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Application of the Gutzwiller Method to Antiferromagnetism

Fumihiko TAKANO* and Mamoru UCHINAMI

*Department of Physics, Tokyo University of Education, Tokyo
and*

**Department of Physics, University of Tsukuba,
Academy Town, Ibaraki.*

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The method of Gutzwiller in the problem of electron correlation in the Hubbard model is extended to the antiferromagnetic state. It is shown that the transition from the paramagnetic to the antiferromagnetic state occurs at a certain value of U (intraatomic Coulomb energy) for a fixed value of the electron concentration. In contrast to the result in the Hartree-Fock approximation, this value of U does not vanish even in the case when the magnetic zone boundary coincides with the Fermi surface. For extremely large values of U , the critical electron concentration is shown to approach to $1/2$.

Special care is taken in the case of the half-filled band, and our ground state energy is compared with that in the Hartree-Fock approximation. It is shown that for large value of U the Hartree-Fock energy is lower, but that for intermediate value of U our energy becomes lower for the special band structure.

§ 1. Introduction

The effect of the electron correlation in a narrow band has often been investigated by using the Hubbard model.¹⁾ Various methods have been employed to discuss the ferro- or antiferromagnetic ordering and the metal-nonmetal transition in this model.

While the ferromagnetic ordering has been discussed by many authors,²⁾ however, the antiferromagnetic phase has been discussed by only a few authors^{3),4)} beyond the Hartree-Fock approximation. Caron and Kemeny³⁾ have used the perturbation technique up to second order, and Bernasconi⁴⁾ has used the method of cluster expansion. Both treated only the case of half-filled band, and they obtained different results in some respect. Thus, it is desirable to investigate the antiferromagnetic ordering in this model more thoroughly by using a different method and without the restriction of the half-filled band.

The method used in this paper is the extension of that of Gutzwiller,⁵⁾ who takes the correlation effect into account by putting the special Ansatz for the form of the density matrix. This method has been applied to the problem of the metal-nonmetal transition⁶⁾ and extended to the case of the degenerate band.⁷⁾

We extend the method of Gutzwiller to the antiferromagnetic (AF) phase and discuss the instability of the paramagnetic and AF phases. The boundary

curve between two phases is drawn on the phase plane of the electron concentration and the energy parameter. Special care will be paid to the case of the half-filled band and the result will be compared with those of other approximations.

Recently, Ogawa et al.⁸⁾ have made the similar investigation, but their extension of the method of Gutzwiller is based on the different idea from ours. Their result is qualitatively the same as ours in some respect but is different in other respect.

In § 2, the reformulation of the Gutzwiller method in the paramagnetic state is given in order to make its extension easy. The extension to the more general state is made in § 3, and the discussion of the AF state is given in § 4. In § 5, our result is compared with others.

§ 2. Reformulation of the Gutzwiller method

The Hubbard model is expressed by the Hamiltonian

$$H = \sum_{i,j} \sum_{\sigma} t_{i,j} a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2.1)$$

where $a_{i\sigma}^{\dagger}$ ($a_{i\sigma}$) is the creation (annihilation) operator of an electron at the i -th lattice site with spin σ , and $n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$ is the number operator. $t_{i,j}$ is the transfer integral whose Fourier component is written as $\epsilon_{\mathbf{k}}$,

$$\epsilon_{\mathbf{k}} = \sum_j t_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \quad (2.2)$$

The last term in the Hamiltonian (2.1) is the intraatomic Coulomb energy.

We define the density matrix in the ground state $|\Psi\rangle$ as

$$\begin{aligned} \rho_{n,m}(h_1, \dots, h_n; p_1, \dots, p_m; f_1, \dots, f_n; q_1, \dots, q_m) \\ = \langle \Psi | a_{h_1\uparrow}^{\dagger} \dots a_{h_n\uparrow}^{\dagger} a_{p_1\downarrow}^{\dagger} \dots a_{p_m\downarrow}^{\dagger} a_{q_1\downarrow} a_{f_n\uparrow} \dots a_{f_1\uparrow} | \Psi \rangle \end{aligned} \quad (2.3)$$

and express the ground state energy as

$$E = \sum_{i,j} t_{i,j} (\rho_{1,0}(i;j) + \rho_{0,1}(i;j)) + U \sum_i \rho_{1,1}(i;i;i;i). \quad (2.4)$$

Thus, we need $\rho_{1,0}$, $\rho_{0,1}$ and $\rho_{1,1}$ for the calculation of E , and Gutzwiller assumes the form for the density matrices $\rho_{n,0}$ ($\rho_{0,n}$) and $\rho_{n,1}$ in the following form:

$$\rho_{n,0}(h_1 \dots h_n; f_1 \dots f_n) = C_n \begin{pmatrix} w_{\uparrow}(i-j) & h_1 \dots h_n \\ & f_1 \dots f_n \end{pmatrix} \quad (2.5)$$

and

$$\begin{aligned} \rho_{n,1}(gh_1 \dots h_{n-1}; g: g f_1 \dots f_{n-1}; g) = C_n' \begin{pmatrix} w_{\uparrow}(i-j) & gh_1 \dots h_{n-1} \\ & g f_1 \dots f_{n-1} \end{pmatrix} \\ \times w_{\downarrow}(g-g). \end{aligned} \quad (2.6)$$

In Eqs. (2.5) and (2.6), $\left(f(i-j) \begin{vmatrix} x_1 \dots x_n \\ y_1 \dots y_n \end{vmatrix} \right)$ is the determinant whose (i, j) el-

ement is given by $f(x_i - y_j)$, and $w_\sigma(i - j)$ is defined by

$$w_\sigma(i - j) = \frac{1}{L} \sum_{(\mathbf{k}\sigma)} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \tag{2.7}$$

L being the total number of lattice sites, and the summation $(\mathbf{k}\sigma)$ being taken over the occupied Bloch states with spin σ . The similar expression is also assumed for the density matrices with the down spin.

The density matrix satisfies the following recurrence formula:

$$\begin{aligned} \sum_g \rho_{n+1,m}(h_1 \cdots h_n g; p_1 \cdots p_m; f_1 \cdots f_n g; q_1 \cdots q_m) \\ = \langle \Psi | a_{h_1 \uparrow}^\dagger \cdots a_{h_n \uparrow}^\dagger \sum_g a_{g \uparrow}^\dagger a_{g \uparrow} a_{f_n \uparrow} \cdots a_{f_1 \uparrow} a_{p_1 \downarrow}^\dagger \cdots a_{p_m \downarrow}^\dagger a_{q_m \downarrow} \cdots a_{q_1 \downarrow} | \Psi \rangle \\ = (N_\uparrow - n) \rho_{n,m}(h_1 \cdots h_n; p_1 \cdots p_m; f_1 \cdots f_n; q_1 \cdots q_m), \end{aligned} \tag{2.8}$$

where N_σ is the total number of electrons with spin σ .

The function w_σ given by Eq. (2.7) has the following properties:

$$\begin{aligned} w_\sigma(i - i) &= \frac{N_\sigma}{L}, \\ \sum_l w_\sigma(i - l) w_\sigma(l - j) &= w_\sigma(i - j). \end{aligned} \tag{2.9}$$

If we use the above properties of $w_\sigma(i - j)$, it is easy to show that the determinant $\left(w(i - j) \begin{matrix} h_1 \cdots h_n \\ f_1 \cdots f_n \end{matrix} \right)$ satisfies the same recurrence formula as Eq. (2.8).

