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 on the interplay between hybridization and correlation we investigate a simple model system consisting of two nondegenerate hybridized bands, one strongly correlated and the other one quasifree. To solve this extended Hubbard model, we apply simple approximations, namely the spectral density approach and the modified alloy analogy, 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 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 interband particle fluctuations cause a spin-dependent band shift and a spin-dependent band broadening of the Hubbard bands. The shift stabilizes and the broadening tends to destabilize ferromagnetism. Stabilization requires relatively high band distances and small hybridization matrix elements. Superexchange and Ruderman-Kittel-Kasuya-Yosida coupling are of minor importance.

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I. INTRODUCTION

The issue of magnetism in band ferromagnets such as 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 aspect is the single-band Hubbard model. Although it was introduced to gain a first qualitative understanding of band ferromagnetism [1–3] it took almost 30 years to answer the question whether it is a generic model for ferromagnetism at all. About 10 years ago a dynamical mean field theory[4–7] (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.[8–10] 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 nondegenerate 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 multiband models. Let us mention the Gutzwiller approximation[11] or various treatments within the DMFT frame.[12,13]

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 3*d* 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[14] and is the central point of widely used models such as 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[15–17] as shown rigorously for the one-dimensional case at quarter filling.[18] This indicates that uncorrelated bands may influence the magnetic phase diagram of the Hubbard model, too, and this most likely occurs if the band distance is smaller than the on-site Coulomb energy (charge-transfer regime[19]). Recent experiments indeed seem to indicate that ferromagnetism can be stabilized if additional *p* orbitals are doped into a $R\mathrm{Co}_2$ system ($R=\mathrm{Ho,Er}$).[20] The aim of this paper is to decide, whether the neglect of *s* and *p* bands is justified when modeling band ferromagnets such as 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 Sec. III 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 this reason we will formulate the much simpler Hubbard-I decoupling[2] (Hu-I), the spectral density approach[21] (SDA), and the modified alloy analogy[22] (MAA) for the described multiband model. These theories are conceptually restricted to high-energy excitations in the strong-coupling regime. This is, however, the interesting regime, where band ferromagnetism occurs. 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.[23] It is found that the SDA as well as the MAA systematically overestimates magnetic quantities such as the Curie temperature but turns out to give a qualitative satisfying description of band ferromagnetism.[23,17] For our purpose the main advan-

tage of these theories is the possibility for analytical estimations.

In Sec. 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 interband 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, such as superexchange and Rudermann-Kittel-Kasuya-Yosida (RKKY) coupling.

II. GENERAL CONSIDERATIONS

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

$$H=\sum_{ij\sigma}(T_{ij}^{d}-\mu)d_{i\sigma}^{\dagger}d_{j\sigma}+\frac{U}{2}\sum_{i\sigma}n_{i\sigma}^{d}n_{i-\sigma}^{d}$$

$$+\sum_{ij\sigma}(T_{ij}^{p}-\mu)p_{i\sigma}^{\dagger}p_{j\sigma}+V\sum_{i\sigma}(d_{i\sigma}^{\dagger}p_{i\sigma}+p_{i\sigma}^{\dagger}d_{i\sigma}). \quad (1)$$

This Hamiltonian is similar to those used, e.g., in Ref. 19 and reduces to the periodic Anderson model (PAM) in the limit $T_{ij}^{d}\rightarrow 0$ for $i\neq j$. The weakly correlated electrons are described by a quasifree ''*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 μ denotes the chemical potential. the free band structure $\epsilon_{k}^{p;d}$ 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 ΔT_0 and the ratio of the free bandwidths α:

$$\Delta T_0=T_0^{p}-T_0^{d}, \quad \alpha=\frac{\mathcal{W}_0^{p}}{\mathcal{W}_0^{d}}. \quad (2)$$

$T_0^{p,d}=T_{ii}^{p,d}$ 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

$$\epsilon_k^{p}=T_0^{p}+\alpha(\epsilon_k^{d}-T_0^{d}). \quad (3)$$

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.[24] 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 ΔT_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 noninteger 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* ''nonmagnetic'' *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 shape of the density of states.[25] 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 $U\rightarrow 0$. For small hybridizations the excitation energies are

