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The 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 a Ruderman–Kittel–Kasuya–Yosida-like (RKKY-like) magnetic ordering mechanism is also observed.

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. Unlike 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 [1–7]. 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 fairly oversimplified theoretical models. In this paper, we want to provide another small piece of the puzzle for the d-band metals.

The investigation of ferromagnetism in the Hubbard model has a long history. In fact, it was the original intention in 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-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 subjected to extensive investigation. For example, 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

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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 fivefold degeneracy of the d bands. How does this fact influence ferromagnetism? In atoms, Hund's rules will favour 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 [14, 21]). 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 transverse (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 the interband exchange constant J, thus fulfilling the predictions made by analogy to the atomic behaviour. This is most obvious in mean-field theory, where the transverse part vanishes, and a magnetization-dependent band shift 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 of ferromagnetism [2, 3, 6, 7]. This leads to the following Hamiltonian:

$$H = H_0 + H_U + H_J \tag{1}$$

where

$$H_0 = \sum_{\boldsymbol{k},m,\sigma} \epsilon_m(\boldsymbol{k}) a^{\dagger}_{\boldsymbol{k},m,\sigma} a_{\boldsymbol{k},m,\sigma} \tag{2}$$

$$H_U = \frac{1}{2} U \sum_{i,m,\sigma} n_{i,m,\sigma} n_{i,m,-\sigma} \tag{3}$$

$$H_J = -\frac{1}{2} J \sum_{i,m} \boldsymbol{\sigma}_{i,m} \cdot \boldsymbol{\sigma}_{i,\bar{m}}. \tag{4}$$

We use the usual notation for the electron annihilation (creation) operators $a^{(\dagger)}_{\boldsymbol{k},m,\sigma}$ with wavevector $\boldsymbol{k}$, band index m ($\bar{m}$ being the complementary band of the two-band system), and spin σ. The free bands are described by the dispersion $\epsilon_m(\boldsymbol{k})$; 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

$$\sigma^{\sigma}_{i,m} = a^{\dagger}_{i,m,\sigma} a_{i,m,-\sigma}$$
$$\sigma^{z}_{i,m} = \frac{1}{2} \sum_{\sigma} z_{\sigma} n_{i,m,\sigma} \tag{5}$$

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:

$$H_J = -\frac{1}{4} J \sum_{i,m,\sigma} (\sigma^{\sigma}_{i,m} \sigma^{-\sigma}_{i,\bar{m}} + \sigma^{z}_{i,m} \sigma^{z}_{i,\bar{m}}) \tag{6}$$

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 [10,22–24]. In this paper, we want to trace both parts of the interband interaction (6) with identical quality.

It goes without saying that (2) and (4) do not represent the full set of local Coulomb interactions between d electrons. Our previous studies [2, 6, 7, 27], however, have given evidence 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*' band-structure 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 (2) and (4) should be most important while, e.g., the interband Coulomb interaction (denoted by $\bar{U}$ in our previous studies [6]) 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. Our present model investigation is to be understood in this sense. 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 of *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 lines of references [2, 6, 7], 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. The effective-medium approach

Even though we restricted consideration to a rather simple model Hamiltonian, we need 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 [29].

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 $\Sigma_{\boldsymbol{k},m,\sigma}(E)$ can be defined using the equation of motion of the single-electron Green's function $G_{\boldsymbol{k},m,\sigma}(E) = \langle\langle a_{\boldsymbol{k},m,\sigma}; a^{\dagger}_{\boldsymbol{k},m,\sigma}\rangle\rangle$:

$$\begin{aligned} EG_{\boldsymbol{k},m,\sigma}(E) &= \hbar + \epsilon_m(\boldsymbol{k})G_{\boldsymbol{k},m,\sigma}(E) + \langle\langle [a_{\boldsymbol{k},m,\sigma}, H_U + H_J]_-; a^{\dagger}_{\boldsymbol{k},m,\sigma}\rangle\rangle \\ &= \hbar + \epsilon_m(\boldsymbol{k})G_{\boldsymbol{k},m,\sigma}(E) + \Sigma_{\boldsymbol{k},m,\sigma}(E)G_{\boldsymbol{k},m,\sigma}(E). \end{aligned} \tag{7}$$

