Influence of spin-flip scattering on the stability of ferromagnetism in a two-band Hubbard model

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Abstract. We investigate the influence of an interband exchange interaction on magnetism in a two-band Hubbard model. Our main emphasis lies on spin-flip scattering which is often neglected but is necessary to retain the full rotational symmetry of the Hamiltonian. We find a striking dependence of the magnetization on the interband exchange coupling constant $J$ and a substantial suppression of ferromagnetic order for a large range of values of $J$. The onset of an RKKY-like magnetic ordering mechanism is also observed.

PACS numbers: 71.10.Fd, 71.20.Be, 75.10.Lp

1. Introduction

Electronic correlations in the transition metals $Fe$, $Co$, $Ni$ still present a major challenge in condensed matter physics. The stability of ferromagnetism in these materials is not yet fully understood. Contrary to rare-earth systems, these materials have no localized magnetic moments on “atomic” orbitals. The formation of finite magnetic moments in an itinerant electron system has to be explained.

In the past, there have been many attempts to describe transition metals theoretically $[1, 2, 3, 4, 5, 6, 7]$. Virtually all of these are based on a modification of the multi-band Hubbard model $[8, 9]$, in which only the on-site Coulomb interaction is considered. Recently, the importance of band degeneracy for correctly describing ferromagnetism has been confirmed by Quantum Monte Carlo (QMC) calculations $[10, 11]$. But since all calculations mentioned above rely on some approximations (even the quasi-exact QMC calculation works only on a simplified Hamiltonian), no complete understanding of the complicated $d$-band metals is reached yet. The only way to gain a picture of the complex physics of these systems is to consider partial problems for which conclusions can be drawn from the available approximate approaches to more or less oversimplified theoretical models. In this paper, we want to provide another small piece belonging to the puzzle of the $d$-band metals.

The investigation of ferromagnetism in the Hubbard model has a long history. In fact, it was the original intention introducing this model $[8, 12]$. It is known for a long time that for a band filling of one electron above (above or below) half
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filling in the limit \( U \to \infty \), the ground state is ferromagnetic for a fcc- (sc- or bcc-) lattice (Nagaoka state) \([13, 14]\). The stability of the Nagaoka state was subject to extensive investigations. E.g. in infinite dimensions \((d = \infty)\), its stability could be proven for a wider range of band fillings and finite \( U \) \([15]\). Using variational treatments, further limits could be set on its stability on various lattice structures in two or three dimensions \([16]\). Related to these statements is the so-called flat-band magnetism \([14, 17]\). Here, a ferromagnetic ground state could be rigorously proven for a dispersionless band structure. Furthermore, for finite temperatures, the existence of a ferromagnetic phase for certain parameter ranges has been established using dynamical mean-field theory \([18, 19]\). We therefore believe that the intraband Coulomb interaction as described by the single-band Hubbard model is one major ingredient for itinerant ferromagnetism.

However, besides the strong on-site Coulomb interaction, transition metal systems are also characterized by the 5-fold degeneracy of the \( d \)-bands. How does this fact influence ferromagnetism? In atoms, Hund’s rules will favor a parallel alignment of the spins of electrons on degenerate levels. That orbital degeneracy will enhance ferromagnetic stability also in lattice systems appears to be a fact. The general validity of Hund’s rule for the ground state of a degenerate Hubbard model has indeed been proven \([20]\) (for further statements concerning ferromagnetism in degenerate Hubbard models see \([21, 14]\)). Often, this is the justification for using a simplified interband exchange interaction, which is restricted to a longitudinal Ising-like spin exchange. The full SU(2)-symmetric interband exchange interaction can be separated into a longitudinal (Ising) and a transversal (spin-flip) term as will be shown below (see equation (6)). The longitudinal interaction will try to align the \( z \)-components of the spins due to the energy gain connected with a positive value of interband exchange constant \( J \), thus fulfilling the predictions made by the analogy to the atomic behaviour. This is most obvious in mean-field theory, where the transverse part vanishes, and a magnetization-dependent bandshift is induced by the longitudinal component.

In several recently published papers, more sophisticated calculations for multi-band Hubbard models were presented, as e.g. in Quantum Monte Carlo \([10, 22]\), slave-boson \([23]\) or Gutzwiller-variational ansatz methods \([24]\). But many of these neglected the transverse part of the spin exchange with the reasoning explained above. Up to now it is not clear what the influences of the disregarded terms are.

A valuable contribution to the problem of ferromagnetism in orbitally degenerate Hubbard models was given in \([25]\), where the authors use an exact diagonalization method on a restricted Hilbert space of an in the limit of \( d = \infty \) equivalent impurity model.