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

$$E_{k2}(V)=\epsilon_k^{p}+\frac{V^2}{|\epsilon_k^{p}-\epsilon_k^{d}|}. \quad (4)$$

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 nonoverlapping bands, i.e., $\Delta T_0>\max(\epsilon_k^{p}-T_0^{p})$, we insert Eq. (3) into Eq. (4) and expand $E_{k1}(V)$ in powers of $(\alpha-1)(\epsilon_k^{d}-T_0^{d})/\Delta T_0$. Equation (4) becomes

$$E_{k1}(V)=T_0^{d}+\Delta T_V^{d}+(\epsilon_k^{d}-T_0^{d})x_V^{d} \quad (5)$$

with the band shift

$$\Delta T_V^{d}=-\frac{V^2}{\Delta T_0} \quad (6)$$

and the band broadening factor

$$x_V^{d}=1+\frac{V^2}{\Delta T_0^{2}}(\alpha-1). \quad (7)$$

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 Eq. (1) with the intersite hoppings t^{d} and t^{p}

$=\alpha t^d$. For small V one can perform a canonical transformation that decouples the p and d band to first order in V. The calculation is lengthy but straightforward. For $U\to\infty$, $\Delta T_0 > t^{(p;d)}$, and $T_0^d < \mu < T_0^p$ the d electrons are well approximated by a two-site Hubbard Hamiltonian with a renormalized center of gravity $\hat{T}_0^d(V)$, renormalized hopping integrals $\hat{t}^d(V)$, and a renormalized interaction $\hat{U}(V)$. We find the parameters

$$\hat{T}_0^d(V)=T_0^d-\frac{V^2}{\Delta T_0},$$

$$\hat{t}^d(V)=t^d\left(1+\frac{V^2}{\Delta T_0^2}(\alpha-1)\right), \tag{8}$$

$$\hat{U}(V)=U+\frac{V^2}{\Delta T_0}.$$

The broadening as well as the shift is clearly recognized in Eq. (8). Our preceding qualitative considerations indicate that interband 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 Eq. (1) can be studied using retarded single-electron Green functions

$$G_{k\sigma}^{dd}=\langle\langle d_{k\sigma};d_{k\sigma}^{\dagger}\rangle\rangle,\quad G_{k\sigma}^{pp}=\langle\langle p_{k\sigma};p_{k\sigma}^{\dagger}\rangle\rangle,$$

$$G_{k\sigma}^{dp}=G_{k\sigma}^{pd}=\langle\langle d_{k\sigma};p_{k\sigma}^{\dagger}\rangle\rangle=\langle\langle p_{k\sigma};d_{k\sigma}^{\dagger}\rangle\rangle,$$

which fulfill the following equations of motion (natural units are used throughout this paper; hence $\hbar=1$):

$$\begin{aligned}
EG_{k\sigma}^{dd}&=1+(\epsilon_k^d-\mu)G_{k\sigma}^{dd}+\Sigma_{k\sigma}G_{k\sigma}^{dd}+VG_{k\sigma}^{pd},\\
EG_{k\sigma}^{pd}&=(\epsilon_k^p-\mu)G_{k\sigma}^{pd}+VG_{k\sigma}^{dd},\\
EG_{k\sigma}^{pp}&=1+(\epsilon_k^p-\mu)G_{k\sigma}^{pp}+VG_{k\sigma}^{dp}.
\end{aligned} \tag{9}$$

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

$$\Sigma_{k\sigma}G_{k\sigma}^{dd}=\left\langle\left\langle\left[d_{k\sigma},\frac{U}{2}\sum_{i\sigma}n_{i\sigma}^d n_{i-\sigma}^d\right]_-;d_{k\sigma}^{\dagger}\right\rangle\right\rangle, \tag{10}$$

where $[\ldots,\ldots]_-$ denotes the commutator. Solving Eq. (9) gives all Green functions:

$$\begin{pmatrix} G_{k\sigma}^{dd} & G_{k\sigma}^{dp}\\ G_{k\sigma}^{pd} & G_{k\sigma}^{pp}\end{pmatrix}^{-1}=\begin{pmatrix} E-\epsilon_k'^{p} & -V\\ -V & E-\epsilon_k'^{d}-\Sigma_{k\sigma}\end{pmatrix}, \tag{11}$$

where ϵ_k' is used as an abbreviation for $\epsilon_k-\mu$.

