

Metallic Ferromagnetism: Progress in our Understanding of an Old Strong-Coupling Problem

D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, M. Ulmke, and J. Wahle*

Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, D-86135 Augsburg, Germany

* Present address: Theoretische Physik, Universität Duisburg, Lotharstr. 1, D-47048 Duisburg, Germany

Abstract: Metallic ferromagnetism is in general an intermediate to strong coupling phenomenon. Since there do not exist systematic analytic methods to investigate such types of problems, the microscopic origin of metallic ferromagnetism is still not sufficiently understood. However, during the last two or three years remarkable progress was made in this field: It is now certain that even in the one-band Hubbard model metallic ferromagnetism is stable in dimensions $d = 1, 2$, and ∞ on regular lattices and at intermediate values of the interaction U and density n . In this paper, the basic questions and recent insights regarding the microscopic conditions favoring metallic ferromagnetism in this model are reviewed. These findings are contrasted with the results for the orbitally degenerate case.

1 Introduction

What is the microscopic origin of ferromagnetism? Exactly seventy years ago, in 1928, Heisenberg addressed this question [1] after having discovered the phenomenon of quantum mechanical exchange and the corresponding exchange interaction. He formulated a spin model (the Heisenberg model), hoping to be able to answer precisely this question. However, it was pointed out by Bloch [2] that a model of localized spins cannot explain *metallic* ferromagnetism as observed in iron, cobalt, and nickel, and that a proper model would have to include the itineracy of the electrons, i.e. the band aspect. Based on the observation that the Curie temperature $T_c \sim 10^3$ K ~ 0.1 eV in these systems it is clear that the kinetic energy and the spin-independent Coulomb interaction, together with the Pauli principle, must ultimately be responsible for metallic ferromagnetism. Ever since one has been looking for the simplest microscopic model and mechanism explaining the origin of metallic ferromagnetism and, equally important, for analytic solutions or at least controlled approximations for these models [3]. Today we know that even with the “right” model these answers are not easily obtained since metallic ferromagnetism generally occurs only at *intermediate* to *strong* coupling and off half filling [4,5]. Thus, it belongs to the class of problems for which systematic theoretical approaches do not exist. Namely, weak-coupling theories or renormalization group approaches [6] which are so effective in detecting instabilities with respect to antiferromagnetism or superconductivity, do not work in this case. Instead, *nonperturbative* methods are required.

During the last two or three years significant progress was made in our understanding of the microscopic foundations of metallic ferromagnetism. These insights were made possible by both new analytic methods and new numerical techniques. In this paper, some of these recent developments will be reviewed. In particular, the microscopic conditions for metallic ferromagnetism in the one-band Hubbard model (Section 2) and in the case of orbital degeneracy (Section 3) are explained and the differences discussed. A conclusion (Section 4) closes the presentation.

2 The One-Band Hubbard Model

The simplest lattice model for correlated electrons, the one-band Hubbard model

$$H_{\text{Hub}} = - \sum_{i,j,\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (2.1)$$

was proposed independently by Gutzwiller [7], Hubbard [8], and Kanamori [9] in 1963, with the explanation of metallic ferromagnetism in 3d transition metals in mind. Concerning the suitability of (2.1) to describe metallic ferromagnetism for general U and electron densities n the three authors came to different conclusions. In any case, the theoretical methods used at that time were not controlled enough to provide definitive conclusions. This is also true for most of the research following their original work, with a few exceptions such as Nagaoka's theorem for a single hole at $U = \infty$ [10]. We note that in the past the kinetic energy in (2.1) was usually restricted to nearest-neighbor (NN) hopping; then it is useful to divide the underlying lattices into bipartite and nonbipartite ones. About ten years ago the interest in the subject started to rise again [11]. In particular, by reducing Kanamori's [9] model density of states (DOS) of noninteracting electrons, $N^0(E)$ (Fig. 1a), to its barest minimum (Fig. 1b) Mielke [12] began to investigate the stability of ferromagnetism in systems with flat, i.e. dispersionless, bands. He [13] and Tasaki [14] were able to derive rigorous criteria for the existence of ferromagnetism in these particular systems [15]. Generalizations to nearly-flat bands are also possible [16]. Ferromagnetism is proven to exist when the lowest band is half-filled and the system is insulating, as well as close to half filling. Due to the pathological degeneracy of the ground state it is still not exactly clear whether away from half filling one really obtains *metallic* ferromagnetism [17].

A different route to ferromagnetism was taken by Müller-Hartmann [18] who investigated the t - t' Hubbard model

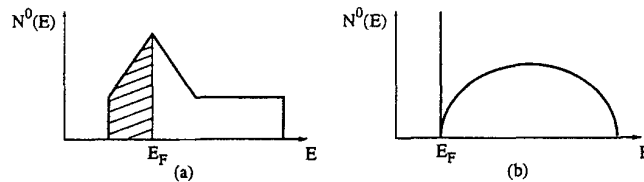


Figure 1 (a) Model DOS favoring ferromagnetism in the Hubbard model as suggested by Kanamori [9]; (b) DOS for flat-band ferromagnetism (schematic) [15].

$$H_{\text{Hub}}^{t,t'} = -t \sum_{\text{NN},\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\text{NNN},\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2.2)$$

i.e. model (2.1) with NN and next-nearest neighbor (NNN) hopping. He found that in $d = 1$ at $U = \infty$ ferromagnetism becomes possible in the low-density limit ($n \rightarrow 0$). This scenario was extended by Pieri et al. [19] and, in particular, by Penc et al. [20] who introduced a generalized model which can be shown to have a metallic phase in $d = 1$.