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

$$\langle\langle [a_{\boldsymbol{k},m,\sigma}, H_U]_-; a^{\dagger}_{\boldsymbol{k},m,\sigma}\rangle\rangle = \Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E)G_{\boldsymbol{k},m,\sigma}(E) \tag{8}$$

$$\langle\langle [a_{\boldsymbol{k},m,\sigma}, H_J]_-; a^{\dagger}_{\boldsymbol{k},m,\sigma}\rangle\rangle = \Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(E)G_{\boldsymbol{k},m,\sigma}(E) \tag{9}$$

with

$$\Sigma_{\boldsymbol{k},m,\sigma}(E) = \Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E) + \Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(E).$$

Assuming the knowledge of either one of these self-energy parts, one can introduce the following effective Hamiltonians:

$$H^{(U,\eta)}_{\text{eff}} = \sum_{\boldsymbol{k}}(\epsilon_m(\boldsymbol{k}) + \Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(\eta))a^{\dagger}_{\boldsymbol{k},m,\sigma}a_{\boldsymbol{k},m,\sigma} + H_U \tag{10}$$

$$H^{(J,\eta)}_{\text{eff}} = \sum_{\boldsymbol{k}}(\epsilon_m(\boldsymbol{k}) + \Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(\eta))a^{\dagger}_{\boldsymbol{k},m,\sigma}a_{\boldsymbol{k},m,\sigma} + H_J \tag{11}$$

which formally depend on a parameter η. By solving each of these Hamiltonians for all values of η, one can obtain the missing self-energy part using the following identities:

$$\Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E) = \Sigma^{(\text{eff},U,\eta)}_{\boldsymbol{k},m,\sigma}(E)\big|_{\eta=E} \tag{12}$$

$$\Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(E) = \Sigma^{(\text{eff},J,\eta)}_{\boldsymbol{k},m,\sigma}(E)\big|_{\eta=E} \tag{13}$$

with $\Sigma^{(\text{eff},U,\eta)}_{\boldsymbol{k},m,\sigma}(E)$ being the self-energy of the effective Hamiltonian (10) and $\Sigma^{(\text{eff},J,\eta)}_{\boldsymbol{k},m,\sigma}(E)$ that of Hamiltonian (11). The introduction of the energy parameter η in the effective Hamiltonians (10) and (11) is necessary in order to distinguish two different kinds of energy. The effective-medium energy parameter η should not be confused with the energy as the dynamic variable of e.g. an equation-of-motion method for solving the corresponding 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:

$$G_{\boldsymbol{k},m,\sigma}(E) = \frac{\hbar}{E - (\epsilon_m(\boldsymbol{k}) + \Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E) + \Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(E))}. \tag{14}$$

The two problems posed by the Hamiltonians (10) and (11) are strongly related to each other. The solution of one in the 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 already been analysed very well 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 the sf model or ferromagnetic

Kondo lattice [30, 31]. So for both partial problems, existing 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 being mathematically 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 section. The sf model has also attracted much interest. A very promising interpolating, moment-conserving, equation-of-motion-decoupling scheme has been developed in references [35–37]. 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. The spectral density approach

According to the effective-medium *ansatz*, the self-energy part $\Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E)$ connected with the intraband Hubbard interaction will be calculated using 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 brief outline of the calculations. The starting point is the single-electron spectral density, defined by

$$S_{\boldsymbol{k},m,\sigma}(E) = \frac{1}{N}\sum_{i,j}\exp(\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j))\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}E\ \exp\left(-\frac{\mathrm{i}}{\hbar}Et\right)\langle[a_{i,m,\sigma}(t),a^{\dagger}_{j,m,\sigma}(0)]_+\rangle \tag{15}$$

where $[\ldots,\ldots]_+$ denotes the anticommutator and $\langle\cdots\rangle$ 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 $U\to\infty$:

$$S_{\boldsymbol{k},m,\sigma}(E) = \sum_{j=1,2}\hbar\alpha^{(j)}_{\boldsymbol{k},m,\sigma}\delta(E-E^{(j)}_{\boldsymbol{k},m,\sigma}). \tag{16}$$