Then, in order that the assumed forms of the density matrices, Eqs. (2.5) and (2.6), may satisfy the relation (2.8), C_n and C_n' in Eqs. (2.5) and (2.6) must be independent of n .

Gutzwiller has determined the value of C_n or C_n' in the following way: Because C_n is independent of n , we have only to consider the case $n = N_\uparrow$ in Eq. (2.5). The value of C_{N_\uparrow} depends on the number of lattice sites involved in ρ_{N_\uparrow} , and is taken to be proportional to the number of all possible configurations of down spin electrons with the weight $\eta^{\nu+\nu'}$, where η is a variational parameter, ν is the number of doubly occupied sites of $h_1, h_2, \dots, h_{N_\uparrow}$ in each configuration, and ν' is the corresponding number of $f_1, f_2, \dots, f_{N_\uparrow}$.

For example, the coefficient C of the diagonal density matrix, (i.e., when $h_1 = f_1, h_2 = f_2, \dots, h_{N_\uparrow} = f_{N_\uparrow}$ in Eq. (2.5)) is taken as

$$C = C_0 \sum_\nu \eta^{2\nu} \binom{N_\uparrow}{\nu} \binom{L - N_\uparrow}{N_\downarrow - \nu}. \tag{2.10}$$

When $h_1 \neq f_1, h_2 = f_2, \dots, h_{N_\uparrow} = f_{N_\uparrow}$, on the other hand, the coefficient C' is taken as

$$C' = C_0 \sum_\nu \left\{ \eta^{2(\nu+1)} \binom{N_\uparrow - 1}{\nu} \binom{L - N_\uparrow - 2}{N_\downarrow - \nu - 2} \right\}$$

$$+ 2\eta^{2\nu+1} \binom{N_{\uparrow}-1}{\nu} \binom{L-N_{\uparrow}-2}{N_{\downarrow}-\nu-1} + \eta^{2\nu} \binom{N_{\uparrow}-1}{\nu} \binom{L-N_{\uparrow}-2}{N_{\downarrow}-\nu} \Big\}. \quad (2.11)$$

In both Eqs. (2.10) and (2.11) C_0 is assumed to be the same, and can be determined from the normalization condition

$$\rho_0 = 1. \quad (2.12)$$

Each summation in Eqs. (2.10) and (2.11) can be replaced by the maximum term, and we can obtain the necessary density matrix for the calculation of the ground state energy (2.4) as follows:

$$\rho_{1,0}(i:i) = w_{\uparrow}(i-i) = \frac{N_{\uparrow}}{L}, \quad (2.13)$$

$$\rho_{1,0}(i:j) = q_{\uparrow} w_{\uparrow}(i-j) \quad \text{for } i \neq j. \quad (2.14)$$

In Eq. (2.14), q_{\uparrow} is given by

$$q_{\uparrow} = \frac{N_{\uparrow}-\nu}{N_{\uparrow}} \cdot \frac{[L-N_{\uparrow}-N_{\downarrow}+\nu+\eta(N_{\downarrow}-\nu)]^2}{(L-N_{\uparrow})(L-N_{\uparrow}-N_{\downarrow}+\nu)}, \quad (2.15)$$

where the value of ν is determined from the equation

$$\eta^2 \frac{(N_{\uparrow}-\nu)(N_{\downarrow}-\nu)}{\nu(L-N_{\uparrow}-N_{\downarrow}+\nu)} = 1. \quad (2.16)$$

The similar expressions for $\rho_{0,1}(i:i)$ and $\rho_{0,1}(i:j)$ is obtained by interchanging the suffix \uparrow and \downarrow .

The two-particle density matrix $\rho_{1,1}(i:i;i;i)$, Eq. (2.6), can be calculated in the similar way, and the result is

$$\rho_{1,1}(i:i;i;i) = \frac{\nu}{L}. \quad (2.17)$$

The value of ν is the same as the one given by Eq. (2.16).

Using Eqs. (2.14) and (2.17), the ground state energy, Eq. (2.4), is expressed as

$$E = q_{\uparrow} \sum_{(\mathbf{k}\uparrow)} \epsilon_{\mathbf{k}} + q_{\downarrow} \sum_{(\mathbf{k}\downarrow)} \epsilon_{\mathbf{k}} + U\nu. \quad (2.18)$$

This energy is to be minimized with respect to η .

Using the above expression for E , Gutzwiller⁵⁾ discussed the possibility of ferromagnetic ground state. Brinkman and Rice,⁶⁾ on the other hand, discussed the metal-insulator transition in the paramagnetic state ($N_{\uparrow}=N_{\downarrow}$). They assumed that the state with $q_{\uparrow}=q_{\downarrow}=0$ corresponds to the insulator, and the state with $q_{\uparrow}=q_{\downarrow} \neq 0$ to the metal. The reason for this is that the discontinuity of the occupation number at the Fermi surface in the \mathbf{k} space is given by q_{σ} .

The magnetic ordering, especially AF ordering, however, plays an important role in the metal-insulator transition. Thus, in the next section, we extend the

method of Gutzwiller to the AF state and discuss the phase boundary between the AF and paramagnetic states.

§ 3. Extension of the Gutzwiller method to more general state

The formulation given in the previous section can be applied only to the para- and ferromagnetic states in which lattice sites are all equivalent. In the AF state, however, we have two sublattices *A* and *B*, and we must change some of the previous arguments.

First we assume the expression for the density matrix corresponding to Eqs. (2.5) and (2.6) in the following form:

$$\rho_{n,0}(h_1 \cdots h_n; f_1 \cdots f_n) = C_n(n_1, n_1') \left(w_{\uparrow}(i-j) \begin{vmatrix} h_1 \cdots h_n \\ f_1 \cdots f_n \end{vmatrix} \right), \tag{3.1}$$

$$\begin{aligned} \rho_{n+1,1}(gh_1 \cdots h_n; g: gf_1 \cdots f_n; g) &= C'_{n+1}(n_1, n_1'; \alpha_g) \\ &\times \left(w_{\uparrow}(i-j) \begin{vmatrix} gh_1 \cdots h_n \\ g f_1 \cdots f_n \end{vmatrix} w_{\downarrow}(g-g) \right). \end{aligned} \tag{3.2}$$

In the above equations, n_1 and n_1' are the numbers of *A* sites involved in $(h_1 \cdots h_n)$ and $(f_1 \cdots f_n)$, respectively, and α_g denotes the type of sublattice to which g belongs,

$$\begin{aligned} \alpha_g &= A, \quad \text{if } g \in A, \\ &= B, \quad \text{if } g \in B. \end{aligned} \tag{3.3}$$

