Non-perturbative approaches to magnetism in strongly correlated electron systems

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Abstract. The microscopic basis for the stability of itinerant ferromagnetism in correlated electron systems is examined. To this end several routes to ferromagnetism are explored, using both rigorous methods valid in arbitrary spatial dimensions, as well as Quantum Monte Carlo investigations in the limit of infinite dimensions (dynamical mean-field theory). In particular we discuss the qualitative and quantitative importance of (i) the direct Heisenberg exchange coupling, (ii) band degeneracy plus Hund's rule coupling, and (iii) a high spectral density near the band edges caused by an appropriate lattice structure and/or kinetic energy of the electrons. We furnish evidence of the stability of itinerant ferromagnetism in the pure Hubbard model for appropriate lattices at electronic densities not too close to half-filling and large enough U. Already a weak direct exchange interaction, as well as band degeneracy, is found to reduce the critical value of U above which ferromagnetism becomes stable considerably. Using similar numerical techniques the Hubbard model with an easy axis is studied to explain metamagnetism in strongly anisotropic antiferromagnets from a unifying microscopic point of view.

PACS: 71.27.+a;75.10.Lp

1. Introduction

Even after several decades of research the microscopic foundations of itinerant ferromagnetism are not sufficiently understood. Indeed, in contrast to other collective electronic phenomena such as antiferromagnetism or conventional superconductivity there exists a remarkable gap between theory and experiment in this field. This has mainly to do with the fact that itinerant ferromagnetism is a quantum-mechanical *strong-coupling* phenomenon whose explanation requires the application of *non-perturbative* techniques. Thus it belongs into the class of the most difficult many-body problems in condensed-matter physics. Significant progress was made in this field in the last few years due to the development and application of several new analytic and numerical approaches. It is the purpose of this paper to present and discuss some of these new, exciting results.

In Sect. 2 we recapitulate the derivation of a general lattice model for correlated electrons starting from a continuum model, and discuss the various truncation steps which eventually lead to the Hubbard model. In particular, the implications of the Lieb-Mattis theorem on the impossibility of ferromagnetism in these truncated models in $d = 1$ dimension are analyzed. In Sect. 3 several microscopic mechanisms favoring ferromagnetism are discussed. New and very recent results concerning ferromagnetism in Hubbard-type models obtained by various non-perturbative methods are presented and put into perspective. Metamagnetic phase transitions and the need for the application of non-perturbative techniques for these investigations are the subject of Sect. 4. Finally, a conclusion is presented in Sect. 5.

2. Electronic correlations and magnetism

2.1. General lattice model

Within the occupation number formalism the Hamiltonian for electrons with spin σ interacting via a *spin-independent* interaction $V^{ee}(\mathbf{r}-\mathbf{r}')$ in the presence of an ionic lattice potential $V^{ion}(\mathbf{r})$ has the form [1, 2] $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, where

$$\hat{H}_0 = \sum_\sigma \int d^3r \hat{\psi}^+_\sigma(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\Delta + V^{ion}(\mathbf{r}) \right] \hat{\psi}_\sigma(\mathbf{r}) \qquad (1)$$

$$\hat{H}_{int} = \frac{1}{2}\sum_{\sigma\sigma'} \int d^3r \int d^3r' V^{ee}(\mathbf{r}-\mathbf{r}')\hat{n}_\sigma(\mathbf{r})\hat{n}_{\sigma'}(\mathbf{r}')\,. \qquad (2)$$

Here $\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}^+_\sigma(\mathbf{r})$ are the usual field operators and $\hat{n}_\sigma(\mathbf{r}) = \hat{\psi}^+_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})$ is the local density. We note that the interaction term is diagonal in the space variables $\mathbf{r}, \mathbf{r}'$, i.e. it depends only on the (operator-valued) densities of the electrons at site $\mathbf{r}, \mathbf{r}'$ which interact via $V^{ee}(\mathbf{r}-\mathbf{r}')$. The lattice potential entering the non-interacting part (1) leads to a splitting of the parabolic dispersion into infinitely many bands which we enumerate by the index α. The non-interacting problem is then characterized by the Bloch wave functions $\phi_{\alpha\mathbf{k}}(\mathbf{r})$ and the band energies $\epsilon_{\alpha\mathbf{k}}$. We may introduce Wannier functions localized at site $\mathbf{R_i}$ by

$$\chi_{\alpha i}(\mathbf{r}) = \frac{1}{\sqrt{L}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R_i}}\ \phi_{\alpha\mathbf{k}}(\mathbf{r})\,, \tag{3}$$

where L is the number of lattice sites, and thus construct creation and annihilation operators $\hat{c}^{+}_{\alpha i\sigma}, \hat{c}_{\alpha i\sigma}$ for electrons with spin σ in the band α at site $\mathbf{R_i}$ as

$$\begin{aligned} \hat{c}^{+}_{\alpha i\sigma} &= \int d^3r\ \chi_{\alpha i}(\mathbf{r})\ \hat{\psi}^{+}_{\sigma}(\mathbf{r}) \\ \longleftrightarrow \hat{\psi}^{+}_{\sigma}(\mathbf{r}) &= \sum_{i\alpha}\ \chi^{*}_{\alpha i}(\mathbf{r})\hat{c}^{+}_{\alpha i\sigma}\,. \end{aligned} \tag{4}$$

Thereby the Hamiltonian may be written in lattice representation as [2]

$$\begin{aligned} \hat{H} = &\sum_{\alpha ij\sigma} t_{\alpha ij}\hat{c}^{+}_{\alpha i\sigma}\ \hat{c}_{\alpha j\sigma} \\ &+\ \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\sum_{ijmn}\sum_{\sigma\sigma'} \mathscr{V}^{\alpha\beta\gamma\delta}_{ijmn}\ \hat{c}^{+}_{\alpha i\sigma}\ \hat{c}^{+}_{\beta j\sigma'}\ \hat{c}_{\delta n\sigma'}\ \hat{c}_{\gamma m\sigma}\,, \end{aligned} \tag{5}$$

where the matrix elements are given by

$$t_{\alpha ij} = \int d^3r\ \chi^{*}_{\alpha i}(\mathbf{r})\left[-\frac{\hbar^2}{2m}\Delta + V^{ion}(\mathbf{r})\right]\chi_{\alpha i}(\mathbf{r}) \tag{6}$$

$$\begin{aligned} \mathscr{V}^{\alpha\beta\gamma\delta}_{ijmn} = &\int d^3r \int d^3r\,' V^{ee}(\mathbf{r}-\mathbf{r}\,') \\ &\chi^{*}_{\alpha i}(\mathbf{r})\ \chi^{*}_{\beta j}(\mathbf{r}\,')\ \chi_{\delta n}(\mathbf{r}\,')\ \chi_{\gamma m}(\mathbf{r})\,. \end{aligned} \tag{7}$$

We note that in contrast to the field-operator representation defined in the continuum, the Wannier representation does *not* lead to a site-diagonal form of the electron-electron interaction, i.e. the interaction does not only depend on the *densities* $\hat{n}_{i\sigma} = \hat{c}^{+}_{i\sigma}\hat{c}_{i\sigma}$ but contains explicit off-diagonal contributions which will be discussed later.

