Two Theorems on the Hubbard Model

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In the attractive Hubbard model (and some extended versions of it), the ground state is proved to have spin angular momentum $S=0$ for every (even) electron filling. In the repulsive case, and with a bipartite lattice and a half-filled band, the ground state has $S=\frac{1}{2}\,||B|-|A||$, where $|B|$ ($|A|$) is the number of sites in the B (A) sublattice. In both cases the ground state is unique. The second theorem confirms an old, unproved conjecture in the $|B|=|A|$ case and yields, with $|B|\neq|A|$, the first provable example of itinerant-electron ferromagnetism. The theorems hold in all dimensions without even the necessity of a periodic lattice structure.

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The importance of the Hubbard model of itinerant electrons is increasingly being appreciated. Because of the model's subtlety, rigorous results and exact solutions are clearly useful bench marks, but these are rare. Two theorems about the ground states are stated and proved here. Parts of them are resolutions of old conjectures while other parts are new. In particular, the assertion that certain versions of the model show ferromagnetic behavior for the half-filled band is, I believe, new and yields the first provable example of itinerant-electron ferromagnetism with finite forces and without *ad hoc* assumptions.

After some preliminary definitions, the two theorems are stated. Each is followed by some remarks about their significance. Finally, the proofs are given. The proofs utilize a new kind of reflection positivity which does not involve the usual spatial reflections but rather reflections in spin space. In fact, spatial symmetry plays no role whatsoever and therefore the theorems apply in the widest generality to any collection of sites; all dimensions and topologies are included. The Hubbard model is not known to satisfy any kind of spatial reflection positivity or infrared bounds and this unfortunate fact has prevented the application of the usual proof techniques[1-3] for establishing the existence of long-range order in periodic lattices.

The Hubbard model on a finite lattice Λ is defined by the Hamiltonian

$$H=\sum_{\sigma}\sum_{x,y\in\Lambda}t_{xy}c_{x\sigma}^{\dagger}c_{y\sigma}+\sum_{x\in\Lambda}U_x n_{x\uparrow}n_{x\downarrow}\,, \tag{1}$$

with the following notation. The operators $c_{x\uparrow}$ and $c_{x\downarrow}$ and their adjoints $c_{x\sigma}^{\dagger}$ satisfy the usual fermion anticommutation relations $\{c_{x\sigma}^{\dagger},c_{y\tau}\}=\delta_{xy}\delta_{\sigma\tau}$ and $\{c_{x\sigma},c_{y\tau}\}=0$. The hopping matrix elements t_{xy} are required to be real and satisfy $t_{xy}=t_{yx}$, but no other *a priori* assumption is made about them (e.g., the condition $t_{xx}=0$ is not assumed, which means that an x-dependent single-particle potential $\sum_{x\sigma}t_{xx}n_{x\sigma}$ is allowed). The reality of the t_{xy}'s is consistent with their interpretation as overlap matrix elements of real operators in real, localized orbitals. The number operators are $n_{x\sigma}=c_{x\sigma}^{\dagger}c_{x\sigma}$, while U_x is the on-site energy which, for theorem 1, is allowed to depend on the site x. The word "lattice" is certainly a misnomer because no particular topology (i.e., periodicity or dimensionality) is assumed; the generality assumed here is that Λ is merely a collection of sites. The number of these sites is denoted by $|\Lambda|$. There is said to be a *bond* between sites x and y if $t_{xy}\neq0$, and Λ is said to be *connected* if there is a connected path of bonds between every pair of sites. Obviously it is no loss in generality to assume that Λ is connected, and this will always be done here. Finally, Λ is said to be *bipartite* if the sites of Λ can be divided into two disjoint sets A and B such that $t_{xy}=0$ whenever $x\in A$ and $y\in A$ or $x\in B$ and $y\in B$. The bipartite condition is really an assertion about the t_{xy}'s and not about Λ, but the terminology is conventional; it implies, in particular, that $t_{xx}=0$ for each $x\in\Lambda$. The symbols $|A|$ and $|B|$ denote the number of sites in A and B in this case, whence $|\Lambda|=|A|+|B|$. The number of electrons is denoted by N; necessarily $N\leq2|\Lambda|$.