In the ferro- and paramagnetic phase we can calculate the spin-dependent average occupation numbers $n_\sigma^d=\langle n_{i\sigma}^d\rangle$ and $n_\sigma^p=\langle n_{i\sigma}^p\rangle$ using the Green functions (11):

$$n_\sigma^{(p;d)}=-\mathrm{Im}\left(\frac{1}{\pi}\int_{-\infty}^{\infty}dE\,f_-(E)G_{ii\sigma}^{(pp;dd)}(E-\mu)\right). \tag{12}$$

$f_-(E)$ is the Fermi function and $G_{ii\sigma}^{(pp;dd)}$ 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 (1). 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 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.

A. Hubbard-I decoupling

Let us start with the Hubbard-I approximation. Straightforward decoupling of the real space equations of motion for the Green's functions (11) yields the Hu-I self-energy

$${}^{\text{Hu-I}}\Sigma_\sigma=Un_{-\sigma}^d\frac{E-T_0^d+\mu}{E-T_0^d+\mu-U(1-n_{-\sigma}^d)}, \tag{13}$$

which is formally identical to the single-band case. The self-energy is V dependent via $n_{-\sigma}^d$, which is calculated using Eqs. (11) and (12). 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 $V\to 0$, $T_{ij}^{i\neq j}\to 0$. Finite values of the hopping and hybridization change the positions and weights of the δ peaks and lead to a mixing of p and d spectral density.

B. SDA

For the single-band model, the SDA is the simplest theory that yields the correct strong-coupling and high-energy behavior, 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:

$$
{}^{dd}M^{(m)}_{k\sigma} = \int_{-\infty}^{\infty} dE\, E^m S^{dd}_{k\sigma}(E)
$$

$$
= \langle \underbrace{[[[[d_{k\sigma}, H]_- H]_- \ldots H]_-}_{m-fold}, d^+_{k\sigma}]_+ \rangle . \quad (14)
$$

$[\ldots,\ldots]_+$ is the anticommutator. 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 Eq. (13) for a SDA self-energy ansatz:

$$
{}^{\mathrm{SDA}}\Sigma_{k\sigma} \overset{!}{=} \gamma_1 \frac{E-\gamma_2}{E-\gamma_3}. \quad (15)
$$

The parameters γ_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 $1/E$:

$$
G^{dd}_{k\sigma} = \sum_{n=0}^{\infty} \frac{{}^{dd}M^{(n)}_{k\sigma}}{E^{n+1}}; \quad \Sigma_{k\sigma} = \sum_{n=0}^{\infty} \frac{C^{(n)}_{k\sigma}}{E^n}. \quad (16)
$$

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

$$
G^{dd}_{k\sigma}(E) = \int_{-\infty}^{\infty} dE' \frac{S^{dd}_{k\sigma}(E')}{E - E' + i0^+} \quad (17)
$$

with respect to $1/E$ and comparing the resulting expressions with the definition of the moments (14). The self-energy coefficients $C^{(n)}_{k\sigma}$ are obtained as functions of the moments ${}^{dd}M^{(0)}_{k\sigma} \ldots {}^{dd}M^{(n+1)}_{k\sigma}$ by inserting the expansions (16) into Eq. (11) (or equivalently into the Dyson equation) and by comparing the coefficients of the $1/E^n$ terms. With the right-hand side (r.h.s.) of Eq. (14), we find the first four correlated spectral moments:

$$
\begin{aligned}
{}^{dd}M^{(0)}_{k\sigma} &= 1, \\
{}^{dd}M^{(1)}_{k\sigma} &= \epsilon'^{d}_k + U n^d_{-\sigma}, \\
{}^{dd}M^{(2)}_{k\sigma} &= (\epsilon'^{d}_k)^2 + 2U n^d_{-\sigma}\epsilon'^{d}_k + U^2 n^d_{-\sigma} + V^2, \\
{}^{dd}M^{(3)}_{k\sigma} &= (\epsilon'^{d}_k)^3 + 3U n^d_{-\sigma}(\epsilon'^{d}_k)^2 + U^2[2n_{-\sigma} + (n^d_{-\sigma})^2] \\
&\quad + U^2 n^d_{-\sigma}(1 - n^d_{-\sigma})(B^{2-\mathrm{band}}_{k-\sigma} + T'_0) + U^3 n^d_{-\sigma} \\
&\quad + V^2(2\epsilon'^{d}_k + \epsilon'^{p}_k + 2U n^d_{-\sigma}). \quad (18)
\end{aligned}
$$

The self-energy coefficients read

$$
\begin{aligned}
C^{(0)}_{\sigma} &= U n^d_{-\sigma}, \\
C^{(1)}_{\sigma} &= U^2 n^d_{-\sigma}(1 - n^d_{-\sigma}), \\
C^{(2)}_{k\sigma} &= U^2 n^d_{-\sigma}(1 - n^d_{-\sigma})[B^{2\text{-band}}_{k-\sigma} + T'_0 + U(1 - n^d_{-\sigma})].
\end{aligned}
$$

$B^{2\text{-band}}_{k\sigma} = B^{2b}_{\sigma} + F^{2b}_{k\sigma}$ is a higher correlation function with the local part B^{2b}_{σ} and a k-dependent part $F^{2b}_{k\sigma}$. For the single-band model, the influence of both terms is discussed in detail in Ref. 26. It turns out that the most important term is the local B_σ, which leads to a spin-dependent band shift in the ferromagnetic phase. With regard to ferromagnetism the nonlocal part $F_{k\sigma}$ seems to be of minor importance. Therefore we will neglect it in the following. From Eq. (14) we find for the local part B^{2b}_{σ}

$$
\begin{aligned}
B^{2b}_{\sigma} = \frac{1}{n^d_\sigma(1-n^d_\sigma)} \Bigg(& \frac{1}{N} \sum_{ij}^{i \neq j} T^d_{ij} \langle d^\dagger_{i\sigma} d_{j\sigma} (2 n^d_{i-\sigma} - 1) \rangle \\
& + \frac{2V}{UN} \sum_{ij} (T^p_{ij} - T^d_{ij}) \langle d^\dagger_{i\sigma} p_{j\sigma} \rangle - V \langle d^\dagger_{i\sigma} p_{i\sigma} \rangle \\
& + \frac{2V^2}{U}(n^d_\sigma - n^p_\sigma) \Bigg).
\end{aligned}
$$

Although B^{2b}_{σ} 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:

$$
\begin{aligned}
B^{2b}_{\sigma} = \mathrm{Im} \Bigg[& -\frac{1}{n_\sigma(1-n_\sigma)\pi} \int_{-\infty}^{\infty} dE\, f_-(E) \left(\frac{2\Sigma_\sigma(E)}{U} - 1 \right) \\
& \times \{ [E - \Sigma_\sigma(E) - T_0] G^{dd}_{ii\sigma}(E - \mu) - 1 \} \Bigg]. \quad (19)
\end{aligned}
$$

The correlation function B^{2b}_{σ} and the self-energy coefficients $C^{(0;1;2)}_{\sigma}$ turn out to be the same functionals of the correlated Green function $G^{dd}_{ii\sigma}$ as in the single-band model. While determining the self-energy coefficients, the whole V dependence in the moments ${}^{dd}M^{(0)}_{k\sigma} \ldots {}^{dd}M^{(3)}_{k\sigma}$ (18) is canceled by the explicit V dependence of the correlated Green function (11). Thus, as in the Hu-I approximation, the SDA self-energy is formally identical to the single-band case:

$$
{}^{\mathrm{SDA}}\Sigma_\sigma = U n^d_{-\sigma} \frac{E - T_0 + \mu - B^{2b}_{-\sigma}}{E - T_0 + \mu - B^{2b}_{-\sigma} - U(1 - n^d_{-\sigma})}. \quad (20)
$$

The V dependence comes again into play by the expectation values $n^d_{-\sigma}$ and $B^{2b}_{-\sigma}$ being evaluated via Eqs. (11), (12), and (19).