2.2. One-band models

The Hamiltonian (5) is too general to be tractable in dimensions $d > 1$. Hence it has to be simplified using physically motivated truncations [2]. In particular, if the Fermi surface lies within a single conduction band, and if this band is well separated from the other bands and the interaction is not too strong, it may be justified to restrict the discussion to a *single* band ($\alpha = \beta = \gamma = \delta = 1$). In this case (5) reduces to

$$\begin{aligned} \hat{H}_{1\text{-}band} = &\sum_{ij\sigma} t_{ij}\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} \\ &+\frac{1}{2}\sum_{ijmn}\sum_{\sigma\sigma'}\mathscr{V}_{ijmn}\hat{c}^{+}_{i\sigma}\hat{c}^{+}_{j\sigma'}\hat{c}_{n\sigma'}\hat{c}_{m\sigma}\,. \end{aligned} \tag{8}$$

For most purposes this single-band Hamiltonian is still too complicated. Taking into account the weak overlap between neighboring orbitals in a tight-binding description one may expect that the overlap between nearest-neighbors is most important. Hence the site-indices in (8) are restricted to nearest-neighbor positions. In the interaction this leaves us with a purely local contribution $\mathscr{V}_{iiii} = U$, the Hubbard term, and the four nearest-neighbor contributions $\mathscr{V}_{ijij} = V$, $\mathscr{V}_{iiij} = X$, $\mathscr{V}_{ijji} = F$, and $\mathscr{V}_{iijj} = F'$, which are *off*-diagonal in the site indices. The remaining one-band, nearest-neighbor Hamiltonian has the form [2–9]

$$\hat{H}^{NN}_{1\text{-}band} = \hat{H}_{Hub} + \hat{V}^{NN}_{1\text{-}band} \tag{9}$$

where

$$\hat{H}_{Hub} = -t\sum_{\langle i,j\rangle,\sigma}(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{10}$$

is the Hubbard model and

$$\begin{aligned} \hat{V}^{NN}_{1\text{-}band} = &\sum_{\langle i,j\rangle}\ [V\hat{n}_i\hat{n}_j \\ &+X\sum_{\sigma}(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.})(\hat{n}_{i\,-\sigma} + \hat{n}_{j\,-\sigma}) \\ &+F'(\hat{c}^{+}_{i\uparrow}\hat{c}^{+}_{i\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} + \text{h.c.}) \\ &-2F(\hat{\mathbf{S}}_i\hat{\mathbf{S}}_j + \frac{1}{4}\hat{n}_i\hat{n}_j)] \end{aligned} \tag{11}$$

is the contribution of nearest-neighbor interactions. Here $\hat{n}_i = \sum_{\sigma}\hat{n}_{i\sigma}$ and $\hat{\mathbf{S}}_i = 1/2\sum_{\sigma\sigma'}\hat{c}^{+}_{i\sigma}\tau_{\sigma\sigma'}\hat{c}_{i\sigma'}$, where τ denotes the vector of Pauli matrices. In (11) the V-term describes a density-density interaction, the X-term is a bond-charge–site-charge interaction ("density-dependent hopping"), the F'-term describes the hopping of local pairs consisting of an up and a down electron and, finally, the F-term corresponds to the *direct* Heisenberg exchange which is generically ferromagnetic in nature. The occupation number formalism illustrates particularly clearly that a spin-independent interaction plus the Pauli principle is able to lead to a mutual orientation of spins. Of all interactions in (9) the Hubbard interaction U is certainly the strongest. Hence, in a final truncation step one may try to neglect even the nearest-neighbor interactions and retain only the on-site interaction U. This leaves us with the Hubbard model (10), the simplest correlation model for lattice electrons [2, 10, 11].

2.2.1. The Hubbard model. The Hubbard model was originally introduced in an attempt to understand itinerant ferromagnetism in 3d-transition metals [2, 10, 11]. The expectation was that in this model ferromagnetism would arise naturally since in a polarized state the electrons do not interact at all. However, it soon became clear that in a ferromagnetic state the *kinetic* energy is also reduced. This makes the stability of ferromagnetism in the Hubbard model a particularly delicate problem. Indeed, the kinetic energy with nearest-neighbor hopping usually favors *anti*-ferromagnetism. At half-filling ($n = 1$) and on bipartite lattices antiferromagnetism is a generic effect since it appears both at weak coupling (Hartree-Fock or Slater mean-field theory) and strong coupling (Anderson's "superexchange" mechanism). Hence it arises naturally in any perturbational approach and, in particular, is tractable by renormalization group methods [12]. By contrast, ferromagnetism is a non-trivial strong-coupling phenomenon which cannot be investigated by any standard perturbation theory.

The above discussion shows that, to understand the microscopic origin of itinerant ferromagnetism, non-perturbative techniques are required. Unfortunately, there are not many controlled approaches [13] of this type available; rigorous mathematical methods (for recent reviews see [14–16]), large-scale numerical methods [5, 17–20], and variational approaches [21–28] are the ones most frequently used.

As to rigorous results about ferromagnetism in the Hubbard model the Lieb-Mattis theorem [1] of 1962 is one

of the most famous. It proves that for spin- and velocity-independent forces between electrons ferromagnetism cannot occur in one spatial dimension. This theorem applies to the general Hamiltonian (5) with infinitely many bands. On the other hand the general *single*-band model (8) is *not* covered by the theorem unless (a) the interaction matrix element $\mathscr{V}_{ijmn}$ is site-diagonal such that the interaction depends only on densities $\hat{n}_i$, and (b) the hopping and interaction does not extend beyond nearest neighbors. Hence the theorem applies to the model (9) with $U, V \neq 0$ but $X, F, F' = 0$, and thereby also to the Hubbard model ($V = 0$). We note that any critique of the single-band model (9) in view of the fact that it can lead to ferromagnetism in $d = 1$ in contrast to the Lieb-Mattis theorem would apply even more so to the Hubbard model since the latter is a particularly special single-band model. In other words: the fact that the Lieb-Mattis theorem applies to the Hubbard model but *not* to the *general* single-band model (9) does not make the Hubbard model a "more physical" model than (9); after all it is only a special case of (9).

Another well-known theorem, that by Nagaoka [29] of 1966, provides explicit, albeit highly idealized, conditions under which ferromagnetism *is* stable in the Hubbard model with nearest-neighbor hopping. It proves that for $U = \infty$ the macroscopic degeneracy of the ground state at half-filling (number of electrons N = number of lattice sites L) is lifted by a single hole, i.e. when one electron is removed ($N = L - 1$). In this case a saturated ferromagnetic ground state is stable for any value of the hopping t on simple cubic and bcc lattices, and for $t < 0$ on fcc and hcp lattices. For the Nagaoka mechanism to work the lattice needs to contain loops along which the holes can move. Once the hole moves, the maximal overlap between the initial and final state clearly occurs in a *ferromagnetic* configuration. The problem is that Nagoaka's proof does not even extend to two holes, that a single hole is thermodynamically irrelevant, and that the limit of $U = \infty$ is highly unrealistic.