The aim of this paper is to investigate the influence of spin-exchange processes originating from the transverse part of the interband interaction on ferromagnetic stability. We examine a minimal two-band model which includes those parts of the general Coulomb interaction that we believe to be the most important for the stability
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This leads to the following Hamiltonian:

\[ H = H_0 + H_U + H_J \]  

\[ H_0 = \sum_{k,m,\sigma} \epsilon_m(k) a_{k,m,\sigma}^\dagger a_{k,m,\sigma} \]  

\[ H_U = \frac{1}{2} U \sum_{i,m,\sigma} n_{i,m,\sigma} n_{i,m,-\sigma} \]  

\[ H_J = -\frac{1}{2} J \sum_{i,m} \sigma_{i,m} \cdot \sigma_{i,m} \]  

We use the usual notation for the electron annihilation (creation) operators \( a_{k,m,\sigma}^\dagger \) with wavevector \( k \), band index \( m \) (\( m \) being the complementary band of the two-band system) and spin \( \sigma \). The free bands are described by the dispersion \( \epsilon_m(k) \), \( U \) and \( J \) are combinations of the appropriate Coulomb matrix elements as introduced e.g. in \[2, 6, 7\]. The spin operators in \( H_J \) are defined as

\[ \sigma_{i,m} = a_{i,m,\sigma}^\dagger a_{i,m,-\sigma} \]  

\[ \sigma_{i,m}^z = \frac{1}{2} \sum_{\sigma} z_{\sigma} n_{i,m,\sigma} \]  

with \( z_{\sigma} = +1 \) (\( -1 \)) for spin \( \uparrow \) (spin \( \downarrow \)). Within this Hubbard-type Hamiltonian, the intraband part \( H_U \) is able to produce ferromagnetism for sufficiently large \( U \) \[18, 19, 26\]. The second interaction, \( H_J \) introduces interband exchange processes of two different kinds, as already mentioned above. This can be seen in the following decomposition of \( H_J \)

\[ H_J = -\frac{1}{4} J \sum_{i,m,\sigma} \left( \sigma_{i,m}^\sigma \sigma_{i,m}^{-\sigma} + \sigma_{i,m}^\sigma \sigma_{i,m}^{-\sigma} \right) \]  

The first term (transverse part) represents spin-flip scattering and the second one (longitudinal) an “Ising-like” exchange, which tends to stabilize spontaneous ferromagnetic order. Many calculations on multi-band Hubbard models only consider the Ising term and neglect the spin-flip part of the interaction \[10, 22, 23, 24\]. In this paper, we want to trace both parts of the interband interaction (6) with identical quality.

It goes without saying that (3) and (4) do not represent the full set of local Coulomb interactions between \( d \)-electrons. Our previous studies \[4, 8, 9, 27\], however, have evidenced that they are most important for treating magnetic phenomena in transition metals. The final goal of our investigation will be the more or less quantitative description of real substances such as Fe \[6\], Co \[7\], Ni \[2\], and Gd \[28\]. For this purpose we combine many-body model methods with “ab-initio”-bandstructure calculations. By definition the underlying many-body model incorporates only those interactions which are believed to be decisive for the collective magnetism with respect to temperature dependencies and typical correlation effects, and which are probably not properly taken into account by usual LSDA-treatments. According to our previous calculations the interactions (3) and (4) should be most important while, e.g., the interband Coulomb
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interaction (denoted by $U$ in our previous studies) turns out to be not that decisive for the band-ferromagnetism of transition metals. It can be assumed that this part of the local Coulomb interaction is sufficiently well covered by an LSDA calculation. In this sense our present model investigation is to be understood. Instead of tackling a more complicated, but probably still insufficient Hamiltonian, we aim at a better understanding of those interactions which might be the roots of the phenomenon ferromagnetism, without referring to a real system. The description of more realistic systems seems possible by a combination of our model study with LDA calculations along the kines of ref. [2, 3, 4], which is intended for the future.

In the following section, we introduce an effective medium method to decompose the complicated many-body problem of the Hamiltonian (1) into two separately solvable problems of simpler structure. After that we introduce the approximations that lead us to a fully self-consistent solution for the two-band model. In section 3, we present and discuss our results.

2. Theory

2.1. Effective Medium Approach

Even though we restricted ourselves to a rather simple model Hamiltonian, one is in need of a convincing approximation method to solve the problem. We propose a method based on an effective medium ansatz. This ansatz will map the original problem of Hamiltonian (1) onto a set of simpler model Hamiltonians, for which well tested standard approximations exist. These can be put together in an appropriate way to get a solution of the original problem. This method is generalizable to many different models, a similar approach applied to the periodic Anderson model was recently published [23].