In the Hubbard model the interaction term is completely independent of lattice and dimension. Therefore the kinetic energy, or dispersion, of the electrons and the underlying lattice must play an important role for the stability of metallic ferromagnetism. This is indeed seen explicitly in all of the above-mentioned investigations and is also apparent in the studies of the single spin-flip instability of the Nagaoka state for which Hanisch et al. [21] recently derived significantly improved bounds for various lattices in $d = 2$ in $d = 3$, and which was solved analytically by Uhrig [22] in the limit of $d = \infty$ for several nonbipartite lattices.

2.1 Routes to Ferromagnetism

On bipartite lattices the t' -hopping term destroys the antiferromagnetic nesting instability at small U [23]. In $d > 1$ it shifts spectral weight to the band edges and thereby introduces an asymmetry into the otherwise symmetric DOS. It will be shown below that a high spectral weight at the band edge (more precisely: the *lower* band edge for $n < 1$) minimizes the loss of kinetic energy of the overturned spins in the magnetic state and is hence energetically favorable. Therefore, frustrated, i.e. nonbipartite lattices, or bipartite lattices with frustration due to hopping (e.g. $t' \neq 0$) support the stabilization of metallic ferromagnetism. The fcc lattice is an example for a frustrated lattice in $d = 3$. The corresponding DOS of the noninteracting particles is shown in Fig. 2. Switching on an additional NNN hopping t' is seen to further increase the spectral weight at the lower band edge. For $t' = t/2$ one even obtains a square-root-like divergence.

To understand why a high spectral weight at the band edge is favorable for the kinetic energy we first consider the case $U = 0$, $n < 1$ [5]. Let us consider a flat, symmetric DOS as in Figs. 3a, b. Fig. 3a describes the paramagnetic state. The fully polarized state is obtained by inverting the spin of the down electrons, which due to the Pauli principle have to occupy higher energy states. Counting the energy from the lower band edge the Fermi energy of the polarized state, μ_\uparrow , is seen to be twice that of the unpolarized state (Fig. 3b). This should be contrasted with the DOS having large spectral weight at the lower band edge shown in Figs. 3c and 3d. Here the Fermi level of the polarized state

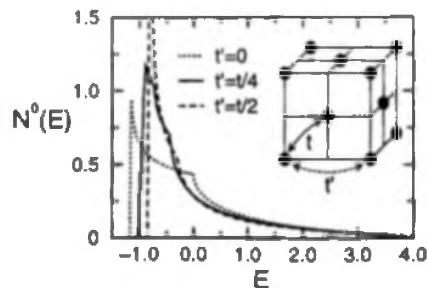


Figure 2
DOS of noninteracting electrons on a fcc lattice in $d = 3$ with and without additional NNN-hopping t' .

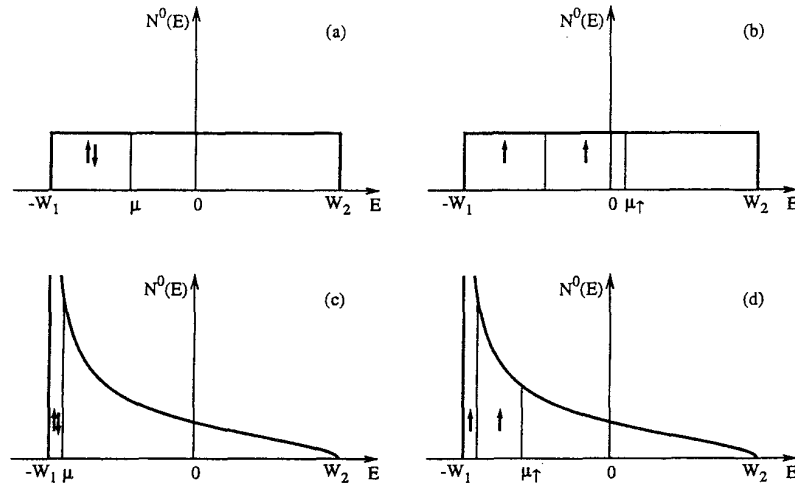


Figure 3 Flat, symmetric DOS for (a) unpolarized and (b) fully polarized electrons; (c) and (d): same as in (a), (b) but for a strongly peaked DOS.

is not so strongly shifted upwards, i.e. fewer high energy states are populated, which is clearly energetically favorable. The energy difference between the fully polarized state and the unpolarized state

$$\Delta E = \left[\int_{-W_1}^{\mu_{\uparrow}} - 2 \int_{-W_1}^{\mu} \right] dE N^0(E) E \quad (2.3)$$

must become negative for the ferromagnetic state to be stable. Of course, in the noninteracting case $\Delta E > 0$ [24]. Nevertheless, even for $U = 0$, ΔE attains its lowest value for a DOS with peaked spectral weight at the lower band edge for all n [5]. To show that $\Delta E < 0$ for $U > 0$ requires a good estimate of the energy of the *correlated paramagnet* – this is indeed a central problem of any correlation theory. It should be noted that the above discussion concerning the shape of the DOS goes beyond the well-known Stoner criterion which predicts an instability of the paramagnet for U equal to the inverse of the DOS precisely *at* the Fermi level.

