybridization (where additionally all other effects resulting from the two-band situation are taken into account). To compare these cases properly we have to fix the d-particle density in our calculations. What further effects can be expected? Naively, one would believe that an uncorrelated and therefore a priori "non-magnetic" p-band would destabilize ferromagnetism by "reducing the average correlation". This reasoning, however, is too simple. Particle fluctuations between the bands will influence the propagation of electrons within the d-band and thus the d-projected density of states. It is known that ferromagnetism depends sensitively on the total density of states. This effect will be most important if the fluctuation rate is spin-dependent. This would cause different alterations of the spin-up and spin-down density of states and directly influence its spin asymmetry.

Let us look at this mechanism in the trivial limiting case of uncorrelated bands \( U \to 0 \). For small hybridizations the excitation energies are:

\[ E_{k1}(V) = \epsilon_k^d - \frac{V^2}{|\epsilon_k^p - \epsilon_k^d|} \]

\[ E_{k2}(V) = \epsilon_k^p + \frac{V^2}{|\epsilon_k^p - \epsilon_k^d|} \]

For the lower band \( E_{k1}(V) \) this causes a band asymmetry, a band shift to lower energies, and a band broadening in the quasiparticle density of states. For non-overlapping bands, i.e. \( \Delta T_0 > \max(\epsilon_k^p - T_0^p) \), we insert (3) into (4) and expand \( E_{k1}(V) \) in powers of \( \frac{(\alpha-1)(\epsilon_k^d - T_0^d)}{\Delta T_0^d} \). Equation (4) becomes

\[ E_{k1}(V) = T_0^d + \Delta T_0^d + (\epsilon_k^d - T_0^d) \cdot x_V^d \]

with the band shift

\[ \Delta T_0^d = -\frac{V^2}{\Delta T_0^d} \]

and the band broadening factor

\[ x_V^d = 1 + \frac{V^2}{\Delta T_0^d} (\alpha - 1) \]
The broadening as well as the shift are also present if the $d$-electrons are correlated as can be seen by studying a two-site cluster out of (1) with the inter-site hoppings $t^d$ and $t^p = \alpha \cdot t^d$. For small $V$ one can perform a canonical transformation that decouples the $p$- and $d$-band in first order in $V$. The calculation is lengthy but straightforward. For $U \to \infty$, $\Delta T_0 > t^{(p,d)}$, and $T_0^p < \mu < T_0^d$ the $d$-electrons are well approximated by a two-site Hubbard Hamiltonian with a renormalized center of gravity $\hat{d}$ which fulfill the following equations of motion

\[ \tilde{T}_0^d(V) = T_0^d - \frac{V^2}{\Delta T_0} \]
\[ \tilde{T}^d(V) = t^d(1 + \frac{V^2}{\Delta T_0} (\alpha - 1)) \]
\[ \tilde{U}(V) = U + \frac{V^2}{\Delta T_0} \].

The broadening as well as the shift is clearly recognized in (8). Our preceding, qualitative considerations indicate that inter-band particle fluctuations indeed modify the $d$-projected density of states. These modifications are expected to influence also the magnetic properties. Up to now we only investigated spin-symmetric limiting cases allowing only a spin symmetric fluctuation rate. Regarding ferromagnetism it will be most important whether one of the effects becomes spin-dependent in the full system.

III. THEORY

The magnetic properties of (1) can be studied using retarded single electron Green functions

\[ G^p_{\sigma \sigma} = \langle \langle \hat{n}_{\sigma \sigma} \rangle \rangle \quad G^{pp}_{\sigma \sigma} = \langle \langle \hat{p}_{\sigma \sigma} \rangle \rangle \]
\[ G^{dp}_{\sigma \sigma} = C^{dp}_{\sigma \sigma} = \langle \langle \hat{d}_{\sigma \sigma} \hat{p}_{\sigma \sigma} \rangle \rangle = \langle \langle \hat{p}_{\sigma \sigma} \hat{d}_{\sigma \sigma} \rangle \rangle \],

which fulfill the following equations of motion [2]:

\[ E_{\Sigma_{k\sigma}^{dd}} = 1 + (\epsilon_k^d - \mu)G_{\sigma \sigma}^{dd} + \Sigma_{k\sigma}G_{\sigma \sigma}^{dd} + V G_{\sigma \sigma}^{dp} \]
\[ E_{\Sigma_{k\sigma}^{pd}} = (\epsilon_k^d - \mu)G_{\sigma \sigma}^{dp} + V G_{\sigma \sigma}^{dd} \]
\[ E_{\Sigma_{k\sigma}^{pp}} = 1 + (\epsilon_k^p - \mu)G_{\sigma \sigma}^{pp} + V G_{\sigma \sigma}^{dp} \].