The function $w_{\sigma}(i-j)$ is given by

$$w_{\sigma}(i-j) = \frac{2}{L} \sum_{(k\sigma)} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} p_{ki}^{\sigma} p_{kj}^{\sigma}, \tag{3.4}$$

where we have assumed the form of the Bloch state in the AF state as

$$a_{k\sigma} = \frac{1}{\sqrt{L/2}} \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} a_{i\sigma} p_{ki}^{\sigma} \tag{3.5}$$

and p_{ki}^{σ} is given by

$$p_{ki}^{\sigma} = \begin{cases} u_{\mathbf{k}}^{\sigma}, & \text{if } i \in A, \\ v_{\mathbf{k}}^{\sigma}, & \text{if } i \in B, \end{cases} \tag{3.6}$$

and $u_{\mathbf{k}}^{\sigma}, v_{\mathbf{k}}^{\sigma}$ are the variational parameters with the condition

$$(u_{\mathbf{k}}^{\sigma})^2 + (v_{\mathbf{k}}^{\sigma})^2 = 1. \tag{3.7}$$

The density matrix should satisfy the recurrence relation, Eq. (2.8). In order that our assumed forms, Eqs. (3.1) and (3.2), may satisfy this relation we neglect the \mathbf{k} -dependence of $u_{\mathbf{k}}^{\sigma}$ and $v_{\mathbf{k}}^{\sigma}$, and the coefficients $C_n(n_1, n_1')$ and $C'_n(n_1, n_1'; \alpha_g)$ in Eqs. (3.1) and (3.2) should satisfy the following recurrence

relations:

$$\begin{aligned} C_n(n_1, n_1') &= (u^\dagger)^2 C_{n+1}(n_1+1, n_1'+1) + (v^\dagger)^2 C_{n+1}(n_1, n_1'), \\ C_n'(n_1, n_1'; \alpha_g) &= (u^\dagger)^2 C_{n+1}'(n_1+1, n_1'+1; \alpha_g) + (v^\dagger)^2 C_{n+1}'(n_1, n_1'; \alpha_g). \end{aligned} \quad (3.8)$$

These relations have been obtained by separating the summation over g in Eq. (2.8) into two sublattices and by using the properties of $w_\sigma(i-j)$

$$w_\sigma(i-i) = \frac{2N_\sigma}{L} (p_i^\sigma)^2, \quad (3.9)$$

$$\begin{aligned} \sum_{i \in A} w_\sigma(i-l) w_\sigma(l-j) &= (u^\sigma)^2 w_\sigma(i-j), \\ \sum_{i \in B} w_\sigma(i-l) w_\sigma(l-j) &= (v^\sigma)^2 w_\sigma(i-j), \end{aligned} \quad (3.10)$$

which are valid if $u_{\mathbf{k}^\sigma}$ and $v_{\mathbf{k}^\sigma}$ are independent of \mathbf{k} .

The values of the coefficient $C_n(n_1, n_1')$ or $C_n'(n_1, n_1'; \alpha_g)$ can be determined in a similar way to that in the previous section. First we consider the diagonal density matrix $\rho_{n,0}(h_1 \cdots h_n; h_1 \cdots h_n)$. In this case, $n_1 = n_1'$ and we simply denote $C_n(n_1)$ instead of $C_n(n_1, n_1)$. The recurrence relation for $C_n(n_1)$ can be written as

$$C_n(n_1) = (u^\dagger)^2 C_{n+1}(n_1+1) + (v^\dagger)^2 C_{n+1}(n_1). \quad (3.11)$$

Repeated use of Eq. (3.11) gives the expression for $C_n(n_1)$ as

$$C_n(n_1) = (v^\dagger)^{2(N_\uparrow - n)} \left(\frac{v^\dagger}{u^\dagger} \right)^{2n_1} \sum_{m_\uparrow = n_1}^{N_\uparrow} C_{N_\uparrow}(m_\uparrow) \binom{N_\uparrow - n}{m_\uparrow - n_1} \left(\frac{u^\dagger}{v^\dagger} \right)^{2m_\uparrow}. \quad (3.12)$$

In the paramagnetic state, we have $u^\dagger = v^\dagger = 1/\sqrt{2}$, and it is shown that the above equation has a solution $C_n = C_{N_\uparrow}$ which is the result in § 2 that C_n is independent of n .

Here, we assume that $C_{N_\uparrow}(m_\uparrow)$ is proportional to the number of configurations of down spin electrons with the weight $\eta^{2\nu} \eta'^{2\nu'} x^{m_\downarrow}$, where η, η' and x are variational parameters and $\nu(\nu')$ is the number of doubly occupied sites in the $A(B)$ sublattice in each configuration. m_\downarrow is the number of down spin electrons on the B sublattice in each configuration. Then, $C_{N_\uparrow}(m_\uparrow)$ can be expressed as

$$\begin{aligned} C_{N_\uparrow}(m_\uparrow) &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} \left[\sum_{\nu} \eta^{2\nu} \binom{m_\uparrow}{\nu} \binom{(L/2) - m_\uparrow}{N_\downarrow - m_\downarrow - \nu} \right] \\ &\quad \times \left[\sum_{\nu'} \eta'^{2\nu'} \binom{N_\uparrow - m_\uparrow}{\nu'} \binom{(L/2) - N_\uparrow + m_\uparrow}{m_\downarrow - \nu'} \right]. \end{aligned} \quad (3.13)$$

The value of the proportional constant C_0 is to be determined from the condition

$$C_0(0) = 1.$$

Next we consider the density matrix which is diagonal except one element, and write

$$\rho_{n+1,0}(hh_1 \cdots h_n : fh_1 \cdots h_n) = C_{n+1}(n_1; \alpha_h, \alpha_f) \begin{pmatrix} zh_1 \cdots h_n \\ fh_1 \cdots h_n \end{pmatrix}, \quad (3.14)$$

where n_1 is the number of A sites in h_1, h_2, \dots, h_n , and α_h is defined in Eq. (3.3). From the recurrence formula for $C_{n+1}(n_1; \alpha_h, \alpha_f)$, we obtain

$$C_n(n_1; \alpha_h, \alpha_f) = (v^\dagger)^{2(N_\uparrow - n)} \left(\frac{v^\dagger}{u^\dagger} \right)^{2n_1} \sum_{m_\uparrow} C_{N_\uparrow}(m_\uparrow; \alpha_h, \alpha_f) \begin{pmatrix} N_\uparrow - n \\ m_\uparrow - n_1 \end{pmatrix} \left(\frac{u^\dagger}{v^\dagger} \right)^{2m_\uparrow}. \quad (3.15)$$

The value of $C_{N_\uparrow}(m_\uparrow; \alpha_h, \alpha_f)$ can be determined in the same way as before and is shown to be written as

$$\begin{aligned} C_{N_\uparrow}(m_\uparrow - 1; A, A) &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} \left[\eta^2 \sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow - 1 \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow - 1 \\ N_\downarrow - m_\downarrow - \nu - 2 \end{pmatrix} \right. \\ &\quad \left. + 2\eta \sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow - 1 \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow - 1 \\ N_\downarrow - m_\downarrow - \nu - 1 \end{pmatrix} + \sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow - 1 \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow - 1 \\ N_\downarrow - m_\downarrow - \nu \end{pmatrix} \right] \\ &\quad \times \left[\sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N_\uparrow - m_\uparrow \\ \nu' \end{pmatrix} \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow \\ m_\downarrow - \nu' \end{pmatrix} \right], \\ C_{N_\uparrow}(m_\uparrow - 1; A, B) &= C_{N_\uparrow}(m_\uparrow - 1; B, A) = C_0 \sum_{m_\downarrow} x^{m_\downarrow} \\ &\quad \times \left[\eta \sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow - 1 \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow \\ N_\downarrow - m_\downarrow - \nu - 1 \end{pmatrix} + \sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow - 1 \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow \\ N_\downarrow - m_\downarrow - \nu \end{pmatrix} \right] \\ &\quad \times \left[\eta' \sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N - m_\uparrow \\ \nu' \end{pmatrix} \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow - 1 \\ m_\downarrow - \nu' - 1 \end{pmatrix} \right. \\ &\quad \left. + \sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N_\uparrow - m_\uparrow \\ \nu' \end{pmatrix} \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow - 1 \\ m_\downarrow - \nu' \end{pmatrix} \right], \\ C_{N_\uparrow}(m_\uparrow; B, B) &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} \left[\sum_{\nu} \eta^{2\nu} \begin{pmatrix} m_\uparrow \\ \nu \end{pmatrix} \begin{pmatrix} (L/2) - m_\uparrow \\ N_\downarrow - m_\downarrow - \nu \end{pmatrix} \right] \\ &\quad \times \left[\eta'^2 \sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N_\uparrow - m_\uparrow - 1 \\ \nu' \end{pmatrix} \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow - 1 \\ m_\downarrow - \nu' - 2 \end{pmatrix} + 2\eta' \sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N_\uparrow - m_\uparrow - 1 \\ \nu' \end{pmatrix} \right. \\ &\quad \left. \times \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow - 1 \\ m_\downarrow - \nu' - 1 \end{pmatrix} + \sum_{\nu'} \eta'^{2\nu'} \begin{pmatrix} N_\uparrow - m_\uparrow - 1 \\ \nu' \end{pmatrix} \begin{pmatrix} (L/2) - N_\uparrow + m_\uparrow - 1 \\ m_\downarrow - \nu' \end{pmatrix} \right], \end{aligned} \quad (3.16)$$