Another possibility to stabilize ferromagnetism is to consider those interactions which are neglected in the Hubbard interaction, in particular the NN direct-exchange interaction. The effect of this and other terms will be discussed in Section 2.3.

2.2 Numerical Investigation of the Hubbard Model on Frustrated Lattices in $d=1, 2$, and ∞

Since metallic ferromagnetism is an intermediate coupling problem purely analytic approaches meet only with limited success, in particular in dimensions $d > 1$. In this situation the development of new numerical techniques in the last few years was of crucial importance for progress in this field. In particular, the density matrix renormalization group (DMRG), applicable mostly in $d = 1$, the projector quantum Monte Carlo method, and

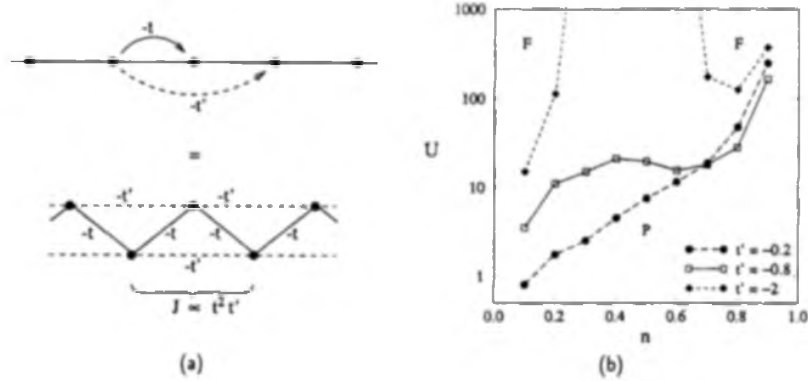


Figure 4 (a) t - t' Hubbard model in $d = 1$. (b) Ground state phase diagram U vs. n for the t - t' Hubbard model in $d = 1$ for several values of t' (after Daul and Noack [26]). P: paramagnetic phase, F: ferromagnetic phase.

the dynamic mean-field theory (DMFT), i.e. the large d limit, in connection with quantum Monte Carlo (QMC) have led to explicit, reliable results in dimensions $d = 1, 2, \infty$.

$d=1$: In one dimension the t - t' Hubbard model may be viewed as a zig-zag chain made of triangular units (Fig. 4a). Taking one of these units by itself the effective exchange interaction between the spins of two electrons due to hopping of an electron or hole along the triangle is $J \propto t^2 t'$ [20,25]. It clearly shows that the sign of t' is crucial: only for $t' < 0$ does one obtain a ferromagnetic exchange; this seems to hold even in the extended system. Of course, $d = 1$ is a special dimension, since (i) ferromagnetic order is only possible at $T = 0$ and $t' \neq 0$ [24], and (ii) the DOS is always large at the band edges.

The t - t' Hubbard model was studied in detail by Daul and Noack [26] using DMRG for systems as large as 140 sites. The resulting magnetic phase diagram is shown in Fig. 4b. Even at small $|t'|$ a large ferromagnetic region in the U vs. n phase diagram is found to exist. As $|t'|$ increases the region of stability shrinks. This is due to the fact that for $|t'| \rightarrow \infty$ the zig-zag chain separates into two unconnected chains with t' as pure NN hopping; in this case the Lieb-Mattis theorem [24] rules out a ferromagnetic state.

$d=2$: The t - t' Hubbard model on a square lattice was investigated by Hlubina et al. [27]. At $T = 0$, using projector QMC on systems as large as 20×20 sites and working at specific “van Hove densities” for which the Fermi energy coincides with the divergence in the noninteracting DOS, these authors found a region of metallic ferromagnetism, e.g. at $|t'| = 0.47t$.

$d=\infty$: Already in three dimensions the coordination number of a fcc lattice is $Z = 12$. It is therefore quite natural to view Z as a large number, and to consider the limit $Z \rightarrow \infty$ [28]. In this case one has to scale the hopping, e.g. as $t = t^*/\sqrt{Z}$ (in the following $t^* = 1$), and thus obtains a purely local theory where the self energy becomes \vec{k} independent and where the propagator $G(\vec{k}, \omega) = G^0(\vec{k}, \omega - \Sigma(\omega))$ may be represented by the noninteracting propagator at a shifted frequency [29]. In this limit the dynamics of the quantum mechanical

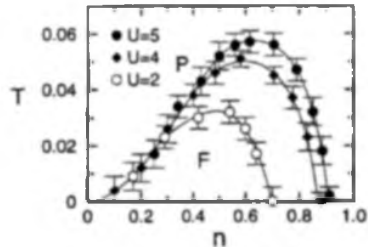


Figure 5
 T vs. n phase diagram of the Hubbard model for a fcc lattice in $d = \infty$ for several values of U [31].

correlation problem is fully included, but due to the local nature of the theory there is no *short-range* order in position space. The dependence on the lattice or the dispersion is then encoded in the DOS $N^0(E)$ of the noninteracting particles. In view of these properties the $d \rightarrow \infty$ limit is now generally referred to as “dynamical mean-field theory” (DMFT) [30].