The aim here is to study the ground state (or states if there is more than one) of H for a given N. Of central importance is the total spin S which is a conserved quantity. The spin operators are the quadratic operators

$$S^{z}=\tfrac{1}{2}\sum_{x\in\Lambda}(n_{x\uparrow}-n_{x\downarrow}),\quad S^{+}=(S^{-})^{\dagger}=\sum_{x\in\Lambda}c_{x\uparrow}^{\dagger}c_{x\downarrow}\,, \tag{2}$$

and $(S_{\rm op})^2=(S^z)^2+\frac{1}{2}S^+S^-+\frac{1}{2}S^-S^+$, with eigenvalues $S(S+1)$.

Theorem 1 (attractive case).—Assume $U_x\leq0$ for every x (but U_x is not necessarily constant) and that N is even. No extra assumption about Λ or the t_{xy}'s is made. Then (a) among the ground states of H there is one with spin $S=0$; (b) if $U_x<0$ for every x, the ground state is unique (and hence has $S=0$).

Remarks.—(1) The theorem is "obvious" if all the U_x's are very large, for then the ground state consists of paired electrons on $N/2$ sites of Λ. In the other extreme that each $U_x=0$, theorem 1 is also obvious because one just fills the lowest $N/2$ levels of the $|\Lambda|\times|\Lambda|$ Hermi-

tian hopping matrix $T=\{t_{xy}\}$.

(2) Theorem 1 can be considerably generalized to what is called an *extended Hubbard model,* and more. We can add any *real* operator M to H provided that M satisfies the following two conditions. (A real operator is polynomial in the $c_{x\sigma}$'s and $c_{x\sigma}^{\dagger}$'s with real coefficients.) (i) M commutes with the spin operators S^z and $S^{\pm}$ and conserves both spin-up and spin-down particle numbers; (ii) M can be written as $M^{\uparrow}+M^{\downarrow}-M^{\uparrow\downarrow}$. Here $M^{\uparrow}$ ($M^{\downarrow}$) is real, Hermitian, involves only spin-up (spin-down) operators, and $M^{\uparrow}$ is identical to $M^{\downarrow}$ when the spins are flipped (i.e., $c_{x\uparrow}$ and $c_{x\downarrow}$ are interchanged). The up-down interaction $M^{\uparrow\downarrow}$ can be written as a sum of terms of the form (in which μ merely denotes a summation index) $M^{\uparrow\downarrow}=\sum_{\mu}V_{\mu}^{\uparrow}(V_{\mu}^{\downarrow})^{\dagger}$ in which each V_{μ} operator is real (but not necessarily Hermitian) and involves only operators for one kind of electron. Again, $V_{\mu}^{\uparrow}$ must be the spin reflection of $V_{\mu}^{\downarrow}$ for each μ. The necessary changes in the proof are straightforward (see Ref. 4). It is also easy to extend the proof to some multiband Hubbard models; the details are left to the reader.

Theorem 2 (repulsive case).—Assume $U_x=U$ =positive constant, independent of x. Assume $|\Lambda|$ is even, Λ is bipartite (so that the t_{xy}'s couple only A and B) and $|B|\geq|A|$. No other assumption about Λ or the t_{xy}'s is made. Let $N=|\Lambda|$ (half-filled band). Then the ground state of H is unique [apart from the trivial $(2S+1)$-fold degeneracy] and has spin $S=\frac{1}{2}\times(|B|-|A|)$.

Remarks.—(3) Theorem 2 is considerably more subtle than theorem 1. The assumptions are more stringent. The theorem has long been assumed to be true in the $|B|=|A|$ case ("the half-filled band has spin zero"), but its proof has been elusive.

(4) The fact that $2S=|B|-|A|$ should be no surprise. In the limit $U=0$ we fill the levels of the matrix $T=\{t_{xy}\}$ and one might hastily conclude that S must be zero in this limit. If so, theorem 2 would be contradicted by a continuity argument with respect to U. However, the rank of T is at most $2|A|$ and so T has at least $|\Lambda|-2|A|=|B|-|A|$ zero eigenvalues. The remaining eigenvalues of T come in plus-minus pairs, so that T has at most $|A|$ negative eigenvalues. To achieve $2S=|B|-|A|$, we fill the negative levels twice with opposite spins and place the remaining electrons in the zero levels with a common spin, say, spin up. Thus the ground state is degenerate when $U=0$, but $S=\frac{1}{2}(|B|-|A|)$ is among them. Therefore, there is no contradiction with the continuity argument mentioned above. If, on the other hand, U is very large we know[5] from second-order perturbation theory that H is effectively an isotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet with Hamiltonian

$$h=(2/U)\sum_{x,y}t_{xy}^{2}(\mathbf{S}_x\cdot\mathbf{S}_y-\tfrac{1}{4}).$$

For such models it is also known[6] that the ground state is unique and has $2S=|B|-|A|$.