We want to introduce the method using the two-band Hamiltonian (1) with the two interaction terms $H_U$ and $H_J$. The self-energy $\Sigma_{k,m,\sigma}(E)$ can be defined using the equation of motion of the single-electron Green’s function $G_{k,m,\sigma}(E) = \langle \langle a_{k,m,\sigma}; a_{k,m,\sigma}^\dagger \rangle \rangle$:

$$EG_{k,m,\sigma}(E) = \hbar + \epsilon_m(k)G_{k,m,\sigma}(E) + \langle [a_{k,m,\sigma}, H_U + H_J]; a_{k,m,\sigma}^\dagger \rangle$$

$$= \hbar + \epsilon_m(k)G_{k,m,\sigma}(E) + \Sigma_{k,m,\sigma}(E)G_{k,m,\sigma}(E)$$

(7)

Using the linearity of the commutator and the Green’s function, one can define “self-energy parts”:

$$\langle [a_{k,m,\sigma}, H_U]; a_{k,m,\sigma}^\dagger \rangle = \Sigma_{k,m,\sigma}^{(U)}G_{k,m,\sigma}(E)$$

(8)

$$\langle [a_{k,m,\sigma}, H_J]; a_{k,m,\sigma}^\dagger \rangle = \Sigma_{k,m,\sigma}^{(J)}G_{k,m,\sigma}(E)$$

(9)

with $\Sigma_{k,m,\sigma}(E) = \Sigma_{k,m,\sigma}^{(U)}(E) + \Sigma_{k,m,\sigma}^{(J)}(E)$. Assuming the knowledge of either one of these self-energy parts, one can introduce the following effective Hamiltonians:

$$H_{\text{eff}}^{(U,\eta)} = \sum_k \left( \epsilon_m(k) + \Sigma_{k,m,\sigma}^{(J)}(\eta) \right) a_{k,m,\sigma}^\dagger a_{k,m,\sigma} + U$$

(10)

$$H_{\text{eff}}^{(J,\eta)} = \sum_k \left( \epsilon_m(k) + \Sigma_{k,m,\sigma}^{(U)}(\eta) \right) a_{k,m,\sigma}^\dagger a_{k,m,\sigma} + J$$

(11)
which formally depend on a parameter $\eta$. By solving each of these Hamiltonians for all values of $\eta$, one can obtain the respectively missing self-energy part using the following identities:

\[
\Sigma_{k,m,\sigma}^{(U)}(E) = \left. \Sigma_{k,m,\sigma}^{(\text{eff},U,\eta)}(E) \right|_{\eta=E} \tag{12}
\]

\[
\Sigma_{k,m,\sigma}^{(J)}(E) = \left. \Sigma_{k,m,\sigma}^{(\text{eff},J,\eta)}(E) \right|_{\eta=E} \tag{13}
\]

with $\Sigma_{k,m,\sigma}^{(\text{eff},U,\eta)}(E)$ being the self-energy of the effective Hamiltonian (10) and $\Sigma_{k,m,\sigma}^{(\text{eff},J,\eta)}(E)$ of Hamiltonian (11). The introduction of the energy-parameter $\eta$ in the effective Hamiltonians (10) and (11) is necessary in order to distinguish two different kinds of energy. The effective medium energy parameter $\eta$ should not be confused with the energy as dynamic variable of e.g. an equation of motion method to solve the respective partial many-body problem. This distinction is mandatory since otherwise, the system could show unphysical behaviour. Furthermore, for the same reasoning it is necessary to calculate expectation values in the full system, e.g. by using the formal solution of equation (7) for the single-electron Green’s function:

\[
G_{k,m,\sigma}(E) = \frac{\hbar}{E - (\epsilon_m(k) + \Sigma_{k,m,\sigma}^{(U)}(E) + \Sigma_{k,m,\sigma}^{(J)}(E))} \tag{14}
\]

The two problems posed by the Hamiltonians (10) and (11) are strongly related to each other. The solution of one in form of the respective self-energy (12) or (13) is needed as input for the other. This implies a self-consistency condition on the two self-energy parts which can only be fulfilled in an iterative way. But the advantage of the effective medium ansatz is also rather obvious: The two Hamiltonians (10) and (11) have been analyzed very well by now since they are both standard models of many-body-theory. Model (10) is essentially the single-band Hubbard model [8], and model (11) is known as $sf$-model or ferromagnetic Kondo-lattice [30, 31]. So for both partial problems already known approximation schemes can be used.

For the Hubbard-model, many useful approximations exist. We use the spectral density approximation (SDA) [26, 32, 33], which has to be considered as a strong-coupling theory. Although this choice prohibits an investigation of the small-$U$ behaviour, its advantages are enormous. Besides of being mathematical simple and numerically reasonably fast, it has proven to give a qualitatively correct picture of ferromagnetism in the strong-coupling regime and compares to more sophisticated approaches [34]. It will be described in the following chapter. The $sf$-model has also attracted much interest. A very promising interpolating, moment-conserving equation-of-motion decoupling scheme has been developed in refs. [35, 36, 37]. This method will be discussed in section 2.3. The combination of these two calculations along the lines described above as effective medium approach will lead us to the solution of the full problem posed by Hamiltonian (1).
2.2. Spectral density approach

According to the effective medium ansatz, the self-energy part $\Sigma^{(U)}_{k,m,\sigma}(E)$ connected with the intraband Hubbard interaction will be calculated using the Hamiltonian \([10]\). We use the spectral density approach (SDA) to solve this problem. This method is numerically simple and fast, and, as shown in the limit of infinite dimensions, its magnetic properties resemble qualitatively the quasi-exact Quantum Monte Carlo calculation \([18, 34, 38]\). The SDA has been studied for the single-band Hubbard model extensively \([26, 32, 33]\).