3. Microscopic mechanisms favoring ferromagnetism

The Hubbard interaction is the result of an extreme truncation of the interaction in the general Hamiltonian (5). All interactions beyond the purely local part (e.g. nearest-neighbor density-density interactions, direct exchange, band degeneracy and the associated Hund's rule couplings) are totally neglected. The Hubbard interaction is therefore very unspecific — it does not depend on the lattice at all and hence not on the spatial dimension. The lattice structure only enters via the kinetic energy. Therefore the stability of ferromagnetism in the Hubbard model can be expected to depend in a sensitive way on the precise form of the kinetic energy [14, 15, 29–33]. Strategies to find the essential "kick" for ferromagnetism in the Hubbard model and more general models should then proceed in different directions: one may (i) keep interactions beyond the Hubbard-U (in particular the direct exchange term F in (9)), (ii) keep band degeneracy and Hund's rule couplings, or (iii) find an appropriate kinetic energy and lattice structure. We will now discuss several recent results obtained along these lines.

3.1. The importance of the Heisenberg exchange interaction

The Heisenberg exchange interaction, caused by direct quantum-mechanical exchange of electrons at nearest-neighbor positions (the F-Term in (11) with $F > 0$), favors the alignment of the electronic spins and hence supports ferromagnetism in a straightforward way [7, 9, 16]. However, since this interaction is rather weak (Hubbard [2] estimated $F \sim \frac{1}{40}$ eV for $3d$-metals, such that $F \ll U$) it cannot be the *sole* origin of itinerant ferromagnetism in systems like Fe, Co, Ni. Nevertheless it may be qualitatively important, since it may well give a correlated system with more or less strong ferromagnetic tendencies the ultimate push and trigger ferromagnetism in spite of its smallness. It is therefore unjustified to neglect the exchange interaction for merely *quantitative* reasons. This becomes particularly clear in the limit of large U (with $U \gg |t|, |V|, |X|, F, F'$) close to $n = 1$, when the one-band model (9) can be transformed into an effective t-J-model [5, 34]

$$\hat{H}^{NN}_{1\text{-band},tJ} = -t \sum_{\langle i,j\rangle,\sigma} \hat{P}(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.})\hat{P} + J \sum_{\langle i,j\rangle} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j \qquad (12)$$

where $\hat{P}$ projects onto the subspace without doubly occupied sites. The effective exchange coupling

$$J = \frac{4t^2}{U}\Big[\Big(1 - \frac{X}{t}\Big)^2 - \frac{FU}{2t^2}\Big] \qquad (13)$$

has an antiferromagnetic part, due to Anderson's superexchange but modified by the X-term, and a ferromagnetic part, due to the direct Heisenberg exchange. Hence for large enough Heisenberg exchange F and/or Hubbard repulsion U the exchange becomes effectively ferromagnetic. This effect is completely neglected in the Hubbard model where even in the Nagaoka-limit ($U = \infty$) the dimensionless parameter FU/t^2 is kept zero!

3.1.1. Generalization of Nagaoka's theorem. If the Heisenberg exchange coupling is taken into account, it is possible to generalize Nagaoka's theorem to $U < \infty$ [35]. We start with the Hamiltonian $\hat{H}^{NN}_{1\text{-band}}$, (9). This Hamiltonian, like the Hubbard Hamiltonian, commutes with the total spin $\hat{\mathbf{S}} = \sum_i \hat{\mathbf{S}}_i$. The eigenvalues of $\hat{\mathbf{S}}^2$ are denoted by $S(S+1)$. We are concerned with saturated ferromagnetic states with one hole below half-filling, i.e. with largest possible eigenvalue $S_{max} \equiv N/2 = (L-1)/2$. There are $2S_{max}+1 = L$ such states with the same energy eigenvalue. It can be shown that the ground states of $\hat{H}_{NN}$ with one hole (i. e. $N = L - 1$) have maximum total spin $S = S_{max} = (L-1)/2$ and are non-degenerate (apart from the above-mentioned $(2S_{max}+1)$-fold spin degeneracy) in the following cases [35]:

Case 1: On any lattice, if $F > 0$, $t \leq 0$ and (a) $X \neq t$ and $U > U_c^{(1)}$, or (b) $X = t$ and $U \geq U_c^{(2)}$.

Case 2: On lattices with loops, if $X = t < 0$, $F = 0$, and $U > U_c^{(2)}$.

In both cases $t > 0$ is allowed if the lattice is bipartite.

These results are summarized in Table 1. The constants $U_c^{(1)}$ and $U_c^{(2)}$ are given by

$$U_c^{(1)} = Z\Big(2|t| + \Big|V - F - 2|t|\Big|$$

Table 1. Sufficient conditions for ferromagnetic ground states with one hole

1a	$F > 0$, $X \neq t$, $U > U_c^{(1)}$	any t	bipartite lattice
		$t \leq 0$	non-bip. lattice
1b	$F > 0$, $X = t$, $U \geq U_c^{(2)}$	any t	bipartite lattice
		$t \leq 0$	non-bip. lattice
2	$F = 0$, $X = t$, $U > U_c^{(2)}$	$t \neq 0$	bipartite, with loops
		$t < 0$	non-bip., with loops

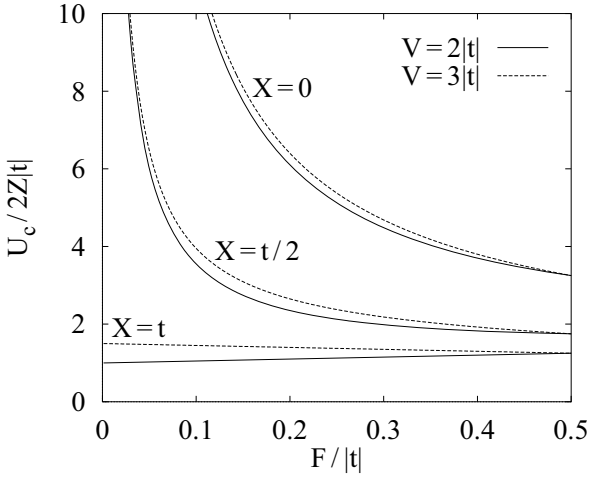

Fig. 1. Critical value U_c vs. exchange interaction F for different t, V, X, and $F' = 0$. For $U > U_c$ the ground state is ferromagnetic. See Table 1 for details

$$+ \frac{(X-t)^2}{F} + \left| F' - \frac{(X-t)^2}{F} \right| \Big), \tag{14}$$

$$U_c^{(2)} = Z\Big(2|t| + \Big|V - \frac{F}{2} - 2|t|\Big| + |F'|\Big) \tag{15}$$

where Z is the number of nearest neighbors. Hence, if $F > 0$ ferromagnetic ground states are stable on any lattice for U larger than a *finite* critical value. For $F \to 0^+$ we have $U_c^{(1)} \to \infty$, thus yielding Nagaoka's condition for the pure Hubbard model. This shows once more that the Heisenberg interaction F, which is neglected in the Hubbard model, provides an obvious mechanism for stabilizing ferromagnetic ground states at finite U. Note that since X and t are expected to be of the same order of magnitude, the sensitive dependence on F, due to the term $(X-t)^2/F$, may cancel from $U_c^{(1)}$. The dependence of U_c on t, V, F is depicted in Fig. 1. The case $X = t$ is special, since in this case the stability of ferromagnetism can be achieved either by $F > 0$, or by $F \geq 0$ and $t < 0$ if the lattice has loops. Note that the case $F > 0$ is *not connected* to the case $F = 0$ by a limiting procedure, since only in the latter case the lattice is required to have loops.