(5) It is easy to construct many regular, periodic lattices in every dimension greater than one with $|B|\neq|A|$. A classic (high-T_c superconductor) two-dimensional example is to start with a square lattice and then intercalate one site in the middle of each bond. The original vertices of the squares are A sites (copper) and the intercalated sites are B sites (oxygen). The half-filled band has three electrons per unit cell and theorem 2 says that then the total net magnetization is $S=\frac{1}{2}(2-1)=\frac{1}{2}$ times the number of unit cells. This was already observed for this lattice in the large-U limit by Mattis.[7]

Whether or not this example is physically realizable is less important than the fact that theorem 2 applied to a periodic lattice with $|B|>|A|$ yields, for the first time, a natural, provable example of an *itinerant-electron model of ferromagnetism.* I use the word ferromagnetism here only in the sense that the spin is extensive, i.e., it is proportional to the number of particles (or cells). Spatial ordering is not implied. A more accurate appelation might be unsaturated ferromagnetism. Still more accurately, ferromagnetism might be the right word—but technically that word implies a spatial ordering that I am not prepared to prove. In one dimension $|B|=|A|$ by definition and therefore $S=0$; this conclusion coincides with the known result[8] that S is always zero in one dimension with nearest-neighbor nonpositive hopping $t_{xy}\leq 0$ and for *any many-body potential.* There is also the example of Thouless and Nagaoka[9-11] with $N=|\Lambda|-1$, $U=\infty$, and $2S=|\Lambda|-1$, but infinite potentials are crucial for this example.

(6) Theorem 2 also has some extensions similar to some of those described in remark (2) above; hole-particle symmetry is required.

Proof of theorem 1.—S^2 and S^z are conserved and I work in the $S^z=0$ subspace since all competitors have a representative there. That is to say, each eigenstate with a given S value can (by the well known properties of angular momentum) be rotated in spin space to a state with $S_z=0$ without changing its energy. Then there are $n=\frac{1}{2}N$ electrons of each type, spin up and spin down. Let $\{\psi^{\alpha}\}$ be any orthonormal basis for *one species* of n spinless fermions; there are

$$m=\binom{|\Lambda|}{n}$$

of these and I require that they be *real* (i.e., each ψ^{α} is a *real,* homogeneous polynomial of order n in the $c_x^{\dagger}$'s acting on the vacuum). A ground state ψ can then be written as $\psi=\sum_{\alpha,\beta}W_{\alpha\beta}\psi_{\uparrow}^{\alpha}\otimes\psi_{\downarrow}^{\beta}$ with $W_{\alpha\beta}$ as coefficients. This $W_{\alpha\beta}$ is here viewed as a $m\times m$ matrix. Because all operators and basis vectors are real and because the Hamiltonian is symmetric between the up and the down spins, it is obvious that if $W_{\alpha\beta}$ corresponds to a ground state then so does $W_{\beta\alpha}^{*}=(W^{\dagger})_{\alpha\beta}$, and hence (by linearity) so does $W+W^{\dagger}$ and $i(W-W^{\dagger})$. Thus, for conveni-

ence, we may henceforth assume $W=W^\dagger$ (but $W_{\alpha\beta}$ is not assumed to be real). The norm of ψ squared is $\langle\psi|\psi\rangle=\sum_{\alpha,\beta}|W_{\alpha\beta}|^2=\mathrm{Tr}W^2$ and I assume that this is unity. The hopping energy part of $\langle\psi|H|\psi\rangle$ is easily found to be $2\,\mathrm{Tr}KW^2$ where

$$K_{\alpha\beta}=\langle\psi^\beta|\sum_{x,y}t_{xy}c_x^\dagger c_y|\psi^\alpha\rangle .$$

Clearly K is real and symmetric since each t_{xy} is real. The on-site energy is given by $-\sum_x U_x\,\mathrm{Tr}(WL_xWL_x)$ with $(L_x)_{\alpha\beta}=\langle\psi^\beta|n_x|\psi^\alpha\rangle$, which is also real and symmetric. The total energy is then

$$E(W)=\langle\psi|H|\psi\rangle=2\,\mathrm{Tr}KW^2+\sum_x U_x\,\mathrm{Tr}(WL_xWL_x)\,, \quad (3)$$

and the equation for W, corresponding to the eigenvalue equation $H\psi=e\psi$, is

