

COMMENT

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To cite this article: Guang-Shan Tian 1990 *J. Phys. A: Math. Gen.* **23** 2231

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COMMENT

A simplified proof of Nagaoka's theorem

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Received 15 December 1989, in final form 13 February 1990

Abstract. We study a special case of the Hubbard model in which the on-site interaction U is infinite and there is exactly one hole. Nagaoka has shown that the ground state in this case has the maximum total spin. In this comment, we give Nagaoka's theorem another proof which is simpler, in some respects, than the original one.

It is well known that the Hubbard model plays a very important role in the study of metallic ferromagnetism, the metal-insulator transition and high temperature superconductivity. It is a relatively simple model but there are unfortunately few rigorous results known [1–4]. Nagaoka's theorem is one of them. In Nagaoka's original paper [1], he considered a special case of the Hubbard model, in which the on-site interaction is infinite and there is exactly one hole, and showed that the unique ground state has the maximum total spin. Considering the fact that the state with S_{\max} can never be the ground state when the band is half filled [4], the result of Nagaoka's theorem is surely very interesting.

In this comment, we shall give Nagaoka's theorem another proof. It is simpler than the original one in some respects.

For the reader's convenience, let us first recall Nagaoka's theorem. The Hamiltonian of the Hubbard model can be written as

$$H = \sum_{\sigma} \sum_{\langle ij \rangle} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are, respectively, creation and annihilation operators for an electron of spin σ at the i th lattice site; U is the on-site Coulomb repulsion interaction parameter which is positive; t_{ij} is the hopping matrix element defined by

$$t_{ij} = \begin{cases} t & \text{if site } i \text{ and } j \text{ are nearest neighbours} \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

Letting U be infinite, there can be at most one electron at each site. Let N be the total number of lattice sites and N_e the total number of electrons. Then it is necessary that $N \geq N_e$. Nagaoka studied a special case in which $N - N_e = 1$. He showed the following.

Theorem. If the crystal structure is simple cubic (sc), body centred cubic (bcc), face centred cubic (fcc), or hexagonal closed packed (hcp) and the parameter $t > 0$, then the ground state has the maximum total spin $S_{\max} = \frac{1}{2} N_e$.

Remark 1. It is worthwhile noticing that sc and bcc can be divided into two sublattices such that all the nearest neighbours of a lattice point on one sublattice belong to the other sublattice. If we introduce an extra phase factor to the atomic wavefunctions at the lattice points on one sublattice, t changes its sign. Since the transformation is canonical, the spectrum of the Hamiltonian H' does not change. Therefore, for sc and bcc lattices, the parameter t can be either positive or negative.

Remark 2. We always assume that the lattice is connected, i.e. given any two sites h and k , there exists a path from h to k along which t_{ij} is never zero.

For the original proof, one can read reference [1]. Nagaoka exploited heavily series expansion in his proof.

Before proceeding to our proof, we would like to introduce some useful notation and terminologies.

(a) Since we are only interested in the case in which U is infinite, we can write the Hamiltonian in the following form

$$H' = t \sum_{\sigma} \sum_{\langle ij \rangle} c_{i\sigma}^+ c_{j\sigma} \quad (3)$$

subject to the condition that there can exist at most one electron at each lattice site.

(b) Take a lattice site k . Let

$$\begin{aligned} s_{kx} &= \frac{1}{2}(c_{k\uparrow}^+ c_{k\downarrow} + c_{k\downarrow}^+ c_{k\uparrow}) \\ s_{ky} &= \frac{1}{2i}(c_{k\uparrow}^+ c_{k\downarrow} - c_{k\downarrow}^+ c_{k\uparrow}) \\ s_{kz} &= \frac{1}{2}(n_{k\uparrow} - n_{k\downarrow}) \end{aligned} \quad (4)$$

where $i = \sqrt{-1}$. It is quite easy to check that

$$[s_{k\alpha}, s_{k\beta}] = i\epsilon_{\alpha\beta\gamma} s_{k\gamma}. \quad (5)$$

These are the commutation relations satisfied by the spin operators of electron. Naturally, we define

$$S^2 = \left(\sum_k s_{kx} \right)^2 + \left(\sum_k s_{ky} \right)^2 + \left(\sum_k s_{kz} \right)^2$$

and

$$S_z = \sum_k s_{kz} = \frac{1}{2} \sum_k (n_{k\uparrow} - n_{k\downarrow}) \quad (6)$$

to be the total spin and total spin z -component operators. Furthermore, a little algebra shows that

$$[H', S^2] = 0 \quad \text{and} \quad [H', S_z] = 0 \quad (7)$$

i.e. they are conserved quantities.

