Ferromagnetism in Single-Band Hubbard Models with a Partially Flat Band

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(Received 18 December 1998)

A Hubbard model with a single, partially flat band has ferromagnetic ground states. It is shown that local stability of ferromagnetism implies its global stability in such a model: The model has only ferromagnetic ground states if there are no single spin-flip ground states. Since a single-band Hubbard model away from half filling describes a metal, this result may open a route to metallic ferromagnetism in single-band Hubbard models. [S0031-9007(99)09222-4]

PACS numbers: 75.10.Lp, 71.10.Fd

Ferromagnetism of itinerant electrons is an old and still unsolved problem in theoretical physics. One of the motivations to introduce the Hubbard model [1] more than 30 years ago has been to understand this problem [2]. Conceptually, the Hubbard model is very simple. It describes electrons on a lattice interacting via a repulsive, purely local Coulomb interaction. Originally, only a single energy band was considered. But it is relatively easy to generalize the model including more energy bands or further interactions. Despite the simplicity of the model, there are only few rigorous results concerning the existence of ferromagnetism. The first rigorous result is the so-called Nagaoka theorem [3]. It states that on certain lattices, for an infinitely large Coulomb repulsion, and close to half filling, the ground state is ferromagnetic. But the problem is that this ferromagnetic state disappears if the repulsion has realistic values or if the number of electrons is varied [4,5], at least for usual cubic lattices in d dimensions [6].

Ferromagnetic ground states also occur if one of several bands of the Hubbard model is dispersionless (Lieb's ferrimagnetism [7] and the flat-band ferromagnetism [8]). Tasaki [9] was able to show the local stability of ferromagnetic ground states in related models with a nearly flat band. But these models (as well as the flat-band ferromagnetism) are already extensions of the single-band Hubbard model since they contain more than one band. Furthermore, these models show characteristic features of an insulator: The (nearly) flat band is half filled and there is a gap in the single-particle spectrum. Other extensions of the Hubbard model have been proposed as well, for instance an additional ferromagnetic interaction between the electrons [10] or degenerate bands with Hund's coupling between the bands [11].

The question, if and under which conditions a simple, *single*-band Hubbard model can show ferromagnetism, is still open. Ferromagnetism is a strong coupling phenomenon. To obtain ferromagnetism within usual mean field theory the dimensionless parameter $\rho_F U$ has to be large, where ρ_F is the density of states at the Fermi level. But it should be noted that a large value of $\rho_F U$ is not sufficient for the existence of ferromagnetism (counterexamples with $\rho_F = \infty$ and $U = \infty$ can be found in [12]). On the other hand, it seems to be clear that a strong asymmetry of the band, together with a large density of states near the Fermi energy, is a condition that favors ferromagnetism. This view is supported by the variational calculations by Hanisch *et al.* [5] and as well by the dynamical mean field analysis by Wahle *et al.* [10]. In this Letter I discuss the extreme limit of this situation, namely a Hubbard model with a partially flat band. The main result is that local stability of ferromagnetism implies its global stability in such models.

At first glance a single, partially flat band seems to be similar to the flat-band ferromagnetism mentioned above. But there are important differences: As already mentioned, the models with a nearly flat band have a gap in the single particle spectrum and the band is half filled [9]. This is a typical situation for an insulator. In the flat band case, it was possible to go away from half filling [8], but if an entire band is flat, single particle eigenstates may be localized. In fact, the existence of a localized basis was an essential point in the proofs [8]. Localized states are as well typical for an insulator. In the present case, the energy band is not half filled and there is no gap in the single particle spectrum. A localized eigenbasis of single particle states does not exist; instead the translational invariance will be important. These are typical properties of a metal.

