Exact Results on Ferromagnetism in Correlated Electron Systems

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Exact results, both old and new, on the stability of saturated ferromagnetism in the Hubbard model and its extensions are discussed. For the Hubbard model with all nearest-neighbor interactions a new set of rigorous criteria, valid at half filling, is derived and a generalization of Nagaoka's theorem to finite interactions is presented. Of all coupling parameters only the on-site and the exchange interaction are found to be essential. At strong coupling comparison with the effective $t-J$ model is made. Further extensions, e.g. to the band-degenerate case, are discussed.

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1. INTRODUCTION

Of all cooperative electronic phenomena *ferromagnetism* is perhaps the one longest known to mankind. Already more than 2800 years ago the unusual properties of magnetite were described and ever since explanations of its origin were offered. A fascinating survey of the history of magnetism can be found in Mattis' book.[1]

A modern microscopic theory of ferromagnetism has to take into account two basic facts: (i) Magnetic phenomena are quantum mechanical by nature, and (ii) magnetic phenomena require electronic interactions. The first is a consequence of the Bohr-van-Leeuwen theorem which proves that within classical theory the magnetization of a system in thermodynamic equilibrium is zero, and the second follows essentially from the Pauli principle which implies that for *non*-interacting electrons the ground state energy obeys $E(S) \leq E(S+1)$, regardless of the external potential, where S is the total spin of the system.[2] As to the interaction responsible for ferromagnetism it is well-known that the perhaps most obvious candidate – the interaction between the *magnetic* moments of the electrons – is not able to explain ferromagnetism in the transition metals Co, Ni, Fe. The energy of the dipole-dipole interaction is of the order of $E_{dipole} \sim \alpha^2 (a_o/r)^3 Ryd \sim 10^{-5} eV$, where α is the fine-structure constant, a_o is the Bohr radius and r is the average separation between the electrons. This corresponds to a temperature $T_{dipole} \sim 0.1K$, which is obviously by a factor 10^4 too low to explain the onset of ferromagnetism in transition metals

where the Curie temperature is of the order of *electrostatic* energies, i.e. $T_{c,Fe} = 1043K, T_{c,Co} = 1388K, T_{c,Ni} = 627K$. This was already known to Heisenberg[3] who therefore proposed that it is the spin-*in*dependent Coulomb interaction which, in conjunction with the Pauli-principle, gives rise to an "effective interaction" between electronic spins (which he assumed to be localized). Bloch[4] stressed that electrons in transition metals are not localized but are mobile. Clearly, the ensueing problem of *itinerant* electrons interacting via a Coulomb interaction leads to an even harder quantum mechanical many-body problem than that for localized spins. This makes it necessary to introduce approximations. In particular, the Hartree-Fock mean field approach and its extensions that take into account the explicit band structure, such as the "local (spin)-density approximation", have led to many approximate and often surprisingly good results for the ground state properties of ferromagnetic transition metals.[5,6] However, in view of the neglect of genuine correlation effects within Hartree-Fock and the fact that it violates the important $SU(2)$ invariance of non-relativistic Hamiltonians under rotations of the spin or the angular momentum, (finite-temperature) mean-field results must be taken with caution. In spite of its undisputable success Hartree-Fock theory and its extensions is *per se* not able to answer conclusively the question whether or not the Coulomb interaction is the origin of ferromagnetism in *real* materials; for a discussion of this fundamental point see ref. 7.

In 1963 the simplest lattice model for correlated electrons, the single-band Hubbard model, was introduced in a modern attempt to clarify the conditions for the occurrence of ferromagnetism in transition metals.[8–10] These metals are characterized by correlation-induced, narrow (degenerate) energy bands. It soon turned out, however, that this model does not provide the hoped-for answer. In fact, 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,[11] Lieb,[12] Mielke[13] and Tasaki[14] apply under conditions which are more specific with regard to the *lattice structure* than the values of the *interaction*. Indeed, the saturated ferromagnetic state (Nagaoka state) was proved to be stable either at $U = \infty$ (in the case of a single hole moving on certain lattices with loops in dimensions $d \geq 2$)[11] or else for *all* $U > 0$ (in the case of special ("decorated") lattices where the single-electron ground state has bulk degeneracy) at sufficiently large filling.[7] For details we refer to the recent reviews by Lieb[15] and Mielke and Tasaki.[7]