The critical couplings $U_c^{(1)}$ and $U_c^{(2)}$ are sums of terms, each of which corresponds to a typical energy scale. This means that the on-site interaction U has to be larger than the energy describing the paramagnetic state (bandwidth $\sim Z|t|$), as well as the threshold energies for the onset of a charge-density wave or phase separation ($\sim Z|V|$), η-pairing superconductivity [36] ($\sim Z|F'|$), and a spin-density wave ($\sim (X-t)^2/F$). However, these terms do not enter separately, but appear in combinations, i. e. the effects interfere, as should be expected.

The above conditions are *sufficient* conditions. The occurrence of ground states with maximum spin outside the above parameter region is not ruled out. As in Nagaoka's theorem for the pure Hubbard model, the ferromagnetic ground state is an itinerant state with non-zero kinetic energy, but the proof of its stability cannot yet be extended to doping beyond a single hole.

3.1.2. Magnetic phase diagram within the dynamical mean-field theory. Even for the simplest electronic correlation model, the Hubbard model, exact solutions are not available in $d = 2, 3$ dimensions, and numerical methods – whether exact diagonalizations or Quantum Monte Carlo (QMC) techniques – are limited by the smallness of the systems that can be studied. Hence one would like to construct, at least, a thermodynamically consistent mean-field theory which is valid also at strong coupling. Such a (non-perturbative) approximation is provided by the exact solution of a model in $d = \infty$. It is now known that in the limit $d \to \infty$ [37] one obtains a *dynamical* mean-field theory for Hubbard-type models where the spatial dependencies become local, but all quantum fluctuations of the d-dimensional model are included [38–42]. In fact the problem is equivalent to an Anderson impurity model complemented by a self-consistency condition [40, 41], leading to dynamical mean-field equations which can be solved numerically, e.g. within a finite-temperature QMC scheme [43]; for reviews see [44, 45]. We employed this numerical approach (for details see [46]) to investigate the influence of the direct exchange interaction F on the stabilization of ferromagnetism in the Hubbard model, using the one-band Hamiltonian (9)-(11) with $X = F' = 0$ [47]. To take the limit $d \to \infty$ the couplings in (9)-(11) have to be scaled appropriately [37, 38], i.e.

$$t = \frac{t^*}{\sqrt{Z}}, \; F = \frac{F^*}{Z}, \; V = \frac{V^*}{Z}. \tag{16}$$

In the following we set $t^* \equiv 1$. In the limit $d \to \infty$ the V^*-term [38] and F^*-term reduce to their Hartree-contributions. Hence their influence is that of a generalized, i.e. spin- and site-dependent, chemical potential. In the homogeneous phase the spin- and site-dependent terms vanish. This implies that the nearest-neighbor interactions F^* and V^* become important only in the symmetry-*broken* phase. Consequently the susceptibilities of the model (9)-(11) with $X = F' = 0$ may be calculated from the pure Hubbard model [47]; this simplifies the matter considerably.

The phase boundaries between the paramagnetic, antiferromagnetic and ferromagnetic phases may then be calculated in principle as follows [47]: (i) QMC simulations are performed in the homogeneous phase of the pure Hubbard model for given U, temperature T, filling n, and number of Matsubara frequencies Λ; (ii) for arbitrary values of F^*, V^* the appropriate susceptibilities are calculated; (iii) the inverse susceptibilities are extrapolated to $\Lambda \to \infty$, if they are negative the homogeneous phase is found to be unstable; (iv) to obtain ground state properties the calculated quantities have to be extrapolated to $T \to 0$. The results of these calculations for $n = 1$, $T = 0$ and a semi-elliptic DOS are collected in Fig. 2, where the exchange coupling F^* is plotted versus the Hubbard interaction U. We neglect the density-density terms in (11), since they become important

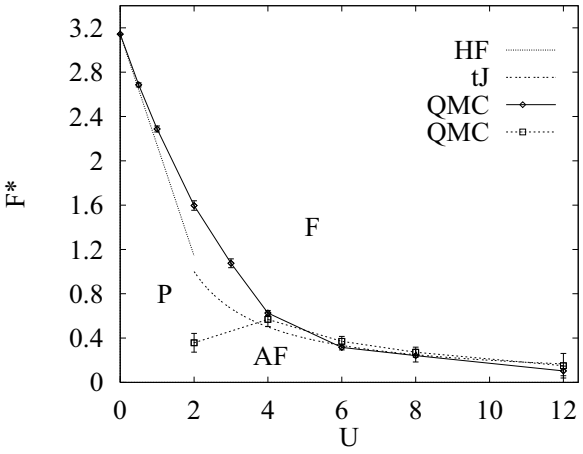

Fig. 2. Critical value of the direct exchange coupling F^* above which ferromagnetism is stable vs. Hubbard interaction U. The phase boundaries were calculated from the divergence of the ferromagnetic (diamonds) and antiferromagnetic (squares) susceptibilities, respectively. The QMC results were extrapolated to $T = 0$, the filling is $n = 1$ (F: ferromagnetic phase, AF: antiferromagnetic phase, P: paramagnetic phase). Dotted line: Hartree(-Fock) theory; dashed line: Heisenberg limit

only for $V^* - F^*/2 > U$ [47, 48]. The solid line marks the phase boundary to the ferromagnetic phase. As expected the critical value of F^*, F_c^*, decreases with U: it depends on U as $(F_c^*(0) - F_c^*(U)) \propto U$ for small U (Hartree-Fock limit) and as $F_c^*(U) \propto 1/U$ for large U (Heisenberg limit). At $U = 12$ the value of F^* necessary to induce ferromagnetism is seen to be as small as $F_c^* \sim 0.1$. This shows how important even a weak exchange coupling F is for the stability of ferromagnetism. For $U > 4$ there may well be a direct transition between the antiferromagnetic and the ferromagnetic phases.

The shape of the DOS and the band filling n are very important factors concerning the stability of ferromagnetism, as will be discussed below (Sect. 3.3). Indeed, a *symmetric* DOS and filling $n = 1$, as used in the above calculation, are especially disadvantageous for ferromagnetism, partly because antiferromagnetism will be the generic magnetic order in this case.

3.2. Band degeneracy and Hund's rule coupling

Another important route to ferromagnetism may be taken by considering more than one energy band, namely by starting from $M > 1$ Wannier (or tight-binding) orbitals. It is known from atomic magnetism that there are ferromagnetic couplings between electrons on the same atom leading to Hund's rules. These on-site "Hund's rule couplings" express the fact that by putting electrons in a maximum spin state an atomic exchange energy may be gained by the following mechanism. A spin wave function with maximum spin is always symmetric. Therefore, for the total wave function to be antisymmetric, the coordinate wave function must be antisymmetric. This reduces the probability for electrons to come close to each other which in turn lowers the Coulomb energy between them. This consideration establishes that in general there will be ferromagnetic on-site interactions *even in a bulk system.* Whether the presence of these terms is sufficient for ferromagnetism to appear in the ground state is, however, strongly dependent on their relative strength compared with the kinetic energy, on the lattice structure, electron density, etc.

