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Stability of ferromagnetism in Hubbard models with degenerate single-particle ground states

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Abstract. A Hubbard model with a $N_{\rm d}$-fold degenerate single-particle ground state has ferromagnetic ground states if the number of electrons is less than or equal to $N_{\rm d}$. It is shown rigorously that the local stability of ferromagnetism in such a model implies global stability: the model has only ferromagnetic ground states, if there are no single spin–flip ground states. If the number of electrons is equal to $N_{\rm d}$, it is well known that the ferromagnetic ground state is unique if and only if the single-particle density matrix is irreducible. We present a simplified proof for this result.

1. Introduction

The problem of ferromagnetism in itinerant electron systems has a long history. It is clear that ferromagnetism (as for any other ordering in itinerant electron systems) occurs due to the interaction of the electrons, or, to be more precise, due to a subtle interplay between the kinetic motion of the electrons and the interaction. In 1963, Hubbard [1], Kanamori [2] and Gutzwiller [3] formulated and studied a simple tight-binding model of electrons with an on-site Coulomb repulsion of strength U. This model is usually called the Hubbard model. Although the assumption, that a realistic system can be described by a purely local repulsion of the electrons is artificial, the Hubbard model became a paradigm for the study of correlated electron systems. The reason is that already a pure on-site interaction can produce many ordering effects that have been observed in electronic systems. The mechanisms that are responsible for some long-range order in the ground state of the Hubbard model are probably also responsible for long-range order in more complicated (and more realistic) models. From a theoretical point of view the Hubbard model is very interesting, because it offers the possibility to derive ordering phenomena in a simple model that does not contain special interactions favouring this order.

In this paper we present a result on ferromagnetism in the Hubbard model. This is an old problem, which has been studied extensively using various approximative methods. The simplest approach is the Hartree–Fock approximation. It yields the Stoner criterion $U\rho_{\rm F} > 1$ for the occurrence of ferromagnetism in the Hubbard model. $\rho_{\rm F}$ is the density of states at the Fermi energy. It is well known that this criterion overestimates the occurrence of ferromagnetism. There are situations where $\rho_{\rm F}U$ is infinite and the ground state of the Hubbard model is not ferromagnetic. Ferromagnetism is not a universal property of the Hubbard model. As far as we know it occurs on special lattices and in special regions of the parameter space.

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In the discussion of ferromagnetism in correlated electron systems, more realistic models with, for example, an additional ferromagnetic interaction between the electrons [4] or a Hund's coupling between several bands in a multi-band system [5] have also been discussed. It is clear that in a realistic description of itinerant ferromagnetism such additional interactions are present and may favour the occurrence of ferromagnetism. However, it is a challenging problem to derive conditions for the occurrence of ferromagnetism in a Hubbard model, which does not explicitly contain such interactions. The hope is that results for this model will yield an important contribution to the understanding of ferromagnetism in more realistic models.

The first rigorous results on ferromagnetism in the Hubbard model is the so-called theorem of Nagaoka [6]. On a large class of lattices, the Hubbard model has a ferromagnetic ground state if the Coulomb repulsion is infinite and if there is one electron less than lattice sites. A very general proof of this theorem has been given by Tasaki [7].

A second class of systems, for which the existence of ferromagnetic ground states has been shown rigorously, are the so-called flat-band models. In 1989, Lieb [8] proved an important theorem on the Hubbard model: at half filling and on a bipartite lattice (one electron per lattice site) the ground state of the Hubbard model is unique up to the usual spin degeneracy. The spin of the ground state is given by $S = \frac{1}{2}||A| - |B||$, where $|A|$ and $|B|$ are the numbers of lattice sites of the two sublattices of the bipartite lattice. When this quantity is extensive, the system is ferromagnetic. In that case, the model has strongly degenerate single-particle eigenstates at the Fermi level, ρ_F is infinite. For a Hubbard model on a translationally invariant lattice such a model has several bands, one of which is flat. Later, it was shown that a multiband Hubbard model for which the lowest band is flat shows ferromagnetism [9–14]. These lattices are not bipartite, generally they contain triangles or next-nearest-neighbour hoppings. A typical example is the Hubbard model on the kagomé lattice [11].