Nagaoka's proof for the stability of ferromagnetism is not applicable in the thermodynamic limit and it has not been possible so far to generalize it to a finite density of holes, $\delta > 0$. Therefore an opposite route was taken by trying to determine the critical hole density, δ_{cr}, above which the Nagaoka state is definitely *unstable*. One method is to use suitable variational ("spin flip") wave functions. By building-in local correlations around the flipped spin Müller-Hartmann and collaborators[16,17] were recently able to bring δ_{cr} down to $\delta_{cr} = 0.29$ for a square lattice in the ther-

modynamic limit; this coincides with the result obtained by von der Linden and Edwards[18] for finite lattices using a more general ansatz. Exact diagonalization studies[19] suggest that δ_{cr} is even lower. Hence at present it cannot be ruled out that for bipartite lattices, e.g. simple cubic and bcc, $\delta_{cr} = 0$ (as in the case of the hypercubic lattice in infinite dimensions[20]), i.e. that the fully polarized ferromagnetic state is never stable for such lattices. By constrast, for non-bipartite lattices, e.g. hcp and fcc, the Nagaoka state appears to be stable for $\delta > 0$ and $t < 0$ (t is the hopping amplitude), or $\delta < 0$ and $t > 0$.[16] As pointed out by Müller-Hartmann et al.[16] such a lattice-dependence of the stability of the fully polarized ferromagnetic state is indeed observed in transition metals: while in their ferromagnetic phase Co (hcp structure) and Ni (fcc structure) are fully polarized, Fe (bcc structure) is not. In view of the utter simplicity of the underlying *single-band* Hubbard model this agreement is quite surprising.

For one-dimensional systems a theorem by Lieb and Mattis[2] puts strong limitations on the stability of ferromagnetism. They proved that for any real and particle-symmetric, but otherwise arbitrary interaction the ground state is unmagnetized. The theorem extends to single-band lattice systems in $d = 1$ without change, provided (i) the hopping is only between nearest neighbors, and (ii) the interaction involves only densities. Both conditions are fulfilled in the case of the Hubbard model, whose ground state in $d = 1$ can therefore not be ferromagnetic.

The rigorous investigations of the single-band Hubbard model described above cannot – and are not expected to – explain experimentally relevant details of ferromagnetism in transition metals. Their only intention is to provide *secure* knowledge about preconditions and possible mechanisms for the formation of electronic ferromagnetism. The price one has to pay is that the models under investigation are usually quite simple and/or that answers are rather limited. The more details one puts into a model to come as close as possible to the physics of *real* materials (band degeneracy, lattice structure, filling, atomic structure etc.) the more approximate the solution of the many-body correlation problem will necessarily have to be, and the more difficult it becomes to distinguish between various physical effects. There is a marked complementarity here – not only, but also in the case of metallic ferromagnetism. For a review of the progress made in the "realistic" theory of metallic magnetism in the 3*d*-transition series see ref. 21. –

One of the obvious features missing in the single-band Hubbard model is band degeneracy – a characteristic of all ferromagnetic metals. Already in 1936/37 Slater[22] suggested that the forces leading to "Hund's rule atomic magnetism" on an individual atom, might also be responsible for bulk ferromagnetism.[1] That is, the coupling of individually ordered atoms, mediated by the hopping of electrons or holes between these atoms, might lead to a coherent alignment and hence trigger bulk ordering. In 1964 Hubbard[23] proposed an extension of his one-band model[9] applicable to narrow degenerate electron bands, where electronic interactions within and between different orbitals only take place on the same atom. This model is still the basis of many present-day investigations. In view of the difficulties that rigorous investigations encounter already in the much simpler single-band model it is perhaps not surprising that almost no results exist for the degenerate-band model. An exception is the one-dimensional case at infinite coupling for certain fillings.[24]

In the following we will derive precise conditions for the stability of saturated

ferromagnetism in a generalized single-band Hubbard model, where longer-range than on-site interactions are explicitly taken into account. The multi-band case can be studied by the same method, leading to explicit results, too (see sect. 6), which will be discussed in detail elsewhere.[25]

2. THE HUBBARD MODEL WITH ALL NEAREST-NEIGHBOR INTERACTIONS

Although the on-site interaction between electrons with opposite spin can be expected to dominate quantitatively,[9] the neglect of all nearest-neighbor (NN) interactions in the single-band 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 between 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,[26] who supplemented the Hubbard model by a NN Coulomb exchange interaction and a pair hopping term; see also Tang and Hirsch.[27] 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. The proposition by Hirsch[26] that the ferromagnetic state found in his model can explain metallic ferromagnetism in *real* solids was called in question by Campbell et al.[28]

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..