In the following we will give only a short outline of the calculations. Starting point is the single-electron spectral density being defined by

$$S_{k,m,\sigma}(E) = \frac{1}{N} \sum_{i,j} \exp(ik(R_i - R_j)) \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE \exp(-i\frac{\hbar}{\epsilon}E) \langle [a_{i,m,\sigma}(t), a_{j,m,\sigma}^+(0)]_+ \rangle$$ \(15\)

where $[\ldots, \ldots]_+$ denotes the anticommutator and $\langle \ldots \rangle$ the thermodynamic average. The construction operators are taken to be in the Heisenberg time-dependent picture.

In an exact spectral-moment analysis in the limit $U \to \infty$, Harris and Lange have shown that the spectral density essentially consists of a two-peak structure \([39]\). Since ferromagnetism is widely believed to be a strong coupling phenomenon, any reasonable approximation aiming at ferromagnetism should contain this limiting case \([34]\).

In the SDA, one makes the following ansatz for the spectral density, which will turn out to correctly reproduce the positions and weights of the quasiparticle peaks according to the Harris- and Lange-calculation in the limit of $U \to \infty$.

$$S_{k,m,\sigma}(E) = \sum_{j=1,2} \hbar \alpha_{k,m,\sigma}^{(j)} \delta(E - E_{k,m,\sigma}^{(j)})$$ \(16\)

The unknown parameters $E_{k,m,\sigma}^{(j)}$ and $\alpha_{k,m,\sigma}^{(j)}$ of the quasiparticle energy and spectral weight can be calculated by the moment method. That means they are fitted by the use of the first four moments of the spectral density, which represent several sum rules, and which can be calculated directly from the Hamiltonian.

$$M_{k,m,\sigma}^{(n)} = \int_{-\infty}^{+\infty} dE E^n S_{k,m,\sigma}(E)$$ \(17\)

$$= \langle [\ldots [a_{k,m,\sigma}, H], \ldots, H], a_{k,m,\sigma}^+ \rangle_{n\text{-fold commutator}}$$ \(18\)

This procedure is identical to the one performed in \([26]\) for the conventional Hubbard problem. An explicit description of the calculation is presented there. As a result one obtains a self-energy of the following structure:

$$\Sigma^{(U)}_{k,m,\sigma}(E) = U \langle n_{i,m,-\sigma} \rangle \frac{E - B_{m,-\sigma} - F_{k,m,-\sigma}}{E - B_{m,-\sigma} - F_{k,m,-\sigma} - U(1 - \langle n_{i,m,-\sigma} \rangle)}$$ \(19\)

The decisive terms are $B_{m,-\sigma}$ and $F_{k,m,-\sigma}$ which distinguish this self-energy from the Hubbard-I solution \([8]\). There these terms would be replaced simply by the center of gravity of the appropriate Bloch band. $B_{m,-\sigma}$ and $F_{k,m,-\sigma}$ mainly consist of higher
correlation functions. They may provoke a spin-dependent shift and/or deformation of the bands and may therefore be responsible for the existence of spontaneous magnetism \[26, 34, 40\]. The \( k \)-dependent term \( F_{k,m,-\sigma} \) seems to be of minor importance for the magnetic behaviour \[26\]. Since \( \sum_k F_{k,m,-\sigma} = 0 \) it does not change the center of gravity of the density of states. It is mainly responsible for a deformation and narrowing of the bands. We have therefore neglected this term in the following calculations. The term \( B_{m,-\sigma} \) has the following structure:

\[
B_{m,\sigma} = \frac{1}{N} \sum_{i,j} \left( \sum_k \exp(-ik(\mathbf{R}_i - \mathbf{R}_j))\epsilon_{m,\sigma}(k) \right) \langle a_{i,m,\sigma}^\dagger a_{j,m,\sigma}(2n_{i,m,-\sigma} - 1) \rangle \tag{20}
\]

with \( \epsilon_{m,\sigma}(k) = \epsilon_m(k) + \epsilon_{k,m,\sigma}(\eta) \). Fortunately, this two-particle correlation function is accessible via the single-electron spectral density, no higher Green’s functions have to be calculated \[41\]. One obtains the following expression:

\[
B_{m,\sigma} = \frac{1}{N} \sum_k \epsilon_{m,\sigma}(k) + \frac{1}{\langle n_{m,\sigma} \rangle (1 - \langle n_{m,\sigma} \rangle)} \frac{1}{N}\hbar \sum_k \left( \epsilon_{m,\sigma}(k) - \frac{1}{N} \sum_{k'} \epsilon_{m,\sigma}(k') \right) \times \int_{-\infty}^{+\infty} d\tilde{E} \frac{S_{k,m,\sigma}(\tilde{E})}{e^{\beta(\tilde{E}-\mu)} + 1} \left( \frac{2}{U_m} (\tilde{E} - \epsilon_{m,\sigma}(k)) - 1 \right) \tag{21}
\]

This leads to a set of equations which can be solved self-consistently. Despite its obvious restrictions, e.g. the complete neglect of quasiparticle damping, the two-pole approximation together with the moment method is able to describe the magnetic properties of the Hubbard model surprisingly well \[26, 38\]. Since the subject of this paper is the influence of the spin-flip processes on the ferromagnetism introduced by the on-site intraband Hubbard interaction, this choice of a numerically simple procedure here seems reasonable. However, one should bear in mind that conceptually, the SDA is a strong coupling method which surely becomes questionable for intermediate to weak couplings. Consequently, we restrict all the following considerations to situations with \( U_m \) substantially larger than the free bandwidth \( W_m \).

