FERROMAGNETISM IN CORRELATED ELECTRON SYSTEMS: A NEW CLASS OF RIGOROUS CRITERIA

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INTRODUCTION

Even after several decades of theoretical work the conditions for the occurence of ferromagnetism in itinerant electron systems, e.g. in the transition metals, are still not well understood. In particular, the simplest lattice model for interacting electrons, the Hubbard model (Gutzwiller, 1963; Hubbard, 1963; Kanamori, 1963), which was originally introduced to clarify precisely this problem, did not provide the hoped-for answer. We now know that the single-band Hubbard model is a generic model for the description of a correlation-induced metal-insulator transition, as well as for the formation of antiferromagnetic order, but *not* for ferromagnetism. Apparently the on-site interaction, which is totally independent of any lattice properties, does not easily provide a mechanism for the generation of ferromagnetism. In the Hubbard model the lattice structure enters only via the kinetic energy due to nearest-neighbor hopping. It is therefore perhaps not surprising that the rigorous proofs of the stability of ferromagnetism in this model by Nagaoka (1966), Lieb (1989), Mielke (1991, 1992) and Tasaki (1992) apply under conditions which are more specific with regard to the *lattice structure* than the values of the *interaction.* Indeed, ferromagnetism was proved to be stable either at $U = \infty$ (in the case of a single hole moving on certain lattices with loops (Nagaoka, 1966)), or else for *all* $U > 0$ (namely in the case of asymmetric bipartite lattices in arbitrary dimensions $d > 1$ at half filling (Lieb,1989), or for special ("decorated") lattices where the single-electron ground state has bulk degeneracy, at sufficiently large filling (Mielke, 1991, 1992; Tasaki, 1992)). For details we refer to the recent reviews by Lieb (1993) and Mielke and Tasaki (1993). Investigations of the stability of the Nagaoka state have recently led to increasingly refined bounds for the critical hole density (Hanisch and Müller-Hartmann, 1993). Nevertheless there still does not exist a rigorous proof of the stability of ferromagnetism in the Hubbard model for conventional lattices (e.g. hypercubic, bcc, fcc) and thermodynamically relevant band fillings $n \lesssim 1$.

Although the on-site interaction between electrons with opposite spin can be expected to dominate quantitatively (Hubbard, 1963), the neglect of all nearest neighbor (NN) interactions in the Hubbard model is certainly a drastic simplification. There remains the question about the *qualitative* importance of NN terms even if they are weak. After all, in the limit $n = 1, U = \infty$ for example, the ground state has a macroscopic degeneracy which may naturally be lifted even by an arbitrarily weak NN interaction. Besides that, the Heisenberg interaction, i.e. the direct quantum-mechanical exchange interaction on NN-sites, should be able to lead to ferromagnetism in a rather straightforward way, even in the case of itinerant electrons. In a series of papers this question was recently taken up by Hirsch (1989a, b; 1991), who supplemented the Hubbard model by a NN Coulomb exchange interaction and a pair hopping term; see also Tang and Hirsch (1990). On the basis of a mean-field decoupling approximation, as well as numerical investigations in $d = 1$, he found that, at half-filling, this single-band model can have a ferromagnetic ground state. In particular, by considering the consequences of a single spin-flip Hirsch (1990a) derived an important condition for the (in)stability of the fully polarized ferromagnetic state in the Hubbard model with NN Coulomb exchange on a d-dimensional hypercubic lattice at half filling. Mean-field theory is found to reproduce this condition over an increasing parameter range as d increases. Unless the instability is of first order the condition provides the exact value of the exchange coupling required to produce saturated ferromagnetism. The proposition by Hirsch (1989a, b; 1990b) that the ferromagnetic state found in his model can explain metallic ferromagnetism in *real* solids was called in question by Campbell et al. (1990). Based on a thorough investigation of a Peierls-Hubbard model in $d = 1$ where all nearest neighbors are included these authors argued that the values of the interaction parameters are all related (being mainly determined by the rate of fall-off of the Wannier functions and the screening length of the electronic interaction) and cannot be "dialed at will ". They conclude that, although ferromagnetism is a possible ground state of Hirsch's model, the interaction values required for its stability are unlikely to occur in a real system.