where the constant C_0 is taken to be the same as in Eq. (3.13).

If we substitute Eq. (3.13) into Eq. (3.12), or Eq. (3.16) into Eq. (3.15),

the expression of $C_n(n_1)$ or $C_n(n_1; \alpha_h, \alpha_f)$ contains four summations, each of which can be replaced by the maximum term. Then if we write for Eq. (3.13)

$$C_{N_\uparrow}(m_\uparrow) = C_0 \sum_{m_\downarrow} x^{m_\downarrow} Q Q', \quad (3.17)$$

Eq. (3.16) becomes

$$\begin{aligned} C_{N_\uparrow}(m_\uparrow-1; A, A) &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} Q Q' \left(\frac{m_\uparrow - \nu}{m_\uparrow} \right) \\ &\quad \times \frac{[(L/2) - m_\uparrow + (\eta - 1)(N_\downarrow - m_\downarrow - \nu)]^2}{((L/2) - m_\uparrow)((L/2) - m_\uparrow - (N_\downarrow - m_\downarrow - \nu))}, \\ C_{N_\uparrow}(m_\uparrow-1; A, B) &= C_{N_\uparrow}(m_\uparrow-1; B, A) \\ &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} Q Q' \left(\frac{m_\uparrow - \nu}{m_\uparrow} \right) \cdot \left(\frac{(L/2) - m_\uparrow + (\eta - 1)(N_\downarrow - m_\downarrow - \nu)}{(L/2) - m_\uparrow - (N_\downarrow - m_\downarrow - \nu)} \right) \\ &\quad \times \left(\frac{(L/2) - (N_\uparrow - m_\uparrow) + (\eta' - 1)(m_\downarrow - \nu')}{(L/2) - (N_\uparrow - m_\uparrow)} \right), \end{aligned} \quad (3.18)$$

$$\begin{aligned} C_{N_\uparrow}^\#(m_\uparrow; B, B) &= C_0 \sum_{m_\downarrow} x^{m_\downarrow} Q Q' \left(\frac{N_\uparrow - m_\uparrow - \nu'}{N_\uparrow - m_\uparrow} \right) \\ &\quad \times \frac{[(L/2) - (N_\uparrow - m_\uparrow) + (\eta' - 1)(m_\downarrow - \nu')]^2}{((L/2) - (N_\uparrow - m_\uparrow))((L/2) - (N_\uparrow - m_\uparrow - \nu') - m_\downarrow)}, \end{aligned}$$

where Q or Q' is the maximum term of the summation over ν or ν' in Eq. (3.13). The values of ν, ν' are determined from

$$\begin{aligned} \eta^2 &= \frac{\nu[(L/2) - m_\uparrow - (N_\downarrow - m_\downarrow) + \nu]}{(m_\uparrow - \nu)(N_\downarrow - m_\downarrow + \nu)}, \\ \eta'^2 &= \frac{\nu'[(L/2) - (N_\uparrow - m_\uparrow) - m_\downarrow + \nu']}{(N_\uparrow - m_\uparrow - \nu')(m_\downarrow - \nu')}. \end{aligned} \quad (3.19)$$

Putting Eq. (3.17) into Eq. (3.12), we have

$$C_0(0) = C_0 (v^\uparrow)^{2N_\uparrow} \sum_{m_\uparrow} \sum_{m_\downarrow} \left(\frac{u^\uparrow}{v^\uparrow} \right)^{2m_\uparrow} x^{m_\downarrow} \binom{N_\uparrow}{m_\uparrow} Q Q' \quad (3.20)$$

and

$$\begin{aligned} C_1(1) &= C_0 (v^\uparrow)^{2(N_\uparrow-1)} \left(\frac{v^\uparrow}{u^\uparrow} \right)^2 \sum_{m_\uparrow} \sum_{m_\downarrow} \left(\frac{u^\uparrow}{v^\uparrow} \right)^{2m_\uparrow} x^{m_\downarrow} \binom{N_\uparrow-1}{m_\uparrow-1} Q Q', \\ C_1(0) &= C_0 (v^\uparrow)^{2(N_\uparrow-1)} \sum_{m_\uparrow} \sum_{m_\downarrow} \left(\frac{u^\uparrow}{v^\uparrow} \right)^{2m_\uparrow} x^{m_\downarrow} \binom{N_\uparrow-1}{m_\uparrow} Q Q'. \end{aligned} \quad (3.21)$$

Replacing the summations over m_\uparrow and m_\downarrow by their maximum terms and using the normalization condition $C_0(0) = 1$, Eq. (3.21) can be simplified as

$$C_1(1) = \frac{m_\uparrow}{N_\uparrow} \cdot \frac{1}{(u^\dagger)^2},$$

$$C_1(0) = \frac{N_\uparrow - m_\uparrow}{N_\uparrow} \cdot \frac{1}{(v^\dagger)^2}, \tag{3.22}$$

where the values of m_\uparrow and m_\downarrow corresponding to the maximum term is given by

$$\left(\frac{u^\dagger}{v^\dagger}\right)^2 = \frac{(m_\uparrow - \nu) ((L/2) - m_\uparrow) ((L/2) - N_\uparrow + m_\uparrow - m_\downarrow + \nu')}{(N_\uparrow - m_\uparrow - \nu') ((L/2) - N_\uparrow + m_\uparrow) ((L/2) - m_\uparrow - N_\downarrow + m_\downarrow + \nu)},$$

$$x = \frac{(m_\downarrow - \nu') ((L/2) - m_\uparrow - N_\downarrow + m_\downarrow + \nu)}{(N_\downarrow - m_\downarrow - \nu) ((L/2) - N_\uparrow + m_\uparrow - m_\downarrow + \nu')}. \tag{3.23}$$

Thus, we have

$$\rho_{1,0}(i:i) = \begin{cases} \frac{m_\uparrow}{L/2} & \text{for } i \in A, \\ \frac{N_\uparrow - m_\uparrow}{L/2} & \text{for } i \in B, \end{cases} \tag{3.24}$$

which is the expected result.