$$KW+WK+\sum_x U_xL_xWL_x-eW\,. \quad (4)$$

Now consider the positive semidefinite matrix $|W|$ defined by $|W|^2=W^2$. Obviously, $\mathrm{Tr}W^2=\mathrm{Tr}|W|^2$. Moreover, in an orthonormal basis (not to be confused with the ψ^α basis for the electrons) in which the Hermitian $m\times m$ matrix W is diagonal, with diagonal elements w_i, the Hermitian matrix $|W|$ is also diagonal with elements $|w_i|$. In this diagonal basis I compute

$$\mathrm{Tr}WL_xWL_x=\sum_{i,j}w_iw_j|(L_x)_{ij}|^2\le\sum_{i,j}|w_i||w_j||(L_x)_{ij}|^2$$
$$=\mathrm{Tr}|W|L_x|W|L_x\,.$$

Since $U_x\le 0$, I conclude that $E(W)\ge E(|W|)$ and therefore that *among the ground states there is one satisfying* $W=|W|\ge 0$. This is the "spin-space reflection positivity" mentioned in the second paragraph. (This part of the proof is an adaptation of that given in Ref. 4.) I choose this positive (possibly semidefinite) matrix W and now make the choice that the ψ^α's are the natural x-space basis for the electrons, i.e., α denotes n points in Λ and $\psi^\alpha=\prod_{x\in\alpha}c_x^\dagger|0\rangle$. (Some arbitrary convention for the sign of the ψ^α's can be made here.) Since $W\ge 0$, it follows that $W_{\alpha\alpha}>0$ for at least one α, for otherwise W vanishes identically. However, the vector $\phi^\alpha=\psi_\uparrow^\alpha\otimes\psi_\downarrow^\alpha$ satisfies $(S_{\mathrm{op}})^2\phi^\alpha=0$ and therefore this ground state ψ has a nonzero projection onto the eigenspace of $(S_{\mathrm{op}})^2$ in which $S=0$. This would be impossible if conclusion (a) were false and thus conclusion (a) must be true.

To prove conclusion (b) I shall prove that necessarily a Hermitian W satisfies $W=|W|$ or $W=-|W|$ for every ground state when $U_x<0$ for every x. This will prove conclusion (b) for the following reason. If there were two normalized, Hermitian ground state W's, say W^1 and W^2 with $W^1\neq\pm W^2$, then for every real constant d, the Hermitian matrix $W^1+dW^2\equiv W_d$ is not zero and defines (after normalization) a ground state, by virtue of the linearity of the eigenvalue Eq. (4). It is easy to verify that there must be a d for which W_d is neither positive nor negative semidefinite, and this contradicts the assertion that the ground state W_d satisfies $W_d=\pm|W_d|$.

With W given then, consider the Hermitian, positive semidefinite matrix $R\equiv|W|-W$ which is also a multiple of a ground state and satisfies (4). If Q denotes the kernel of R, i.e., $Q=\{\text{vectors } V \text{ such that } RV=0\}$, then the assertion $W=\pm|W|$ is implied by the following statement which I shall prove: Q is either just the zero vector or else every vector is in Q. Let V be in Q and take the expectation of (4) in this state V, i.e.,

$$\langle V|KR+RK+\sum_x U_xL_xRL_x|V\rangle=e\langle V|R|V\rangle .$$

Since $RV=0$ and, for all x, $U_x<0$ and $\langle V|L_xRL_x|V\rangle\ge 0$ by the positive semidefiniteness of R, I conclude that $\langle V|L_xRL_x|V\rangle=0$ for all x. Since R is positive semidefinite, I conclude that $RL_xV=0$. Thus each L_x maps Q into Q. Now let the matrices in (4) act on V (without taking expectation values). Since $RL_xV=0$ and $RV=0$, I conclude that $RKV=0$. Thus K also maps Q into Q. As before, let α denote a collection of n points in Λ and define $L^\alpha=\prod_{x\in\alpha}L_x$, which is the projector onto the basis vector μ^α in C^m [with components $(\mu^\alpha)_\gamma=\delta_{\alpha\gamma}$] and which has matrix elements $(L^\alpha)_{\gamma\delta}=\delta_{\alpha\gamma}\delta_{\gamma\delta}$. Note that the L_x's commute with each other and so the ordering of the L_x's is unimportant in the definition of L^α. Each L^α maps Q into Q because each L_x does. Since Λ is connected by T, it is easy to see that the α's are connected by K, i.e., for all α and β there are indices $\gamma_1,\gamma_2,\ldots,\gamma_p$ for some integer p such that the ordinary (not matrix) product $G_{\beta\alpha}\equiv K_{\beta\gamma_1}K_{\gamma_1\gamma_2}\cdots K_{\gamma_p\alpha}$ is not zero. If Q is not just the zero vector and $V\neq 0$ is in Q then $L^\alpha V\neq 0$ for some fixed choice of α (because $\sum_\alpha L^\alpha$ is the identity). Then $L^\alpha V=z\mu^\alpha$ for some nonzero constant z and with μ^α being the aforementioned basis vector. But then the vector $F\equiv L^\beta KL^{\gamma_1}K\cdots L^{\gamma_p}KL^\alpha V$ is in Q and, in fact, $F=zG_{\beta\alpha}\mu^\beta$. In short, Q contains a complete set of vectors (i.e., every μ^β) because $G_{\beta\alpha}$ is nonzero for every β by virtue of the connectivity. Thus every vector is in Q since Q is a linear space, which implies that $W=\pm|W|$ and which, in turn, implies uniqueness of the ground state. Q.E.D.