Let us therefore take a closer look at the terms in the Hamiltonian (5) in the case of M relevant bands. In this case we have to retain the band index $\alpha = 1, \dots M$. Now there exist important on-site interactions even beyond the Hubbard interaction $U = \mathscr{V}_{iiii}^{\alpha\alpha\alpha\alpha}$, namely the following couplings that are off-diagonal in the *band* indices, and are hence only present for $M > 1$ bands: density-density interaction $V_0 = \mathscr{V}_{iiii}^{\alpha\beta\alpha\beta}$, direct exchange interaction $F_0 = \mathscr{V}_{iiii}^{\alpha\beta\beta\alpha}$, and hopping of double occupancies $F_0' = \mathscr{V}_{iiii}^{\alpha\alpha\beta\beta}$. For simplicity we assume the orbitals to be equivalent, i.e. U is the same for all orbitals α, and V_0, F_0, F_0' each have a fixed value for all pairs of orbitals α, β. Furthermore it should be noted that for equivalent orbitals these parameters are not independent, but are related by $U = V_0 + 2F_0$, $F_0 = F_0'$ [49]. In addition to these Hund's rule couplings there are still the inter-site terms, namely the hopping t_{ij}^{α} which takes place only between like orbitals (this follows from the general derivation above), and the next-neighbor interactions $V_1 = \mathscr{V}_{ijij}^{\alpha\alpha\alpha\alpha}$, $X_1 = \mathscr{V}_{iiij}^{\alpha\alpha\alpha\alpha}$, $F_1 = \mathscr{V}_{ijji}^{\alpha\alpha\alpha\alpha}$, $F_1' = \mathscr{V}_{iijj}^{\alpha\alpha\alpha\alpha}$. For simplicity, these next-neighbor couplings are assumed to be diagonal in the band indices, i.e. they act only between like orbitals on neighboring sites. Finally, since we are dealing with equivalent orbitals, we assume that the next-neighbor parameters t, X_1, F_1, F_1' each have the same value for all bands α. The resulting multi-band Hamiltonian then reads

$$\hat{H}_{M\text{-}band}^{NN} = \sum_{\alpha=1}^{M} \hat{H}_{1\text{-}band,\alpha}^{NN} + \hat{H}_{interband} \tag{17}$$

where

$$\begin{aligned}\hat{H}_{1\text{-}band,\alpha}^{NN} = & -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}_{i\alpha\sigma}^{+}\hat{c}_{j\alpha\sigma} + \text{h.c.}) \\ & + U \sum_{i\sigma} \hat{n}_{i\alpha\downarrow}\hat{n}_{i\alpha\uparrow} + \sum_{\langle i,j\rangle} \Big[V_1 \hat{n}_{i\alpha}\hat{n}_{j\alpha} \\ & + X_1 \sum_{\sigma} (\hat{c}_{i\alpha\sigma}^{+}\hat{c}_{j\alpha\sigma} + \text{h.c.})(\hat{n}_{i\alpha-\sigma} + \hat{n}_{j\alpha-\sigma}) \\ & + F_1' (\hat{c}_{i\alpha\uparrow}^{+}\hat{c}_{i\alpha\downarrow}^{+}\hat{c}_{j\alpha\downarrow}\hat{c}_{j\alpha\uparrow} + \text{h.c.}) \\ & - 2F_1 (\hat{\mathbf{S}}_{i\alpha}\hat{\mathbf{S}}_{j\alpha} + \frac{1}{4}\hat{n}_{i\alpha}\hat{n}_{j\alpha}) \Big]\end{aligned} \tag{18}$$

is a straightforward generalization of the one-band Hamiltonian (9) to more than one band, and

$$\begin{aligned}\hat{H}_{interband} = & \sum_{i;\alpha<\beta} \Big[V_0 \hat{n}_{i\alpha}\hat{n}_{i\beta} \\ & - 2F_0 (\hat{\mathbf{S}}_{i\alpha}\hat{\mathbf{S}}_{i\beta} + \frac{1}{4}\hat{n}_{i\alpha}\hat{n}_{i\beta}) \\ & + F_0' (\hat{c}_{i\alpha\uparrow}^{+}\hat{c}_{i\alpha\downarrow}^{+}\hat{c}_{i\beta\downarrow}\hat{c}_{i\beta\uparrow} + \text{h.c.}) \Big] .\end{aligned} \tag{19}$$

Several of the processes contained in the Hamiltonian (17) are illustrated in Fig. 3.

The physical picture of bulk ferromagnetism, originally put forward by Slater, is the following. If the on-site Hund's rule couplings are strong enough, they lead to an independent ferromagnetic alignment of spins on each atom. In this

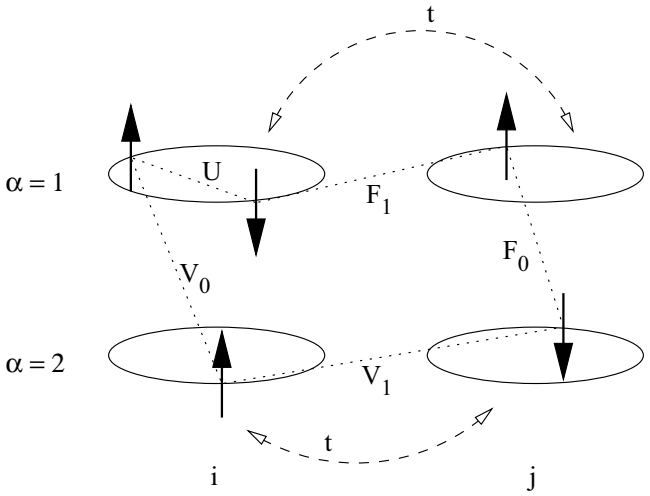

Fig. 3. Illustration of the interaction and kinetic energy in a two-band model: U, V_0, F_0 are the Hubbard interaction, the density-density interaction, and the direct exchange interaction, respectively, acting on the same site, while V_1 and F_1 act between neighboring sites i and j, and t is the hopping

situation the kinetic energy plays a decisive role since it can serve to communicate the spin alignment across the solid. Indeed, if the alignment on neighboring atoms were different, the hopping of electrons from one atom to the next would generate on-site Hund's rule interactions and thus increase the energy. These interactions can only be avoided if the spin alignment on neighboring atoms is the same, implying *global* ferromagnetism. This mechanism for the stabilization of ferromagnetic order works all the better the larger the number M of orbitals, i. e. bands, is onto which an electron can hop; it does not work for a single band ($M = 1$). Therefore one should expect band degeneracy to favor ferromagnetism. This very qualitative picture is indeed found in Stoner mean-field theory [50]: Since the non-interacting DOS is proportional to the number of degenerate bands, the critical interaction decreases as $U_c^{Stoner}(M) \sim 1/M$. On the other hand, few *exact* results are known in the case of degenerate bands. For example, for a one-dimensional chain with two orbitals ($M = 2$) and infinite on-site Coulomb interactions it has been shown that the ground state is ferromagnetic for $N = L + 1$ electrons [51]. This statement has been extended to $L + 1 \leq N \leq 2L - 1$, i.e. up to one electron less than half-filling [52]. The important point is that on a one-dimensional chain with only one orbital and hopping between nearest neighbors, Nagaoka's theorem is not applicable, since the lattice does not have loops. In that case the ground state is degenerate with respect to the total spin S. On the other hand, if there are two orbitals the loop property is restored, and the ferromagnetic states with maximum spin become the only ground states.