The Hamiltonian of a single-band Hubbard model on a d-dimensional translationally invariant lattice with periodic boundary conditions is

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{N_s} \sum_{\delta} \left(\sum_k c_{k+\delta\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) \times \left(\sum_k c_{-k\downarrow} c_{k+\delta\uparrow} \right). \quad (1)$$

$c_{k\sigma}^\dagger$ ($c_{k\sigma}$) creates (annihilates) an electron with spin σ in a single particle eigenstate given by $\psi_k(x) = N_s^{-1/2} \exp(ikx)$, and N_s is the number of sites of the lattice, which is equal to the number of single particle states in the band. The interaction is usually written in the form $U \sum_x c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger c_{x\downarrow} c_{x\uparrow}$. It is repulsive, $U > 0$. The Hamiltonian has the usual SU(2) spin symmetry. Furthermore, due to translational invariance, the total

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momentum is a good quantum number. The wave vectors k are elements of the first Brillouin zone (BZ). More precisely, k is a representative of a class of equivalent wave vectors each belonging to a different BZ. A statement like $k + \delta = k'$ means that $k + \delta$ and k' are both representatives of the same class of wave vectors. I assume that the single particle band is partially flat, a finite fraction of the band energies ϵ_k is degenerate. I assume that the set of degenerate band energies is situated at the bottom of the band, but some comments on other situations are given as well. Shifting the energy scale one can always take $\epsilon_k \geq 0$. As a consequence, $H \geq 0$. Let $\mathcal{L}$ be the subset of wave vectors k with $\epsilon_k = 0$. N_d is the degeneracy, i.e., the number of elements in $\mathcal{L}$. In such a situation the Hamiltonian has ferromagnetic ground states if $N_e \leq N_d$. Let

$$\psi_{0F} = \prod_{k\in\mathcal{L}} c_{k\uparrow}^\dagger |0\rangle \tag{2}$$

be the (only) ground state of H with $S = S_z = N_d/2$, $N_e = N_d$. For $N_e < N_d$ one can construct $\binom{N_d}{N_e}$ ferromagnetic ground states with $S = S_z = N_e/2$ by replacing the product in (2) by a product over an arbitrary subset of $\mathcal{L}$ with N_e elements. Using the SU(2) invariance of the Hamiltonian one can construct further ground states with $S_z < S = N_e/2$. The question is the following: Are there ground states with $S < N_e/2$?

ψ_{0F} has zero energy. Any other ground state with $N_e \leq N_d$ must have zero energy as well. Since both parts of the Hamiltonian, the kinetic energy, and the interaction, are non-negative, the ground states of H are simultaneously ground states of the kinetic energy and of the interaction. This simplifies the situation considerably. Let us assume that H has a ground state with $N_e = N_d - n + m$ electrons ($n \geq m$) and a spin $S = S_z = N_e/2 - m$. Such a state can be written in the form

$$\psi = S_-^{n,m}(\alpha)\psi_{0F}\,, \tag{3}$$

where

$$S_-^{n,m}(\alpha) = \sum_{l_1\cdots l_m;k_1\cdots k_n} \alpha_{l_1\cdots l_m;k_1\cdots k_n} \prod_j c_{l_j\downarrow}^\dagger \prod_j c_{k_j\uparrow}\,. \tag{4}$$

$\alpha_{l_1\cdots l_m;k_1\cdots k_n}$ are antisymmetric in the first m and in the last n indices. ψ should be a state with spin $S = S_z = N_e/2 - m$. This is the case if $S + \psi = 0$ where $S+ = \sum_k c_{k\uparrow}^\dagger c_{k\downarrow}$, which yields $\sum_k \alpha_{k,l_2\cdots l_m;k,k_2\cdots k_n} = 0$. Since the Hamiltonian is translationally invariant, the eigenstates of H are also eigenstates of the momentum operator. Let ψ be a state with momentum p. This means that $\alpha_{l_1\cdots l_m;k_1\cdots k_n}$ vanishes if $\sum_{j=1}^m l_j - \sum_{j=1}^n k_j \neq p$. Since ψ is a ground state of the kinetic energy, $\alpha_{l_1\cdots l_m;k_1\cdots k_n}$ has to vanish if some indices l_j are not in $\mathcal{L}$. Furthermore, I let $\alpha_{l_1\cdots l_m;k_1\cdots k_n} = 0$ if some indices k_j are not in $\mathcal{L}$. ψ is a ground state of the interaction if and only if $\sum_k c_{k+\delta\uparrow} c_{-k\downarrow}\psi = 0$ for all δ. This yields a condition for α, namely

$$\sum_{P\in S_{n+1}} (-1)^P \alpha_{l_1\cdots l_{m-1},-k_{P(n+1)}+\delta;k_{P(1)}\cdots k_{P(n)}} = 0\,, \tag{5}$$