In the similar manner, we can obtain the expression for the density matrix $\rho_{1,0}(i:j)$ as

$$\rho_{1,0} = w_\uparrow(i-j) \sqrt{q_{\alpha_i}^\dagger q_{\alpha_j}^\dagger}, \tag{3.24'}$$

where $q_{\alpha_i}^\dagger$ is given by

$$q_{A^\dagger} = \frac{m_\uparrow - \nu}{N_\uparrow} \frac{[(L/2) - m_\uparrow + (\eta - 1)(N_\downarrow - m_\downarrow - \nu)]^2}{((L/2) - m_\uparrow) ((L/2) - m_\uparrow - N_\downarrow + m_\downarrow + \nu)},$$

$$q_{B^\dagger} = \frac{N_\uparrow - m_\uparrow - \nu'}{N_\uparrow} \frac{[(L/2) - N_\uparrow + m_\uparrow + (\eta' - 1)(m_\downarrow - \nu')]^2}{((L/2) - N_\uparrow + m_\uparrow) ((L/2) - N_\uparrow + m_\uparrow - m_\downarrow + \nu')}. \tag{3.25}$$

The expression for the density matrix of down spin is similar to Eq. (3.24')

$$\rho_{0,1} = w_\downarrow(i-j) \sqrt{q_{\alpha_i}^\dagger q_{\alpha_j}^\dagger}, \tag{3.24''}$$

and $q_{\alpha_i}^\dagger$ is obtained by interchanging the suffices \uparrow and \downarrow , (η, ν) and (η', ν') .

In order to obtain the form of the two-body density matrix, we assume the form of $\rho_{n,1}$ as

$$\rho_{n,1}(h_1 \cdots h_{n-1}g; g; h_1 \cdots h_{n-1}g; g)$$

$$= C_n(m; \alpha_g) \left(w_\uparrow(i-j) \begin{vmatrix} h_1 \cdots h_{n-1}g \\ h_1 \cdots h_{n-1}g \end{vmatrix} \cdot w_\downarrow(g-g) \right), \tag{3.26}$$

where m is the number of A sites in h_1, \dots, h_{n-1} . Then, the recurrence relation (2.8) requires the following relation for $C_n(m; \alpha_g)$;

$$C_n(m; \alpha_g) = (u^\dagger)^2 C_{n+1}(m+1; \alpha_g) + (v^\dagger)^2 C_{n+1}(m; \alpha_g),$$

from which we obtain for the coefficient of $\rho_{1,1}(g; g; g; g)$

$$C_1(0; \alpha_g) = (v^\dagger)^{2(N_\dagger - 1)} \sum_{m_\dagger} C_{N_\dagger}(m_\dagger; \alpha_g) \binom{N_\dagger - 1}{m_\dagger} \left(\frac{u^\dagger}{v^\dagger}\right)^{2m_\dagger}. \quad (3.27)$$

$C_{N_\dagger}(m_\dagger; \alpha_g)$ can be calculated in the similar manner to Eqs. (3.17) and (3.18), and the result is

$$\begin{aligned} C_{N_\dagger}(m_\dagger - 1; A) &= C_0 \sum_{m_\dagger} x^{m_\dagger} Q Q' \frac{\nu}{m_\dagger}, \\ C_{N_\dagger}(m_\dagger; B) &= C_0 \sum_{m_\dagger} x^{m_\dagger} Q Q' \frac{\nu'}{N_\dagger - m_\dagger}, \end{aligned} \quad (3.28)$$

where Q, Q' is defined in the same way as before and the equations for ν and ν' are the same as Eq. (3.19).

Using Eq. (3.28) in Eq. (3.27) and taking the maximum term, we obtain

$$C_1(0; A) = \frac{1}{(u^\dagger)^2} \frac{\nu}{N_\dagger}, \quad C_1(0; B) = \frac{1}{(v^\dagger)^2} \frac{\nu'}{N_\dagger},$$

and the expression for $\rho_{1,1}$ becomes

$$\rho_{1,1}(g; g; g; g) = \begin{cases} \frac{2\nu}{L} & \text{for } g \in A, \\ \frac{2\nu'}{L} & \text{for } g \in B. \end{cases} \quad (3.29)$$

Using the expressions for density matrices, Eqs. (3.24'), (3.24'') and (3.29), it is easy to calculate the ground state energy, Eq. (2.4), and the result is

$$\begin{aligned} E &= \frac{N_\dagger}{2} \{ (\sqrt{q_A^\dagger} + \sqrt{q_B^\dagger})^2 \bar{\epsilon}^\dagger + (\sqrt{q_A^\dagger} - \sqrt{q_B^\dagger})^2 \bar{\epsilon}'^\dagger \} \\ &+ \frac{N_\dagger}{2} \{ (\sqrt{q_A^\dagger} + \sqrt{q_B^\dagger})^2 \bar{\epsilon}^\dagger + (\sqrt{q_A^\dagger} - \sqrt{q_B^\dagger})^2 \bar{\epsilon}'^\dagger \} \\ &+ U(\nu + \nu'), \end{aligned} \quad (3.30)$$

where $\bar{\epsilon}^\sigma$ and $\bar{\epsilon}'^\sigma$ are defined as

$$\bar{\epsilon}^\sigma = \frac{1}{N_\sigma} \sum_{(\mathbf{k}\sigma)} \epsilon_{\mathbf{k}}, \quad \bar{\epsilon}'^\sigma = \frac{1}{N_\sigma} \sum_{(\mathbf{k}\sigma)} \epsilon_{\mathbf{k}+\mathbf{K}} \quad (3.31)$$

and we have assumed $t_{i,i} = 0$ which means $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} = 0$. The vector \mathbf{K} is the wave number satisfying relation

$$e^{i\mathbf{K} \cdot \mathbf{R}_j} = \begin{cases} 1 & \text{for } j \in A, \\ -1 & \text{for } j \in B. \end{cases} \quad (3.32)$$

The expression for the occupation number in the momentum space is similarly calculated and is given by

$$\begin{aligned} \langle n_{\mathbf{k}\sigma} \rangle = & \frac{N_{\sigma}}{L} [1 - (q_A^{\sigma} + q_B^{\sigma})] + \frac{1}{2} (\sqrt{q_A^{\sigma}} + \sqrt{q_B^{\sigma}})^2 \sum_{(\mathbf{k}'\sigma)} \delta_{\mathbf{k}, \mathbf{k}'} \\ & + \frac{1}{2} (\sqrt{q_A^{\sigma}} - \sqrt{q_B^{\sigma}})^2 \sum_{(\mathbf{k}'\sigma)} \delta_{\mathbf{k}, \mathbf{k}'+\mathbf{K}}. \end{aligned} \tag{3.33}$$

In the case of para- or ferromagnetic state, it is easily seen that the expressions (3.30) and (3.33) coincide with those given by Gutzwiller.

The energy is to be minimized with respect to η, η', x and $(u^{\dagger}/v^{\dagger})$. It is, however, more convenient to consider the energy as a function of ν, ν', m_{\uparrow} and m_{\downarrow} , because x and $(u^{\dagger}/v^{\dagger})$ do not appear in Eq. (3.30).*) This is carried out in the next section.