The self-energy $\Sigma_{k\sigma}$ is introduced as usual via

\[ \Sigma_{k\sigma}G_{\sigma \sigma}^{dd} = \langle [\hat{d}_{\sigma \sigma}, \frac{U}{2} \sum_{\sigma} n_{\sigma \sigma}^d n_{\bar{\sigma} \bar{\sigma}}^d \hat{n}_{\bar{\sigma} \bar{\sigma}}^d \hat{a}_{\bar{\sigma} \bar{\sigma}}^d \hat{d}_{\sigma \sigma}] \rangle \]

where $[\ldots , \ldots , \ldots]$ denotes the commutator. Solving (11) gives all Green functions:

\[ \left( \begin{array}{cc} C_{\sigma \sigma}^{dd} & C_{\sigma \sigma}^{dp} \\ C_{\sigma \sigma}^{dp} & C_{\sigma \sigma}^{pp} \end{array} \right)^{-1} = \left( \begin{array}{cc} E - \epsilon_k^p & -V \\ -V & E - \epsilon_k^d - \Sigma_{k\sigma} \end{array} \right) \].

where $\epsilon_k^\prime$ is used as an abbreviation for $\epsilon_k - \mu$. In the ferro- and paramagnetic phase we can calculate the spin-dependent average occupation numbers $n_{\sigma \sigma}^d = \langle n_{\sigma \sigma}^d \rangle$ and $n_{\sigma \sigma}^p = \langle n_{\sigma \sigma}^p \rangle$ using the Green functions (11):

\[ n_{\sigma}^{(p,d)} = \frac{1}{\pi} \int_{-\infty}^{\infty} dE f_-(E) G_{\bar{\sigma} \bar{\sigma}}^{pp}(E - \mu) \].

$f_-(E)$ is the Fermi function and $G_{\bar{\sigma} \bar{\sigma}}^{pp}$ are the local Green functions.

Obviously we can calculate the phase boundary between para- and ferromagnetism as soon as we have found an (approximate) expression for the self-energy.

To this aim we will formulate the Hu-I, SDA, and MAA for the two-band problem (3). By comparing the influence of the hybridization within different approximations we can minimize the risk of an artificial $p$-band influence. The two "simple" approximations Hu-I and SDA can give an excellent insight into the working mechanisms. Due to their explicit structure of the self energy, one can perform some demonstrative analytical estimations. The SDA gives qualitatively convincing results concerning ferromagnetism. This is due to the fact that it reproduces the correct values for the centers of gravity and weights of the Hubbard bands in the strong coupling limit $U \to \infty$. Compared to Hu-I, an additional correlation function is considered that describes the itineracy of electrons of opposite spin direction and allows for a spin-dependent band shift. The MAA is a first systematic improvement of the SDA, since it allows quasiparticle damping, which is completely neglected within the SDA. By comparing MAA- and SDA-results one can see, if the mechanisms derived within the SDA are also present in a more complex theory.

Hubbard-I decoupling: Let us start with the Hubbard-I approximation. Straightforward decoupling of the real space equations of motion in (1) yields the Hu-I self-energy

\[ n_{\Sigma_{\sigma}} = U n_{\sigma}^d - \frac{E - T_0^d + \mu - U (1 - n_{\sigma}^d)}{E - T_0^d + \mu - U (1 - n_{\sigma}^d)} \]

which is formally identical to the single-band case. The self-energy is $V$-dependent via $n_{\sigma}^d$, which is calculated using (11) and (4). Equation (13) gives three excitation energies in every point of the Brillouin-zone, corresponding to the three-peak structure of the spectral density in the atomic limit $V \to 0; V_{ij} \to 0$. Finite values of the hopping and hybridization change the positions and weights of the $\delta$-peaks and lead to a mixing of $p$- and $d$- spectral density.