There are several extensions of the flat-band ferromagnetism. The most important result has been derived by Tasaki [15]. He discussed the question of whether the flat-band ferromagnet is stable with respect to small perturbations. He showed under very general assumptions that for a class of multi-band Hubbard models with a nearly flat lowest band the ferromagnetic state is stable with respect to single spin–flips if the Coulomb repulsion U is sufficiently large and if the nearly flat band is half filled. This local stability of the ferromagnetic state suggests its global stability. The class of models, for which Tasaki was able to prove this important result consists of models, for which the nearly flat, lowest band is separated from the rest of the spectrum by a sufficiently large gap. Therefore, one would expect that these models describe an insulating ferromagnet. This a general problem for the flat-band ferromagnetism as well. The flat-band models show ferromagnetism if the flat band is half filled or less than half filled. Even if the flat band is less than half filled, or if the model has no gap between the flat band the other bands (this is the case for the kagomé lattice), the system may be an insulator. The reason is that for an entire flat band, the system can be described by localized states as well. Furthermore, the existence of a basis of localized states was an essential part of the proofs.

Another extension of the flat-band ferromagnetism are models with a partially flat band. In [13] a general necessary and sufficient condition for the uniqueness of ferromagnetic ground states has been derived for a model with a degenerate single-particle ground state. This result holds only if the number of electrons is equal to the number of degenerate single-particle ground states. However, it does not require a gap in the spectrum or an entirely flat band. A partially flat band is sufficient. A Hubbard model with a single band far away from half filling is expected to be a conductor. This remains true if the band is partially flat. Therefore, these models may describe a metallic ferromagnet. A generalization of this result to a situation where the number of electrons is less than the number of single-particle states has recently been published [16]. The main result of that letter is that in a single-band Hubbard model with a degenerate single partial ground state local stability of ferromagnetism implies global stability, if the number of electrons is less than or equal to the number of degenerate single-particle ground states. Stability is meant here in the sense of absolute stability: the ferromagnetic ground state is the only ground state of the system.

That local stability of ferromagnetism implies global stability has often been assumed but is by no means guaranteed. It would be certainly useful to know, in which situations this is the case. The aim of the present paper is to generalize the result into a general Hubbard model with degenerate single-particle ground states. It is not necessary to have a single-band model. It is even not necessary to have translational invariance, although this would be a natural assumption.

Let us mention that Hubbard models with a partially flat band are not only an academic toy model. Very recently Arita *et al* [17] used such a model to explain the negative magnetoresistance of certain organic conductors. They mention that standard band-structure calculations for these materials yield a partially flat band.

This paper is organized as follows. The next section contains the main definitions and results. The proof of the result combines the ingredients of the proofs in [13] and [16]. The main part of the proof is the choice of a suitable basis. This choice is discussed in section 3. Section 4 contains a new proof of the result in [13]. The proof in [13] used an induction in the number of degenerate single-particle states and was not intuitive at all. On the other hand, the basic idea as to why the condition in [13] should be true is simple. The new proof is based on this basic idea and is much easier. Furthermore, it can be generalized to situations where the number of electrons is less than the number of degenerate single-particle states. This generalization is presented in section 5.

2. Main result

We consider a Hubbard model on a finite lattice with N_s sites. The Hamiltonian is

$$H = H_\mathrm{hop} + H_\mathrm{int} \tag{1}$$

where

$$H_\mathrm{hop} = \sum_{x,y,\sigma} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} \tag{2}$$

and

$$H_\mathrm{int} = \sum_x U_x n_{x\uparrow} n_{x\downarrow} \tag{3}$$

where x and y are lattice sites. As usual $c^\dagger_{x\sigma}$ and $c_{x\sigma}$ are the creation and the annihilation operators of an electron on site x with spin $\sigma = \uparrow, \downarrow$. They satisfy the anticommutation relations $\left[c_{x\sigma}, c^\dagger_{y\tau}\right]_+ = \delta_{xy}\delta_{\sigma\tau}$, and $[c_{x\sigma}, c_{y\tau}]_+ = \left[c^\dagger_{x\sigma}, c^\dagger_{y\tau}\right]_+ = 0$. The number operator is defined as $n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}$. The hopping matrix $T = (t_{xy})$ is real symmetric and the on-site Coulomb repulsion U_x is positive. We do not need to assume any kind of translational symmetry, therefore the lattice is simply a collection of sites. We allow the local Coulomb repulsion to depend on x. The total number of electrons is $N_\mathrm{e} = \sum_{x\in\Lambda}(n_{x\uparrow} + n_{x\downarrow})$.