Proof of theorem 2.— First make the conventional unitary hole-particle transformation for the spin-up electrons followed by a sign change on the B sublattice, i.e., $c_{x\uparrow}\to\epsilon(x)c_{x\uparrow}^\dagger$ and $c_{x\uparrow}^\dagger\to\epsilon(x)c_{x\uparrow}$ with $\epsilon(x)=1$ for $x\in A$, $\epsilon(x)=-1$ for $x\in B$. The spin-down electrons are unaltered, i.e., $c_{x\downarrow}\to c_{x\downarrow}$. Then $n_{x\uparrow}\to 1-n_{x\uparrow}$ and the transformed H is $\tilde{H}+UN_\downarrow$ with

$$\tilde{H}=\sum_\sigma\sum_{x,y\in\Lambda}t_{xy}c_{x\sigma}^\dagger c_{y\sigma}-U\sum_{x\in\Lambda}n_{x\uparrow}n_{x\downarrow}\,, \quad (5)$$

and with $N_\sigma=\sum_x n_{x\sigma}$. The original number operators N_σ transform as $N_\downarrow\to\tilde{N}_\downarrow=N_\downarrow$ and $N_\uparrow\to\tilde{N}_\uparrow=|\Lambda|-N_\uparrow$. The original condition $N=|\Lambda|$ becomes $N_\uparrow=N_\downarrow$. The

spin operators (2) become the *pseudo-spin operators*

$$\tilde{S}^z = \tfrac{1}{2}(|\Lambda| - N_\uparrow - N_\downarrow), \quad \tilde{S}^+ = \sum_{x\in\Lambda} \epsilon(x) c_{x\uparrow} c_{x\downarrow}, \qquad (6)$$

and $S^2 \to (\tilde{S}^z)^2 + \frac{1}{2}\tilde{S}^+\tilde{S}^- + \frac{1}{2}\tilde{S}^+\tilde{S}^+ \equiv (\tilde{S})^2$. The $\tilde{S}$ operators commute with $\tilde{H}$, but so do the spin operators S given in (2). The S operators are the transforms of the pseudo-spin operators in the original variables and are of no special physical interest. The $\tilde{S}$ operators are the ones of interest as far as $\tilde{H}$ is concerned.

As before, I can work in the $\tilde{N}_\uparrow = \tilde{N}_\downarrow = |\Lambda|/2$ subspace, which implies that $N_\uparrow = N_\downarrow = |\Lambda|/2$. The uniqueness part of theorem 2 is then a consequence of conclusion (b) of theorem 1, which also states that the unique ground state $\tilde{\psi}$ of $\tilde{H}$ has $S=0$. This last fact is of secondary importance. The real problem is to prove that $2\tilde{S} = |B| - |A|$. The shortest proof is to return to H and the $S^z=0$ subspace (in the *original variables).* For each $U>0$ the ground state $\psi(U)$ is nondegenerate as has been shown and I want to prove that $2S = |B| - |A|$. The nondegeneracy of the ground state for *all* $U>0$ implies that the S of this unique ground state must be independent of U, for otherwise continuity in U would imply a degeneracy for some value of $U>0$. However, when U is very large, H, as stated before, is equivalent (to leading order in U) to h, the Heisenberg antiferromagnetic Hamiltonian defined in remark (4). As stated there, h *also* has a unique ground state[6] (for $S^z=0$) and this state has $2S = |B| - |A|$. The uniqueness property of h is crucial for it implies a gap (however small it may be) in the spectrum of h. Thus, for large enough U the S value of the ground state of h is identical to that of H. Q.E.D.

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