The above discussion shows that, in spite of some remarkable progress, the conditions for the stability of ferromagnetism in itinerant electron systems are not yet clear. For example, one would like to know reliably how important NN-interactions are in comparison with the Hubbard repulsion in a three-dimensional system, whether among the NN interactions the exchange contribution really dominates, whether interactions beyond NN matter, how important band degeneracy is, etc., etc.

MODEL AND STRATEGY OF SOLUTION

In this paper we show that it is possible, quite surprisingly perhaps, to give an answer to at least some of these questions. Namely, we will derive detailed, rigorous criteria for the stability of saturated ferromagnetism in the most general single-band model of itinerant electrons with spin-independent interactions at half-filling (Strack and Vollhardt, 1994b). These criteria are valid for arbitrary translationally invariant lattices (e.g. with or without loops, bipartite or not) with L sites and coordination number Z. The model has the form

$$\hat{H} = \sum_{i \neq j, \sigma} t_{ij} \hat{c}^{+}_{i\sigma} \hat{c}_{j\sigma} + \frac{1}{2} \sum_{ijmn} \sum_{\sigma\sigma'} v_{ijmn} \hat{c}^{+}_{i\sigma} \hat{c}^{+}_{j\sigma'} \hat{c}_{n\sigma'} \hat{c}_{m\sigma}. \tag{1}$$

The first term is a general kinetic energy due to hopping between two sites i, j, and the second term describes the electronic interaction. The matrix elements

$$
\begin{aligned}
t_{ij} &= \langle i| - \frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})|j\rangle \\
v_{ijmn} &= \langle ij|v_{ee}(\mathbf{r}-\mathbf{r}')|mn\rangle
\end{aligned} \tag{2}
$$

where $U(\mathbf{r})$ is a one-particle potential, are expressed in terms of Wannier orbitals localized at sites i, j, m, n. As usual $\hat{c}^+_{i\sigma}(\hat{c}_{i\sigma})$ creates (annihilates) a σ-electron at site i.

We wish to know under which circumstances the saturated ferromagnetic state

$$
|\Psi_F\rangle = \prod_i \hat{c}^+_{i\uparrow} \mid 0\rangle \tag{3}
$$

is the unique ground state of $\hat{H}$. The central question is then: *for what choice of coupling parameters in (1) does $|\Psi_F\rangle$ become the eigenstate with the lowest energy?* To find an answer we

(i) transform (1) into a sum of positive-semidefinite operators, i.e. construct a lower bound E_l on the ground state energy (this is the hard part),

(ii) show that $|\Psi_F\rangle$ is an eigenstate of (1), i.e. obtain an upper bound E_u,

(iii) determine the conditions for $E_l = E_u$,

(iv) prove the uniqueness of $|\Psi_F\rangle$.

This strategy for searching for eigenstates with the lowest eigenvalue appears rather natural. It was recently introduced by Brandt and Giesekus (1992) into the investigation of the Hubbard model and was used by them to derive exact ground state energies for this model at $U = \infty$ on special lattices. Subsequently Strack (1993) adapted it to the $U = \infty$ limit of the periodic Anderson model in $d = 1$ and the Emery model in $d = 1, 2$; for a restricted parameter range he calculated the exact ground state energy which has a simple algebraic structure, i. e. exponentially small terms do not enter (Strack and Vollhardt, 1994a).