(c) Following Nagaoka, we introduce a complete set of orthogonal state vectors. In terms of them, we can write the Hamiltonian H' in a suitable matrix form.

First, we order the lattice sites in some way. For instance, one can do it in alphabetical order. Then we define

$$\Psi_{i\alpha} = (-1)^i c_{1\sigma_1}^+ c_{2\sigma_2}^+ \cdots c_{(i-1)\sigma_{i-1}}^+ c_{(i+1)\sigma_{i+1}}^+ \cdots c_{N\sigma_N}^+ |0\rangle \quad (8)$$

where α denotes the spin configuration $(\sigma_1, \sigma_2, \dots, \sigma_{(i-1)}, \sigma_{(i+1)}, \dots, \sigma_N)$ and $|0\rangle$ is the vacuum state. It is easy to see that in this state, each site is occupied by one

electron except the i th site which is empty. Therefore, there exists exactly one hole in this state. Letting i and α run over all the possible choices, we obtain the complete set of state vectors. These vectors are orthogonal and normalised.

(d) Consider the matrix elements $\langle \Psi_{i\alpha} | H' | \Psi_{j\beta} \rangle$. If one matrix element $\langle \Psi_{h\gamma} | H' | \Psi_{k\rho} \rangle$ is non-zero, then

(i) the configurations γ and ρ must have the same number of spin-up and spin-down electrons since H' conserves N_\uparrow and N_\downarrow , respectively;

(ii) the sites h and k must be nearest neighbours; furthermore, one of them must be unoccupied while double occupation is forbidden;

(iii) since there exists exactly one hole, only one term of H' contributes to $\langle \Psi_{h\gamma} | H' | \Psi_{k\rho} \rangle$; assume that site h is occupied by a up-spin electron and site k is empty; then the single contributing term is $t c_{k\uparrow}^+ c_{h\uparrow}$;

(iv) noticing that

$$H' = t \sum_{\sigma} \sum_{\langle ij \rangle} c_{i\sigma}^+ c_{j\sigma} = -t \sum_{\sigma} \sum_{\langle ij \rangle} c_{j\sigma} c_{i\sigma}^+ \quad (9)$$

and the fermion operators satisfy the anticommutation relations, we see that any non-zero matrix element

$$\langle \Psi_{h\gamma} | H' | \Psi_{k\rho} \rangle = \langle \Psi_{h\gamma} | t c_{k\uparrow}^+ c_{h\uparrow} | \Psi_{k\rho} \rangle = -t \langle \Psi_{h\gamma} | c_{h\uparrow} c_{k\uparrow}^+ | \Psi_{k\rho} \rangle \quad (10)$$

is equal to $-t$ by our definition of state vectors (that is why we give $\Psi_{i\alpha}$ a phase factor $(-1)^i$).

(e) Given two state vectors $\Psi_{h\gamma}$ and $\Psi_{k\rho}$. If the matrix element

$$\langle \Psi_{h\gamma} | H' | \Psi_{k\rho} \rangle = -t \quad (11)$$

is non-zero, we call them super nearest neighbours.

(f) Given two state vectors $\Psi_{i\alpha}$ and $\Psi_{j\beta}$ which are not super nearest neighbours, i.e. $\langle \Psi_{i\alpha} | H' | \Psi_{j\beta} \rangle = 0$, they are said to be linked if one can find a finite number of intermediate state vectors $\Psi_{m\chi}, \Psi_{n\delta}, \dots, \Psi_{s\tau}$ such that each of $\{(\Psi_{i\alpha}, \Psi_{m\chi}), (\Psi_{m\chi}, \Psi_{n\delta}), \dots, (\Psi_{s\tau}, \Psi_{j\beta})\}$ is a pair of super nearest neighbours. It is equivalent to saying that one can find a positive integer M such that

$$\langle \Psi_{i\alpha} | (H')^M | \Psi_{j\beta} \rangle \neq 0. \quad (12)$$

It is not difficult to see that, for two- or three-dimensional SC, BCC, FCC or HCP lattices, any pair of state vectors which have the same number of up-spin and down-spin electrons, are linked. In the one-dimensional case, some state vectors are not linked even if they have the same N_\uparrow and N_\downarrow . For example, the following two configurations are not linked:



Now, we are ready to prove the theorem.