§ 4. Energy in the AF state

The expression for the ground state energy derived in the previous section is general in the sense that it is applicable to both the ferro and AF states (accordingly to the ferrimagnetic state, too). In this section we confine our discussion to the AF state only and we put

$$N_{\uparrow} = N_{\downarrow} = N.$$

Then, we can expect the relations

$$\eta = \eta', \quad \nu = \nu', \quad m_{\uparrow} = m_{\downarrow} = m \tag{4.1}$$

hold in the ground state, and we have

$$\begin{aligned} q_A^{\uparrow} = q_B^{\downarrow} = & \frac{m - \nu}{N} \cdot \frac{[(L/2) - N + \nu + \eta(N - m - \nu)]^2}{((L/2) - m)((L/2) - N + \nu)} = q, \\ q_B^{\uparrow} = q_A^{\downarrow} = & \frac{N - m - \nu}{N} \cdot \frac{[(L/2) - N + \nu + \eta(m - \nu)]^2}{((L/2) - N + m)((L/2) - N + \nu)} = q', \end{aligned} \tag{4.2}$$

from Eqs. (4.1) and (3.25), and

$$\eta^2 = \frac{\nu((L/2) - N + \nu)}{(m - \nu)(N - m - \nu)} \tag{4.3}$$

from Eq. (3.19). The expression (3.30) for the energy becomes

$$E = N\{(\sqrt{q} + \sqrt{q'})^2 \bar{\epsilon} + (\sqrt{q} - \sqrt{q'})^2 \bar{\epsilon}'\} + 2U\nu. \tag{4.4}$$

First we consider the stability of the paramagnetic phase. For this purpose, it is convenient to use the reduced quantities defined as

$$\frac{L}{N} \equiv z, \quad \frac{m}{N} \equiv \frac{1}{2}(1 + \delta), \quad \frac{2\nu}{N} \equiv \bar{\nu}, \tag{4.5}$$

*) Equation (3.23) is not symmetric with respect to the spin variables, but Eqs. (3.30) and (3.33) are symmetric. This is another reason why we take m_{\uparrow} and m_{\downarrow} as independent variables instead of x and $(u^{\dagger}/v^{\dagger})$.

where $\delta \neq 0$ corresponds to the AF state. In terms of these quantities, Eqs. (4.2) and (4.3) are rewritten as

$$\begin{aligned} q &= \frac{1-\bar{\nu}+\delta}{2} \frac{[z-2+\bar{\nu}+\eta(1-\bar{\nu}-\delta)]^2}{(z-2+\bar{\nu})(z-1-\delta)}, \\ q' &= \frac{1-\bar{\nu}-\delta}{2} \frac{[z-2+\bar{\nu}+\eta(1-\bar{\nu}+\delta)]^2}{(z-2+\bar{\nu})(z-1+\delta)} \end{aligned} \quad (4.6)$$

and

$$\eta^2 = \frac{\bar{\nu}(z-2+\bar{\nu})}{(1-\bar{\nu}+\delta)(1-\bar{\nu}-\delta)}. \quad (4.7)$$

Substituting these expressions into Eq. (4.4) and expanding it in powers of δ , we obtain

$$\begin{aligned} \frac{E}{N} &= 4q_0\bar{\epsilon} + U\bar{\nu} \\ &+ q_0[4\beta\bar{\epsilon} - \alpha^2(\bar{\epsilon} - \bar{\epsilon}')] \delta^2 + \dots, \end{aligned} \quad (4.8)$$

where q_0 is the value of q, q' at $\delta=0$ and is given by

$$q_0 = \frac{1-\bar{\nu}}{2} \frac{[z-2+\bar{\nu}+\eta_0(1-\bar{\nu})]^2}{(z-2+\bar{\nu})(z-1)}, \quad (4.9)$$

and η_0 is given by

$$\eta_0 = \frac{\sqrt{\bar{\nu}(z-2+\bar{\nu})}}{(1-\bar{\nu})}. \quad (4.10)$$

The parameters α and β in Eq. (4.8) are defined as

$$\begin{aligned} \alpha &= \frac{1}{z-1} + \frac{1}{1-\bar{\nu}} - \frac{2\eta_0}{A}, \\ \beta &= \left(\frac{\eta_0}{A} - \frac{1}{z-1} \right) \left(\frac{\eta_0}{A} - \frac{1}{z-1} - \frac{1}{1-\bar{\nu}} \right), \\ A &= z-2+\bar{\nu}+\eta_0(1-\bar{\nu}). \end{aligned} \quad (4.11)$$

From Eq. (4.8), we can see that the phase boundary between para- and antiferromagnetic states is given by

$$4\beta\bar{\epsilon} - \alpha^2(\bar{\epsilon} - \bar{\epsilon}') = 0. \quad (4.12)$$

It is to be noted that the value of $\bar{\nu}$ is determined so as to minimize the energy of the paramagnetic state. That is, $\bar{\nu}$ is determined from the equation

$$\frac{\partial}{\partial \bar{\nu}} [4q_0\bar{\epsilon} + U\bar{\nu}] = 0. \quad (4.13)$$

We can solve Eq. (4.12) numerically, and get the relation between z and

the energy parameter. To do so, we assume the relation

$$\epsilon_{\mathbf{k}+\mathbf{K}} = -\epsilon_{\mathbf{k}} \tag{4.14}$$

which is valid for the simple cubic lattice or the body-centered cubic lattice with only the nearest neighbour transfer. From Eq. (4.14), we have

$$\bar{\epsilon} = -\bar{\epsilon}', \tag{4.15}$$

and Eq. (4.12) becomes

$$\alpha^2 = 2\beta. \tag{4.16}$$

Special care is needed in the case of the half-filled band, $z=2$. In this case, Eqs. (4.9) and (4.10) become very simple as

$$\begin{aligned} q_0 &= 2\bar{\nu}(1-\bar{\nu}), \\ \eta_0 &= \frac{\bar{\nu}}{1-\bar{\nu}}, \end{aligned} \tag{4.17}$$

and Eq. (4.11) becomes

$$\begin{aligned} \alpha &= 1, \\ \beta &= \frac{(1-2\bar{\nu})(2-3\bar{\nu})}{4(1-\bar{\nu})^2}. \end{aligned} \tag{4.18}$$

Then, the solution of Eq. (4.16) is shown to be given by

$$\bar{\nu} = 1 - \frac{1}{\sqrt{2}}. \tag{4.19}$$

The value of $\bar{\nu}$ which is determined from Eq. (4.13) is

$$\bar{\nu} = \begin{cases} 0 & \text{for } \frac{U}{|\bar{\epsilon}|} > 8, \\ \frac{1}{2} \left(1 - \frac{U}{8|\bar{\epsilon}|} \right) & \text{for } \frac{U}{|\bar{\epsilon}|} < 8, \end{cases} \tag{4.20}$$

as was obtained by Brinkman and Rice.

It is, however, noted that E is proportional to $\bar{\nu}$ when $z=2$. Thus, the difference between the paramagnetic and AF states vanishes when $U/|\epsilon| > 8$.