We now write (1) as $\hat{H} = \hat{H}^{1,2} + \hat{H}^{3,4}$ where $\hat{H}^{1,2}$ contains the sum over all 1- and 2-site terms and $\hat{H}^{3,4}$ involves all interactions involving 3 and 4 different sites. We first solve the problem for $\hat{H}^{1,2}$ and then include $\hat{H}^{3,4}$ afterwards. Due to translational invariance the (real) matrix elements in (1) depend only on the separation between sites, i.e. $t_{ij} \equiv t_{j-i}, v_{ijmn} \equiv v_{j-i,m-i,n-i}$. The 1- and 2-site contributions to the interaction are given by

$$
U \equiv v_{iiii}, V_{j-i} \equiv v_{ijij}, X_{j-i} \equiv v_{iiij}, F_{j-i} \equiv v_{ijji}, F'_{j-i} \equiv v_{iijj}. \tag{4}
$$

Then one obtains

$$
\hat{H}^{1,2} = \hat{H}_t + \hat{H}_U + \hat{H}_V + \hat{H}_X + \hat{H}_F + \hat{H}_{F'} \tag{5a}
$$

$$
\begin{aligned}
&= \sum_{i\neq j,\sigma} t_{j-i}\hat{c}^+_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \frac{1}{2}\sum_{i\neq j} V_{j-i}\hat{n}_i\hat{n}_j \\
&+ \frac{1}{2}\sum_{i\neq j,\sigma} X_{j-i}(\hat{c}^+_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^+_{j\sigma}\hat{c}_{i\sigma})(\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma}) \\
&+ \frac{1}{2}\sum_{i\neq j,\sigma\sigma'} F_{j-i}\hat{c}^+_{i\sigma}\hat{c}^+_{j\sigma'}\hat{c}_{i\sigma'}\hat{c}_{j\sigma} + \frac{1}{2}\sum_{i\neq j,\sigma} F'_{j-i}\hat{c}^+_{i\sigma}\hat{c}^+_{i-\sigma}\hat{c}_{j-\sigma}\hat{c}_{j\sigma}
\end{aligned} \tag{5b}
$$

where $\hat{n}_{i\sigma} = \hat{c}^+_{i\sigma}\hat{c}_{i\sigma}$ and $\hat{n}_i = \sum_\sigma \hat{n}_{i\sigma}$. While U parametrizes the on-site interaction and V describes the usual interaction between charges ($\equiv$ densities) at arbitrary sites

$i \neq j$, the remaining interactions are off-diagonal. Hence X_{j-i} corresponds to a density-dependent hopping between i and j. Noting that $\hat{H}_F$ may be written as

$$\hat{H}_F = \sum_{i \neq j} F_{j-i}(-\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4}\hat{n}_i\hat{n}_j), \tag{6}$$

with spin operator $\hat{\mathbf{S}}_i$, we see that F_{j-i} is just the familiar Heisenberg exchange integral, while F'_{j-i} generates hopping of doubly occupied sites.

Special Limits

Let us first discuss some special limits of (5), with $l = j - i$:

1. On-site limit: for $V_l = X_l = F_l = F'_l = 0$ one recovers the Hubbard model with general hopping;

2. Nearest neighbor (NN)-limit: for $\mid l \mid = 1$, with $t_1 \equiv -t, V_1 \equiv V, X_1 \equiv X, F_1 \equiv F, F'_1 \equiv F'$, eq.(5) corresponds to a generalized Hubbard model where all NN interactions are included (Campbell et al., 1988, 1990; Hirsch 1989a, 1990b). Considerable simplifications occur if $X = t$, since in this case the hopping processes interfere in such a way that the number of doubly occupied sites stays constant. In this limit and $F = F' = 0$, we recently showed that the exact ground state solution may be obtained in a wide range of the parameters U, V (Strack and Vollhardt, 1993). The ground state is either a highly degenerate state with singly occupied sites, or corresponds to a charge-density wave. The range of parameters where these states are stable was extended by Ovchinnikov (1993). – At the point $t = X = -V = -F = -F' = 1, U \to U - Z$ one obtains the exactly solvable supersymmetric model of Essler et al. (1992, 1993) which exhibits superconductivity. We note already here that the operators (8a,b,d) introduced below are linear combinations of the generators of the algebra relevant for their model.