Furthermore, the following rigorous result can be established for the Hamiltonian (17) at half-filling [53]. For $N = ML$ electrons, the ground states of $\hat{H}_{M\text{-}band}$ have maximum spin $S = S_{max} = ML/2$ if

$$2V_0 \geq F_0 \geq \frac{U_c^{(1,2)}}{1 + M/2} \quad \text{and} \quad F_1 > 0 \tag{20}$$

where $U_c^{(1,2)}$ are the critical values for U in the *single* band system, as given in (14)–(15). The meaning of these bounds is the following. The requirement that $2V_0 \geq F_0$ and F_0 be greater than a certain threshold leads to an alignment of the electronic spins on an isolated atom. On the other hand, ferromagnetism within each band is brought about by the next-neighbor exchange $F_1 > 0$ and the Hubbard interaction U larger than a threshold related to $U_c^{(1,2)}$. The combination of these two effects (using the fact that $U = V_0 + 2F_0$ for equivalent bands) leads to a critical value for the Hund's rule coupling F_0, which indeed becomes lower as the number of bands increases.

While this result contains some ideas of Slater's picture, it does not explain the itinerant aspects of multi-band ferromagnetism, since at half-filling the ferromagnetic ground states are insulating. So far, this result can only be modified to apply also to Nagaoka's case (one hole, $N = ML - 1$) [53].

3.3. Kinetic energy and lattice structure

The stability of ferromagnetism is intimately linked with the structure of the underlying lattice and the kinetic energy (i.e. the hopping) of the electrons [18–25, 29–33]. This is supported by several facts: (a) Nagaoka's proof of ferromagnetism in the Hubbard model for a single hole at $U = \infty$ [29] depends on the existence of closed loops along which the hole can move, and (b) on bipartite lattices $anti$ferromagnetism is the generic magnetic state making it hard for ferromagnetism to become stable. Hence non-bipartite lattices with loops (or with a kinetic energy involving hopping between nearest and next-nearest neighbors sites effectively leading to a motion on loops) should be expected to support ferromagnetism because the competing antiferromagnetic tendencies are severely weakened, and because the corresponding DOS of non-interacting electrons is asymmetric and thus has a peak at a non-symmetric position. Indeed, a peak at one of the band edges as in the case of the fcc lattice is favorable for ferromagnetism [10, 17, 18, 21–24]. This is supported by the observation [24] that Co and Ni, having non-bipartite hcp and fcc lattice structure, respectively, show a full magnetization while bcc-Fe has only a partial magnetization.

3.3.1. A model density of states. To gain insight into why a DOS with a peak (or more precisely with a high spectral density) at the band edge, e.g. at the lower band edge for $n < 1$, may be favorable for ferromagnetism, we study non-interacting electrons with the following model DOS:

$$N^0(E) = \frac{1}{\Delta}\left(1 + \frac{1}{3}A^2 + \frac{2A}{\Delta}E\right) \tag{21}$$

where Δ is the width of the band and A parameterizes the asymmetry. The lower band edge is $-(A+3)\Delta/6$ such that the first moment of $N^0(E)$ vanishes. For $A = -1(+1)$ the DOS has a triangular shape with the peak at the lower (upper) edge, while for $A = 0$ it is flat. We wish to calculate the energy difference $\delta\epsilon$ between the fully polarized and the paramagnetic state

$$\delta\epsilon \equiv \epsilon_{ferro}(n, A) - \epsilon_{para}(n, A) \tag{22}$$

as a function of A and the band filling. It is easy to confirm that for all n $\delta\epsilon$ is lowest for $A = -1$. The reason is this: In the paramagnetic state N non-interacting electrons ($N/2$ electrons with spin up and down each) fill the lowest $N/2$ **k**-states up to an energy E_F^{para}, while in the ferromagnetic state the N singly occupied **k**-states below $E_F^{ferro} > E_F^{para}$ are filled, i.e. the $N/2$ **k**-states with energy above E_F^{para} are also occupied. The higher the DOS is at the lower edge the less the additional $N/2$ **k**-states are forced into high-energy states, i.e. the lower E_F^{ferro} will be. Then $\delta\epsilon$ is kept at a minimum.

3.3.2. The Hubbard model on fcc type lattices. As explained in the previous section, a lattice structure which gives a high DOS at low energies is expected to be favorable for ferromagnetism (at $n < 1$) because this situation reduces the loss in kinetic energy. The question remains: is a strongly peaked DOS *sufficient* to induce ferromagnetic order in the single band Hubbard model without additional interactions?

In this section we discuss the results of a QMC-investigation of the stability of ferromagnetism in the single band Hubbard model in the limit of infinite dimensions.

Based on the considerations in Sect. 3.3.1, the fcc lattice is expected to be a good candidate for ferromagnetism because of its high (divergent) DOS at the lower band edge. The fcc-lattice can be generalized to higher dimensions in different ways [23, 54]. Here we use the definition of an fcc lattice as the set of all points with integer cubic coordinates summing up to an even integer [23]. It is a non-bipartite Bravais lattice for any dimension $d > 2$. For $d = 2$ it is identical to the square lattice. Nearest neighbors are connected by *two different* unit vectors on a simple hypercubic (hc) lattice. The coordination number is hence $Z = 2d(d-1)$. With the proper scaling of the hopping term, (16), the non-interacting DOS of the generalized fcc lattice can be calculated in $d = \infty$ [23] as:

$$N^0_{gfcc}(E) = e^{-(1+\sqrt{2}E)/2}/\sqrt{\pi(1+\sqrt{2}E)} \tag{23}$$

which has a strong square-root divergency at the lower band edge, $-1/\sqrt{2}$, and no upper band edge. Since we choose a *positive* hopping integral ($-t > 0$), $N^0_{gfcc}(E)$ might be regarded as the DOS of holes rather than electrons. A full polarization of holes would hence correspond to a *maximal* (though not full) polarization in a more than half-filled band.

While the three dimensional fcc lattice has no square-root but only a logarithmic divergency at the band edge it is worth mentioning that a square-root divergency arises on the fcc lattice in any dimension if there is an additional next nearest neighbor hopping of the size $t' = t/2$ between sites that are linked by two unit vectors in the *same* direction on the hc lattice. The energy dispersion and the DOS of this so-called "half-hypercubic" (hh) lattice [54] can easily be obtained from the hc lattice as:

$$\epsilon_{hh}(k) = \frac{t}{2t_{hc}}\epsilon^2_{hc}(k) - 3t \tag{24}$$

$$N^0_{hh}(E) = \frac{2t^2_{hc}}{t}\frac{N^0_{hc}(\sqrt{E+3t})}{\sqrt{E+3t}}\ . \tag{25}$$

In the limit $d \to \infty$, the hh and fcc lattices become equivalent.