The Hubbard model has an $SU(2)$ spin symmetry, it commutes with the spin operators

$$\vec{S} = \sum_x \sum_{\sigma,\tau=\uparrow,\downarrow} c^\dagger_{x\sigma} (\vec{p})_{\sigma\tau} c_{x\tau}/2 \tag{4}$$

where $\vec{p}$ is the vector of Pauli matrices,

$$p_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad p_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad p_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5}$$

We denote by $S(S+1)$ the eigenvalue of $\vec{S}^2$.

The eigenstates of the hopping matrix T are φ^i, the corresponding eigenvalues are ϵ_i, $i = 1, \ldots, N_\mathrm{s}$. Let $\epsilon_i \leqslant \epsilon_j$ for $i < j$. In the following we will discuss a Hubbard model with N_d degenerate single-particle ground states. The energy scale is chosen such that $\epsilon_i = 0$ for $i \leqslant N_\mathrm{d}$.

The main result of the present paper can now be formulated.

Theorem. *In a Hubbard model with N_d degenerate single-particle ground states and $N_\mathrm{e} \leqslant N_\mathrm{d}$ electrons, local stability of ferromagnetism implies global stability: the model has only ferromagnetic ground states with a spin $S = \frac{1}{2}N_\mathrm{e}$, if and only if there are no single spin–flip ground states (ground states with a spin $S = \frac{1}{2}N_\mathrm{e} - 1$).*

This theorem is true for any positive Coulomb repulsion U_x. The existence of ferromagnetic ground states is indeed trivial. Any multi-particle state that contains only electrons with spin up in single-particle states φ^i, $i \leqslant N_\mathrm{d}$ is a ground state of the Hamiltonian. It is even a ground state of the kinetic part and of the interaction part of the Hamiltonian separately. The problem is to show that there are no further ground states. The above theorem yields a necessary and sufficient condition for the existence of non-ferromagnetic ground states.

As already mentioned in [13], one can use degenerate perturbation theory to generalize the result to a situation where the flat part of the band does not lie at the bottom of the single-particle spectrum. A concrete model, where such a situation occurs, has been investigated by Arita *et al* [18]. They investigated a special type of one-dimensional Hubbard model used for the description of atomic quantum wires. These models have a flat band that is not situated at the bottom of the spectrum.

3. Choice of the basis

The main part of the proof of the theorem is the choice of an appropriate basis. It turns out that the choice of the single-particle basis used in [13] is useful. In this section we give a detailed construction of such a basis. The starting point is the representation

$$T = \begin{pmatrix} C^\dagger T_0 C & C^\dagger T_0 \\ T_0 C & T_0 \end{pmatrix} \tag{6}$$

of the hopping matrix. Here T_0 is a positive $(N_\mathrm{s} - N_\mathrm{d}) \times (N_\mathrm{s} - N_\mathrm{d})$-matrix, rank $T_0 = N_\mathrm{s} - N_\mathrm{d}$. C is an $(N_\mathrm{s} - N_\mathrm{d}) \times N_\mathrm{d}$-matrix. This representation of T can be obtained as follows: since rank $T = N_\mathrm{s} - N_\mathrm{d}$, one can find $N_\mathrm{s} - N_\mathrm{d}$ rows (or columns) of T which are linear independent. We label the corresponding sites by $x = N_\mathrm{d} + 1, \ldots, N_\mathrm{s}$. T_0 is the submatrix $(t_{xy})_{x,y \in \{N_\mathrm{d}+1,\ldots,N_\mathrm{s}\}}$. Since T is non-negative, T_0 is positive. The matrix C is given by $(T_0)^{-1} T_{01}$ where $T_{01} = (t_{xy})_{x \in \{N_\mathrm{d}+1,\ldots,N_\mathrm{s}\}, y \in \{1,\ldots,N_\mathrm{d}\}}$. The other matrix elements of T are fixed, since T is symmetric and since the other rows of T are linear dependent.