Investigations of the stability of metallic ferromagnetism on fcc-type lattices in large dimensions, obtained by solving the DMFT equations by finite-temperature QMC techniques, were first performed by Ulmke [31]. The resulting T vs. n phase diagram is shown in Fig. 5 for different values of the interaction parameter U . At $T = 0$ the critical interaction $U_c(n)$ (Fig. 5) is consistent with the analytically obtained spin-flip results by Uhrig [22]. The region of stability is seen to increase with U . By using an improved iterated perturbation theory to solve the DMFT equations Nolting et al. [32] obtained a similar phase diagram. To make contact with $d = 3$ we now use the corresponding fcc DOS shown in Fig. 2. For $t' = 0$ no instability is found at temperatures accessible to QMC. However, already a small contribution of t' -hopping (which is present in any real system) is enough to produce a large region of stability for metallic ferromagnetism in addition to an antiferromagnetic phase close to half filling (Fig. 6a) [31]. This shows the strong and subtle dependence of the stability on the dispersion and the distribution of spectral weight in the DOS. The maximal transition temperature is $T_c^{\max} = 0.05 \simeq 500$ K for a band width $W = 4$ eV. This is well within the range of real transition temperatures, e.g. in nickel.

So far we only argued on the basis of the shape of the DOS of the *noninteracting* electrons, $N^0(E)$. On the other hand the interaction will renormalize the band and relocate spectral weight. Therefore it is not *a priori* clear at all whether the arguments concerning the kinetic energy etc. (Fig. 3) still hold even at finite U . To settle this point we calculate the DOS of the interacting system, $N(E)$, by the maximum entropy method. In Fig. 6b we show $N(E)$ corresponding to the parameter values leading to the phase diagram in Fig. 6a. Clearly the ferromagnetic system is metallic since there is appreciable weight at the Fermi level ($E = \mu$). Furthermore, the spectrum of the majority spins is seen to be only slightly affected by the interaction, the overall shape of the noninteracting DOS being almost unchanged (the magnetization is quite large ($m = 0.56$ at $n = 0.66$) and hence the electrons in the majority band are almost noninteracting). This implies that the arguments concerning the distribution of spectral weight in the noninteracting case and the corresponding kinetic energy are even applicable to the polarized, interacting case. The spectrum of the minority spins is slightly shifted to higher energies and has a pronounced peak around $E - \mu \simeq U = 6$.

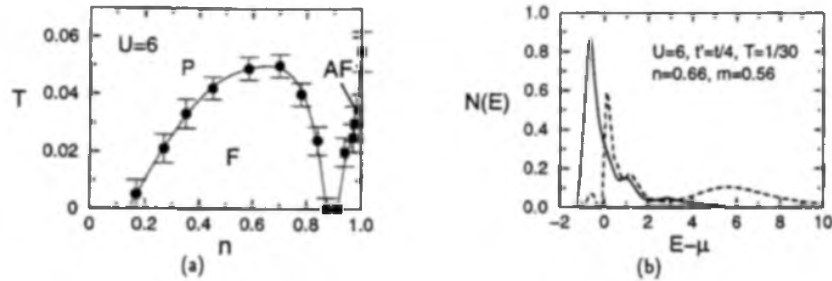


Figure 6 (a) T vs. n phase diagram of the Hubbard model as obtained within DMFT for the DOS corresponding to a three-dimensional fcc lattice with NN-hopping $t' = t/4$ (see Fig. 2) [31]; (b) DOS of the interacting electrons in the ferromagnetic phase of (a), solid line: majority spin, dashed line: minority spin.

To study the influence of the distribution of spectral weight on the stability of ferromagnetism within the DMFT systematically Wahle et al. [33] recently solved the DMFT equations with a tunable model DOS (Fig. 7),

$$N^0(E) = c \frac{\sqrt{D^2 - E^2}}{D + aE}. \quad (2.4)$$

with $c = (1 + \sqrt{1 - a^2})/(\pi D)$ and half-bandwidth $D \equiv 2$. Here a is an asymmetry parameter which can be used to change the DOS continuously from a symmetric, Bethe lattice DOS ($a = 0$) to a DOS with a square-root divergence at the lower band edge ($a = 1$), corresponding to a fcc lattice with $t' = t/4$ in $d = 3$ (Fig. 2). It is possible, in principle, to map any $N^0(E)$ to a dispersion $E(\vec{k})$ (although not uniquely).

The strong dependence of the stability of metallic ferromagnetism on the distribution of spectral weight is shown in Fig. 8a. Already a minute increase in spectral weight near the band edge of the noninteracting DOS, obtained by changing a from 0.97 to 0.98 (see Fig. 8b) is enough to almost double the stability region of the ferromagnetic phase. It should be mentioned that Obermeier et al. [34] found ferromagnetism even on a hypercubic, i.e. bipartite, lattice, but only at very large U values ($U > 30$).