C. MAA

Besides the restriction to strong interaction strengths a drawback of SDA and Hu-I is the exclusion of scattering processes that 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.[27] With this approach one can account for electron scattering at the potentials formed by the distribution of electrons of opposite spin direction. The main excitation energies of the many-body system are modeled 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 (10)

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

$$0=\sum_{p\sigma}^{p=1,2} x_{p\sigma}\frac{E_{p\sigma}-T_0^d-\Sigma_\sigma(E)}{1-G_{ii\sigma}^{dd}(E)[E_{p\sigma}-\Sigma_\sigma(E)-T_0^d]}. \quad (21)$$

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

$$\gamma_1=x_{1\sigma}(E_{1\sigma}-T_0^d)+x_{2\sigma}(E_{2\sigma}-T_0^d),$$

$$\gamma_2=\frac{(E_{1\sigma}-T_0^d)(E_{2\sigma}-T_0^d)}{\gamma_1},$$

$$\gamma_3=x_{1\sigma}(E_{2\sigma}-T_0^d)+x_{2\sigma}(E_{1\sigma}-T_0^d),$$

Eq. (21) becomes

$$\Sigma_\sigma(E)=\gamma_1\frac{1+G_{ii\sigma}^{dd}(E)[\Sigma_\sigma(E)-\gamma_2]}{1+G_{ii\sigma}^{dd}(E)[\Sigma_\sigma(E)-\gamma_3]}. \quad (22)$$

Here $x_{1\sigma}+x_{2\sigma}=1$ is already used. To complete the theory, we now have to adjust the parameters γ_1, γ_2, and γ_3. Similar to the SDA these parameters can be fitted to the on-site spectral moments $M_{ii\sigma}^{(m)}$ and on-site self-energy coefficients $C_{ii\sigma}^{(m)}$. The latter two are defined analogously to $M_{k\sigma}$ and $C_{k\sigma}$ in Eq. (14). To this purpose one has to expand the local Green function $G_{ii\sigma}^{dd}$ and the local self-energy Σ_σ in powers of $1/E$ analogously to Eq. (16). Then one inserts these expansions into Eq. (22) and compares the coefficients of the $1/E^n$ terms up to $n=2$ which is best to be done in the form $\Sigma_\sigma-\gamma_1+G_{ii\sigma}[\Sigma_\sigma(\Sigma_\sigma-\gamma_3)-\gamma_1(\Sigma_\sigma-\gamma_2)]=0$. Using the abbreviation ${}^{\mathrm{MAA}}\Sigma_\sigma\rightarrow\Sigma_\sigma$, we finally find for the MAA self-energy

$$\Sigma_\sigma=Un_{-\sigma}^d\frac{(G_{ii\sigma}^{dd})^{-1}+\Sigma_\sigma-B_{-\sigma}^{2b}}{(G_{ii\sigma}^{dd})^{-1}+\Sigma_\sigma-B_{-\sigma}^{2b}-U(1-n_{-\sigma}^d)}. \quad (23)$$

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 $G_{ii\sigma}^{dd}$ and the expectation values n_σ^d and B_σ^{2b}.

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.

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 Ref. 23 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

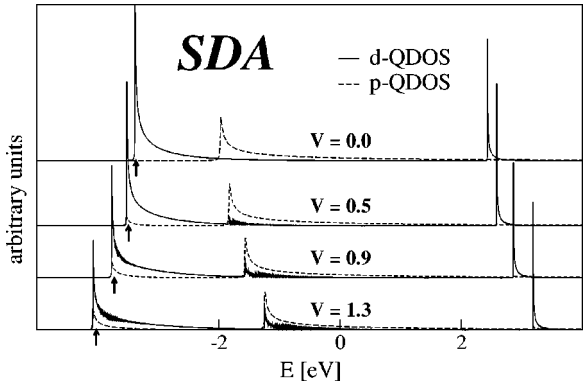

FIG. 1. Quasiparticle density of states (QDOS) as a function of the energy E at different V. The system is forced to be paramagnetic. Parameters: $U=5.0$, $n=0.25$, $\alpha=4.0$, $\Delta T_0=3.0$, $T=0$ K, fcc(∞) lattice; see Eq. (24). The arrows show the position of the Fermi energy. With rising V the distance between the subbands increases quadratically.