By construction, the single-particle ground states obey $T\psi = 0$. This holds if and only if

$$\psi = \begin{pmatrix} \bar{\psi} \\ -C\bar{\psi} \end{pmatrix}. \tag{7}$$

A basis of single-particle ground states can be obtained by choosing an arbitrary set of N_d linear independent vectors $\bar{\psi}$. We choose the basis $\mathcal{B} = \{\psi_i : \bar{\psi}_i(x) = \delta_{x,i}\}$. Since t_{xy}

are real, $\psi_i(x)$ are real. This basis is not orthonormal. The matrix $B = (b_{ij})_{i,j=1,\ldots,N_{\rm d}}$ with $b_{ij} = \sum_x \psi_i(x)\,\psi_j(x)$ is positive and the dual basis is formed by $\psi_i^d(x) = \sum_j (B^{-1})_{ij}\psi_j(x)$. One has $\sum_x \psi_i^d(x)\,\psi_j(x) = \delta_{i,j}$. We introduce creation operators for electrons in the state $\psi_i(x)$,

$$a_{i\sigma}^\dagger = \sum_x \psi_i(x)\, c_x^\dagger \tag{8}$$

and the corresponding dual operators

$$a_{i\sigma} = \sum_x \psi_i^d(x)\, c_x^\dagger. \tag{9}$$

They obey the commutation relations $[a_{i\sigma}, a_{j\tau}^\dagger] = \delta_{i,j}\delta_{\sigma,\tau}$. These creation and annihilation operators can now be used to construct multi-particle states. The unique ferromagnetic ground state with $N_{\rm e} = N_{\rm d}$ electrons and $S = S_3 = N_{\rm d}/2$ is

$$\psi_{0\rm F} = \prod_i a_{i\uparrow}^\dagger |0\rangle. \tag{10}$$

A general ground state of the kinetic part of the Hamiltonian is given by

$$\psi^{n,m}(\alpha) = S_-^{n,m}(\alpha)\,\psi_{0\rm F} \tag{11}$$

where

$$S_-^{n,m}(\alpha) = \sum_{j_1\ldots j_m;i_1\ldots i_n} \alpha_{j_1\ldots j_m;i_1\ldots i_n} \prod_k a_{j_k\downarrow}^\dagger \prod_k a_{i_k\uparrow}. \tag{12}$$

This state has $N_{\rm e} = N_{\rm d} - n + m$ electrons. In the following I assume that $N_{\rm e} \leqslant N_{\rm d}$, i.e. $m \leqslant n$. $\psi^{n,m}(\alpha)$ is a state with $S_3 = (N_{\rm d} - n - m)/2 = N_{\rm e}/2 - m$. It obeys $S_+\psi^{n,m}(\alpha) = 0$ if and only if

$$\sum_k \alpha_{k,j_1\ldots j_{m-1};k,i_1\ldots i_{n-1}} = 0. \tag{13}$$

In that case it is a state with a spin $S = S_3$. We want to derive a condition for $\psi^{n,m}(\alpha)$ to be a ground state of the Hamiltonian. A necessary and sufficient condition is

$$c_{x\uparrow}c_{x\downarrow}\psi^{n,m}(\alpha) = 0 \tag{14}$$

for all x. For $x \leqslant N_{\rm d}$ one obtains $a_{i\uparrow}a_{i\downarrow}\psi^{n,m}(\alpha) = 0$. Therefore, $\alpha_{j_1\ldots j_m;i_1\ldots i_n} = 0$ if $\{j_1 \ldots j_m\}$ is not a subset of $\{i_1 \ldots i_n\}$. It turns out that this fact is important since it simplifies the proof substantially.