The importance of genuine correlations for the stability of ferromagnetism is apparent from Fig. 9, where the DMFT results are compared with Hartree-Fock theory [33]. The quantum fluctuations, absent in Hartree-Fock theory, are seen to reduce the stability regime of ferromagnetism drastically. Spatial fluctuations (e.g. spin waves), absent also in the DMFT, should be expected to reduce that stability regime further.

2.3 Additional Interactions

In the one-band Hubbard model only the local interaction is retained. Thereby, several interactions which naturally arise when the Coulomb interaction is expressed in Wannier representation are neglected. Even in the limit of a single band and taking into account only NN contributions, four additional interactions appear [35,36,5]:

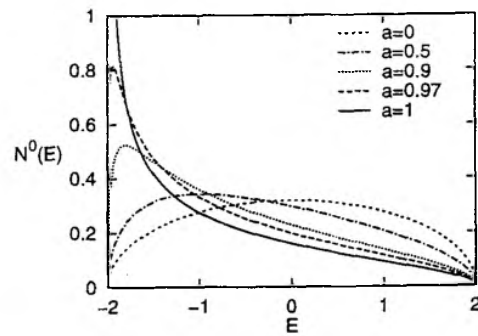


Figure 7
Model DOS, Eq. (2.4), shown
for different values of the
asymmetry parameter a [33].

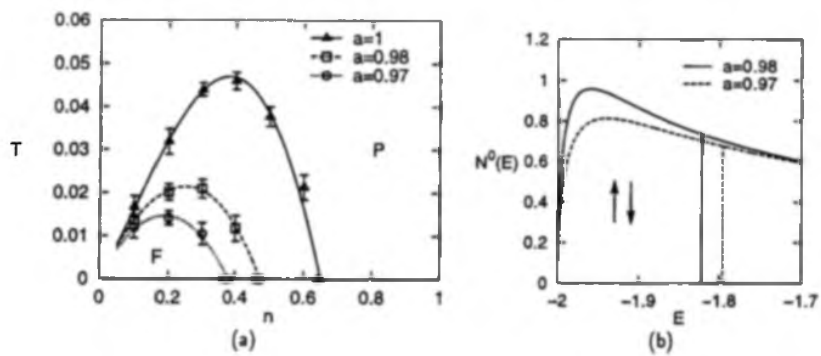


Figure 8 (a) T vs. n phase diagram of the Hubbard model as obtained within DMFT; (b) corresponding shapes of the noninteracting DOS; Fermi energies for $n = 0.3$ are indicated by vertical lines [33].

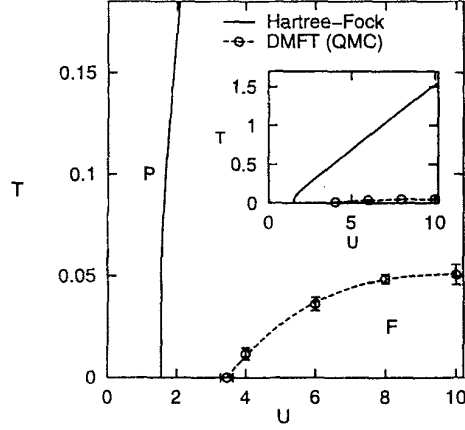


Figure 9
 T vs. U phase diagram for a strongly peaked DOS ($a = 0.98$, see Fig. 8b) at $n = 0.4$ within DMFT (circles; dashed line is guide to the eyes only) in comparison with Hartree-Fock (solid line) [33].

$$V_{1\text{-band}}^{\text{NN}} = \sum_{\text{NN}} \left[V n_i n_j + X \sum_{\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) (n_{i,-\sigma} + n_{j,-\sigma}) - 2F (\vec{S}_i \cdot \vec{S}_j + \frac{1}{4} n_i n_j) + F' (c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{j\downarrow} c_{j\uparrow} + \text{h.c.}) \right]. \quad (2.5)$$

Here the first term corresponds to a density-density interaction, the second term to a density-dependent hopping, and the fourth term describes the hopping of doubly occupied sites. In particular, the third term (with $F = F^*/Z > 0$)

$$H_F = -2 \frac{F^*}{Z} \sum_{\text{NN}} \vec{S}_i \cdot \vec{S}_j \quad (2.6)$$

describes the direct ferromagnetic exchange between electrons on NN sites. It is this spin-type interaction which Heisenberg in his original model singled out as the main source of ferromagnetism. It should be noted, however, that this interaction is present even when the electrons are not localized but are free to move. The exchange interaction will be quite small, but nevertheless it favors ferromagnetic ordering in the most obvious way. Hirsch [36] argued that this term is the main driving force for metallic ferromagnetism in systems like iron, cobalt, and nickel. Indeed, one can show rigorously that a next-neighbor direct exchange interaction, if chosen large enough, can easily trigger the ferromagnetic instability [37,5]. To investigate the importance of the direct exchange interaction we supplement the Hubbard model by this term, $H = H_{\text{Hub}} + H_F$, neglecting all the other NN interactions. We note that within the DMFT the Heisenberg exchange reduces to the Weiss/Hartree-Fock contribution. In Fig. 10 the influence of the exchange interaction on the stability regime of ferromagnetism is depicted [33]. For $F^* = 0$ ferromagnetism is unstable down to the lowest temperatures for $U = 4$. However, by taking into account a small value of $F^* \simeq 0.15 \ll U$ at $T = 0$, the ferromagnetic phase is stabilized. Likewise, at larger values of U the critical temperature for the onset of ferromagnetism is significantly enhanced. Hence, F^* (and also the other neglected interactions) may well be important for systems on the verge of a ferromagnetic instability. Nevertheless, since we now know that the Hubbard interaction U together with a suitable kinetic energy is sufficient to trigger a ferromagnetic instability the ferromagnetic exchange interaction does not, in general, play an unrenounceable role and is thus less important than U itself.