$$\rho^{(0)}(E)=\frac{e^{-(1+\sqrt{2}E/t^*)/2}}{t^*\sqrt{\pi(1+\sqrt{2}E/t^*)}}. \quad (24)$$

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 stabilize 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.[25] Figures 1 and 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 subbands are broadened. One can see that the band

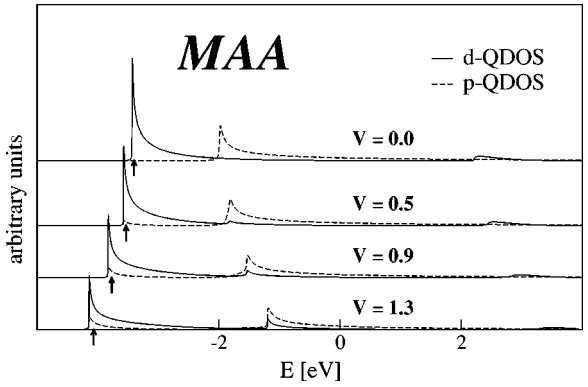

FIG. 2. Same as in Fig. 1, but calculated with the MAA. The peaks are broader than those in Fig. 1 due to quasiparticle damping. This is most pronounced in the upper Hubbard band.

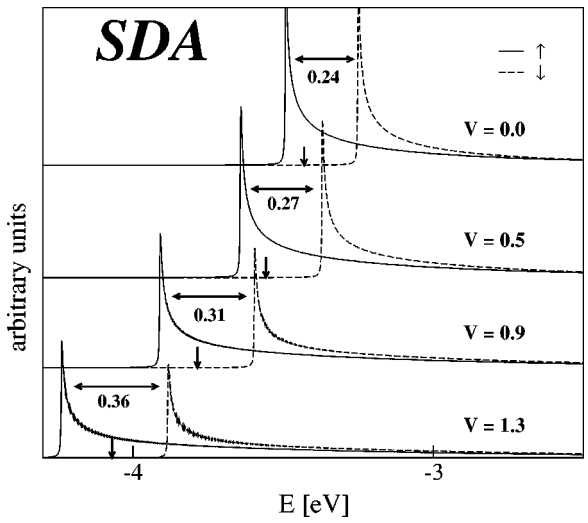

FIG. 3. Lower Hubbard band of the ↑- and ↓*d* QDOS in the ferromagnetic phase. Parameters as in Figs. 1 and 2. The distance between the ↑ and ↓ bands increases with *V*.

shifts are proportional to V^2, which agrees perfectly with the results for free bands [Eqs. (5)–(7)] and the two-site cluster [Eq. (8)].

Figure 3 displays the lower Hubbard band (SDA) of the *d* 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 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 Eq. (11) with $\Sigma_{k\sigma}=\Sigma_{\sigma}^{SDA}$. For $U\rightarrow\infty$ we find

$$E_{1k\sigma}^{\mathrm{SDA}}=T_0^d+U+(\epsilon_k^d-T_0^d)n_{-\sigma}^d+B_{-\sigma}^{2b}(1-n_{-\sigma}^d),$$

$$E_{2k\sigma}^{\mathrm{SDA}}=\epsilon_k^p+V^2X_{k\sigma},$$

$$E_{3k\sigma}^{\mathrm{SDA}}=T_0^d+(\epsilon_k-T_0^d)(1-n_{-\sigma}^d)+B_{-\sigma}^{2b}n_{-\sigma}^d-V^2X_{k\sigma},$$

where

$$V^2X_{k\sigma}=V^2\frac{1-n_{-\sigma}^d}{\epsilon_k^p-T_0^d-(\epsilon_k^d-T_0^d)(1-n_{-\sigma}^d)-B_{-\sigma}^{2b}n_{-\sigma}^d} \tag{25}$$