In this context one should also mention the NN-model introduced by Castellani et al. (1979) to investigate the metal-insulator transition in systems like V_2O_3. They suggested to start with the Hubbard model on a bipartite lattice at half filling, and then to construct an *effective* NN-Hamiltonian $\hat{H}_{eff}$ by a decimation procedure defined by a partial trace over the degrees of freedom on one of the sublattices. In view of the symmetry properties of the Hubbard model, $\hat{H}_{eff}$ must be invariant under uniform rotations in spin and charge space, separately. This implies the form

$$\begin{aligned}\hat{H}_{eff} &= -4J\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + I\sum_{\langle i,j\rangle}\hat{\boldsymbol{\rho}}_i \cdot \hat{\boldsymbol{\rho}}_j - 16K\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i^2\hat{\mathbf{S}}_j^2 \\ &+ 4\Delta\sum_i \hat{\mathbf{S}}_i^2 + D\sum_{\langle i,j\rangle,\sigma}(\hat{c}_{i\sigma}^+\hat{c}_{j\sigma} + \hat{c}_{j\sigma}^+\hat{c}_{i\sigma})(1 - \hat{n}_{i-\sigma} - \hat{n}_{j-\sigma})\end{aligned} \tag{7}$$

where $\hat{\boldsymbol{\rho}}_i$ are charge operators, $\hat{\rho}_i^+ = \hat{c}_{i\uparrow}^+\hat{c}_{i\downarrow}^+, \hat{\rho}_i^- = \hat{c}_{i\downarrow}\hat{c}_{i\uparrow}, \hat{\rho}_i^z = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 1$, and the factor of 2 in the definition of $\hat{\mathbf{S}}_i$ by Castellani et al. (1979) was taken into account. This effective model is a generalization of the Blume-Emery-Griffiths model for ^{3}He-^{4}He mixtures (Blume et al., 1971) and contains a 6- and 8-Fermion term (the K-term). For $K = 0$, however, (7) is a special limit of the Hubbard model with all NN interactions at $X = t$. Therefore, as noted by Castellani et al. (1994), the model of Essler et al. (1992, 1993) is also particular case of (7).

We now recast (5). Introducing the non-local operators

$$
\begin{aligned}
\hat{P}_{ij,\sigma} &= (1-\hat{n}_{i-\sigma})\hat{c}_{i\sigma} + \lambda_1(1-\hat{n}_{j-\sigma})\hat{c}_{j\sigma} && \text{(8a)}\\
\hat{Q}_{ij,\sigma} &= \hat{n}_{i-\sigma}\hat{c}_{i\sigma} + \lambda_1\hat{n}_{j-\sigma}\hat{c}_{j\sigma} && \text{(8b)}\\
\hat{A}_{ij} &= \alpha_{j-i}^{-1}(\hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}) + \lambda_2\alpha_{j-i}(\hat{c}_{j\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{i\downarrow}\hat{c}_{j\uparrow}) && \text{(8c)}\\
\hat{B}_{ij} &= \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \lambda_3\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} && \text{(8d)}
\end{aligned}
$$

where

$$
\begin{aligned}
\lambda_1 &= -sgn(t_{j-i}),\\
\lambda_2 &= sgn(X_{j-i}+t_{j-i}),\\
\lambda_3 &= sgn(F'_{j-i} - \alpha_{j-i}^{-2}|X_{j-i}+t_{j-i}|), && \text{(9)}
\end{aligned}
$$

and $\alpha_{j-i} \neq 0$ is real but otherwise arbitrary, and rewriting (8c) by use of the operator identity