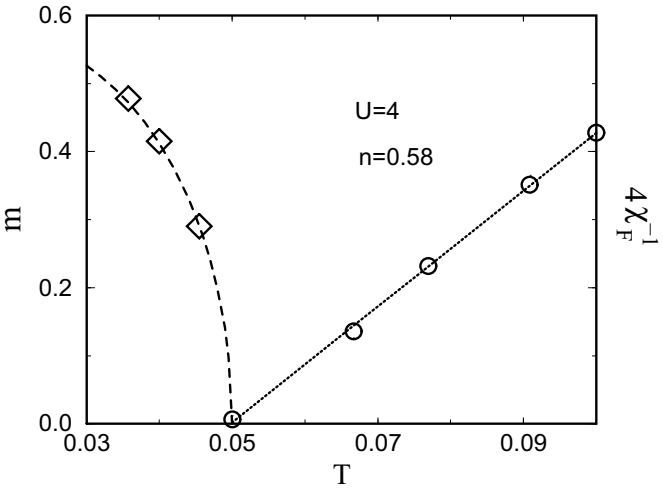

Fig. 4. Magnetization m (diamonds) and inverse ferromagnetic susceptibility χ_F^{-1} (circles; values multiplied by a factor of 4 to use the same scale) for $U = 4$ and $n = 0.58$. Error-bars are of the size of the symbols or smaller. (Note that the value of χ_F^{-1} at $T = 0.05$ is a data point, not an extrapolation.) The dotted line is a linear fit to χ_F^{-1}, the dashed line a fit with a Brillouin function to m

The fact that the fcc lattice provides a good 'environment' for ferromagnetism has also been supported by variational studies of the stability of the Nagaoka state [21, 24]. Variational calculations provide limits for the critical density n_c and the critical interaction U_c where saturated ferromagnetism becomes unstable: While for the hc lattice in $d = \infty$ the stability regime shrinks to the point $U_c = \infty$, $\delta_c = 0$ [22], for the fcc DOS (23) there is a critical line $U_c(n)$ with $U_c(0) = 0$ and $U_c(1) = \infty$ [55]. The Nagaoka state is always unstable in the case of electron doping ($n > 1$).

Recently, these variational boundaries were qualitatively confirmed by Uhrig's calculation of the exact single spin-flip energy of the Nagaoka state in $d = \infty$ [54]. While on the hh lattice U_c vanishes at low densities, U_c remains finite for all densities in the case of the "laminated" lattice which is a different generalization of the fcc lattice without a divergent DOS at the band edge. His results, too, emphasize the subtle dependence of the stability of ferromagnetism on the lattice structure.

Antiferromagnetism is not expected on the fcc-lattice in high dimensions because the difference of the numbers of not frustrated bonds and frustrated bonds is only of the order of d resulting in an effective field of the order of $t^2 d \propto 1/d$ [55]. Even in $d = 3$ antiferromagnetism is frustrated and is expected only very close to half-filling.

To detect a ferromagnetic instability we calculated the temperature dependence of the uniform static susceptibility, χ_F, from the two-particle correlation functions [46]. At an intermediate interaction strength of $U = 4$ we found the ferromagnetic response to be strongest around quarter filling ($n \simeq 0.5$). χ_F obeys a Curie-Weiss law (Fig. 4) and the Curie temperature T_c can safely be extrapolated from the zero of χ_F^{-1} to a value of $T_c = 0.051(2)$ at $n = 0.58$. Below T_c the magnetization m grows rapidly, reaching more than 80% of the fully polarized value ($m_{max} = n = 0.58$) at the lowest temperature which is only 30% below T_c. The three data points $m(T)$ (Fig. 4) are consistent with a Brillouin

function with the same critical temperature of $T_c = 0.05$ and an extrapolated full polarization at $T = 0$. A saturated ground state magnetization is also consistent with the single spin-flip energy of the fully polarized state which is positive at the present parameter values [54].

Translated to the three dimensional fcc lattice with $Z = 12$ nearest neighbors and a bandwidth of $W = 16t$, the critical temperature becomes $T_c(3D) \approx 0.011W$ [56]. Thus, despite the oversimplifications of the single band Hubbard model, the resulting Curie temperature has a realistic order of magnitude of 500-800K for typical values of W around 5 eV.

In order to answer the question if the system is still metallic we also calculated the single particle spectrum [57]. We find that the system is metallic since both spectra have a finite value at the Fermi level.

We conclude that within the dynamical mean-field theory a DOS with sufficiently large spectral weight at low energies is able to induce itinerant ferromagnetism in the single band Hubbard model. Detailed investigations of the dependence of ferromagnetism on the electronic density, the interaction strength, and in particular the extension to more realistic densities of states (e.g. fcc lattice in $d = 3$) is under progress and will be presented elsewhere [57].

In the $d = \infty$ limit the dynamics of the correlated system is fully taken into account, while spatial fluctuations are suppressed [38–42]. One might therefore suspect that the stability of ferromagnetism is somehow *over*estimated in this approach (in particular since the rivaling antiferromagnetism is completely absent on the fcc lattice). However, most recently similar results were reported for the Hubbard model with nearest and next-nearest neighbor hopping t and t', respectively, in dimensions $d = 1$ [20] and $d = 2$ [19], which are consistent with the results in $d = \infty$. Hence the existence of itinerant ferromagnetism in the pure Hubbard model with a suitable kinetic energy seems to be established at last.

4. Metamagnetic phase transitions

An issue related to the stability of (itinerant) ferromagnetism in the Hubbard model is the question concerning metamagnetism [58] in this and other models. Here it is an external magnetic field H which helps to suppress the (not necessary long-range) antiferromagnetic correlations in the system and thereby induces a pronounced transition from a state with low magnetization to one with high magnetization. At the metamagnetic transition the magnetization curve $m(H)$ shows an up-turn such that the susceptibility $\chi(H) = \partial m/\partial H$ has some kind of maximum. This feature serves as a convenient general definition for "metamagnetism". Metamagnetic transitions were first observed in strongly anisotropic antiferromagnets of which $FeCl_2$ and $Dy_3Al_5O_{12}$ (DAG) are well-studied prototypes [59]. These materials are insulators where the valence electrons are localized at the Fe and Dy ions, respectively. The arising local moments order antiferromagnetically and are strongly anisotropic in the sense that they are constrained to lie along an easy axis **e**. In this case a spin-flop transition in an external magnetic field $\mathbf{H} \parallel \mathbf{e}$ cannot occur. Apart from the above materials there are also conducting systems that most probably belong to this class, e.g. the conductors $UA_{1-x}B_x$ (where A = P, As; B = S, Se) [59], $SmMn_2Ge_2$ [60] and $TbRh_{2-x}Ir_xSi_2$ [61].