Proof of Nagaoka's theorem. For simplicity, we take a two-dimensional simple lattice as an example.

Our strategy of proof is as follows. We first find a lower bound λ_0 for the eigenvalues of the Hamiltonian matrix. Then we show that there is a unique (apart from trivial $(2S+1)$ -fold spin degeneracy) vector Ψ_0 such that $H'\Psi_0 = \lambda_0\Psi_0$, i.e. λ_0 is, in fact, the lowest eigenvalue of the Hamiltonian. Then we show that the ground-state vector Ψ_0

can be explicitly expressed as a linear combination of state vectors $\{\Psi_{i\alpha}\}$. Finally, we show that Ψ_0 has total spin S_{\max} by applying the operator S^2 to it.

Let $\langle \Psi_{i\alpha} | H' | \Psi_{j\beta} \rangle$ be the matrix element at the intersection of row $(i\alpha)$ and column $(j\beta)$. We write H' into a $(N2^{N-1}) \times (N2^{N-1})$ matrix. Since H' preserves N_{\uparrow} and N_{\downarrow} , the matrix has the following block form

$$H' = \begin{pmatrix} H(N-1, 0) & & 0 \\ & H(N-2, 1) & \\ & & \ddots \\ 0 & & & H(0, N-1) \end{pmatrix} \quad (13)$$

where $H(n_1, n_2)$ denotes the submatrix with n_1 up-spin and n_2 down-spin electrons.

Take an arbitrary submatrix $H(n_1, n_2)$. The elements in each row of it are either 0 or $-t$. The non-zero elements are contributed by the super-nearest-neighbour state vectors as we have said above. Let z be the number of the nearest neighbours of each site in the two-dimensional simple lattice. It is not difficult to see that any state vector has also z super nearest neighbours if we impose the periodic boundary condition on the lattice. Therefore, in each row of $H(n_1, n_2)$, there are exactly z non-zero elements $-t$. On the other hand, all the elements on the principal diagonal line must be zero because H' only contains hopping terms. These conclusions hold for any partition (n_1, n_2) .

Let λ be an eigenvalue of $H(n_1, n_2)$ and u_{λ} be the corresponding eigenvector. Then

$$\lambda u_{\lambda} = H(n_1, n_2) u_{\lambda}. \quad (14)$$

Let

$$|u_m| = \max_{1 \leq j \leq N_{\lambda}} |u_j| \quad (15)$$

where N_{λ} is the number of components of u_{λ} . The m th row of equation (14) is

$$\lambda u_m = \sum_{k=1}^{N_{\lambda}} H(n_1, n_2)_{mk} u_k \quad (16)$$

therefore

$$|\lambda| |u_m| = \left| \sum_{k=1}^{N_{\lambda}} H(n_1, n_2)_{mk} u_k \right| \leq \sum_{k=1}^{N_{\lambda}} |H(n_1, n_2)_{mk}| |u_k| \leq \sum_{k=1}^{N_{\lambda}} |H(n_1, n_2)| |u_m|. \quad (17)$$

Dividing (17) by $|u_m| > 0$, we find

$$|\lambda| \leq \sum_{k=1}^{N_{\lambda}} |H(n_1, n_2)_{mk}| = zt. \quad (18)$$

Since λ is real (H' is Hermitian),

$$\lambda \geq -zt \quad (19)$$

therefore, the eigenvalues of $H(n_1, n_2)$ as well as H' are indeed bounded below by $-zt$.