$$
\langle\hat{\Omega}^+\hat{\Lambda} + \hat{\Lambda}^+\hat{\Omega}\rangle = \langle(\alpha\hat{\Omega}^+ + \alpha^{-1}\hat{\Lambda}^+)(\alpha\hat{\Omega} + \alpha^{-1}\hat{\Lambda})\rangle - \alpha^2\langle\hat{\Omega}^+\hat{\Omega}\rangle - \alpha^{-2}\langle\hat{\Lambda}^+\hat{\Lambda}\rangle \qquad (10)
$$

which holds for all $\alpha \neq 0$, it can be verified that

$$
\begin{aligned}
\hat{H}^{1,2} &= \frac{1}{2}\sum_{i\neq j}\Big[|t_{j-i}|\sum_\sigma(\hat{P}_{ij,\sigma}\hat{P}^+_{ij,\sigma} + \hat{Q}^+_{ij,\sigma}\hat{Q}_{ij,\sigma}) + |X_{j-i}+t_{j-i}|\hat{A}^+_{ij}\hat{A}_{ij} + |\widetilde{F}'_{j-i}|\hat{B}^+_{ij}\hat{B}_{ij}\Big]\\
&+ \widetilde{U}\hat{D} + \frac{1}{4}\sum_{i\neq j}|\widetilde{V}_{j-i}|[\hat{n}_i + sgn(\widetilde{V}_{j-i})\hat{n}_j]^2 + \hat{C}_1 - \sum_{i\neq j}\widetilde{F}_{j-i}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j. \qquad (11)
\end{aligned}
$$

Here $\hat{D} = \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the number operator for doubly occupied sites and $\hat{C}_1 = -\frac{1}{2}L\sum_{l\neq 0}\big[\,|\widetilde{V}_l|\,\hat{n} + 4|t_l|(1-\hat{n})\big]$, with $\hat{n} = (1/L)\sum_{i\sigma}\hat{n}_{i\sigma}$; furthermore

$$
\begin{aligned}
\widetilde{F}'_l &= F'_l - |\,X_l + t_l\,|/\alpha_l^2\,,\\
\widetilde{F}_l &= F_l - \alpha_l^2|X_l + t_l|,\\
\widetilde{V}_l &= V_l - \frac{1}{2}(F_l + \alpha_l^2|X_l+t_l|) && \text{(12a)}
\end{aligned}
$$

for all $l \neq 0$, and

$$
\widetilde{U} = U - \sum_{l\neq 0}(4|t_l| + |\widetilde{V}_l| + |X_l+t_l|/\alpha_l^2 + |\widetilde{F}'_l|). \qquad (12b)
$$

Except for the $\widetilde{U}$- and $\widetilde{F}$-terms and the unimportant $\hat{C}_1$ all terms in (11) are positive-semidefinite. For $n=1$ it is seen that $|\Psi_F\rangle$ is an eigenstate of $\hat{H}^{1,2}$: (i) the P, Q, A, B-terms have zero eigenvalue and hence $|\Psi_F\rangle$ even represents a ground state of these terms; (ii) from $\hat{D}|\Psi_F\rangle = 0$ it follows that, for $\widetilde{U} \geq 0, |\Psi_F\rangle$ is also a ground state of this term; (iii) the $\widetilde{V}$-term has eigenvalues $L\sum_{l\neq 0}|\widetilde{V}_l|$ for $\widetilde{V}_l > 0$ and zero for $\widetilde{V}_l \leq 0$; since these values coincide with the lower bound of that term obtained by application of the Schwarz inequality $|\Psi_F\rangle$ is a ground state of the $\widetilde{V}$- term, too; (iv) $|\Psi_F\rangle$ is the unique ground state of the Heisenberg term provided $\widetilde{F}_l > 0$. For $\widetilde{F}_l > 0$ it is then clear that $|\Psi_F\rangle$ is the unique ground state of (11). That this is true even for $\widetilde{F}_l = 0$, provided $X_l \neq -t_l$ at least for $l=1$, can be proved by induction as follows: For $\hat{H}^{1,2}$, (11), without the A-term the set of all states with singly occupied sites represents a complete set of ground states (GS). We will prove that of these states only $|\Psi_F\rangle$ is a