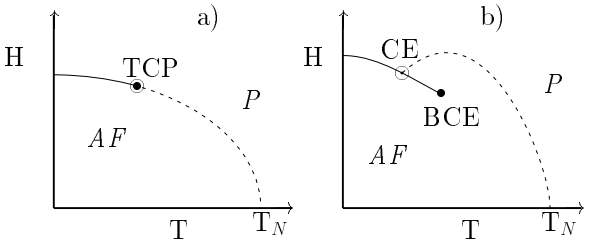

Fig. 5. Schematic $H - T$ phase diagram for a) a typical Ising-type metamagnet (TCP: tricritical point), b) the Ising model (26) in mean-field theory with $R < 3/5$ (CE: critical endpoint, BCE: bicritical endpoint) [63]. Full lines: first order transition, broken lines: second order transition; AF: antiferromagnetic phase, P: paramagnetic phase

Hitherto completely different theories are employed to describe metamagnetic phase transitions in these different, strongly anisotropic antiferromagnets. Investigations of localized systems are usually based on the Ising model, where more than one interaction has to be introduced to describe the experimentally observed first order phase transitions [62]. With antiferromagnetic coupling J between the Z nearest-neighbor (NN) spins and a ferromagnetic coupling J' between the Z' next-nearest-neighbors (NNN) one obtains

$$H_{Ising} = J \sum_{NN} S_i S_j - J' \sum_{NNN} S_i S_j - 2H \sum_i S_i \ . \qquad (26)$$

In Weiss mean-field theory this model shows two different types of phase diagrams depending on the parameter $R \equiv Z'J'/(ZJ)$ [63]. For $R > 3/5$ the first and second order phase transition line join smoothly at the same point, producing a tricritical point (TCP), while for $R < 3/5$ there is no common endpoint (see Fig. 5). However the scenario of Fig. 5b was not found when evaluating (26) beyond mean-field theory [64].

For *itinerant electron metamagnetism* (IEM) Moriya and Usami [65] proposed a Landau theory, where the parameters have to be deduced from microscopic models. The idea is to calculate first the independent electron band structure and to introduce the Coulomb interaction within the random phase approximation.

It is our purpose to investigate the origin of metamagnetism in strongly anisotropic antiferromagnets from a microscopic, quantum-mechanical point of view, and to describe different kinds of metamagnets (i.e. metallic *and* insulating, band-like *and* localized systems) qualitatively within a single model. To this end we study the Hubbard model (10) with the additional constraint that the antiferromagnetic magnetization $\mathbf{m}_{st}$ lies *parallel* to the external magnetic field **H** [66]. In this way the existence of an easy axis **e** along which **H** is directed, such that $\mathbf{e} \parallel \mathbf{m}_{st} \parallel \mathbf{H}$, is incorporated in a natural way. By this approach, both kinetic energy and Coulomb interaction are captured microscopically, whereas the relativistic corrections (responsible for the easy axis) are not. This procedure is justified since the relativistic corrections are of $\mathcal{O}(10^{-2}$ eV) and are thus small compared to the kinetic and Coulomb energy which are of $\mathcal{O}$(1eV). Therefore the existence of an anisotropy axis **e** and the correlations

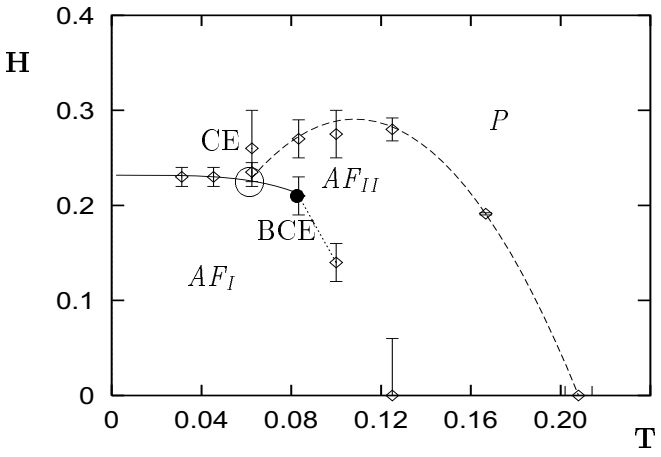

Fig. 6. $H-T$ phase diagram for the $d=\infty$ Hubbard model with easy axis along H at $n=1$ and $U=4$ [67]; same notation as in Fig. 5b

described by the Hubbard model are quite unrelated. Note, that the existing Ising and IEM theories do not treat the kinetic energy and Coulomb interaction microscopically, but within an effective model.

A perturbative treatment of the Hubbard model with easy axis in the weak and strong coupling limit shows that the appearance of a tri- or multicritical point is a delicate matter, since neither of these two limits is able to describe a change of the transition from first to second order [67]. Apparently the entire transition scenario depends sensitively on the value of the electronic on-site interaction U. To study this point in greater detail we have to go to intermediate coupling. In this non-perturbative regime we employ again QMC simulations to calculate the magnetization $m(H)$ and the staggered magnetization $m_{st}(H)$ of the Hubbard model (10) in $d=\infty$ [67]. As the results do not much depend on the precise form of the density of states we choose $N^0(\epsilon)=[(2t^*)^2-\epsilon^2]^{1/2}/(2\pi t^{*2})$, setting $t^*\equiv 1$ in the following. All calculations are performed at half-filling.

The results for $m(H)$ and $m_{st}(H)$ are used to construct the $H-T$ phase diagram at $U=4$ (Fig. 6). It displays all the features of Fig. 5b. In particular, the first order line continues *into* the ordered phase, separating two different AF phases: AF_I (where $m\simeq 0$) and AF_{II} (where $m>0$). The position of its endpoint cannot, at present, be determined accurately (dotted line). This phase diagram is surprisingly similar to the experimental phase diagram of $FeBr_2$ [68].

A change in U and the filling n will affect the phase diagram quantitatively and qualitatively. These results will be reported elsewhere [69].

5. Conclusion

In the last few years, and especially most recently, considerable progress was made in our understanding of the microscopic origin of itinerant ferromagnetism. These results were obtained on the basis of well-defined lattice models of correlated electrons, of which the one-band Hubbard model is a particularly important ingredient, by applying new, non-perturbative techniques, ranging from rigorous to large-scale numerical methods. There exists convincing evidence now that on appropriate, non-artificial lattices, or for an appropriate kinetic energy, itinerant ferromagnetism is stable even in the pure Hubbard model, for electronic densities not too close to half-filling and large enough U. Important ingredients are:
(i) lattices with loops (or a kinetic energy allowing for motion on loops, e.g. with t,t' hopping) such that the Nagaoka mechanism works and antiferromagnetism is suppressed,
(ii) a large spectral weight near the band edge. (We note that this condition goes far beyond the mean-field Stoner criterion for ferromagnetism, $UN(0)=1$, where $N(0)$ is the DOS at the Fermi energy.)

The direct exchange interaction, as well as band degeneracy, will strongly reduce the critical value of U above which ferromagnetism becomes stable.

Furthermore, using the dynamical mean-field theory to solve the Hubbard model with easy-axis in the intermediate coupling regime, it appears to be possible to describe various, different forms of metamagnetism within a single microscopic theory.

The development and application of controlled, non-perturbative techniques will continue to be of particular importance for the investigation of correlated electron systems.

One of us (DV) thanks Elliott Lieb for very useful discussions. In its early stages this work was supported in part by the Deutsche Forschungsgemeinschaft under SFB 341.

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