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 nonoverlapping bands [i.e., $\Delta T_0>\max(\epsilon_k^p-T_0^p)$], we can rewrite $E_{3k\sigma}^{\mathrm{SDA}}$ in terms of a band shift $\Delta T_{V\sigma}$ and a band broadening factor $x_{V\sigma}$

$$E_{3k\sigma}^{\mathrm{SDA}}=T_0^d+\Delta T_{V\sigma}+n_{-\sigma}^dB_{-\sigma}^{2b}+(\epsilon_k^d-T_0^d)(1-n_{-\sigma}^d)x_{V\sigma}.$$

Both are spin dependent:

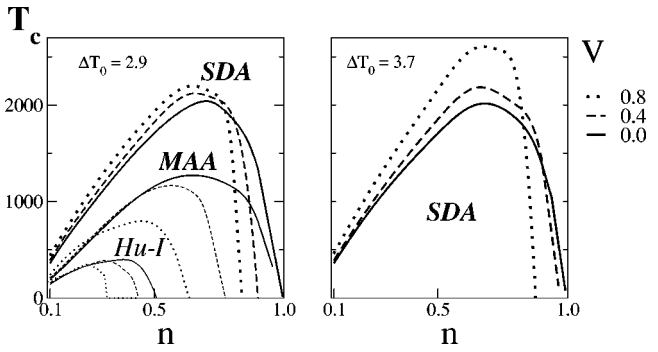

FIG. 4. *n*-*T* phase diagram for different values of *V* and different band distances ΔT_0. Other parameters as in the previous figures.

$$\Delta T_{V\sigma}=-\frac{V^2}{\Delta T_0-n_{-\sigma}^dB_{-\sigma}^{2b}}(1-n_{-\sigma}^d),$$

$$x_{V\sigma}=1+\frac{V^2}{(\Delta T_0-n_{-\sigma}^dB_{-\sigma}^{2b})^2}(\alpha-1+n_{-\sigma}^d). \tag{26}$$

α is the ratio of the free bandwidths as defined in Eq. (2). Thus a hybridization with an uncorrelated band causes alterations in the band structure similar to the noninteracting case [Eqs. (6) and (7)], i.e., a band shift and a band broadening for the correlated *d* subband. The important difference is the *spin dependence* of both quantities in the full system. Equation (26) describes two competing effects. The shift to lower energies $\Delta T_{V\sigma}^d$ 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 the 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). Figure 5 gives a systematic overview of the *V* dependence of the Curie temperature for different band distances ΔT_0.

There exists a critical band distance ΔT_0^c that separates regimes with qualitatively different behavior 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. ΔT_0^c is characterized by the following:

(i) Above the critical band distance (up triangles) 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 $\Delta T_0<\Delta T_0^c$ (down triangles). We are now in the destabilizing

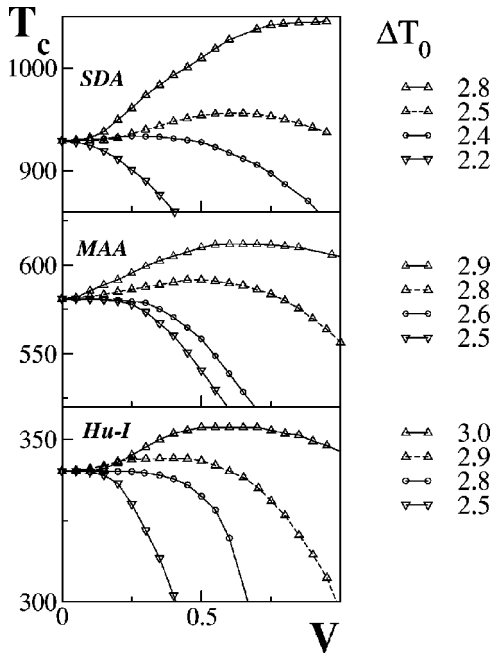

FIG. 5. Curie temperatures in dependence of V calculated within different theories. Up triangles: stabilization of ferromagnetism for small V; down triangles: destabilization of ferromagnetism. Other parameters as in the previous figures.