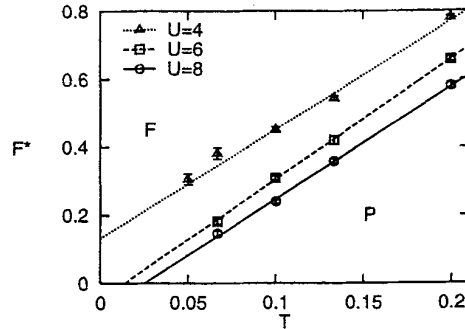


Figure 10
Direct exchange F^* vs. T phase diagram for the generalized model $H = H_{\text{Hubb}} + H_F$ for different values of U in the case of a strongly peaked DOS ($a = 0.98$, see Fig. 8b) at $n = 0.6$. The linear extrapolation to $T = 0$ shows that there exists a critical value of U above which ferromagnetism is stable even in the absence of the direct exchange [33].

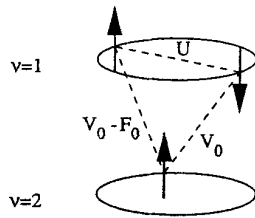


Figure 11
Illustration of the local interactions between electrons in a two-band model.

3 Orbital Degeneracy

The properties of the metallic ferromagnets iron, cobalt, and nickel are determined by 3d electrons, implying a five-fold degeneracy. Therefore it has long been speculated that band degeneracy is an essential precondition for metallic ferromagnetism. Band degeneracy leads to additional on-site matrix elements of the Coulomb interaction describing intra-atomic interactions

$$V_{\text{interband}} = \sum_i \left[\sum_{\nu < \nu'; \sigma \sigma'} (V_0 - \delta_{\sigma \sigma'} F_0) n_{i\nu \sigma} n_{i\nu' \sigma'} - F_0 \sum_{\nu < \nu'; \sigma \neq \sigma'} c_{i\nu \sigma}^\dagger c_{i\nu \sigma'} c_{i\nu' \sigma'}^\dagger c_{i\nu' \sigma} \right] \quad (3.7)$$

as shown in Fig. 11 in the case of a two-fold degeneracy. In particular, they imply a density-density interaction V_0 and a (ferromagnetic) exchange interaction F_0 between electrons on different orbitals. These ‘‘Hund’s rule couplings’’ are responsible for the ferromagnetic alignment of the spins on an isolated atom. Slater [38] and van Vleck [39] suggested that this ‘‘atomic magnetism’’ may be transmitted from one atom to another by the kinetic energy, leading to coherent bulk order in the system. The relevant Hamiltonian is then a sum of Hubbard models for each orbital, complemented by the purely local interband coupling terms in (3.7):

$$H = \sum_{\nu} \left[-t \sum_{\text{NN}, \sigma} c_{i\nu \sigma}^\dagger c_{j\nu \sigma} + U \sum_i n_{i\nu \uparrow} n_{i\nu \downarrow} \right] + V_{\text{interband}}. \quad (3.8)$$

This model has received wide attention [40], especially most recently [41]. Away from quarter or half filling the model is particularly difficult to treat due to the high degeneracy in the atomic limit. Quite generally ferromagnetism is found to be stabilized by Hund’s

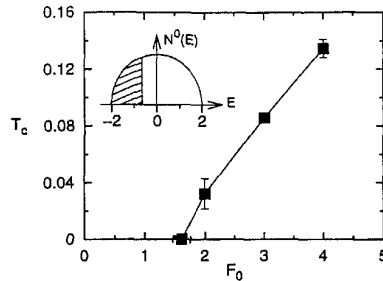


Figure 12
Curie temperature T_c vs. Hund's rule exchange coupling F_0 for a two-band Hubbard model with symmetric noninteracting DOS (see inset) as obtained within DMFT at $U = 9$, $V_0 = 5$, and $n = 1.25$ [42].

rule coupling at intermediate to strong interactions. In this regime the DMFT, solved by QMC, once more provides a powerful method for the investigation of (3.8) [42].