Next we take a special vector

$$u_0 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \quad (20)$$

Obviously,

$$H(n_1, n_2)u_0 = -zt u_0 \quad (21)$$

since there are exactly z non-zero elements ($-t$) in each row of $H(n_1, n_2)$. Therefore, $-zt$ is the lowest eigenvalue of $H(n_1, n_2)$ as well as H' . It is easy to see that u_0 corresponds to the state vector

$$\Psi_0(n_1, n_2) = \sum_{\{\alpha\}} \Psi_{i\alpha}(n_1, n_2) \quad (22)$$

in the subspace (n_1, n_2) . In particular,

$$\Psi_0(N-1, 0) = \sum_i (-1)^i c_1^+, \dots, c_{(i-1)}^+ c_{(i+1)}^+, \dots, c_N^+ |0\rangle. \quad (23)$$

In (23), we dropped the index α because there is only one spin configuration ($\uparrow, \uparrow, \dots, \uparrow$) in this subspace. Applying the operators S^2 and S_z to $\Psi_0(N-1, 0)$, we find

$$S^2 = \frac{1}{4}(N-1)(N+1) = S_{\max}(S_{\max} + 1) \quad (24)$$

and

$$S_z = S_{\max} = \frac{1}{2}N_e = \frac{1}{2}(N-1). \quad (25)$$

On the other hand, one of the lowest eigenvalue states in each subspace (n_1, n_2) must have total spin S_{\max} since $[H', S^2] = 0$ and $[H', S_z] = 0$. Therefore, one of the ground states of H' has the maximum spin.

Finally, we show that the ground state is non-degenerate. In fact, it is a direct corollary of the following theorem.

Theorem (Perron). Let A be a square matrix with all $a_{ij} \geq 0$. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A and $\rho = \max_{1 \leq v \leq n} |\lambda_v|$. If A is irreducible, i.e. for any pair (i, j) , there is a positive integer M such that $\{A^M\}_{ij}$ is non-zero, then ρ is an eigenvalue of A and has multiplicity one.

(One can find a proof of this theorem in reference [5] p 182.)

Consider $H(n_1, n_2)$. The negative of it, $-H(n_1, n_2)$ certainly has only positive elements and is irreducible in two- or three-dimensional lattices as we discussed in (f). The largest eigenvalue of $-H(n_1, n_2)$ is zt . By Perron's theorem, it has multiplicity one. This eigenvalue corresponds to the lowest eigenvalue $-zt$ of $H(n_1, n_2)$ as well as H' . Therefore, the ground state has multiplicity 1, i.e. it is non-degenerate. QED.

Some remarks are in order.

Remark 1. In the one-dimensional case, the Hamiltonian matrix is not irreducible. Therefore, the ground states may be degenerate.

Remark 2. The fact that all the non-zero matrix elements of the Hamiltonian are negative plays an important role in our proof. In the two-hole case, we could not find a set of orthogonal-state vectors such that the signs of the non-zero matrix elements are the same. It makes our method useless for this case. At present physicists are vigorously debating the two-hole case [6].

Before finishing this comment, we would like to compare briefly Nagaoka's ferromagnetic ground state with the ground states of the Hubbard model with finite Coulomb repulsion U .

It is folklore among physicists that the ground states of the Hubbard model would be antiferromagnetic rather than ferromagnetic when U is sufficiently large and $n = N - N_c$ is small. When $U \gg t$ and $n \ll N$, we know from the second-order perturbation theory that the model may be described by the following effective Hamiltonian [7]:

$$H_{\text{eff}} = T_h + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) \quad (26)$$

where

$$T_h = -t \sum_{\sigma} \sum_{\langle ij \rangle} (1 - n_{i,-\sigma}) c_{i\sigma}^+ c_{j\sigma} (1 - n_{j,-\sigma}) + \text{HC} \quad (27)$$

and $J = 4t^2/U > 0$. The second term of H_{eff} is the well known isotropic spin- $\frac{1}{2}$ Heisenberg antiferromagnetic Hamiltonian whose ground state has spin 0 [8]. In fact, by calculating the spin-wave spectrum to the first-order terms in nt and t^2/U , Nagaoka also showed that the ferromagnetic state with $S = S_{\text{max}}$ cannot be the ground state for an SC lattice if

$$U < Nt/\alpha \quad (28)$$

with $\alpha = 0.246$. Therefore, Nagaoka's ferromagnetic ground state will eventually be destroyed when the thermodynamic limit is taken. We see that infinite potential is really crucial for the proof of Nagaoka's ferromagnetism.

We would like to thank our referee for his valuable suggestions.

Note added. After submission of this work, we found an article by Tasaki [9]. He used a quite different method and could prove Nagaoka's theorem for more general cases.

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