SDA For the single-band model, the SDA is the simplest theory that yields the correct strong coupling and high energy behaviour, which seems to be decisive for the existence of ferromagnetism. The general structure of the spectral density and the self-energy is the
same as in *Hu-I*. The energy-positions and weights of the δ-peaks in the spectral density are obtained by fitting it to the first four spectral moments:

\[
\begin{align*}
\frac{dd M_{k\sigma}^{(m)}}{E_n}&= \int_{-\infty}^{\infty} dE E^m S_{k\sigma}^{dd}(E) \\
&= \langle \{[[[d_{k\sigma}, H] \ldots H] \ldots H] \ldots d_{k\sigma}^+ \} \rangle .
\end{align*}
\]

\[\text{[......]} \] is the anti-commutator. For the two-band model we will apply this concept directly to the self-energy rather than to the spectral density. Therefore we choose the same structure as in (14) for a self-energy ansatz:

\[
SDA \Sigma_{k\sigma} = \gamma \frac{E - \gamma_2}{E - \gamma_3} .
\]

The parameters \(\gamma_i\) shall now be fitted to the spectral moments. To this end we expand the Green function and the self-energy with respect to powers of \(\frac{1}{E}\):

\[
G_{k\sigma}^{dd} = \sum_{n=0}^{\infty} \frac{dd M_{k\sigma}^{(n)}}{E^{n+1}}, \quad \Sigma_{k\sigma} = \sum_{n=0}^{\infty} \frac{C_{k\sigma}^{(n)}}{E^n} ,
\]

(15)

The high-energy coefficients of the Green function are the spectral moments (14). This can easily be seen by expanding the spectral representation of the Green function

\[
G_{k\sigma}^{dd}(E) = \int_{-\infty}^{\infty} dE' \frac{S_{k\sigma}^{dd}(E')}{E - E' + i0^+}
\]

with respect to \(\frac{1}{E}\) and comparing the resulting expressions with the definition of the moments (14). The self-energy coefficients \(C_{k\sigma}^{(n)}\) are obtained as functions of the moments \(dd M_{k\sigma}^{(0)} \ldots dd M_{k\sigma}^{(n+1)}\) by inserting the expansions (13) into (11) (or equivalently into the Dyson equation) and by comparing the coefficients of the \(\frac{1}{E}\) terms. With the r.h.s. of (14), we find the first four correlated spectral moments:

\[
\begin{align*}
\frac{dd M_{k\sigma}^{(0)}}{E_n} &= 1 \\
\frac{dd M_{k\sigma}^{(1)}}{E_n} &= \epsilon_k + U n_{-\sigma}^d \\
\frac{dd M_{k\sigma}^{(2)}}{E_n} &= (\epsilon_k^d)^2 + 2Un_{-\sigma}^d \epsilon_k^d + U^2 n_{-\sigma}^d + V^2 \\
\frac{dd M_{k\sigma}^{(3)}}{E_n} &= (\epsilon_k^d)^3 + 3U n_{-\sigma}^d (\epsilon_k^d)^2 + U^2 (2n_{-\sigma} + (n_{-\sigma}^d)^2) \\
&\quad+ U^2 n_{-\sigma}^d (1 - n_{-\sigma}^d) (B_{2-band}^2 + T_0') \\
&\quad+ U^3 n_{-\sigma}^d + V^2 (2\epsilon_k^d + \epsilon_k^p + 2Un_{-\sigma}^d) .
\end{align*}
\]

(16)

The self-energy coefficients read:

\[
\begin{align*}
C^{(0)}_{k\sigma} &= U n_{-\sigma}^d \\
C^{(1)}_{k\sigma} &= U^2 n_{-\sigma}^d (1 - n_{-\sigma}^d) \\
C^{(2)}_{k\sigma} &= U^2 n_{-\sigma}^d (1 - n_{-\sigma}^d) (B_{2-band}^2 + T_0' + U(1 - n_{-\sigma}^d)) .
\end{align*}
\]