To identify the main mechanism responsible for ferromagnetism in the band-degenerate model and to distinguish it from that relevant for the one-band Hubbard model (namely, the strongly peaked DOS near the band edge) we here choose a featureless, symmetric Bethe-DOS as shown in the inset of Fig. 12. For such a DOS no ferromagnetic instability was found in the one-band model up to the largest U values within the DMFT [33] (see also [34]). In the following we restrict our discussion to a two-fold degeneracy. As can be seen from Fig. 12 no ferromagnetism occurs in the orbitally degenerate model even at $U = 9$ if the Hund's rule exchange interaction F_0 is absent. However, already a comparatively small value of F_0 is sufficient to make the ferromagnetic state favorable. The magnetic phase diagram T vs. n is shown in Fig. 13a for the same interaction parameters as in Fig. 12 at $F_0 = 4$ [42] (here we took into account the relation $U = V_0 + F_0$ which makes (3.8) form-invariant with respect to orbital rotations). Close to half filling ($n = 2$) the antiferromagnetic state is found to be stable, while for lower filling ferromagnetism is stable in a broad range of densities. The maximum critical temperature is $T_c^{\max} \sim 0.1$ which, for a band width of 4 eV, corresponds to about 1000 K. This result should be compared with the Hartree-Fock result (Fig. 13b) which is both qualitatively and quantitatively insufficient. In particular, Hartree-Fock theory does not describe the suppression of T_c caused by the antiferromagnetic super-exchange near half filling. Furthermore, the critical temperatures are by more than an order of magnitude too high, reflecting the absence of dynamical fluctuations in this approximation. Fig. 12 clearly shows that already moderately large Hund's rule couplings are able to mediate metallic ferromagnetism even in a system with an unspecific, symmetric DOS. It is interesting to see that the magnetic phase diagrams T vs. n for the one-band model (Fig. 6a) and the band-degenerate model (Fig. 13a) look very similar, although the origin for the ferromagnetic phase is quite different.

Here we did not discuss the possibility of orbital ordering where the electron densities alternate on the two orbitals on neighboring sites. In [42] it is found that orbital ordering sets in around quarter filling ($n = 1$) when F_0 is decreased.

4 Discussion

In this paper we discussed recent developments in our understanding of the origin of metallic ferromagnetism both in the one-band Hubbard model and the band-degenerate

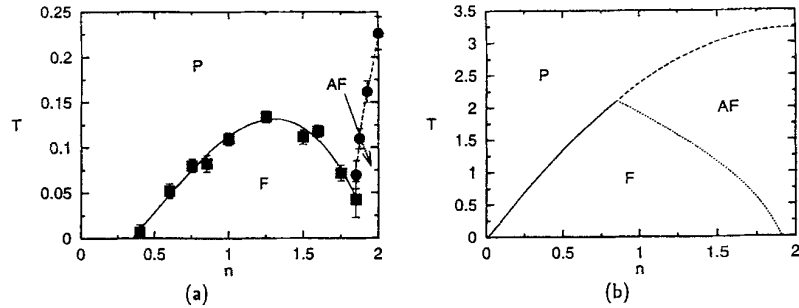


Figure 13 Magnetic phase diagram T vs. n of a two-band Hubbard model for the same U and V_0 as in Fig. 12, and $F_0 = 4$: (a) DMFT, (b) Hartree-Fock [42].

model. Analytical results for $d = 1$ and, in particular, numerical results for $d = 1, 2$, and ∞ were finally able to show convincingly that the one-band Hubbard model has a metallic ferromagnetic phase in a surprisingly large region of the on-site interaction U and density n . A stabilization of this phase at intermediate U values requires a sufficiently large spectral weight near the band edge. Such a DOS is typical for frustrated lattices which optimize the kinetic energy of the polarized state and at the same time frustrate the parasitic antiferromagnetic ordering. By contrast, the origin of metallic ferromagnetism in the band-degenerate Hubbard model need not primarily be due to a DOS effect but is rather caused by (moderate) Hund's rule couplings. In this respect the origin of ferromagnetism in the orbitally degenerate model is more straightforward than in the one-band case. In the absence of orbital ordering the resulting magnetic phase diagrams are remarkably similar.

The identification of a single main driving force for the stabilization of metallic ferromagnetism in the one-band and the band-degenerate model, respectively, helps to differentiate between different effects. In real systems these effects will tend to conspire, as is evident, for example, in nickel where an fcc lattice leads to a strongly asymmetric DOS and the band degeneracy provides for Hund's rule couplings. The combination of these effects will be investigated in the future.

Bibliography

- [1] W. Heisenberg, *Z. Physik* **49**, 619 (1928).
- [2] F. Bloch, *Z. Phys.* **57**, 545 (1929).
- [3] D. C. Mattis, *The Theory of Magnetism I*, Springer, Berlin, 1988.
- [4] E. H. Lieb, in *The Hubbard Model: Its Physics and Mathematical Physics*, edited by D. Baeriswyl et al., page 1, Plenum, New York, 1995; P. Fazekas, *Phil. Mag. B* **76**, 797 (1997).
- [5] D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, M. Ulmke, *Z. Phys. B* **103**, 283 (1997).
- [6] R. Shankar, *Rev. Mod. Phys.* **66**, 129 (1994).
- [7] M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 59 (1963).
- [8] J. Hubbard, *Proc. Roy. Soc. London A* **276**, 238 (1963).