4. The case $N_{\rm e} = N_{\rm d}$

This case has already been discussed in [13]. In the following we obtain a simplified proof of the result in [13]. Let us first discuss the stability with respect to single spin–flips. A ferromagnetic ground state is called stable with respect to a single spin–flip, if there is no single spin–flip state with the same energy. I derive a necessary and sufficient condition for $\psi_{0\rm F}$ to be stable with respect to a single spin–flip. A general state with a single spin–flip can be written in the form

$$\psi = \sum_{j,k} \alpha_{j;k} c_{j\downarrow}^\dagger c_{k\uparrow}\psi_{0\rm F}. \tag{15}$$

If and only if $\alpha_{j;k} \propto \delta_{j,k}$, is ψ the unique ferromagnetic ground state with $S = N_{\mathrm{d}}/2$, $S_z = N_{\mathrm{d}}/2 - 1$. If and only if $\sum_j \alpha_{j;j} = 0$, is ψ a state with $S = S_z = N_{\mathrm{d}}/2 - 1$. Therefore, I assume $\sum_j \alpha_{j;j} = 0$. ψ is a ground state if and only if $c_{x\uparrow} c_{x\downarrow} \psi = 0$,

$$c_{x\uparrow} c_{x\downarrow} \psi = \sum_{j,k,l} \alpha_{j;k}\, \psi_j(x)\, \psi_l(x)\, c_{l\uparrow} c_{k\uparrow} \psi_{0\mathrm{F}}. \tag{16}$$

The right-hand side vanishes if and only if

$$\sum_j \psi_j(x)(\alpha_{j;k}\, \psi_l(x) - \alpha_{j;l}\, \psi_k(x)) = 0 \qquad \forall\, k, l. \tag{17}$$

I introduce

$$\tilde{\psi}_k(x) = \sum_j \alpha_{j;k}\, \psi_j(x). \tag{18}$$

The condition for $\alpha_{j,k}$ yields

$$\tilde{\psi}_k(x)\, \psi_l(x) - \tilde{\psi}_l(x)\, \psi_k(x) = 0 \qquad \forall\, k, l, x. \tag{19}$$

A trivial solution is $\tilde{\psi}_k(x) = \psi_k(x)$. It corresponds to $\alpha_{j,k} \propto \delta_{j,k}$ and has been excluded above. Multiplying the condition for $\tilde{\psi}_k(x)$ by $\psi_l^d(y)\, \psi_k^d(z)$ and summing over k and l yields

$$\tilde{\rho}_{y,x} \rho_{x,z} - \rho_{y,x} \tilde{\rho}_{x,z} = 0 \tag{20}$$

where $\rho_{y,x} = \sum_j \psi_j(x)\, \psi_j^d(y)$, $\tilde{\rho}_{y,x} = \sum_j \tilde{\psi}_j(x)\, \psi_j^d(y)$. If the matrix $\rho_{x,y}$ is irreducible, the only solution is $\tilde{\rho}_{y,x} = \rho_{y,x}$. It corresponds to $\alpha_{j,k} \propto \delta_{j,k}$ and has been excluded above. If the matrix $\rho_{x,y}$ is reducible, the equation for $\tilde{\rho}_{y,x}$ has another non-trivial solution. From the non-trivial solution for $\tilde{\rho}_{y,x}$ one obtains a solution for $\alpha_{j,k}$ from which one can easily construct a solution with $\sum_j \alpha_{j,j} = 0$. Thus $\psi_{0\mathrm{F}}$ is stable with respect to a single spin–flip if and only if $\rho_{x,y}$ is irreducible. This is the condition derived previously in [13]. To derive this condition, it was not necessary to use the special single-particle basis introduced in section 3. The use of this basis is useful for the investigation of multi-spin–flip states.