GS of the A-term in (11), so that $|\Psi_F\rangle$ is the unique GS of the entire Hamiltonian (11). With $|\Psi_{F,L}\rangle = \prod_{i=1}^{L} \hat{c}_{i\uparrow}^{+}|0\rangle$ as the saturated ferromagnetic state for L sites we define $|\Psi_{L+1,\sigma}\rangle = \hat{c}_{L+1,\sigma}^{+}|\Psi_{F,L}\rangle$ as a wave function for the $(L+1)$-site model. For two sites we find $|X_1 + t_1|\ \hat{A}_{12}^{+}\hat{A}_{12}|\Psi_{2,\sigma}\rangle = 0$ for $\sigma =\uparrow$ and $\neq 0$ for $\sigma =\downarrow$. Hence $|\Psi_{F,2}\rangle$ is a GS of the A-term and thereby the unique GS of (11) with $\widetilde{F} = 0$. Let $|\Psi_{F,L}\rangle$ be the unique GS of the L-site model. For the $(L+1)$-site model it is easy to show that $|X_1 + t_1|\hat{A}_{L,L+1}^{+}\hat{A}_{L,L+1}|\Psi_{L+1,\sigma}\rangle = 0$ for $\sigma =\uparrow$ and $\neq 0$ for $\sigma =\downarrow$. Hence $|\ \Psi_{F,L+1}\rangle$ is also the unique GS of the $(L+1)$-site model. Q.E.D.

Hence for $n = 1$, arbitrary $\alpha_l \neq 0$ and in the parameter regime

$$F_1 > 0, \quad \text{for } X_1 = -t_1$$
$$F_l \geq \alpha_l^2 |X_l + t_l|\,, \text{ otherwise} \tag{13a}$$

$$U \geq \sum_{l\neq 0} \left[4|t_l| + \left| V_l - \frac{F_l + \alpha_l^2|X_l + t_l|}{2} \right| + \frac{|X_l + t_l|}{\alpha_l^2} + \left| F_l' - \frac{|X_l + t_l|}{\alpha_l^2} \right| \right] \tag{13b}$$

the unique ground state of the Hamiltonian (5) is a fully polarized ferromagnetic state (Strack and Vollhardt, 1994b). The ground state energy is given by

$$E = \frac{1}{2} L \sum_{l\neq 0} (V_l - F_l). \tag{14}$$

It may be shown that (13) also holds for complex hopping elements t_l. -

The above procedure can even be extended to include $\hat{H}^{3,4}$. In this case one has to introduce operators as in (8) that depend on 3 and 4 different site-indices. Details will be presented elsewhere (Strack and Vollhardt, 1994c). These contributions only *renormalize* the 2-site terms, i.e. lead to the replacements $t_l \rightarrow t_l - \frac{1}{2}\sum_i' v_{iil}, V_l \rightarrow V_l + \frac{1}{2}W_l$ in (13a,b) and $F_l \rightarrow F_l - W_l - 4\sum_i' |v_{l0i}|$ in (13a), where $W_l = \sum_i'(|v_{0li}| + |v_{lli}|) + \sum_{i,j}'' |v_{ilj}|$ and the prime (double prime) on the sum implies $i \neq 0, l$ $(i \neq 0, l, j)$. This means that under the above conditions, given only by inequalities, the ground state of the general Hamiltonian (1) has saturated magnetization. This rigorous result holds for arbitrary translationally invariant lattices, i.e. even in $d = 1$ (the theorem of Lieb and Mattis (1962) on the absence of ferromagnetism does not apply when $X_l, F_l, F_l' \neq 0$). Note that these are *sufficient* conditions, i.e. they do not rule out the stability of saturated ferromagnetism outside the above parameter range, e.g. in models where F is put to zero as in the Hubbard model.