Below we will show that it is possible to give an answer to at least some of these questions. Namely, we will derive[29] detailed, rigorous criteria for the stability of saturated ferromagnetism in an extended Hubbard model where all NN-interactions are included, at half filling. 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[9,26,28,29]

$$\begin{aligned}
\hat{H} &= \hat{H}_t + \hat{H}_U + \hat{H}_V + \hat{H}_X + \hat{H}_F + \hat{H}_{F'} \\
&= -t \sum_{\langle i,j\rangle,\sigma} \hat{c}^+_{i\sigma}\hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V \sum_{\langle i,j\rangle} \hat{n}_i\hat{n}_j \\
&+ X \sum_{\langle i,j\rangle,\sigma} (\hat{c}^+_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^+_{j\sigma}\hat{c}_{i\sigma})(\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma}) \\
&+ F \sum_{\langle i,j\rangle,\sigma\sigma'} \hat{c}^+_{i\sigma}\hat{c}^+_{j\sigma'}\hat{c}_{i\sigma'}\hat{c}_{j\sigma} + F' \sum_{\langle i,j\rangle,\sigma} (\hat{c}^+_{i\sigma}\hat{c}^+_{i-\sigma}\hat{c}_{j-\sigma}\hat{c}_{j\sigma} + h.c.) \qquad (1)
\end{aligned}$$

where operators are indicated by a hat. Here $\hat{n}_{i\sigma} = \hat{c}^+_{i\sigma}\hat{c}_{i\sigma}$, $\hat{n}_i = \sum_\sigma \hat{n}_{i\sigma}$ and the summation extends over NN-bonds. While U parametrizes the on-site interaction and V describes the usual interaction between charges ($\equiv$ densities) at NN-sites, the remaining interactions are off-diagonal. Hence X corresponds to a density-dependent hopping between NN-sites. Noting that $\hat{H}_F$ may be written as

$$\hat{H}_F = 2F \sum_{(i,j)} (-\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j - \frac{1}{4}\hat{n}_i\hat{n}_j), \tag{2}$$

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

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.[30] 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.[31] At the point $t = X = -V = -F = -F' = 1, U \to U - Z$ one obtains the exactly solvable supersymmetric model of Essler et al.[32] which exhibits a particular kind of superconductivity where Cooper-pairs are purely local ("η-pairing"). We note that for $X = t$ and $n = 1$ there exists a one-to-one correspondence (via a particle-hole transformation only for up-spins[33]) between saturated ferromagnetism and η-pairing and, hence, between the rigorous conditions for their stability.[34]

In this context one should also mention the NN-model introduced by Castellani et al.[35] some time ago 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 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

$$\begin{aligned} \hat{H}_{eff} &= -4J \sum_{(i,j)} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j + I \sum_{(i,j)} \hat{\vec{\rho}}_i \cdot \hat{\vec{\rho}}_j - 16K \sum_{(i,j)} \hat{\vec{S}}_i^2 \hat{\vec{S}}_j^2 \\ &+ 4\Delta \sum_i \hat{\vec{S}}_i^2 + D \sum_{(i,j),\sigma} (\hat{c}^+_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^+_{j\sigma}\hat{c}_{i\sigma})(1 - \hat{n}_{i-\sigma} - \hat{n}_{j-\sigma}) \end{aligned} \tag{3}$$

where $\hat{\vec{\rho}}_i$ is a vector of 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 $\hat{\vec{S}}_i$ in ref.[35] was taken into account. This effective model is a generalization of the Blume-Emery-Griffiths model for ^{3}He-^{4}He mixtures[36] and contains a 6- and 8-Fermion term (the K-term). For $K = 0$, however, (3) is a special limit of the Hubbard model with all NN interactions at $X = t$. Therefore, as noted by Castellani et al.,[37] the model of Essler et al.[32] is also a particular case of (3).