The unknown parameters $E^{(j)}_{\boldsymbol{k},m,\sigma}$ and $\alpha^{(j)}_{\boldsymbol{k},m,\sigma}$, the quasiparticle energy and the spectral weight, can be calculated by the moment method. This means they are fitted by the use of the first four moments of the spectral density, which represent several sum rules:

$$M^{(n)}_{\boldsymbol{k},m,\sigma} = \int_{-\infty}^{+\infty}\mathrm{d}E\ E^n S_{\boldsymbol{k},m,\sigma}(E) \tag{17}$$

and which can be calculated directly from the Hamiltonian:

$$M^{(n)}_{\boldsymbol{k},m,\sigma} = \langle[\underbrace{[\ldots[a_{\boldsymbol{k},m,\sigma},H]_-,\ldots,H]_-}_{n-\text{fold commutator}},a^{\dagger}_{\boldsymbol{k},m,\sigma}]_+\rangle. \tag{18}$$

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:

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

The decisive terms are $B_{m,-\sigma}$ and $F_{\boldsymbol{k},m,-\sigma}$ which distinguish this self-energy from the Hubbard-I solution [8]. There these terms would be replaced simply by the centre of gravity of the appropriate Bloch band. $B_{m,-\sigma}$ and $F_{\boldsymbol{k},m,-\sigma}$ 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 $\boldsymbol{k}$-dependent term $F_{\boldsymbol{k},m,-\sigma}$ seems to be of minor importance for the magnetic behaviour [26]. Since $\sum_{\boldsymbol{k}} F_{\boldsymbol{k},m,-\sigma} = 0$, it does not change the centre 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:

$$B_{m,\sigma} = \frac{1}{N}\sum_{i,j}\left(\sum_{\boldsymbol{k}} \exp(-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j))\epsilon_{m,\sigma}(\boldsymbol{k})\right)\langle a^{\dagger}_{i,m,\sigma} a_{j,m,\sigma}(2n_{i,m,-\sigma} - 1)\rangle \tag{20}$$

with $\epsilon_{m,\sigma}(\boldsymbol{k}) = \epsilon_m(\boldsymbol{k}) + \Sigma^{(J)}_{\boldsymbol{k},m,\sigma}(\eta)$. 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:

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

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 certainly becomes questionable for intermediate to weak couplings. Consequently, we restrict all of the following considerations to situations with U_m substantially larger than the free bandwidth W_m.

2.3. The rigid-spin approximation

Next, we have to solve Hamiltonian (11). 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 for solving 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 $\boldsymbol{\sigma}_{i,\bar{m}}$. 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 between the two models can be reached if one artificially fixes the operator $\boldsymbol{\sigma}_{i,\bar{m}}$ to its spin degrees of freedom. This can be done in

an iterative way for both bands separately. This means that for calculating the self-energy for band m one has to fix the spin operator of the other band ($\boldsymbol{\sigma}_{i,\bar{m}}$) and vice versa. Thus no constraints are introduced concerning the quantum mechanical attributes of the partial electron system under consideration, such as the indistinguishability of the particles. In our opinion, the name *rigid-spin approximation* (RSA) is an appropriate for this method.

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

$$EG_{i,j,m,\sigma}(E) = \overline{h} + \sum_{l}\left(\sum_{\boldsymbol{k}} \exp(\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_l))(\epsilon_m(\boldsymbol{k}) + \Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(\eta))\right)G_{l,j,m,\sigma}(E)$$
$$-\frac{1}{2}J\left(F_{i,i,j,m,\sigma}(E) + z_{\sigma}\Gamma_{i,i,j,m,\sigma}(E)\right) \tag{22}$$

two higher Green's functions are introduced, the 'spin-flip' function $F_{i,l,j,m,\sigma}(E) = \langle\langle \sigma^{-\sigma}_{i,\bar{m}} a_{l,m,-\sigma}; a^{\dagger}_{j,m,\sigma}\rangle\rangle$ and the 'Ising' function $\Gamma_{i,l,j,m,\sigma}(E) = \langle\langle \sigma^{z}_{i,\bar{m}} a_{l,m,\sigma}; a^{\dagger}_{j,m,\sigma}\rangle\rangle$. For these two Green's functions, the respective equations of motion can be obtained without difficulty. 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 functions in the equations of motion of the spin-flip and Ising function by '*ansatze*' interpolating between several non-trivial limiting cases, such as $S = \frac{1}{2}$, ferromagnetic saturation of one band, empty band, 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 self-energy of the following structure:

$$\Sigma^{(J)}_{m,\sigma}(E) = J\langle\sigma^{z}_{i,\bar{m}}\rangle + J^2\mathcal{F}(\Sigma^{(J)}_{m,\sigma}(E), \langle n_{m,\sigma}\rangle, \langle\sigma^{+}_{i,\bar{m}}\sigma^{-}_{i,m}\rangle, \ldots). \tag{23}$$