\(B_{2-band}^2 = B_{2b}^2 + F_{2b}^2\) is a higher correlation function with the local part \(B_{2b}^2\) and a \(k\)-dependent part \(F_{2b}^2\). For the single-band model, the influence of both terms is discussed in detail in reference [1]. It turns out that the most important term is the local \(B_{2}\), which leads to a spin-dependent band shift in the ferromagnetic phase. With regard to ferromagnetism the non-local part \(F_{2b}\) seems to be of minor importance. Therefore we will neglect it in the following. From (14) we find for the local part \(B_{2b}^2\):

\[
\begin{align*}
B_{2b}^2 &= \frac{1}{n_{-\sigma}^d (1 - n_{-\sigma}^d)} \left( \frac{1}{N} \sum_{ij} \left( T_{ij}^d (d_{i\sigma}^+ d_{j\sigma} (2n_{-\sigma}^d - 1)) + 2V \sum_{ij} (T_{ij}^p - T_{ij}^d) \langle d_{i\sigma}^+ p_{j\sigma} \rangle - V \langle d_{i\sigma}^+ p_{j\sigma} \rangle \right) \right) .
\end{align*}
\]

Although \(B_{2b}^2\) contains expectation values of the uncorrelated band and higher correlation functions, it can be expressed as a functional of the correlated single-electron Green function only:

\[
\begin{align*}
B_{2b}^2 &= \frac{- n_{\sigma}^d - n_{\sigma}^d}{n_{\sigma}^d (1 - n_{\sigma}^d)} \int_{-\infty}^{\infty} dE j_{-\sigma}(E) \left( \frac{2\Sigma_{\sigma}(E)}{U} \right) - 1 .
\end{align*}
\]

(17)

The correlation-function \(B_{2b}^2\) and the self-energy coefficients \(C_{\sigma}^{(0:1:2)}\) turn out to be the same functional as the correlated Green function \(G_{\sigma}^{dd}\) as in the single-band model. While determining the self-energy coefficients, the whole \(V\)-dependence in the moments \(dd M_{k\sigma}^{(0)} \ldots dd M_{k\sigma}^{(n+1)}\) (16) is cancelled by the explicit \(V\)-dependence of the correlated Green function (11). Thus, like in the *Hu-I* approximation, the SDA self-energy is formally identical to the single-band case:

\[
\begin{align*}
SDA \Sigma_{\sigma} &= \frac{U n_{-\sigma}^d}{E - T_0 + \mu - B_{2b}^2} E - T_0 + \mu - B_{2b}^2 - U(1 - n_{-\sigma}^d) .
\end{align*}
\]

The \(V\)-dependence comes again into play by the expectation values \(n_{-\sigma}^d\) and \(B_{2b}^2\) being evaluated via (14), (13), and (17).

**MAA**

Besides the restriction to strong interaction strengths a drawback of SDA and *Hu-I* is the exclusion of scattering processes, which lead to quasiparticle damping. The correlated \(d\)-system is described by two quasiparticles with infinite lifetime corresponding to singly or doubly occupied sites. One possibility to include quasiparticle damping is the description of the system by a fictitious alloy (alloy analogy) which is a standard method in many-body physics.[3] With this approach one can account for electron scattering at the potentials formed by the distribution of the
electrons of opposite spin direction. Main excitation energies of the many body system are modelled by atomic energy levels of a fictitious alloy. Correlation effects are then described by the properties of this alloy and its self-energy is identified with the self-energy of the many body problem. Since the self-energy of electrons exclusively characterizes correlated electrons, we will only describe the correlated subsystem by a fictitious alloy. In the strong coupling limit we have two main excitation energies within the correlated subsystem. Consequently we will describe it by a two-component alloy. The resulting effective alloy problem can be solved by the Coherent Potential Approximation (CPA), which yields the CPA self-energy

\[ 0 = \sum_{p=\sigma} x_{p\sigma} \frac{E_{p\sigma} - T^{d}_0 - \sigma(E)}{1 - G^{dd}_{i\sigma}(E)(E_{p\sigma} - \sigma(E) - T^{d}_0)}. \]  

(18)