2.3. Rigid Spin Approximation

Next, we have to solve the Hamiltonian \([14]\). The approximation scheme for this effective problem has to be chosen very carefully since our investigation aims at effects directly induced by the interaction \([4]\). There is no standard method to solve this model beyond mean-field level. In the following, we want to apply a non-perturbative, moment-conserving, self-consistent method which explicitly includes spin exchange scattering.

The basis of the approximation scheme is the similarity between the interaction \([4]\) and the well-known \( sf \)- or Kondo-lattice model. The difference of the two models lies in the electron spin operator \( \sigma_{i,m} \). In our model, this operator is built from electron construction operators. In the Kondo model, the charge degrees of freedom of the \( f \)-spin have been projected out. Only a pure spin operator remains. A formal equivalency
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between both models can be reached if one artificially fixes the operator $\sigma_{i,m}$ to its spin degrees of freedom. This can be done in an iterative way for both bands separately. That means for calculating the self-energy for band $m$ one has to fix the spin-operator of the other band ($\sigma_{i,m}$) and vica versa. Thus no constraints are introduced concerning the quantum mechanical attributes of the partial electron system under consideration, as e.g. the non-distinguishability of the particles. In our opinion, the name Rigid Spin Approximation (RSA) is an appropriate denotation for this method.

Now we can apply a proper approximation developed for the $sf$-model. We use a moment-conserving, self-consistent interpolating equation-of-motion decoupling scheme \cite{35,36,37}. A discussion of the neccessary approximations and their implications can be found there, so that we can restrict ourselves to a short summary in this paper. In the equation of motion for the single-electron Green’s function $G_{i,j,m,\sigma}(E) = \langle \langle a_{i,m,\sigma}; a_{j,m,\sigma}^\dagger \rangle \rangle$, 

$$EG_{i,j,m,\sigma}(E) = \hbar + \sum_l \left( \sum_k \exp(i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_l))(\epsilon_m(\mathbf{k}) + \Sigma_{k,m,\sigma}(\eta)) \right) G_{l,j,m,\sigma}(E)$$

$$-\frac{1}{2}J(F_{i,i,j,m,\sigma}(E) + z\sigma \Gamma_{i,i,j,m,\sigma}(E))$$ (22)

two higher Green’s functions are introduced, the “spin-flip” function $F_{i,i,j,m,\sigma}(E) = \langle \langle \sigma_{i,m}^\dagger a_{i,m,-\sigma}; a_{j,m,\sigma}^\dagger \rangle \rangle$ and the “Ising” function $\Gamma_{i,i,j,m,\sigma}(E) = \langle \langle \sigma_{i,m}^z a_{i,m,\sigma}; a_{j,m,\sigma}^\dagger \rangle \rangle$. For these two Green’s functions, the respective equations of motion can be obtained without problems. In each of them, new Green’s functions are introduced. For these we carefully apply a sophisticated decoupling scheme. The central idea is to express all local higher Green’s function in the equations of motion of the spin-flip and Ising function by interpolation “ansatizes” between several non-trivial limiting cases, such as $S = \frac{1}{2}$, ferromagnetic saturation of one band, empty and full band. The corresponding interpolation parameters can be obtained using a moment method similar to the one described in section 2.2. Within this approximation scheme we obtain a selfenergy of the following structure:

$$\Sigma_{m,\sigma}^{(J)}(E) = J\langle \sigma_{i,m}^z + J^2 F(\Sigma_{m,\sigma}^{(J)}(E), \langle n_{m,\sigma} \rangle, \langle \sigma_{i,m}^\dagger \sigma_{i,m}^- \rangle, \ldots)$$ (23)

The first term corresponds to the mean-field solution. The second part corresponds to higher order terms in $J$. The complex functional $F$ depends on several correlation functions, as e.g. the interband spin-exchange correlation $\langle \sigma_{i,m}^\dagger \sigma_{i,m}^- \rangle$ or the interband Ising correlation $\langle \sigma_{i,m}^z \sigma_{i,m}^\dagger \rangle$, the selfenergy part $\Sigma_{m,\sigma}^{(J)}(E)$ and of course, via the effective medium, on the intraband selfenergy part $\Sigma_{m,\sigma}^{(U)}(E)$. All correlation functions as well as the selfenergy parts have to be determined selfconsistently. The selfenergy part $\Sigma_{m,\sigma}^{(J)}(E)$ is $\mathbf{k}$-independent due to the neglect of magnonic excitation energies, which are small compared to the electronic excitations under consideration \cite{36}. It is worth to mention that this method can be continued smoothly to the exactly solvable non-trivial limiting case of one electron in a ferromagnetic saturated background of $f$-spins.
3. Results and Discussion