In order to investigate the case $z=2$ more carefully, we must use the full expression for the energy. Due to Eq. (4.15), Eq. (4.4) becomes

$$\begin{aligned} \frac{E}{N} &= 4\sqrt{qq'}\bar{\epsilon} + U\bar{\nu} \\ &= 4\bar{\nu} \cdot \frac{1-\bar{\nu} + \sqrt{1-\delta^2 - 2\bar{\nu} + \bar{\nu}^2}}{\sqrt{1-\delta^2}} \cdot \bar{\epsilon} + U\bar{\nu}. \end{aligned} \tag{4.21}$$

First we minimize E/N with respect to δ , and introduce a new variable

$$y = \frac{1}{\sqrt{1-\delta^2}}. \quad (4.22)$$

In terms of y , Eq. (4.21) can be written as

$$\frac{E}{N} = 4\bar{\nu}f(y)\bar{\epsilon} + U\bar{\nu}, \quad (4.23)$$

where $f(y)$ is given by

$$f(y) = (1-\bar{\nu})y + \sqrt{1-\bar{\nu}(2-\bar{\nu})}y^2. \quad (4.24)$$

Because ϵ is negative, the minimum of E/N corresponds to the maximum of $f(y)$. The solution y_0 of the equation $f'(y_0) = 0$ is given by

$$y_0 = \frac{1-\bar{\nu}}{\sqrt{\bar{\nu}(2-\bar{\nu})}}. \quad (4.25)$$

From the definition of y , Eq. (4.22), we have a condition

$$1 \leq y \leq \frac{1}{\sqrt{\bar{\nu}(2-\bar{\nu})}}, \quad (4.26)$$

which corresponds to

$$0 \leq \delta \leq 1-\bar{\nu}. \quad (4.27)$$

It is easily seen that the maximum of $f(y)$ occurs in the above range if and only if

$$0 \leq \bar{\nu} \leq 1 - \frac{1}{\sqrt{2}}. \quad (4.28)$$

When the condition (4.28) is fulfilled, the maximum value of $f(y)$ is given by

$$f(y_0) = \frac{1}{\sqrt{\bar{\nu}(2-\bar{\nu})}},$$

and otherwise the maximum is given by

$$f(1) = 2(1-\bar{\nu}).$$

From the above argument, we can see that the ground state energy is given by

$$\frac{E}{N} = 4\bar{\epsilon} \sqrt{\frac{\bar{\nu}}{2-\bar{\nu}}} + U\bar{\nu}, \quad \text{for } 0 \leq \bar{\nu} < 1 - \frac{1}{\sqrt{2}}, \quad (4.29a)$$

$$= 8\bar{\epsilon}\bar{\nu}(1-\bar{\nu}) + U\bar{\nu}, \quad \text{for } 1 - \frac{1}{\sqrt{2}} \leq \bar{\nu}, \quad (4.29b)$$

and the former case corresponds to the AF state ($\delta \neq 0$) and the latter to the paramagnetic state ($\delta = 0$).

It is shown that the minimum of this energy, Eqs. (4.29a) and (4.29b), is

given by*)

$$\begin{aligned} \frac{E_0}{N} &= 4\bar{\epsilon} \sqrt{\frac{\bar{\nu}_0}{2-\bar{\nu}_0}} + U\bar{\nu}_0, \quad \text{when } \frac{4|\bar{\epsilon}|}{U} < \frac{\sqrt{2}+1}{2}, \quad (\text{AF state}) \\ &= -2|\bar{\epsilon}| \left(1 - \frac{U}{8|\bar{\epsilon}|}\right)^2, \quad \text{when } \frac{4|\bar{\epsilon}|}{U} > \frac{\sqrt{2}+1}{2}, \quad (\text{paramagnetic state}) \end{aligned} \tag{4.30}$$

where $\bar{\nu}_0$ in Eq. (4.30) is given by the solution of

$$\bar{\nu}_0(2-\bar{\nu}_0)^2 = (4|\bar{\epsilon}|/U)^2. \tag{4.31}$$

We can summarize the above result as follows:

(1) When $(U/|\epsilon|) < 8(\sqrt{2}-1)$, the minimum of the ground state energy occurs at

$$\bar{\nu}_0 = \frac{1}{2} \left(1 - \frac{U}{8|\bar{\epsilon}|}\right), \quad \delta_0 = 0 \tag{4.32}$$

and the energy is given by

$$\frac{E_0}{N} = -2|\bar{\epsilon}| \left(1 - \frac{U}{8|\bar{\epsilon}|}\right)^2. \tag{4.33}$$

(2) When $(U/|\epsilon|) > 8(\sqrt{2}-1)$, the minimum of the energy occurs at $\bar{\nu}_0$ and δ_0 which are given by

$$\begin{aligned} \bar{\nu}_0(2-\bar{\nu}_0)^2 &= (4|\bar{\epsilon}|/U)^2, \\ y_0 &= \frac{1}{\sqrt{1-\delta_0^2}} = \frac{1-\bar{\nu}_0}{\sqrt{\bar{\nu}_0(2-\bar{\nu}_0)}}, \\ \delta_0 &= \left[1 - \frac{\bar{\nu}_0(2-\bar{\nu}_0)}{(1-\bar{\nu}_0)^2}\right]^{1/2}, \end{aligned} \tag{4.34}$$

and the energy is given by

$$\frac{E_0}{N} = 4\bar{\epsilon} \sqrt{\frac{\bar{\nu}_0}{2-\bar{\nu}_0}} + U\bar{\nu}_0. \tag{4.35}$$

We can obtain the phase boundary between the paramagnetic and AF states, by using Eq. (4.16) and the value of $(U/|\epsilon|) = 8(\sqrt{2}-1)$ at $z=2$. Equation (4.16) is calculated numerically and the result is shown in Fig. 1, in which the result in the Hartree-Fock approximation is also shown.

§ 5. Comparison with other approximations and discussion

As is seen from Fig. 1, our result differs from that of H-F approximation mainly in two respects. The first is the behaviour of the phase boundary in the

*) The result in the paramagnetic state is nothing but that obtained by Brinkman and Rice.

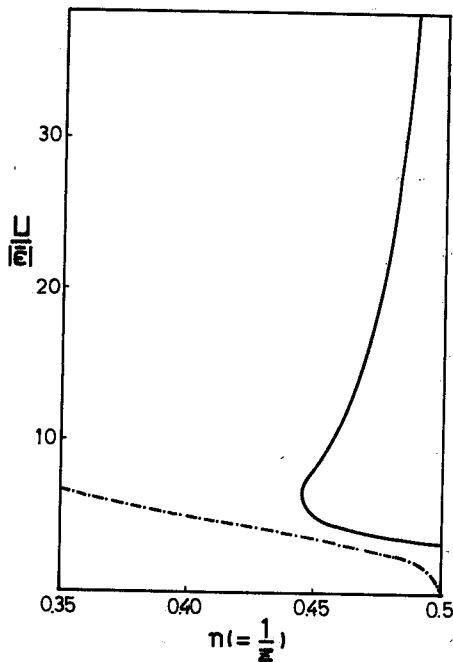


Fig. 1. Phase boundary between para- and antiferromagnetic state. Full line: Present result, Chained line: Result of H-F approximation (assuming the constant density of states).

states at some value of $U/|\epsilon|$, whereas Bernasconi⁴⁾ has shown that the AF state is always stable for any value of $U \neq 0$ when $\epsilon = -\epsilon'$. We cannot give any definite conclusion about this point. The similar phase boundary to ours has also been obtained by Ogawa et al.⁵⁾ Their transition, however, is of first order. The reason of this first order transition is obvious: They have failed to obtain the AF state with the energy lower than the paramagnetic state in extending the method of Gutzwiller. Therefore, they have compared the energy of the paramagnetic state in the Gutzwiller method with that of the AF state in the H-F approximation. Thus, their transition has been obtained by comparing the results in two different approximations and becomes of first order.