\( E_{p\sigma} \) and \( x_{p\sigma} \) are the atomic energy-levels and concentrations of the alloy components. The CPA, being a single-site theory, gives a local self-energy \( \Sigma_\sigma \). After rearranging the terms and setting

\[ \gamma_1 = x_{1\sigma}(E_{1\sigma} - T^{d}_0) + x_{2\sigma}(E_{2\sigma} - T^{d}_0) \]

\[ \gamma_2 = \frac{(E_{1\sigma} - T^{d}_0)(E_{2\sigma} - T^{d}_0)}{\gamma_1} \]

\[ \gamma_3 = x_{1\sigma}(E_{2\sigma} - T^{d}_0) + x_{2\sigma}(E_{1\sigma} - T^{d}_0) \]

, equation (18) becomes

\[ \Sigma_\sigma(E) = \gamma_1 \frac{1 + G^{dd}_{i\sigma}(E)(\Sigma_\sigma(E) - \gamma_2)}{1 + G^{dd}_{i\sigma}(E)(\Sigma_\sigma(E) - \gamma_3)} \].

(19)

Here \( x_{1\sigma} + x_{2\sigma} = 1 \) is already used. To complete the theory, we now have to adjust the parameters \( \gamma_1, \gamma_2, \) and \( \gamma_3 \). Similar to the SDA these parameters can be fitted to the on-site spectral moments \( M^{(m)}_{i\sigma} \) and on-site self-energy coefficients \( G^{(m)}_{i\sigma} \). The two latters are defined analogously to \( M^{\alpha}_{i\sigma} \) and \( C^{\alpha}_{i\sigma} \) (14). To this purpose one has to expand the local Green function \( G^{dd}_{i\sigma} \) and the local self-energy \( \Sigma_\sigma \) in powers of \( n \) analogously to (13). Then one inserts these expansions into (14) and compares the coefficients of the \( \frac{1}{n} \)-terms up to \( n = 2 \). Using the abbreviation \( \Sigma_{AA} \rightarrow \Sigma_\sigma \), we finally find for the MAA self-energy:

\[ \Sigma_\sigma = U n^d \frac{(G^{dd}_{i\sigma})^{-1} + \Sigma_\sigma - B_{2b}^d}{(G^{dd}_{i\sigma})^{-1} + \Sigma_\sigma - B_{2b}^d - U(1 - n^d)}. \]

This is again, as in \( Hu-I \) and SDA, formally identical to the single-band expression, i.e. the self-energy is the same functional of the correlated Green function as in the single-band case. The self-energy is \( V \)-dependent via \( G^{dd}_{i\sigma} \) and the expectation-values \( n^d \) and \( B_{2b}^d \).

The MAA self-energy is still consistent with the high-energy limit and additionally allows for quasiparticle damping, thus being a systematic improvement of the SDA [3].

**IV. RESULTS AND DISCUSSION**

Keeping in mind the scope of the theories used in our approach, we will now investigate the influence of the additional \( p \)-band. In reference [4] these theories are thoroughly evaluated. To gain the best possible comparison with these calculations, we choose the same lattice structure (fcc-tight-binding, \( d \rightarrow \infty \), after particle-hole transformation) for our investigations of the two-band model. The density of states reads

\[ \rho^{(0)}(E) = \frac{e^{-(1 + \sqrt{2}E/t^*)/2}}{t^* \sqrt{\pi(1 + \sqrt{(2)E/t^*)}}}. \]

(20)

In the following all energies will be given in units of \( t^* \). The density of states exhibits a divergence at the lower band edge. This feature is known to stabilizes ferromagnetism. The main trends regarding the influence of the hybridization are also present in other lattice structures (e.g. sc or bcc tight-binding). Ferromagnetism, however, is most certain within the fcc-lattice [4]. Fig. 1 and Fig. 2 show the quasiparticle densities of states calculated with SDA and MAA for different values of \( V \) in the paramagnetic case. In both theories the QDOS consists of two Hubbard-bands and the uncorrelated band. These bands move apart with rising \( V \) while the correlated sub-bands are broadened. One can see that the band shifts are proportional to \( V^2 \), which agrees perfectly with the results for free bands [5, 6, 7] and the two-site cluster [5].