In this section we present the results obtained by the theory described above. The results are compared with the usual mean-field calculation for the spin-exchange interaction. The two-band model under consideration consists of two bands $m = \{0, 1\}$ of unit width ($W_{0,1} = 1.0$) thus defining the energy unit used in this paper. The bands are not degenerate, the centers of gravity are shifted by 0.1. As an example we choose tight-binding bcc free densities of states [42]. In the single-band Hubbard model, the existence of ferromagnetism depends on the lattice structure, as has been shown by various methods (stability of the Nagaoka state [16], SDA [38], QMC in $d = \infty$ [43]). From these investigations, it follows that the system has stronger tendency towards ferromagnetism in non-bipartite lattices (e.g. fcc). It seems reasonable to believe that this will also hold for the two-band model although we did no systematic analysis of the lattice dependence.

![Figure 1](image)

*Figure 1.* Magnetization $m$ as function of band occupation $n$ of a single-band Hubbard model with $U = 5$, $T = 0$ on a bcc-lattice. The dashed line indicates saturation ($m = n$). Antiferromagnetic ordering is expected close to half filling ($n = 1$) which is not considered in this paper. Due to particle-hole-symmetry, it is sufficient to investigate the region of $0 < n < 1$

One expects the local intraband Coulomb matrix element $U$ to be large whereas the interband exchange coupling constant $J$ could be one order of magnitude smaller. As mentioned above the SDA which we use to find the intraband selfenergy part $\Sigma^{(U)}_{k,m,\sigma}(E)$ is basically a strong-coupling theory. In the large-$U$ regime, however, magnetic key quantities such as the Curie-temperature, the $T = 0$-moment, and so on, are already saturated, i.e. no longer $U$-dependent (see e.g. figure 11 in [26]). More interesting is the $J$-dependence. We therefore restrict ourselves to the representative value of $U = 5$ and inspect in detail the influence of the interband interaction $J$. Furthermore, the evaluation is confined to $T = 0$, although the theory of course holds for finite
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temperatures, too.

3.1. The $J = 0$ case

In the case of vanishing interband coupling, $J = 0$, the situation is identical to two separate single-band Hubbard models which are only coupled by a common Fermi energy. It determines the respective partial band occupations $n_{\{0,1\}}$ according to the total number of electrons per site $n_{\text{tot}} = n_0 + n_1$. For the single-band Hubbard model, the existence of ferromagnetism has been since long a matter of controversial discussions, but recent results confirm its stability for certain parameter regimes \[15, 18\]. The SDA has turned out to be able to reproduce the QMC results in this limiting case on a qualitative level \[14, 38\].

First, let us remind of a result obtained within a single-band Hubbard model. In figure 1, the dependence of the magnetization on the electron density (occupation number) is plotted. For $n < n_{\text{c (hub)}}^{(0)} \approx 0.56$ the system is paramagnetic, only for $n > n_{\text{c (hub)}}^{(0)}$ ferromagnetic ordering is possible. With increasing $n$, the system becomes quickly saturated. Antiferromagnetic ordering occurs only in the very vicinity of half filling ($n = 1.0$) which we will never consider in the following discussion. More information on ferromagnetism in the single-band Hubbard model can be found in \[18, 19, 26, 33, 38, 41, 44\].

![Figure 1](image1.png)

**Figure 1.** The magnetization $m$ as function of the electron density $n$ for the single-band situation. Together with the total magnetization $m_{\text{tot}}$, the partial occupation numbers per band $n_0$ and $n_1$ are plotted.

In figure 2, the magnetization as function of the electron density is plotted for the two-band situation. Together with the total magnetization $m_{\text{tot}}$, the partial occupation numbers per band $n_0$ and $n_1$ are plotted.

![Figure 2](image2.png)

**Figure 2.** Magnetization $m$ as function of total occupation $n_{\text{tot}}$ of a two-band system (solid line: total magnetization, dashed line: polarization of the lower band ($m = 0$), chained line: polarization of the upper band ($m = 1$)). The thin lines represent the partial occupation numbers per band. System parameters: $U = 5$, $J = 0$, $T = 0$.
numbers and polarizations per band are shown. The interband interaction is still set to zero \((J = 0)\). As already mentioned above, both bands are coupled only via the chemical potential. Ferromagnetic order sets in in band \(m = 0\), the lower band, when this band reaches a critical occupation of \(n_0 = n_{c,0}^{(J=0)} \approx 0.63 > n_c^{(hub)}\) which is the case for a total occupation of \(n_{tot} \approx 0.98\). The critical electron density of the lower band \(n_{c,0}^{(J=0)}\) is larger than in the single-band case \(n_c^{(hub)}\). Even though the upper band is neither explicitly coupled to the lower band nor is ferromagnetic by itself, it has an influence on the para- to ferromagnetic transition of the lower band. This can be understood, since the upper band can act as source or sink of electrons for the lower band. With the onset of ferromagnetism, a spin-dependent band splitting takes place. This provides for a rearrangement of electrons between the bands due to the same chemical potential for both bands. Now, if the system tries to order ferromagnetically, when band \(m = 0\) reaches the “single-band critical occupation” of approximately \(n_0 \approx 0.56\), the corresponding shift of the densities of states will make the ferromagnetic phase instable. This happens until the real critical value of the two-band situation, \(n_0 = n_{c,0}^{(J=0)} \approx 0.63\) is reached. This effect is analogous to the findings in [45], where a similar situation was examined using a Stoner-like theory.