3. DERIVATION OF RIGOROUS CRITERIA FOR FERROMAGNETISM

We wish to know for which coupling parameters in (1) the saturated ferromagnetic state

$$|\Psi_F\rangle = \prod_i \hat{c}_{i\uparrow}^+ |0\rangle \tag{4}$$

is the unique ground state of $\hat{H}$. 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[38] 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[39] 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.[40]

We now recast (1). Introducing the non-local operators[29]

$$\begin{aligned}
\hat{P}_{ij,\sigma} &= (1-\hat{n}_{i-\sigma})(\hat{c}_{i\sigma} + \lambda_1 \hat{c}_{j\sigma})(1-\hat{n}_{j-\sigma}) \\
\hat{Q}_{ij,\sigma} &= \hat{n}_{i-\sigma}(\hat{c}_{i\sigma} + \lambda_1 \hat{c}_{j\sigma})\hat{n}_{j-\sigma} \\
\hat{A}_{ij} &= \alpha^{-1}(\hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}) + \lambda_2 \alpha(\hat{c}_{j\downarrow}\hat{c}_{i\uparrow} + \hat{c}_{i\downarrow}\hat{c}_{j\uparrow}) \\
\hat{B}_{ij} &= \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \lambda_3 \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}
\end{aligned} \tag{5}$$

where $\lambda_1 = sgn(t), \lambda_2 = sgn(X-t), \lambda_3 = sgn(F' - \alpha^{-2}|X-t|)$, and $\alpha \neq 0$ is real but otherwise arbitrary, and rewriting (5) by use of the operator identity

$$\langle \hat{\Omega}^+\hat{\Lambda} + \hat{\Lambda}^+\hat{\Omega}\rangle = \langle (\alpha\hat{\Omega}^+ + \alpha^{-1}\hat{\Lambda}^+)(\alpha\hat{\Omega} + \alpha^{-1}\hat{\Lambda})\rangle - \alpha^2\langle \hat{\Omega}^+\hat{\Omega}\rangle - \alpha^{-2}\langle \hat{\Lambda}^+\hat{\Lambda}\rangle \tag{6}$$

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

$$\begin{aligned}
\hat{H} &= \sum_{(i,j)} \Big[|t| \sum_\sigma (\hat{P}_{ij,\sigma}\hat{P}^+_{ij,\sigma} + \hat{Q}^+_{ij,\sigma}\hat{Q}_{ij,\sigma}) + |X-t|\hat{A}^+_{ij}\hat{A}_{ij} + |\widetilde{F'}|\hat{B}^+_{ij}\hat{B}_{ij} \Big] \\
&+ \tilde{U}\hat{D} + \frac{1}{2}|\tilde{V}| \sum_{(i,j)} [\hat{n}_i + sgn(\tilde{V})\hat{n}_j]^2 - 2\tilde{F} \sum_{(i,j)} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j + \text{const.}
\end{aligned} \tag{7}$$

Here $\hat{D} = \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the number operator for doubly occupied sites and

$$\begin{aligned}
\tilde{F}' &= F' - |X-t|/\alpha^2, \\
\tilde{F} &= F - \alpha^2|X-t|, \\
\tilde{V} &= V - \frac{1}{2}(F + \alpha^2|X-t|) - 2|t|, \\
\tilde{U} &= U - Z[2|t| + |\tilde{V}| + |X-t|/\alpha^2 + |\widetilde{F'}|].
\end{aligned} \tag{8}$$

Except for the $\widetilde{U}$- and $\widetilde{F}$-term all terms in (7) are positive-semidefinite. Furthermore, for $n = 1$ it is seen that $|\Psi_F\rangle$ is an eigenstate of $\widehat{H}$: (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 $\widehat{D}|\Psi_F\rangle = 0$ 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 $LZ|\widetilde{V}|$ for $\widetilde{V} > 0$ and zero for $\widetilde{V} \leq 0$ – 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 $\widetilde{F} > 0$. For $\widetilde{F} > 0$ it is then clear that $|\Psi_F\rangle$ is the unique ground state of (7). That this is true even for $\widetilde{F} = 0$, provided $X \neq t$, can be proved by induction.[29]

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

$$\begin{aligned} F &> 0, \text{ for } X = t \\ F &\geq \alpha^2 |X - t|, \text{ otherwise} \\ \frac{U}{Z} &\geq 2|t| + \left| V - 2|t| - \frac{F + \alpha^2 |X - t|}{2} \right| + \frac{|X - t|}{\alpha^2} + \left| F' - \frac{|X - t|}{\alpha^2} \right| \end{aligned} \tag{9}$$

the unique ground state of the Hamiltonian (1) is a fully polarized ferromagnetic state. The ground state energy is given by $E = \frac{1}{2} LZ(V - F)$. This rigorous result holds for arbitrary translationally invariant lattices, i.e. even in $d = 1$ (as discussed in the Introduction the theorem of Lieb and Mattis[2] on the absence of ferromagnetism in $d = 1$ does not apply when $X, F, F' \neq 0$). 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.