Fig. 2 displays the lower Hubbard band (SDA) of the correlated density of states in the ferromagnetic case. It turns out, that the hybridization-caused band shift is in fact spin-dependent in the ferromagnetic phase. The shift is larger for majority-spin electrons. The magnetic prop-
properties can thus be changed drastically due to the presence of the uncorrelated band. Within the framework of the SDA we can derive analytical expressions for the shift and the broadening by calculating the poles of \( \Sigma_{k\sigma} = \Sigma_{SDA} \). For \( U \to \infty \) we find:

\[
\begin{align*}
E_{1k\sigma}^{SDA} &= T_0^d + U + (\epsilon_k^d - T_0^d)n_{-\sigma}^d + B_{-\sigma}^{2b}(1 - n_{-\sigma}^d) \\
E_{2k\sigma}^{SDA} &= \epsilon_k^d + V^2X_{k\sigma} \\
E_{3k\sigma}^{SDA} &= T_0^d + (\epsilon_k - T_0^d)(1 - n_{-\sigma}^d) + B_{-\sigma}^{2b}n_{-\sigma}^d - V^2X_{k\sigma}
\end{align*}
\]

where

\[
V^2X_{k\sigma} = V^2\frac{1 - n_{-\sigma}^d}{\epsilon_k^p - T_0^d - (\epsilon_k^d - T_0^d)(1 - n_{-\sigma}^d) - B_{-\sigma}^{2b}n_{-\sigma}^d}
\]

describes the whole influence of the hybridization. The other terms are the well-known SDA-result for the single-band Hubbard model. For band fillings smaller than unity, the most important energies are \( E_{3k\sigma} \) forming the lower Hubbard-band. For non-overlapping bands (i.e. \( \Delta T_0^c > \max(\epsilon_k^d - T_0^d) \)), we can rewrite \( E_{3k\sigma}^{SDA} \) in terms of a band shift \( \Delta T_{V\sigma} \) and a band broadening factor \( x_{V\sigma} \)

\[
E_{3k\sigma}^{SDA} = T_0^d + \Delta T_{V\sigma} + n_{+\sigma}^d B_{+\sigma}^{2b} + (\epsilon_k^d - T_0^d)(1 - n_{-\sigma}^d) \cdot x_{V\sigma}
\]

Both are spin dependent:

\[
\begin{align*}
\Delta T_{V\sigma} &= -\frac{V^2}{\Delta T_0^c - n_{+\sigma}^d B_{+\sigma}^{2b}}(1 - n_{-\sigma}^d) \\
x_{V\sigma} &= 1 + \frac{V^2}{(\Delta T_0^c - n_{+\sigma}^d B_{+\sigma}^{2b})^2}(\alpha - 1 + n_{-\sigma}^d)\tag{21}
\end{align*}
\]

\( \alpha \) is the ratio of the free band widths as defined in \( H_{MAA} \). Thus an hybridization with an uncorrelated band causes alterations in the band structure similar to the non-interacting case \( \Sigma_{k\sigma} = \Sigma_{\sigma} \), i.e. a band shift and a band broadening for the correlated sub-band. The important difference is the spin dependence of both quantities in the full system. Equation (21) describes two competing effects. The shift to lower energies \( \Delta T_{V\sigma} \) supports magnetism since it is larger for majority-spin electrons. The band broadening \( x_{V\sigma} \), in contrast, destabilizes magnetism, since broader bands are known to be inconvenient for band-ferromagnetism. In addition, the spin dependence of \( x_{V\sigma} \) works against ferromagnetism. \( \Delta T_{V\sigma} \) and \( x_{V\sigma} \) constitute the main mechanisms by which the \( p \)-band influences the \( d \)-band magnetism.

In Fig. 4 Curie temperatures are shown in dependence of the band filling \( n^d \) for different parameters \( V \). We find both, stabilization for lower particle densities as well as destabilization for higher ones in all theories. Surprisingly, the stabilization is clearly more pronounced, if the band distance increases (r.h.s of Fig. 4).