Nearest Neighbor Limit

We now consider the NN-limit, i.e. the Hubbard model with all NN-interactions, with $\alpha_l = \alpha$, etc. The sum over l in (13b) then only leads to an overall factor Z, the number of NNs. For $F = F' = 0$ and $X = t$ (13b) reduces to $U - (4t + V)Z \geq 0$ which was derived earlier as a condition for the stability of a 2^L-fold degenerate ground state with singly occupied sites (Strack and Vollhardt, 1993). We now see that for $F > 0$ this degeneracy is lifted. If (13a) is taken as an equality α may be eliminated from (13); the parameter restriction for the stability of the saturated ferromagnet is then given by

$$\frac{U}{Z} \geq 4|t| + |V - F| + \frac{(X - t)^2}{F} + \left| F' - \frac{(X - t)^2}{F} \right| \tag{15}$$

with $F > 0$. For a fcc-lattice this condition can be further improved , i.e. Z can essentially be replaced by $\sqrt{Z}$ (Strack and Vollhardt, 1994c). We observe that of all interaction parameters *two* are most important for the stabilization of ferromagnetism: the on-site repulsion U and the exchange coupling F. As long as F is non-zero (as in *real* physical systems), even if arbitrarily small, there exists a critical value of U above which the fully polarized state is stable. This was already concluded earlier by Hirsch (1989a, b; 1990a, b; 1991) in his investigations of the Hubbard model plus NN-exchange (the F-term in (5)), with and without the F'-term. Our results, where *all* interactions are included rigorously, give qualitative support to his findings. Note, however, that the X-contribution is important, too. In our approach the interdependence of U and F is caused by the operator A_{ij}, (8c), and the invariance property of the operator identity (9) under changes of α. For a cubic lattice ($Z = 6$) and the estimated values $V = 2eV, X = \frac{1}{2}eV, F = F' = \frac{1}{40}eV$ (Hubbard, 1963) with $0.5eV \leq t \leq 1.5eV$ one finds critical values between $U = 24eV$ for $t = 0.5eV$ and $U = 528eV$ for $t = 1.5eV$. These values depend sensitively on t, X and F. In the limit $V = X = F' = 0, F \to 0^+$, i.e. approaching the Hubbard model, the required U-values become arbitrarily large; this is reminiscent of the result by Nagaoka (1966) for the Hubbard model at $U = \infty$ with a single hole.

Equ. (15) provides a rigorous *upper* bound on the critical value of U (or F) that is necessary to stabilize the fully polarized ferromagnet. This leads to the question of how the saturated state can become unstable. Generalizing the single spin-flip analysis of Hirsch (1990a) to the Hubbard model with all NN interactions, van Dongen and Janiš (1994) recently determined *lower* bounds on F. In fact, unless the transition is of first order these bounds are necessary and sufficient.

From (15) we see that the critical value of U required for ferromagnetism to be stable increases with Z. This is contrary to what one expects physically: the larger Z is, the more effective the internal magnetic field experienced by the electrons should become, making it easier to orient the spins. Hence the critical U-value should decrease with Z. The conditions derived above do not show this behavior; in fact, they are completely independent of the actual lattice structure. This is due to the rather coarse treatment of the lattice sums in (1), (5) which, on the other hand, allow one to derive rigorous upper bounds. – These bounds can be further improved by using instead of (8a,b) new operators $\hat{P}_{ij,\sigma} = (1 - \hat{n}_{i-\sigma})(\hat{c}_{i\sigma} + \lambda_1 \hat{c}_{j\sigma})(1 - \hat{n}_{j-\sigma}), \hat{Q}_{ij,\sigma} = \hat{n}_{i-\sigma}(\hat{c}_{i\sigma} + \lambda_1 \hat{c}_{j\sigma})\hat{n}_{j-\sigma}$ (Strack and Vollhardt, 1994c). Then the critical value of U in the above numerical example is lowered to $U = 12eV$ for $t = 0.5eV$, i.e. by a factor of two. This is now already in the range of physically relevant interaction parameters. – In a similar way we also obtain rigorous criteria for the stability of saturated ferromagnetism in the model (7) of Castellani et al. (1979). They read