For $F = F' = 0$ and $X = t$ (9) reduces to a result which was derived earlier as a condition for the stability of a 2^L-fold degenerate ground state with singly occupied sites.[30,31] We now see that for $F > 0$ this degeneracy is lifted.

If (9) is taken as an equality α may be eliminated from (9); the parameter restriction for the stability of the saturated ferromagnet is then given by

$$\frac{U}{Z} \geq 2|t| + \left| V - 2|t| - F \right| + \frac{(X - t)^2}{F} + \left| F' - \frac{(X - t)^2}{F} \right| \tag{10}$$

with $F > 0$. For a fcc-lattice this condition can be further improved , i.e. Z can essentially be replaced by $\sqrt{Z}$. 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[26] in his mean-field and numerical investigations of the Hubbard model plus NN-exchange (the F-term in (1)), with and without the F'-term. Our results, where *all* NN-interactions are included rigorously, give qualitative support to his findings. Note, however, that the X-contribution is quantitatively important, too. In our approach the interdependence of U and F is caused by the operator A_{ij}, (5), and the invariance property of the operator identity (6) under changes of α. For a cubic

lattice ($Z = 6$) and Hubbards[9] estimated values $V = 2eV, X = \frac{1}{2}eV, F = F' = \frac{1}{40}eV$ eq. (10) yields a critical value of $U = 12eV$ for $t = 0.5eV$, which is within the range of realistic energies. This value depends 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-value becomes arbitrarily large; this is already reminiscent of the result by Nagaoka[11] for the Hubbard model at $U = \infty$ with a single hole (see next section). We note that by a different decomposition $|t|$ in (10) may be replaced by $|t - 2X|$.[43]

Eq. (10) 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 discussed earlier in the literature[41] to the Hubbard model with all NN interactions, van Dongen and Janiš[42] recently determined *lower* bounds on U. In fact, unless the transition is of first order these bounds are necessary and sufficient.

From (10) we see that the critical value of U 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 will 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 independent of the actual lattice structure. This is due to the rather coarse treatment of the lattice sums in (1) which, on the other hand, is a precondition for our present derivation of rigorous upper bounds. In a similar way we also obtain rigorous criteria for the stability of saturated ferromagnetism in the effective model (3) of Castellani et al.;[35] they read[43]

$$J > 0\ ,\ K \geq 0\ ,\ -\frac{12\Delta}{Z} \geq |I| + |D| + \frac{1}{2}|I - 2|D||. \tag{11}$$

4. GENERALIZATION OF NAGAOKA'S THEOREM TO $U < \infty$

Nagaoka's theorem proves that the macroscopic degeneracy of the ground state of the half-filled Hubbard model at $U = \infty$ may be lifted by the presence of a single hole, provided the underlying lattice allows for a loop-motion of the hole. In this case it is most favorable for the hole to move in a background of completely aligned spins. Sofar it was not possible to generalize Nagaoka's theorem to finite U. We will now show that such an extension can be obtained using the approach discussed above.

To derive conditions for the stability of saturated ferromagnetism in the Hubbard model with all NN interactions, (1), in the presence of a single hole we investigate instead of (4) the general Nagaoka state

$$|\Psi_N\rangle = \frac{1}{\sqrt{L}} \sum_i a_i \hat{c}_{i\uparrow} |\Psi_F\rangle \tag{12}$$

following the strategy discussed in sect. 3; here a_i is a yet undetermined amplitude. It is seen that now the P-term and the density interaction ($\tilde{V}$) in (7) require explicit consideration. Eq. (12) is found to be the ground state of the P-term provided[43]

$$a_i + sgn(t) a_j = 0 \tag{13}$$

where i and j are NN-sites. For $t < 0$ this requires $a_i = a_j = const.$ while $t > 0$ demands $a_i = -a_j$. For the latter condition to be fulfilled the lattice has to have

$A-B$ structure. Here the explicit lattice structure enters. The above conditions, as well as those required to prove the uniqueness of the ground state, are the same as those derived by Nagaoka,[11] although the proof itself is quite different. Investigation of the $\widetilde{V}$-term then shows that the Nagaoka state is stable under a condition quite similar to (10), namely[43]

$$\frac{U}{Z} \geq 2|t| + \beta\Big|V - 2|t| - \frac{F + \alpha^2|X-t|}{2}\Big| + \frac{|X-t|}{\alpha^2} + \Big|F' - \frac{|X-t|}{\alpha^2}\Big| \qquad (14)$$