Fig. 2 gives a systematic overview of the \( V \)-dependence of the Curie temperature for different band distances \( \Delta T_0^c \). There exists a critical band distance \( \Delta T_0^c \) that separates regimes with qualitatively different behaviour of the Curie temperature (lines with circles). This distance is about 2.8 eV for \( Hu-I \), for \( MAA \) approximately 2.6 eV, while within the SDA the critical band distance is somewhat smaller than 2.4 eV. \( \Delta T_0^c \) is characterized by the following:

(i) Above the critical band distance (triangles up) we are in the stabilizing regime. Here ferromagnetism can be stabilized by the uncorrelated bands for small hybridizations \( V \). The Curie temperature \( T_c \) shows a
maximum as a function of the hybridization $V$.

(ii) The situation is different for small band distances $\Delta T_0 < \Delta T^c_0$ (triangles down). We are now in the destabilizing regime. No enhancement of the Curie temperature is found, only destabilization of magnetism. The different behaviour can be understood by inspecting again the two competing band structure effects (21) of the hybridization: At small band distances $\Delta T_0$ the destabilizing band broadening $x_{V\sigma} \sim 1 + \frac{V^2}{\Delta T_0}$ is more important than the stabilizing shift $\Delta T_{V\sigma} \sim -\frac{V^2}{\Delta T_0}$. We are in the destabilizing regime. As $\Delta T_0$ increases, the shift more and more over-compensates the broadening, though both effects become smaller. Thus ferromagnetism can be stabilized for $\Delta T_0 > \Delta T^c_0$. Large inter-band fluctuations at high values of $V$, however, suppress ferromagnetism also in this regime.

For further investigations we only show $SDA$-results since the dependence of the hybridization strength $V$ is qualitatively the same in all theories. First we want to look at the critical band distance, that separates the stabilizing from the destabilizing regime. It depends sensitively on the band filling $n^d$ (Fig. 4). For densities $n^d$ closer to half filling the critical band distance is enhanced. This could reflect the fact, that the Fermi energy rises with increasing band filling and therefore the gap between the Fermi energy and the uncorrelated states becomes smaller. This enhances the inter-band fluctuation rate and the stabilization of ferromagnetism is more unlikely. As in the single-band model, no ferromagnetism was found at $n^d \geq 1$ for the free density of states (20).

Finally we want to study ground state properties: The $p$-band can induce a ferromagnetic ground-state, if the single-band system is paramagnetic, but close to a ferromagnetic transition (Fig. 5 bcc tight-binding lattice). A ferromagnetic ground state is induced by the $p-d$ hybridization for band distances greater than $\Delta T^f_0 = 0.3 eV$ and for moderate values of $V$. The magnetization shows a distinct maximum as a function of the hybridization strength as shown in the inset of Fig. 5.

V. CONCLUSIONS

Let us summarize our findings. The question, whether and how an uncorrelated band can stabilize band ferromagnetism can now be answered:

Stabilization of ferromagnetism is only found for small hybridization strengths. Strong fluctuations between the bands generally suppress ferromagnetic order. Small fluctuations can stabilize ferromagnetism if the band distance is larger than a critical energy $\Delta T^c_0$, which depends sensitively on the band filling $n$ and on the shape of the free density of states.

The stabilization and the destabilization result from spin-dependent inter-band particle fluctuations. They induce a spin-dependent renormalization of the correlated quasiparticle density of states. This renormalization can be analyzed in terms of a band broadening dominating at small band distances and a band shift dominating at larger ones. The former turns out to suppress, the latter
to stabilize ferromagnetism.

In other words: as usual the system lowers its energy by inter-band particle fluctuations. Because the latters can be spin-dependent, the energy-win is different for the spin-up and the spin-down electrons. This in turn influences the stability of the ferromagnetic phase and e.g. the Curie-temperatures. The described mechanism can also give a "final kick" to a system, that is close to a ferromagnetic transition.

There are various arguments that compared to this mechanism indirect exchange interactions as an RKKY-like coupling of localized $d$-moments are of minor importance: (i) In most of the calculations shown here, the lower band edge of the $p$-band is located above the Fermi-energy (Fig. 1 - Fig. 6). Except for the mixing of $d-$ and $p-$states, this band is therefore empty and no polarization of the $p$-band can be expected. This excludes RKKY-coupling.

(ii) RKKY-coupling results from simultaneous fluctuations at different sites and is thus of order $V^4$ (see e.g. reference [14]). The same holds for other indirect exchange mechanisms as e.g. super-exchange. On the other hand

the band-structure effects we discussed above are based on uncoupled fluctuations and are thus of order $V^2$. Therefore they will dominate the system.