Finally, our energy is compared with that in the H-F approximation. Though our method does not satisfy the variation principle strictly, we have chosen the values of parameters to minimize the energy. Thus, it is interesting to compare the energy obtained with other results. Because we have neglected the \mathbf{k} -dependence of $u_{\mathbf{k}}^{\sigma}, v_{\mathbf{k}}^{\sigma}$, our energy is not necessarily lower than the H-F energy.

In order to compare the energy in both approximations, we take the form of the density of states as

limit of large U , and the second is the finite value of $U/|\epsilon|$ at $z=2$.

The value of $1/z$ on the phase boundary in the H-F approximation decreases monotonically as U increases, but in our curve $1/z$ reaches a minimum value and then increases again up to $1/2$ as U tends to infinity. As was pointed out by Ogawa et al., the physical reason of this increase may be as follows: When U is very large, the effective exchange energy between nearest neighbours, becomes of the order of $-t^2/U$, where t is the transfer integral between nearest neighbours. Because this effective exchange energy becomes smaller, the AF state becomes unstable as U increases.

As for the second difference, it is to be noted that the results of two methods^{3),4)} beyond the H-F approximation are different with each other. Both treated only the half-filled band, and Caron and Kemeny³⁾ have obtained the first order transition between AF and paramagnetic

$$\rho(\epsilon) = \begin{cases} \rho_0 + \alpha|\epsilon|, & |\epsilon| \leq D, \\ 0, & |\epsilon| > D, \end{cases} \quad (5.1)$$

which is normalized such as

$$\rho_0 D + \frac{1}{2} \alpha D^2 = \frac{1}{2}. \quad (5.2)$$

The H-F energy is expressed as

$$\frac{(E_0)_{\text{H-F}}}{L} = -\frac{2}{L} \sum_{\langle k \rangle} \sqrt{\epsilon_k^2 + U^2 n^2 \delta^2} + U n^2 (1 + \delta^2), \quad (5.3)$$

where $n = N_1/L = N_2/L = (1/z)$ and δ is the difference of the average numbers of electrons in two sublattices and is determined by the equation

$$\frac{1}{U} = \frac{1}{L} \sum_{\langle k \rangle} \frac{1}{\sqrt{\epsilon_k^2 + U^2 n^2 \delta^2}}. \quad (5.4)$$

For the sake of simplicity, we restrict the discussion to the case of the half-filled band. In this case, by using the density of states given by Eq. (5.1), Eqs. (5.3) and (5.4) can be rewritten as

$$\begin{aligned} \frac{(E_0)_{\text{H-F}}}{L} = -\rho_0 \left[D\sqrt{D^2 + a^2} + \frac{a^2}{2} \log \frac{\sqrt{D^2 + a^2} + D}{\sqrt{D^2 + a^2} - D} \right] - \frac{2}{3} \alpha [(D^2 + a^2)^{3/2} - a^3] \\ + \frac{1}{4} U + \frac{1}{U} a^2, \end{aligned} \quad (5.5)$$

$$\frac{1}{U} = \frac{1}{2} \rho_0 \log \frac{\sqrt{D^2 + a^2} + D}{\sqrt{D^2 + a^2} - D} + \alpha (\sqrt{D^2 + a^2} - a), \quad (5.6)$$

where we have put

$$\frac{1}{2} U \delta = a. \quad (5.7)$$

On the other hand, our energy has been given by Eqs. (4.33) and (4.35), in which in the same situation as above, $\bar{\epsilon}$ is expressed as

$$\bar{\epsilon} = -\left(\frac{1}{2} \rho_0 D + \frac{1}{3} \alpha D^2\right) D. \quad (5.8)$$

First, we can easily see that Eq. (4.33) gives lower energy than Eq. (5.3) for the small value of U . In fact, for small U , Eq. (5.5) becomes

$$\frac{(E_0)_{\text{H-F}}}{L} = \frac{1}{4} U + \bar{\epsilon} - D(1 + \alpha D^2) \exp[-2/\rho_0 U], \quad (5.9)$$

while Eq. (4.33) gives

$$\frac{E_0}{L} = \frac{1}{4} U + \bar{\epsilon} - \frac{U^2}{32D} \left(1 + \frac{1}{3} \alpha D^2\right), \quad (5.9')$$

which is certainly lower than Eq. (5.9).

In the opposite limit, i.e., when U is very large, Eq. (5.5) becomes

$$\frac{(E_0)_{\text{H-F}}}{L} = -\frac{1}{3} \left(1 + \frac{1}{2} \alpha D^2 \right) \frac{D^2}{U} \quad (5.10)$$

and Eq. (4.35) becomes

$$\frac{E_0}{L} = -\frac{1}{4} \left(1 + \frac{1}{3} \alpha D^2 \right)^2 \frac{D^2}{U}. \quad (5.10')$$

Our energy, Eq. (5.10') is always higher than $E_{\text{H-F}}$, Eq. (5.10) because we have the restriction

$$|\alpha D^2| \leq 1, \quad (5.11)$$

which is obtained from the conditions $\rho(0) \geq 0$ and $\rho(-D) \geq 0$.

From the above argument, we can expect that our energy, Eq. (4.33) and Eq. (4.35) is lower than the H-F energy, Eq. (5.5) for small value of U , and both energies become equal at a certain value of U , and then the H-F energy becomes lower. If this critical value of U is smaller than our critical value, $U/|\bar{\epsilon}| = 8(\sqrt{2}-1)$, our energy in the AF state is always higher than the H-F energy. From the numerical calculation, the condition that our energy is lower than the H-F energy at $U/|\bar{\epsilon}| = 8(\sqrt{2}-1)$ is given by

$$1 > \alpha D^2 > 0.63. \quad (5.12)$$

In other words, our approximation gives lower energy than the H-F approximation in the AF state for some values of U if the condition (5.12) is fulfilled. As mentioned before, however, our procedure does not strictly satisfy the variation principle, and the above argument is only for comparison. We believe that our result in the AF state has the meaning even if the condition (5.12) is not fulfilled.

As for the metal-insulator transition, our result seems to indicate that the transition predicted by Brinkman and Rice does not appear because we have always nonzero value of q or q' . It is, however, not certain that the insulator corresponds to the state with q and $q' = 0$ only. Strictly speaking, we must calculate the excitation energy and check the existence of the energy gap. The extension of the Gutzwiller method to excited states is an interesting problem in this sense and will be our future problem.

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References

- 1) J. Hubbard, Proc. Roy. Soc. **A276** (1963), 238; **A277** (1964), 237; **A281** (1964), 401.
- 2) For example,
J. Kanamori, Prog. Theor. Phys. **30** (1963), 275.
Y. Nagaoka, Phys. Rev. **147** (1966), 392.
- 3) L. G. Caron and G. Kemeny, Phys. Rev. **B3** (1971), 3007.
- 4) J. Bernasconi, Physik. Kond. Materie **14** (1972), 225.
- 5) M. C. Gutzwiller, Phys. Rev. **137** (1965), A1726.
- 6) W. F. Brinkman and T. M. Rice, Phys. Rev. **B2** (1970), 4302.
- 7) K. Chao, J. Phys. **C7** (1974), 127.
K. Chao and M. C. Gutzwiller, J. Appl. Phys. **42** (1971), 1420.
- 8) T. Ogáwa, T. Matsubara and K. Kanda, Prog. Theor. Phys. **53** (1975), 614.
- 9) T. Matsubara and T. Yokota, *Proceedings of the International Conference on Theoretical Physics, Kyoto* (1953), p. 693.
D. R. Penn, Phys. Rev. **142** (1966), 350.