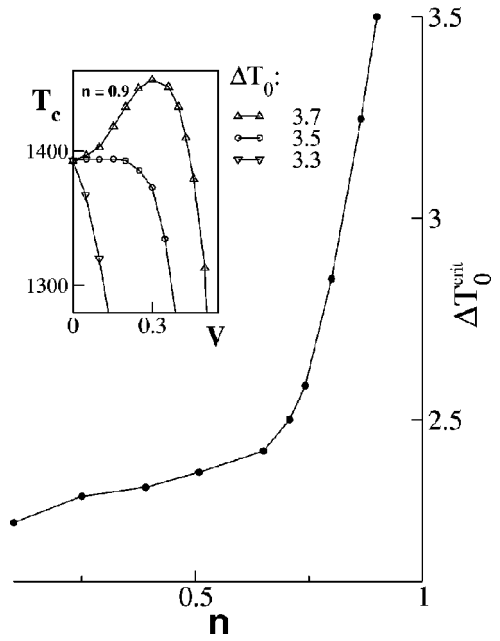

FIG. 6. Critical band distance that separates the stabilizing and the destabilizing regime. Above the line ferromagnetism is stabilized by the uncorrelated band for small V. Below the line ferromagnetism is destabilized. Inset: as in Fig. 5 for $n=0.9$, SDA. Further parameters as in the previous figures.

regime. No enhancement of the Curie temperature is found, only destabilization of magnetism.

The different behavior can be understood by inspecting again the two competing band structure effects (26) of the hybridization: At small band distances ΔT_0 the destabilizing band broadening $x_{V\sigma}\sim 1+V^2/\Delta T_0^2$ is more important than the stabilizing shift $\Delta T_{V\sigma}\sim -V^2/\Delta T_0$. We are in the destabilizing regime. As ΔT_0 increases, the shift more and more overcompensates the broadening, though both effects become smaller. Thus ferromagnetism can be stabilized for $\Delta T_0 > \Delta T_0^c$. Large interband 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. 6).

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 interband fluctuation rate, and the stabilization of ferromagnetism is more unlikely. As in the single-band model, no ferromagnetism was found at $n^d \geqslant 1$ for the free density of states (24).

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. 7, bcc tight-binding lattice). A ferromagnetic ground state is induced by the p-d hybridization for band distances larger than $\Delta T_0^c = 0.3$ 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. 7.

V. CONCLUSIONS

Let us summarize our findings. The questions if 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

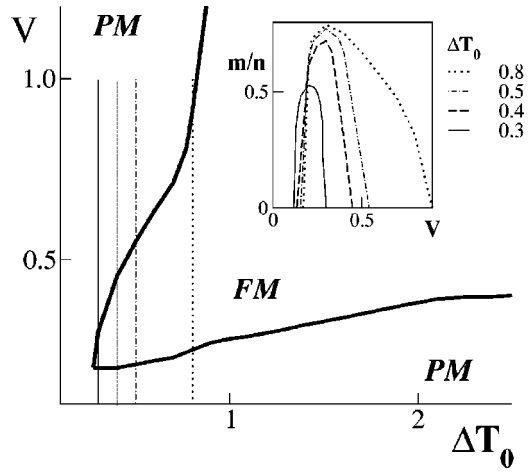

FIG. 7. p-band-induced ferromagnetism for a bcc tight-binding lattice. Inset: Magnetization in dependence of V. Parameters: $T=0$ K, $U=4$, $\mathcal{W}_0=1$, $\alpha=4$, $n=0.55$ (SDA).

distance is larger than a critical energy ΔT_0^c, which depends sensitively on the band filling n and on the shape of the free density of states.

The stabilization and destabilization result from spin-dependent interband 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 and the latter to stabilize ferromagnetism.

In other words, as usual the system lowers its energy by interband particle fluctuations. Because the latter can be spin dependent, the energy gain 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 show that compared to this mechanism indirect exchange interactions such 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 (Figs. 1–6). 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., Ref. 16). The same holds for other indirect exchange mechanisms such as superexchange. 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 considerable influence of the p band on 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 antiferromagnetic phase was left open in our analysis and remains an interesting question to be answered in further investigations.

ACKNOWLEDGMENTS

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