- [9] J. Kanamori, *Prog. Theor. Phys.* **30**, 275 (1963).
- [10] Y. Nagaoka, *Phys. Rev.* **147**, 392 (1966).
- [11] E. H. Lieb, *Phys. Rev. Lett.* **62**, 1201 (1989).
- [12] A. Mielke, *J. Phys. A* **24**, 3311 (1991).
- [13] A. Mielke, *J. Phys. A* **25**, 4335 (1992); A. Mielke, *Phys. Lett. A* **174**, 443 (1993).
- [14] H. Tasaki, *Phys. Rev. Lett.* **69**, 1608 (1992).
- [15] A. Mielke and H. Tasaki, *Commun. Math. Phys.* **158**, 341 (1993).
- [16] H. Tasaki, *Phys. Rev. Lett.* **73**, 1158 (1994); *ibid.* **75**, 4678 (1995).
- [17] H. Tasaki, *Prog. Theor. Phys.* **99**, 489 (1998).
- [18] E. Müller-Hartmann, *J. Low Temp. Phys.* **99**, 349 (1995).
- [19] P. Pieri, S. Daul, D. Baeriswyl, and M. Dzierzawa, *Phys. Rev. B* **54**, 9250 (1996).
- [20] K. Penc, H. Shiba, F. Mila, and T. Tsukagoshi, *Phys. Rev. B* **54**, 4056 (1996).
- [21] T. Hanisch, G. S. Uhrig, and E. Müller-Hartmann, *Phys. Rev. B* **56**, 13960 (1997).
- [22] G. S. Uhrig, *Phys. Rev. Lett.* **77**, 3629 (1996).
- [23] W. Hofstetter and D. Vollhardt, *Ann. Physik* **7**, 48 (1998).
- [24] E. H. Lieb and D. Mattis, *Phys. Rev.* **125**, 164 (1962).
- [25] H. Tasaki, *J. Phys.: Condens. Matter* **10**, 4353 (1998).
- [26] S. Daul and R. Noack, *Z. Phys. B* **103**, 293 (1997). S. Daul and R. Noack, *Phys. Rev. B* **58**, 2635 (1998).
- [27] R. Hlubina, S. Sorella, and F. Guinea, *Phys. Rev. Lett.* **78**, 1343 (1997).
- [28] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).
- [29] D. Vollhardt, in *Correlated Electron Systems*, edited by V. J. Emery, World Scientific, Singapore, 1993.
- [30] T. Pruschke, M. Jarrell, and J. K. Freericks, *Adv. Phys.* **44**, 187 (1995); A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [31] M. Ulmke, *Euro. Phys. J. B* **1**, 301 (1998).
- [32] T. Herrmann and W. Nolting, *J. Magn. Magn. Mater.* **170**, 253 (1997); T. Herrmann and W. Nolting, *Solid State Commun.* **103**, 351 (1997); T. Wegner, M. Potthoff, and W. Nolting, *Phys. Rev. B* **57**, 6211 (1998).
- [33] J. Wahle, N. Blümer, J. Schlipf, K. Held, and D. Vollhardt, *Phys. Rev. B* **58** (1998, in press).
- [34] T. Obermeier, T. Pruschke, and J. Keller, *Phys. Rev. B* **56**, R8479 (1997).
- [35] J. T. Gammel and D. K. Campbell, *Phys. Rev. Lett.* **60**, C 71 (1988); D. K. Campbell, J. T. Gammel, and E. Y. Loh Jr., *Phys. Rev. B* **38**, 12043 (1988).
- [36] J. E. Hirsch, *Phys. Rev. B* **40**, 2354 (1989); *ibid.* **40**, 9061 (1989); S. Tang and J. E. Hirsch, *Phys. Rev. B* **42**, 771 (1990).
- [37] R. Strack and D. Vollhardt, *Phys. Rev. Lett.* **72**, 3425 (1994); M. Kollar, R. Strack, and D. Vollhardt, *Phys. Rev. B* **53**, 9225 (1996).
- [38] J. C. Slater, *Phys. Rev.* **49**, 537 (1936).
- [39] J. H. van Vleck, *Rev. Mod. Phys.* **25**, 220 (1953).
- [40] L. M. Roth, *Phys. Rev.* **149**, 306 (1966); K. I. Kugel' and D. I. Khomskii, *Sov. Phys.-JETP* **37**, 725 (1973); M. Cyrot and C. Lyon-Caen, *J. Phys. C* **36**, 253 (1975); W. Gill and D. J. Scalapino, *Phys. Rev. B* **35**, 215 (1987); A. M. Oleś, *Phys. Rev. B* **23**, 271 (1981); *ibid.* **28**, 327 (1983); A. M. Oleś and G. Stollhoff, *Phys. Rev. B* **29**, 314 (1984); G. Stollhoff and P. Thalmeier, *Z. Phys. B* **43**, 13 (1981).

-
- [41] J. Kuei and R. T. Scalettar, *Phys. Rev. B* **55**, 14968 (1997); J. E. Hirsch, *Phys. Rev. B* **56**, 11022 (1997); M. Fleck, A. M. Oleś, and L. Hedin, *Phys. Rev. B* **56**, 3159 (1997); T. Okabe, *Prog. Theor. Phys.* **98**, 331 (1997); J. Bünemann and W. Weber, *Physica B* **230**, 412 (1997); J. Bünemann, F. Gebhard, and W. Weber, *J. Phys. Condens. Matter* **9**, 7343 (1997); J. Bünemann, W. Weber, and F. Gebhard, *Phys. Rev. B* **57**, 6896 (1998).
- [42] K. Held and D. Vollhardt, *Euri. Phys. J. B* (1998, in press).