Let us now consider a multi-spin–flip state $\psi^{n,m}(\alpha)$. It is a ground state if and only if

$$\sum_P (-1)^P \sum_{j_1} \psi_{j_1}(x)\, \psi_{k_{P(n+1)}} \alpha_{j_1 \ldots j_n; k_{P(1)} \ldots k_{P(n)}} = 0. \tag{21}$$

Since $\alpha_{j_1 \ldots j_n; i_1 \ldots i_n}$ is antisymmetric in the last n indices, it is sufficient to sum over all cyclic permutations.

$$\sum_{r=1}^{n+1} (-1)^{nr} \sum_{j_1} \psi_{j_1}(x)\, \psi_{k_r}(x)\, \alpha_{j_1 \ldots j_n; k_{r+1} \ldots k_{n+1}, k_1 \ldots k_{r-1}} = 0. \tag{22}$$

Since $\alpha_{j_1 \ldots j_n; i_1 \ldots i_n} \neq 0$ only if $\{j_1 \ldots j_n\} = \{i_1 \ldots i_n\}$, we obtain for $n = 1$ (the single spin–flip case)

$$\psi_k(x)\, \psi_{k'}(x)(\alpha_{k;k} - \alpha_{k';k'}) = 0. \tag{23}$$

With $\tilde{\psi}_k(x) = \alpha_{k,k}\, \psi_k(x)$ this yields the original condition (19). This means that with this choice of the basis, the functions $\tilde{\psi}_k(x)$ are either equal to $\psi_k(x)$ or vanish. A solution exists, if the set $\{\psi_k(x), k = 1 \ldots N_{\mathrm{d}}\}$ decays in two subsets such that $\psi_k(x)\, \psi_{k'}(x) = 0$ if the two factors are out of different subsets. This is equivalent to the above condition on the single-particle density matrix $\rho_{x,y}$. For $n > 1$ we now use the fact that the set $\{j_1, \ldots, j_n\}$ is a subset of $\{k_1, \ldots, k_{n+1}\}$. I choose $j_2 = k_1$, $j_3 = k_2$, etc in (22). With this choice only the terms with

$r \geqslant n$ in the sum over r do not vanish. For $r = n$ the only non-vanishing contribution in the sum over j_1 is $j_1 = k_{n+1}$. For $r = n + 1$ one has $j_1 = k_n$. This finally yields

$$\psi_{k_n}(x)\,\psi_{k_{n+1}}(x)(\alpha_{k_1\ldots k_n;k_1\ldots k_n} - \alpha_{k_{n+1}k_1\ldots k_{n-1};k_{n+1}k_1\ldots k_{n-1}}) = 0. \tag{24}$$

For some fixed $k_1, \ldots k_{n-1}$ I let $\alpha_{k;k} = \alpha_{kk_1\ldots k_{n-1};kk_1\ldots k_{n-1}}$. The indices $k_1 \ldots k_{n-1}$ are chosen such that $\alpha_{k;k}$ does not vanish identically, which is possible since $\alpha_{j_1\ldots j_n;i_1\ldots i_n}$ does not vanish identically. This shows that the existence of a multi-spin–flip ground state implies the existence of a single spin–flip ground states. Therefore, the ferromagnetic ground state of the Hubbard model with $N_\mathrm{e} = N_\mathrm{d}$ electrons is the unique ground state (up to the spin degeneracy due to the $SU(2)$ symmetry) if and only if ρ_{xy} is irreducible.

5. The case $N_\mathrm{e} < N_\mathrm{d}$

It is now very easy to generalize the second part of the above derivation to the case $N_\mathrm{e} < N_\mathrm{d}$. We will show that the existence of a multi-spin–flip ground state implies the existence of a single spin–flip ground state. Let $\psi^{1,n}(\alpha)$, $n > 1$ be a single spin–flip ground state for $N_\mathrm{e} = N_\mathrm{d} - n + 1$ electrons. The condition, that this is a ground state, yields

$$\sum_{r=1}^{n+1}(-1)^{nr} \sum_{j_1\in\{k_1,\ldots k_{n+1}\}\setminus\{k_r\}} \psi_{j_1}(x)\,\psi_{k_r}(x)\,\alpha_{j_1;k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}} = 0. \tag{25}$$