for all k_j, l_j, δ. S_{n+1} is the group of all permutations P of $n + 1$ objects and $(-1)^P$ denotes the sign of the permutation P; $(-1)^P = 1$ if P is even and -1 if P is odd. I let $\delta = \sum_{j=1}^{n+1} k_j - \sum_{j=1}^{m-1} l_j + p$, since otherwise (5) is trivial. Using the fact that α is antisymmetric in the last n indices, one can rewrite (5) in the form

$$\sum_{i=1}^{n+1} (-1)^{n(i-1)} \alpha_{l_1\cdots l_{m-1},p+\sum_{j=1}^{n+1} k_j - \sum_{j=1}^{m-1} l_j - k_i;k_{i+1}\cdots k_{n+1},k_1\cdots k_{i-1}} = 0\,. \tag{6}$$

The sum runs now over all cyclic permutations of the indices k_j. I define

$$\tilde{\alpha}_{l_2\cdots l_m;k_2\cdots k_n} = \sum_{k_1} \alpha_{k_1+\tilde{p},l_2\cdots l_m;k_1\cdots k_n}\,, \tag{7}$$

where $\tilde{p} \neq 0$ is chosen such that $\tilde{\alpha}$ is not identically zero. This is possible since for some $k \in \mathcal{L}$, $k + \tilde{p}$ is also in $\mathcal{L}$ and since α is not identically zero [13]. I put $l_1 = k_1 + \tilde{p}$ in (6) and sum over k_1. Using the definition of $\tilde{\alpha}$ and the antisymmetry of α in the last n indices, one obtains

$$\sum_{k_1} \alpha_{k_1,l_2\cdots l_{m-1},p+\sum_{j=2}^{n+1} k_j - \sum_{j=2}^{m-1} l_j - k_1;k_2\cdots k_{n+1}} - \sum_{i=2}^{n+1} (-1)^{(n-1)(i-2)} \tilde{\alpha}_{l_2\cdots l_{m-1},p-\tilde{p}+\sum_{j=2}^{n+1} k_j - \sum_{j=2}^{m-1} l_j - k_i;k_{i+1}\cdots k_{n+1},k_2\cdots k_{i-1}} = 0\,. \tag{8}$$

The first term in this equation vanishes. The reason is that for each k_1 there is a term in the sum over k_1 with k_1 replaced by $p + \sum_{j=2}^{n+1} k_j - \sum_{j=2}^{n-1} l_j - k_1$. Because of the antisymmetry of α in the first m indices, these two terms are equal up to a different sign and annihilate each other. This yields

$$\sum_{i=2}^{n+1} (-1)^{(n-1)(i-2)} \tilde{\alpha}_{l_2\cdots l_{m-1},p-\tilde{p}+\sum_{j=2}^{n+1} k_j - \sum_{j=2}^{m-1} l_j - k_i;k_{i+1}\cdots k_{n+1},k_2\cdots k_{i-1}} = 0\,, \tag{9}$$

which is the same condition as (9) for $\tilde{\alpha}$ instead of α. Consequently, $\tilde{\psi} = S_-^{n-1,m-1}(\tilde{\alpha})\psi_{0F}$ is also a ground state of H. This shows that if H has a ground state with $N_e = N_d - n + m$ electrons ($n \geq m$) and a spin $S = S_z = N_e/2 - m$, it has also a ground state with the same number of electrons and a spin $S = S_z = N_e/2 - m + 1$. One can now iterate this procedure to obtain finally a single spin-flip state with a spin $S = S_z = N_e/2 - 1$:

Theorem.—In a single-band Hubbard model with a N_d-fold degenerate single particle ground state and

$N_e \leq N_d$ electrons local stability of ferromagnetism implies global stability. The model has only ferromagnetic ground states with a spin $S = N_e/2$, if there are no ground states with a single spin flip, i.e., with a spin $S = N_e/2 - 1$.

Remarks.—(i) The existence of single spin-flip ground states is relatively easy if $N_e = N_d$. A general single spin-flip state with momentum p is given by

$$\psi = \sum_k \alpha_{k+p,k} c^{\dagger}_{k+p\downarrow} c_{k\uparrow} \psi_{0F} . \quad (10)$$

This state has a spin $S = N_e/2 - 1$ if $p \neq 0$. The condition (5) shows that this state is a ground state if and only if $\alpha_{k+p,k} = \alpha_{k'+p,k'}$ for all $k, k' \in \mathcal{L}$. Therefore, it is possible to construct a single spin-flip ground state with momentum p if and only if $\epsilon_{k+p} = 0$ for all k with $\epsilon_k = 0$. In that situation, the single particle density matrix in [14] is reducible. Thus, for $N_e = N_d$ our result is as well a consequence of the result in [14], but due to translational invariance, the condition for the occurrence of ferromagnetism is much simpler. For $N_e < N_d$ it is not possible to obtain a similar (simple) condition for the existence of a single spin-flip ground state.