The first term corresponds to the mean-field solution. The second part corresponds to higher-order terms in J. The complex functional $\mathcal{F}$ depends on several correlation functions, such as the interband spin-exchange correlation $\langle\sigma^{+}_{i,\bar{m}}\sigma^{-}_{i,m}\rangle$ and the interband Ising correlation $\langle\sigma^{z}_{i,\bar{m}}\sigma^{z}_{i,m}\rangle$, the self-energy part $\Sigma^{(J)}_{m,\sigma}(E)$, and of course, via the effective medium, the intraband self-energy part $\Sigma^{(U)}_{m,\sigma}(E)$. All correlation functions as well as the self-energy parts have to be determined self-consistently. The self-energy part $\Sigma^{(J)}_{m,\sigma}(E)$ is $\boldsymbol{k}$-independent due to the neglect of magnonic excitation energies, which are small compared to the electronic excitations under consideration [36]. It is worth mentioning 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 centres 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 simulations for $d = \infty$ [43]). From these investigations, it follows that the

system has a stronger tendency towards ferromagnetism in non-bipartite (e.g. fcc) lattices. 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.

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 self-energy part $\Sigma^{(U)}_{\boldsymbol{k},m,\sigma}(E)$ is basically a strong-coupling theory. In the large-U regime, however, magnetic key quantities such as the Curie temperature and the $T = 0$ moment 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 consideration 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 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 $n_{\mathrm{tot}} = n_0 + n_1$. For the single-band Hubbard model, the existence of ferromagnetism has long been a matter of controversial discussion, 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 [34, 38].

First, let us recall 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 $n < n_c^{(\mathrm{Hub})} \approx 0.56$ the system is paramagnetic; only for $n > n_c^{(\mathrm{Hub})}$ is ferromagnetic ordering 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].

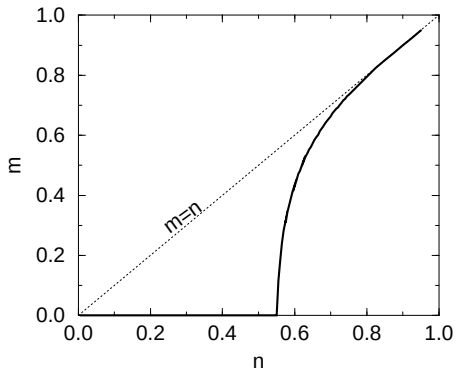

Figure 1. Magnetization m as a function of band occupation n for a single-band Hubbard model with $U = 5$, $T = 0$ on a bcc lattice. The dotted line indicates saturation ($m = n$). Antiferromagnetic ordering is expected close to half-filling ($n = 1$), which is not considered in this paper. Due to particle–hole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

In figure 2, the magnetization as a function of the electron density is plotted for the two-band situation. Together with the total magnetization m_{tot}, the partial occupation numbers and

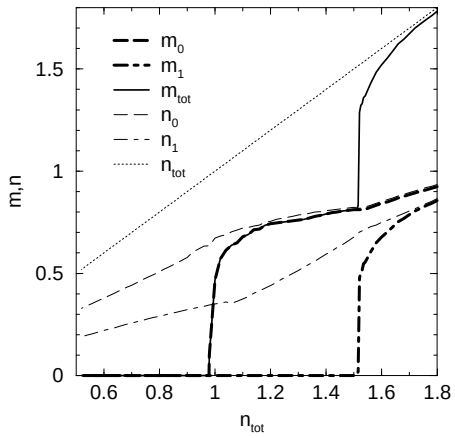

Figure 2. Magnetization m as a function of total occupation n_{tot} for a two-band system (solid curve: total magnetization; dashed curve: polarization of the lower band ($m = 0$); chain curve: polarization of the upper band ($m = 1$)). The thin curves represent the partial occupation numbers per band. System parameters: $U = 5$, $J = 0$, $T = 0$.