The sum over j_1 is restricted to the set $\{k_1, \ldots k_{n+1}\} \setminus \{k_r\}$ since otherwise $\alpha_{j_1;k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}}$ vanishes. The similar condition for a multi-spin–flip ground state $\psi^{m,n+m-1}(\alpha)$ is

$$\sum_{r=1}^{n+m}(-1)^{(n+m-1)r} \sum_{j_1\in\{k_1,\ldots k_{n+m}\}\setminus\{k_r,j_2\ldots j_m\}} \psi_{j_1}(x)\,\psi_{k_r}(x)\,\alpha_{j_1\ldots j_m;k_{r+1}\ldots k_{n+m}k_1\ldots k_{r-1}} = 0. \tag{26}$$

I let $j_r = k_{n+r}$, $r \geqslant 2$. Then the sum over r runs from 1 to $n + 1$ and the sum over j_1 runs over all elements of $\{k_1 \ldots k_{n+1}\} \setminus \{k_r\}$, all other terms vanish identically. One obtains

$$\sum_{r=1}^{n+1}(-1)^{nr} \sum_{j_1\in\{k_1,\ldots k_{n+1}\}\setminus\{k_r\}} \psi_{j_1}(x)\,\psi_{k_r}(x)\,\alpha_{j_1k_{n+2}\ldots k_{n+m};k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}k_{n+2}\ldots k_{n+m}} = 0. \tag{27}$$

Therefore, we can choose $\tilde\alpha_{j_1;k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}} = \alpha_{j_1k_{n+2}\ldots k_{n+m};k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}k_{n+2}\ldots k_{n+m}}$ for some fixed $k_{n+2}, \ldots k_{n+m}$, such that $\tilde\alpha_{j_1;k_{r+1}\ldots k_{n+1}k_1\ldots k_{r-1}}$does not vanish identically. This is possible since $\alpha_{j_1\ldots j_m;k_1\ldots k_n}$ does not vanish identically. The corresponding single spin–flip state $\psi^{1,n}(\tilde\alpha)$ is thus a ground state for $N_\mathrm{e} = N_\mathrm{d} - n + 1$ electrons.

The proof presented here is considerably simpler than the proof in [13]. Compared to the proof in [16] it has the advantage that the existence of the single-spin–flip ground state is trivial, whereas in [16] a lengthy calculation (hidden in footnote 13) was necessary to show that. On the other hand, for a translationally invariant multi-band system the basis used here is clearly artificial. However, if one uses a natural basis of Bloch states, it is very hard to construct the single spin–flip states from multi-spin–flip states.

6. Summary and outlook

In this paper it has been shown that for a general Hubbard model with degenerate single-particle ground states, local stability of ferromagnetism implies global stability of ferromagnetism. To be more precise: if there are no single spin–flip ground states, all ground states have the maximal spin. This result holds if the number of electrons is less than or equal to the number of degenerate single-particle ground states. A similar result has been proven for a single-band Hubbard model in [16] and the present result can be seen as a generalization. It holds for a Hubbard model with more than one band, it holds even if the model does not have translational invariance. Furthermore, the proof presented here is much simpler than the proof in [16].

The result is important since in many cases it is much simpler to show local stability of ferromagnetism than global stability. In [15] it has been shown that under very general conditions the flat-band ferromagnetism can be extended to situations where the lowest band is not flat but has a weak dispersion. He was able to prove that in such a situation the ferromagnetic ground state is locally stable. It would be very interesting to obtain conditions under which in that case the ferromagnetic ground state is globally stable, i.e. where it is the real ground state of the system. This is clearly a very difficult project. The present theorem does not apply since Tasaki's model does not have degenerate single-particle ground states. However, one may hope that a generalization is possible. If in a situation with degenerate single-particle ground states the ferromagnetic ground state is the only one, it is possible that ferromagnetism is stable with respect to small perturbations of the Hamiltonian. The main problem is clearly that for a general model there is no gap in the single-particle spectrum as in the models discussed by Tasaki [15].

From a physics point of view ferromagnetism for models with a partially flat band, as studied in this paper, differs from the flat-band ferromagnetism, since a flat-band ferromagnet is typically an insulator, whereas models with a partially flat band describe metals. Therefore, our new approach is a step towards the understanding of metallic ferromagnetism in the Hubbard model.

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