(ii) Let us consider a situation where the degenerate single particle energy lies at the upper band edge of the single band, and let $N_e \geq 2N_s - N_d$. In this case the model has ferromagnetic ground states with a spin $S = (2N_s - N_e)/2$. Performing a particle-hole transformation one obtains a model that fulfills the conditions of the above theorem. Thus local stability of ferromagnetism implies global stability in this case as well.

(iii) In the above derivation, one uses the fact that the Hamiltonian is translationally invariant. This is a natural assumption. But it is also possible to investigate a more general case. As for $N_e = N_d$ in [14], the proof is much more complicated and less intuitive [15].

(iv) The result is true for any $U > 0$. U may be arbitrarily small. Therefore one may wonder whether this model corresponds to a strong coupling situation. This is indeed the case. The relevant dimensionless parameter is $\rho_F U$. It is infinite in our model for any $U > 0$, since the Fermi level lies in the region where the band is flat. A partially flat band is certainly an unrealistic situation. Typically, this assumption has the consequence that the hopping matrix elements $t_{xy} = N_s^{-1} \sum_k \epsilon_k \exp[ik(x - y)]$ have a longer range than usual. On the other hand, one may hope that as in the flat band case [9] our result extends to a nearly flat case as long as U is not too small. This would be a realistic situation in transition metals.

(v) In most cases it is much simpler to study the stability of the ferromagnetic state with respect to single spin flips than the global stability. In the case of a Hubbard model with a nearly flat band, Tasaki [9] was able to show the stability with respect to single spin flips. In most variational treatments single spin-flip states are used as well [5]. The variational studies of the stability of the Nagaoka state [4,5] are complicated and the general single spin-flip problem is too difficult to be solved completely on usual lattices in $1 < d < \infty$ dimensions. In our case the situation is simpler since we already know that there are ferromagnetic ground states. The aim is only to show under which conditions there are other ground states. If there are further ground states, one should expect that small perturbations are sufficient to destroy ferromagnetism. This would be an instable situation. If there are no other ground states, it is possible that ferromagnetism is stable with respect to small perturbations of the Hamiltonian. But it is difficult to investigate this problem since in the present model there is no gap in the single particle spectrum. This is the main technical difference to the models discussed in [9].

(vi) As in [14] one can generalize the above result to a situation, where the degenerate single particle states are not at the bottom of the band. I assume again that the N_d-fold degenerate single particle state has energy 0 and that $\mathcal{L}$ is the subset of k with $\epsilon_k = 0$. Let $\mathcal{L}_<$ be the subset of k with $\epsilon_k < 0$ and let $N_<$ be the number of elements of $\mathcal{L}_<$. For $U = 0$ and $N_e \leq 2N_< + N_d$ the ground states are highly degenerate: Each single particle state with $k \in \mathcal{L}_<$ contains two electrons and the remaining $N_e - 2N_<$ electrons can be distributed arbitrarily among the states with zero energy. If U is small one can apply degenerate perturbation theory. This means that among these degenerate states one has to find those with a minimal interaction energy. Since the system is translationally invariant the contribution from the single particle states with $k \in \mathcal{L}_<$ is the same for all the degenerate multiparticle states. It is therefore sufficient to minimize the interaction energy of the electrons in single particle states with $k \in \mathcal{L}$. This is equivalent to the above situation, where $\epsilon_k = 0$ was the bottom of the band. If the degeneracy is lifted at first order in U, the ground state is ferromagnetic with a spin $S = (N_e - 2N_<)/2$. Depending on N_e, the spin varies between 0 and $N_d/2$ and may be extensive if N_d is extensive. If the degeneracy is not lifted at first order, another ground state with a smaller spin is usually favored at higher order in U. This argument explains, e.g., the results presented in [16]. But this argument is perturbative and holds only for (very) small U. Is it possible that this ferromagnetism disappears when U becomes larger? At the moment I am not able to answer this question. But if the following conjecture is true, the ferromagnetism is stable for any finite U.