polarizations per band are shown. The interband interaction is still set to zero ($J = 0$). As already mentioned above, the two 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 $n_0 = n_{c,0}^{(J=0)} \approx 0.63 > n_c^{(\mathrm{Hub})}$ which is the case for a total occupation of $n_{\mathrm{tot}} \approx 0.98$. The critical electron density of the lower band $n_{c,0}^{(J=0)}$ is larger than in the single-band case ($n_c^{(\mathrm{Hub})}$). Even though the upper band is neither explicitly coupled to the lower band nor ferromagnetic by itself, it has an influence on the paramagnetic–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 chemical potential being the same for the two 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 unstable. 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

Let us focus on the interband exchange interaction. Figure 3 shows, like figure 2, the magnetization as a function of the 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 section 2.3 was applied.

The mean-field result is easily understood: when the lower band reaches a critical occupation number $n_0 = n_{c,0}^{(\mathrm{mf})} \approx 0.50 < n_{c,0}^{(J=0)}$, a transition to a ferromagnetic state occurs. Now the interband exchange in the 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.

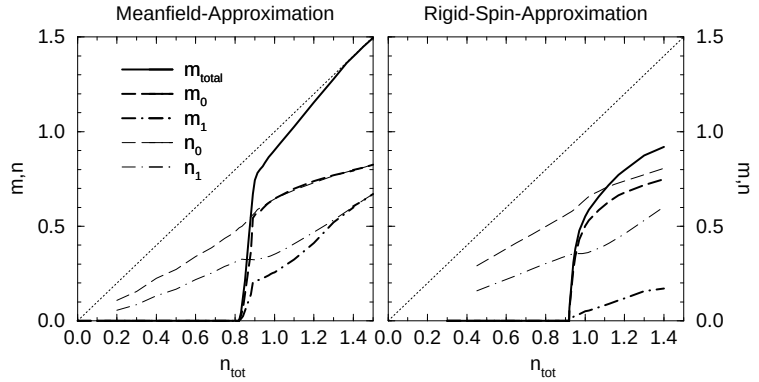

Figure 3. As figure 2, but with finite $J = 0.2$. Left-hand side: the interband exchange interaction in the mean-field approximation; right-hand side: the interband exchange interaction in the RSA.

This induces a polarization of the upper band as well. The same mechanism now works as a feedback on the lower band, increasing the magnetization even more. The lower band thus becomes quickly saturated.

When analysing the same situation using the rigid-spin approximation, the picture is modified in a rather drastic way. The onset of ferromagnetism is indicated by a critical occupation for the lower band $n_c^{(\mathrm{RSA})}$ which is only a little larger than $n_c^{(\mathrm{mf})}$. 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 the two 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

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 a function of J for fixed $U = 5$ and $n_{\mathrm{tot}} = 1.0$. 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 figure 6. For the chosen total occupation number $n_{\mathrm{tot}} = 1.0$, 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 three regions. For very small J the magnetization rises (region A); for intermediate J it decreases (region B); and it shows a re-entrant 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.

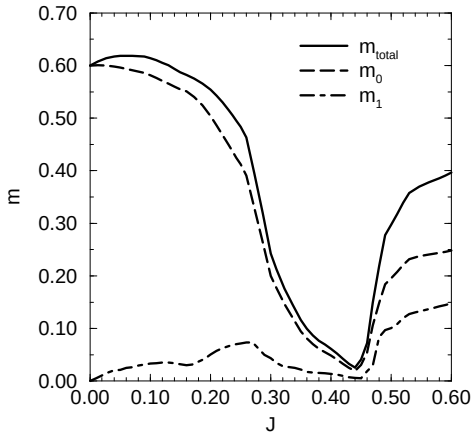

Figure 4. Total magnetization m (solid curve) and partial polarization of the two bands (dashed curve: lower band (0); chain curve: upper band (1)) as functions of the interband coupling constant J for fixed total occupation $n_{\mathrm{tot}} = 1.0$ and $U = 5$, $T = 0$.