$$J > 0\ ,\ K \geq 0\ ,\ -\frac{24\Delta}{Z} \geq 3|I| + 4|D| \tag{16a}$$

The new operators $\hat{P}_{ij,\sigma}, \hat{Q}_{ij,\sigma}$ lead to an even wider range of stability (Strack and Vollhardt, 1994c)

$$J > 0\ ,\ K \geq 0\ ,\ -\frac{12\Delta}{Z} \geq |I| + |D| + \frac{1}{2}\big|I - 2|D|\big|. \tag{16b}$$

LARGE-U LIMIT AND EFFECTIVE $t - J$ MODEL

For $U \gg |t|, |V|, |X|, |F|, |F'|$ the condition (15) may be written as $\widetilde{J} \equiv 4Z(X - t)^2/U - 2F < 0$. In this limit and for $\delta = 1 - n \ll 1$ the Hubbard model with all NN-interactions can itself be transformed into an effective $t - J$ model by use of the usual canonical transformation (Harris and Lange, 1967). The effective Heisenberg coupling is found as

$$J = 4\frac{(X-t)^2}{U} - 2F \tag{17a}$$

$$= \frac{4t^2}{U}\left[\left(1-\frac{X}{t}\right)^2 - \frac{FU}{2t^2}\right] \tag{17b}$$

For $d = 1$ this was already derived by Campbell et al. (1988, 1990) and, for $X = 0$, by Tang and Hirsch (1990). (Note that the additional factor Z of the rigorous result is absent here). We see that J has an antiferromagnetic contribution, reducing to the usual result $4t^2/U$ for $X = 0$, as well as a ferromagnetic one, proportional to FU. Hence there exists a physically important, dimensionless parameter $\lambda \equiv FU/t^2 > 0$ which is not *a priori* small and which may lead to ferromagnetic order. In the Hubbard model, where $F \equiv 0, \lambda$ is kept zero even in the limit $U \to \infty$. This is seen to be quite unrealistic. – If $t \simeq X$ the antiferromagnetic contribution to the effective coupling may, in principle, be very weak even if U is not extremely large. Hence, for $F > 2(X-t)^2/U$ one obtains a *ferromagnetic* $t - J$ model which is worth studying for clear physical reasons (Campbell et al., 1990; Tang and Hirsch, 1990; Putikka et al., 1992). Most importantly this model allows one to treat the more general case $n < 1$ and $T > 0$, e.g. ferromagnetic states without full polarization, and hence to make contact with experiment.

SUMMARY AND OUTLOOK

We derived explicit, rigorous, sufficient conditions for the stability of saturated ferromagnetism in the ground state of the most general one-band model of correlated electrons interacting via spin-independent forces. These criteria, given by inequalities for the interaction parameters, hold for arbitrary, translationally invariant lattices at half filling. A similar analysis can be performed in the case of the pure Hubbard model in an external magnetic field B and the spinless Falicov-Kimball model, both at half filling (Strack and Vollhardt, 1994 b,c). In the latter case the energy of the static electrons, E_f, corresponds to B in the Hubbard model. For this it is necessary to introduce a new set of non-local operators. Then one can show that for any $B > 0 (E_f \neq 0)$ there exists a critical value of $U > 0$ above which the fully polarized ferromagnetic state is stable (above which there are either only mobile or only static electrons). – In the next step the effect of band degeneracy must be investigated. All known ferromagnets have degenerate bands. Hence degeneracy is generally expected to be essential for the stabilization of ferromagnetism in real systems. However, so far there do not exist results that prove its importance beyond doubt.

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