Conjecture.—Let E_{0S} be the smallest eigenenergy of H in the subspace of eigenstates with a spin S. Suppose that for some $U = U_0$ the Hamiltonian has a degenerate ground state with a ground state energy $E_{0S_1} = E_{0S_2}$ and $S_1 \neq S_2$. Then I claim that $E_{0S_1} \leq E_{0S_2}$ for $U > U_0$ if $S_1 > S_2$.

It is sufficient to prove this conjecture for $N_e \leq N_s$, since the result for larger electron numbers can be obtained using a particle-hole transformation. I am not aware of any (rigorous) result for the Hubbard model that is in contradiction to this conjecture. The physical intuition behind it is simply that if for some value U_0 of the interaction a degeneracy occurs, one should expect that the state with a higher spin should have a larger kinetic energy and a smaller interaction energy, so that for higher values of U the higher spin is favored. As far as I know there is no proof for this conjecture. The conjecture is trivial if $S_1 = N_e/2$, since the energy of a state with maximal spin (and $N_e \leq N_s$) does not depend on U, whereas any other eigenenergy is a monotonously increasing function of U.

Let us note that this route to ferromagnetism in single-band Hubbard models naturally leads to nonsaturated ferromagnetic states if the degeneracy is not situated at a band edge. This is similar to Lieb's ferrimagnetism [7]. It is even possible that a single-band Hubbard model on a bipartite lattice has a degeneracy somewhere in the (symmetric) band. But if this degeneracy occurs in the middle of the band Lieb's theorem tells us that the ground state has $S = 0$. This is not a contradiction to the above result. In such a special situation one can easily see that p exists such that for each $k \in \mathcal{L}$, $k + p$ is as well in $\mathcal{L}$. Therefore, as shown in the first remark, the degeneracy is not lifted within a first order perturbational treatment and a second order perturbational treatment favors the singlet state, as predicted by Lieb's theorem. The most simple bipartite lattice, where this situation occurs, is a bipartite lattice where $t_{xy} = t$ if x and y belong to different sublattices and $t = 0$ otherwise. Such a lattice is called a complete bipartite graph.

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[1] J. Hubbard, Proc. R. Soc. London A **276**, 238 (1963).
[2] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).
[3] Y. Nagaoka, Phys. Rev. **147**, 392 (1966); a very general proof is given by H. Tasaki, Phys. Rev. B **40**, 9192 (1989).
[4] A. Sütő, Commun. Math. Phys. **140**, 43 (1991).
[5] T. Hanisch, G. S. Uhrig, and E. Müller-Hartmann, Phys. Rev. B **56**, 13 960 (1997), and references therein.
[6] A special case is the one-dimensional Hubbard model, for which ferromagnetism is unstable in the whole parameter space.
[7] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).
[8] A. Mielke, J. Phys. A **24**, L73 (1991); **24**, 3311 (1991); **25**, 4335 (1991); H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992); A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).
[9] H. Tasaki, J. Stat. Phys. **84**, 535 (1996).
[10] J. Wahle, N. Blümer, J. Schlipf, K. Held, and D. Vollhardt, Phys. Rev. B **58**, 12 749 (1998), and references therein.
[11] K. Held and D. Vollhardt, Eur. Phys. J. B **5**, 473 (1998); K. Kubo, D. M. Edwards, A. C. M. Green, T. Momoi, and H. Sakamoto, cond-mat/9811286 (1998); and references therein.
[12] A. Mielke, J. Phys. A **25**, 6507 (1992).
[13] The existence of $\tilde{\alpha}$ can be shown as follows: Define $\tilde{\psi}_{\tilde{p}} = S_-^{n-1,m-1}(\tilde{\alpha})$ and calculate $\sum_{\tilde{p}} \|\tilde{\psi}_{\tilde{p}}\|^2$. This quantity can be shown to be positive, so that at least for some $\tilde{p}$ one has a nontrivial $\tilde{\alpha}$.
[14] A. Mielke, Phys. Lett. A **174**, 443–448 (1993).
[15] A. Mielke (to be published).
[16] K. Kusakabe and H. Aoki, J. Phys. Soc. Jpn. **61**, 1165 (1992).