where $\beta = 1$ for $V \geq 2|t| + F$, and $\beta = 2$ for $V < 2|t| + F$, with an additional condition depending on the type of (translationally invariant) lattice:

$$\text{lattice} \begin{cases} \text{bipartite} & \begin{cases} \text{with loops} & : \ t \text{ arbitrary}, F \geq \alpha^2|X-t| \\ \text{without loops} & : \ t \text{ arbitrary}, F > \alpha^2|X-t| \end{cases} \\ \text{non} - \text{bipartite} & \begin{cases} \text{with loops} & : \ t < 0\,, \ F \geq \alpha^2|X-t| \\ \text{without loops} & : \ t < 0\,, \ F > \alpha^2|X-t| \end{cases} \end{cases}$$

Here α is a non-zero but otherwise arbitrary parameter. We note that for $F > \alpha^2|X-t|$ this result holds for $d \geq 1$ since in this case the uniqueness is guaranteed by the Heisenberg-term in (7), while for $F = \alpha^2|X-t|$ it requires $d \geq 2$ as in Nagaoka's proof. For $X = V = F' = 0$ and $F \to 0$, i. e. $\alpha \to 0$, the critical value of U approaches infinity. Hence (14) is a generalization of the Nagaoka theorem to finite U-values.

5. EFFECTIVE $t-J$ MODEL

For $U \gg |t|, |V|, |X|, |F|, |F'|$ the condition (10) may be written as $4Z(X - t)^2/U - 2F < 0$. 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.[44] The effective Heisenberg coupling is found as

$$J = \frac{4t^2}{U}\Big[\Big(1 - \frac{X}{t}\Big)^2 - \frac{FU}{2t^2}\Big] \qquad (15)$$

For $d = 1$ this was already derived by Campbell et al.[28] and, for $X = 0$, by Tang and Hirsch.[27] (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 for large enough F and/or U. 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[28,26] which is worth studying for clear physical reasons. Most importantly this model allows one to treat the more general case $n < 1$ and $T > 0$, e.g. ferromagnetic states without full polarization (for a square lattice see Putikka et al.[45]), and hence to make contact with experiment.

6. FURTHER GENERALIZATIONS AND OUTLOOK

Rigorous conditions for the stability of ferromagnetism can even be derived for the most general single-band model of itinerant electrons, i.e. when a reduction of the general interaction matrix element v_{ijmn} to two NN-sites (leading to (1)) is not made.[29] The additional interactions only lead to a renormalization of t and F, but do not change the character of the inequality (9).

An analysis similar to that discussed in sect. 3 and 4 can also be performed[29] in the case of the pure Hubbard model in an external magnetic field B and the spinless Falicov-Kimball model,[43] both at half filling. 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 $B > 0$ (any $E_f \neq 0$) 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).

Rigorous conditions for arbitrary translationally invariant lattices may even be derived for the band-degenerate Hubbard model with all NN interactions at half filling. In this case one has interatomic as well as intraatomic interactions (Hund's rule coupling), i.e. charge-charge, bond-charge, exchange and pair-hopping interactions on the same and between NN-sites. These conditions hinge on the existence of arbitrary, but finite exchange interactions (which will always be present in *real* systems). They are given by (7) with an additional positive-semidefinite term $(N-1)[X_0^2/F_0+|F_0'-X_0^2/F_0|+|V_0-F_0|]$ on the r.h.s. of (7).[25] Here N is the number of bands and the parameters with subscript zero refer to interactions between the orbitals localized on a single site. Since the additional term is proportional to $(N-1)$ the critical U-value, U_c, increases with the band degeneracy. For $F_0 = F_0' \simeq 1eV$,[46] and assuming $V_0 \simeq X_0 \simeq F_0$, this term leads to an additional energy of $\sim 4eV$, increasing U_c to $U_c \simeq 16eV$. Although this is still within a physically relevant range[46] an increase of U_c with increasing degeneracy is not what is commonly expected. Within our approach the origin of this dependence, as well as of that on Z which is quite analogous (see the discussion at the end of sect. 3), is easily traced. We note that the conditions derived by us are *sufficient* and may still be too high for realistic materials. This would be the prize one has to pay for being able to obtain rigorous results on a *very* general electronic correlation model.

It is clear that in spite of its long history the problem of metallic ferromagnetism is still not sufficiently understood – neither from a fundamental nor even from a pragmatic point of view. It is equally clear that this area of research, in particular the controlled investigation of Hubbard-type correlation models with degeneracy, will continue to provide exciting new insight in the future.

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