3.2. The \(n_{tot}\)-dependency of the magnetization

![Figure 3](image-url)  
**Figure 3.** The same as figure 2, but with finite \(J = 0.2\). Left-hand side: Interband exchange interaction in mean-field approximation, right-hand side in RSA

Let us focus on the interband-exchange interaction. Figure 3 shows, similar to figure 2, the magnetization as function of electron occupation but with finite \(J = 0.2\). On the left hand side, calculations were made using the mean-field approximation for the interband-exchange self-energy part, on the right hand side the rigid spin approximation as explained in chapter 2.3 was applied.
The mean-field result is easily understood: When the lower band reaches a critical occupation number \( n_0 = n_{c,0}^{(mf)} \approx 0.50 \) a transition to a ferromagnetic state occurs. Now the interband exchange in mean-field approximation will provide for a rigid spin-dependent shift of the \( m = 1 \) quasiparticle bands proportional to the magnetization of the lower band. This induces a polarization of the upper band as well. The same mechanism now works as a feedback onto the lower band, increasing the magnetization even more. The lower band becomes thus quickly saturated.

When analyzing the same situation using the rigid spin approximation, the picture gets modified in a rather drastic way. The onset of ferromagnetism is indicated by a critical occupation for the lower band \( n_c^{(RSA)} \) which is only a little larger than \( n_{c,0}^{(mf)} \). But the polarization of the upper band is much weaker than in the mean-field case. And furthermore, the lower band never reaches saturation. The latter is not a result of the weak polarization of the \( m = 1 \) band, but both effects have the same origin. Continuous spin-flip scattering prohibits the lower band from reaching saturation. These processes, in addition to the generally stronger quasiparticle damping also reduce the magnetic polarization of the upper band.

### 3.3. The \( J \)-dependence of the magnetization

![Figure 4](image.png)

**Figure 4.** Total magnetization \( m \) (solid line) and partial polarization of the two bands (dashed: lower band \( 0 \), chained: upper band \( 1 \)) as function of the interband coupling constant \( J \) for fixed total occupation \( n_{tot} = 1.0 \) and \( U = 5, T = 0 \).

Next, we want to investigate the \( J \)-dependence of the magnetization. This turns out to yield unexpected, non-trivial results. Figure 4 shows the magnetization as function of \( J \) for fixed \( U = 5 \) and \( n_{tot} = 1.0 \). In figure 5, the behaviour for very small \( J \) is plotted together with results obtained using mean-field approximation for the interband-exchange, and finally, the corresponding quasiparticle densities of states are plotted in...
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Figure 5. The same as figure 3, but zoomed to small values of $J$. Additionally, the results of the mean-field calculation are plotted (thin lines).

figure 5. For the chosen total occupation number $n_{\text{tot}} = 1.0$, the lower band is already ferromagnetically ordered for $J = 0$, whereas the upper band is still paramagnetic (see figure 2).

The magnetization curve in figure 4 can be separated roughly into 3 regions. For very small $J$ the magnetization rises (region A), for intermediate $J$ it decreases (region B) and shows a reentrant behaviour for the largest $J$ under consideration (region C).

3.3.1. Region A: The first of these regions is characterized by an increasing magnetization as seen more clearly in figure 5. There, additionally to the RSA result, the mean-field curves are plotted. These are simply understood, any finite $J$ will induce magnetic polarization into the upper band, and via a feedback, push the lower band into saturation. Band $m = 1$ will become more and more polarized, finally reaching saturation, too (not plotted in figure 5). The same effect can be seen in the RSA calculation, which is in first order of $J$ identical to the mean-field result.

3.3.2. Region B: Already for $J \approx 0.05$, which is still a very small parameter, deviations from the mean-field result are quite strong. This leads to the second regime in figure 5. Here, the magnetization decreases, first slightly, but with increasing $J$ stronger and
Figure 6. Quasiparticle densities of states (QDOS) for certain values of $J$ for the same system parameters as in figure 3 with the chemical potential $\mu = 0$. The $m = 0$ bands are drawn in solid, the $m = 1$ quasiparticle bands in dashed lines. Spin $\uparrow$ and spin $\downarrow$ QDOS are plotted separately as indicated.
stronger. In this parameter regime, the higher-order contributions in $J$ to the self-energy become more and more important. The connection between the reduction of the magnetization and spin-flip processes becomes obvious by a comparison with the conventional $sf$-model. The important observation is the onset of a small dip in the quasiparticle densities of states (QDOS) with increasing $J$ (figure 4). This dip is on a much smaller energy scale than the Hubbard splitting, which is also clearly visible in figure 6.