In conclusion we have found a considerable influence of the $p$-band to $d$-band ferromagnetism in our model.

The involved processes are due to the interplay of correlation and hybridization. Hence our investigations showed that the $p-d$ hybridization should be taken into account in model calculations to achieve a realistic description of real substances. Otherwise magnetic properties may be over- or underestimated.

If and how the $p$-bands influence the anti-ferromagnetic phase was left open in our analysis and remains an interesting question to be answered in further investigations.

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FIG. 7: $p$-band induced ferromagnetism for a bcc tight-binding lattice. Inset: Magnetization in dependence of $V$. Parameters: $T = 0\text{K}$, $U = 4$, $W_0 = 1$, $\alpha = 4$, $n = 0.55$. (SDA).

1 M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).
2 J. Hubbard, Proc. Roy. Soc. A 276, 238 (1963).
3 J. Kanamori, Prog. Theor. Phys. (Kyoto) 30, 275 (1963).
4 W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
5 D. Vollhardt, Int. J. Mod. Phys. B 3, 2189 (1992).
6 M. Jarrell, Phys. Rev. Lett. 69, 168 (1992).
7 A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
8 M. Jarrell and T. Pruschke, Z. Phys. B 90, 187 (1993).
9 D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf and M. Ulmke, Z. Phys. B 103, 283 (1997).
10 M. Ulmke, Europ. Phys. J. B 1, 301 (1998).
11 J. Bünemann, W. Weber and F. Gebhard, Phys. Rev. B 57, 6896 (1998).
12 A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B 57, 6884 (1998).
13 T. Maier, M. B. Zöllf, T. Pruschke and J. Keller, Europ. Phys. J. B 7, 377 (1999).
14 A. C. Hewson, The Kondo Problem to Heavy Fermions, Cambridge University Press (1993).
15 B. Möller and P. Wölfle, Phys. Rev. B 48, 10320 (1993).
16 A. N. Tahvildar-Zadeh, M. Jarrell and J. K. Freericks, Phys. Rev. B 55, R3332 (1997).
17 D. Meyer and W. Nolting, Europ. Phys. J. B 18, 385 (2000).
18 T. Yanagisawa and Y. Shimo, Phys. Rev. B 48, 6104 (1993).
19 This term is usual in the investigation of correlation induced metal-insulator transitions. See e.g.: M. Caffarel and W. Krauth, Phys. Rev. Lett. 72, 1545 (1994); Y. Ono, R. Bulla and A. C. Hewson, Europ. Phys. J. B 19, 375 (2001).
20 V. Sechovsky, A. V. Andreev, Z. Arnold, J. Kamarad, T. D. Cuong, L. Havela and N. H. Duc, J. of Alloys a. Comp. 262, 141 (1997).
21 W. Nolting, Z. Phys. B 25, 255 (1972).
22 T. Herrmann and W. Nolting, Phys. Rev. B 53, 10579 (1996).
23 M. Potthoff, T. Herrmann, T. Wegner and W. Nolting, phys. stat. sol. (b) 210, 199 (1998).
24 An investigation of the pure particle number effect is found in: M. Bünger and R. J. Jelitto, phys. stat. sol. (b) 94, 191 (1979).
25 see e.g. J. Wahle, N. Blümer, J. Schlipf, K. Held and D. Vollhardt, Phys. Rev. B 58, 12749 (1998). 
26 T. Herrmann and W. Nolting, J. Magn. Magn. Mat. 170, 253 (1997).
27 B. Velicky, S. Kirkpatrick and H Ehrenreich, Phys. Rev. 175, 747 (1968).
28 natural units are used throughout this paper, hence $\hbar = 1$.
29 best to be done in the form $\Sigma_{\sigma} - \gamma_{1} + G_{\text{dia}}[\Sigma_{\sigma} (\Sigma_{\sigma} - \gamma_{1}) - \gamma_{1}(\Sigma_{\sigma} - \gamma_{2})] = 0$.
30 However, as in the SDA, the low energy behaviour is described poorly. For instant the imaginary part of the self energy does not vanish at the Fermi energy.