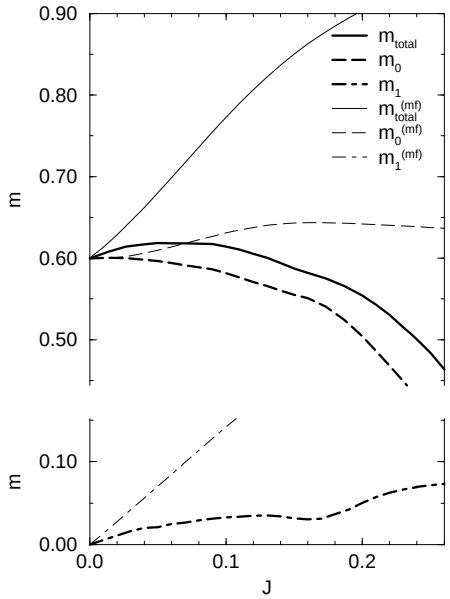

Figure 5. As figure 3, but zoomed to small values of J. Additionally, the results of the mean-field calculation are plotted (thin curves).

3.3.2. Region B. For $J \approx 0.05$, which is still a very small parameter, deviations from the mean-field result are already quite strong. This leads to the second regime in figure 4. Here, the magnetization decreases, first slightly, but with increasing J more and more strongly. 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 from a comparison with the conventional sf model. The important

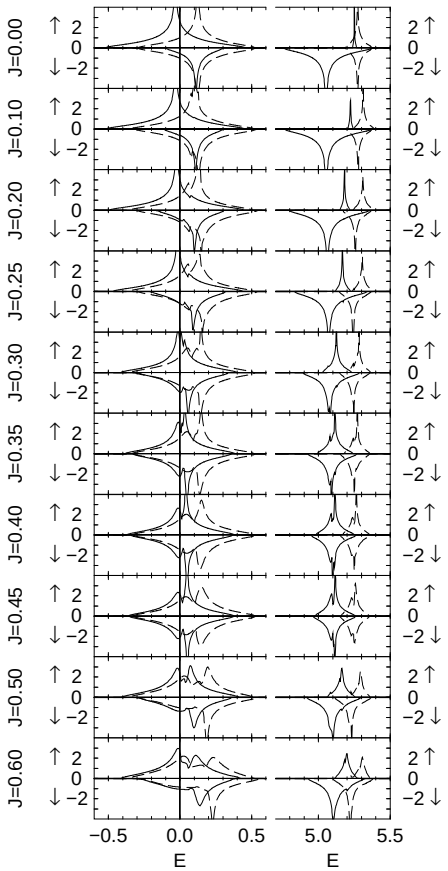

Figure 6. Quasiparticle densities of states (QDOS) for certain values of J for the same system parameters as in figure 3 with the chemical potential $\mu = 0$. The $m = 0$ bands are drawn as solid curves, the $m = 1$ quasiparticle bands as dashed curves. The spin-up and spin-down QDOS are plotted separately as indicated.

observation is the onset of a small dip in the quasiparticle densities of states (QDOS) with increasing J (figure 6). 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 band splitting 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 [36, 46]. 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 corresponding quasiparticle is called a 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 band splitting.

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 achieved 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 re-entrant 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 an RKKY-like interaction mediated by the interband interaction (4). The re-entrant behaviour would indicate that only for $J \gtrsim 0.45$ is the effective RKKY interaction 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 restricted model without direct 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 analysed 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 such as those of 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 represents a promising way to solve these difficulties. The LDA calculation accounts for all interactions on a mean-field level; the many-body treatment should be restricted to just the most important correlations. We believe that the model (1) contains in this sense those interactions whose contributions beyond the mean-field level have the biggest impact on magnetism. A combination of LDA calculations with the model (1) using a simpler approximation for the exchange part yields very good agreement with experimental findings [2, 3, 6, 7]. For example, by fitting the interaction constants U and J to ground-state properties, the Curie temperature can be calculated astonishingly accurately.

In this paper, we introduced a more sophisticated approximation scheme, which is especially an improvement 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 corresponding interband coupling constant, can we verify the mean-field result which leads always to an enhanced stability of spontaneous ferromagnetism. For $J \approx 0.1$, which we call intermediate coupling, the magnetization is already suppressed by spin-flip scattering (using the free bandwidth as the energy scale: $W = 1$). With increasing

J, the ferromagnetic order almost vanishes. The re-entrant behaviour found for even larger J might be due to an RKKY-like ordering mechanism mediated by the interband interaction (4). The regime of J most often attributed to transition metals is that of 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.

Acknowledgments

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