To understand this feature, we want to relate it to a feature known from the conventional $sf$-model. There, a bandsplitting can occur for intermediate to large values of $J$. The size of the gap scales roughly with $J$. The physics causing this gap can be understood best by examining the exactly solvable special case of one electron in a saturated spin background [46, 36]. In this case two different elementary excitations can be observed. One represents the scattering of an electron accompanied by the emission of a magnon, whereas the other can be connected with a bound state of an electron with a cloud of magnons. The latter manifests itself in the spectral density by a delta-like peak splitting of the scattering part for large enough values of $J$. The respective quasiparticle is called magnetic polaron [36]. For the general case of the $sf$-model, i.e. for finite electron density and a not fully polarized spin system, a similar band splitting due to the same two elementary processes will occur for large enough values of $J$ in both spin-resolved sub-bands [37]. The dip seen in the QDOS of figure 6 is a precursor to the magnetic-polaron-induced bandsplitting.

The reduction of the magnetization originates clearly from the spin-flip terms in the Hamiltonian. A further test is the artificial neglect of quasiparticle damping by setting $\Im \Sigma_{\sigma}(E) = 0$. Even then, a reduction, though smaller, of the magnetization with increasing $J$ is found. So additionally to the generic damping effects, explicit spin-flip scattering depolarizes the system.

3.3.3. Region C: Finally, one observes a reentrant behaviour of the ferromagnetic ordering in figure 4, the origin of which is not completely clear. One possible mechanism for supporting magnetic order would be a RKKY-like interaction mediated by the interband interaction (4). The reentrant behaviour would indicate, that only for $J \gtrsim 0.45$, the effective RKKY-interaction is strong enough to have an effect. To support our proposal, we have performed a calculation for the case of $U = 0$ and finite $J$. Even for these more or less unphysical parameters, we find stable ferromagnetic solutions. But as in the finite-$U$ case, these only occur for relatively large values of $J \gtrsim 0.64$. So even this artificially castrated model without direkt Coulomb interaction shows similar behaviour, which is, of course, quantitatively modified in the more realistic model with finite $U$.

How this proposed mechanism is related to an enhanced stability of ferromagnetism due to the two-band situation found in [25] is an interesting, but open question.
4. Conclusions

In this paper, we have analyzed a special multi-band Hubbard model which contains the two interaction terms believed to have the biggest influence on the stability of ferromagnetic ordering.

Our model (1) is clearly insufficient to describe the rich physics of transition metals. But the same applies probably to any other model Hamiltonian which is still tractable within many-body theory. However, ab-initio calculations as e.g. density functional theory applied within the local density approximation (LDA) appear to underestimate just those correlation effects which seem to be decisive for phenomena like ferromagnetism. A proper combination of LDA calculations with a many-body treatment gives a promising way to solve these difficulties. The LDA calculation accounts for all interactions on a mean-field level, the many-body treatment should restrict itself only to the most important correlations. We believe that the model (1) contains in this sense those interactions whose contributions beyond meanfield have the biggest impact on magnetism. A combination of LDA calculations with the model (1) using a simpler approximation on the exchange part yields very good agreement with experimental facts [2, 3, 6, 7]. For example, by fitting the interaction constants U and J to groundstate properties, the Curie-temperature could be calculated astonishingly accurate.

In this paper, we introduced a more sophisticated approximation scheme, which is especially improved on the exchange interaction part of model (1). Our analysis was based on the fact that the intraband Hubbard interaction alone is able to form ordered magnetic moments in a band (itinerant magnetism). We investigated the influence of interband exchange coupling, often referred to as Hund’s rule coupling, on the stability of ferromagnetism. Only for very small values of J, the respective interband coupling constant, we can verify the mean-field result which leads always to an enhanced stability of spontaneous ferromagnetism. Already for J ≈ 0.1 which we call intermediate coupling the magnetization gets suppressed by spin-flip scattering (using the free bandwidth as energy scale: W = 1). With increasing J the ferromagnetic order almost vanishes. The reentrant behaviour found for even larger J might be due to an RKKY-like ordering mechanism mediated by the interband interaction (1). The regime of J most often referred to transition metals belongs to intermediate coupling strengths. Our results indicate that the influence of the spin flip processes can manifest itself in a rather dramatic reduction of the magnetization.

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Acknowledgments

One of us (D.M.) gratefully acknowledges the support of the Friedrich-Naumann foundation. This work also benefitted from the financial support of the Sonderforschungsbereich SFB 290 (“Metallische dünne Schichten: Struktur, Magnetismus und elektronische Eigenschaften”) of the Deutsche Forschungsgemeinschaft.