Gutzwiller Approximation for Antiferromagnetism in Hubbard Model[*]

Tohru OGAWA, Kunihiko KANDA and Takeo MATSUBARA

Department of Physics, Kyoto University, Kyoto

The variational approach initiated by Gutzwiller is extended to include antiferromagnetism. A simplified assumption corresponding to that adopted by him is used in order to evaluate the ground state energy of the Hubbard model and to draw the phase diagram similar to those constructed by Penn on the basis of the Hartree-Fock approximation. It is found that the antiferromagnetic state in the phase diagram is restricted to a narrow region bounded by threshold values for both the coupling constant and electron density. For sufficiently large intraatomic repulsion paramagnetic state becomes more stable than antiferromagnetic state except for the case of one electron per site. The phase transition between paramagnetic and antiferromagnetic states is of first order and the coexistence of these two states with different density occurs.

§ 1. Introduction

Electron correlation in narrow energy bands is one of the most important problem in solid state physics. It is closely connected with the origin of magnetism in solids and it also plays an essntial role in the distinction between metals and insulators.[1]

Single band Hubbard model[2] studied in this paper is the simplest model to treat this problem. It may be an over-simplified one because of the short range of the interaction, non-degeneracy and the s-character of the band and neglection of the other freedoms. Nevertheless, it includes ideal metals as the weak coupling limit and Heisenberg model of magnetism in insulators as the strong coupling limit, and it has possibility of clarifying the interconnection between these two limiting cases. It is important to search for reliable treatment of this model since more complicated realistic models are difficult to be treated satisfactorily without understanding a simple model. One of the promising methods to treat electron correlation arising from repulsive interaction is the variational approach due to Gutzwiller.[3] It enables us to interpolate between the weak and strong coupling limits in the approximation higher than the Hartree-Fock approximation.

The purpose of this paper is to extend Gutzwiller's method to include antiferromagnetism and to draw a ground state phase diagram as the functions of the electron number and a coupling constant within the framework of the single

---

band Hubbard model in an approximation higher than the Hartree-Fock approximation adopted by Penn in the same problem.[4]

Section 2 is devoted to the reformulation of the Gutzwiller approximation and review of the main results obtained by this method. The reformulated method is extended so as to include antiferromagnetism in § 3 and results of the numerical calculation for actual variation procedure are given in § 4. Some problems with relation to the present approximation and the validity of the results are discussed in § 5. In the Appendix, the special case of one electron per site is considered to elucidate the mathematical structure of the present approximation.

§ 2. Reformulation of Gutzwiller approximation

In this section, the Gutzwiller approximation for a single band Hubbard model is reformulated in a rather different form from the original one. We consider a system with the single band Hubbard Hamiltonian given by

$$H = \sum_{ij} \varepsilon_{ij} (a_i^+ a_j + b_i^+ b_j) + U \sum_i a_i^+ a_i b_i^+ b_i , \qquad (2\cdot1)$$

where $a_i^+ (b_i^+)$ and $a_i (b_i)$ are respectively creation and annihilation operators of an electron in Wannier state with up (down) spin on a crystalline lattice site i locating at R_i. $\{i\}$ consist of a set of sites $\mathcal{L}$ whose number of elements is L. ε_{ij} is assumed to be a function of $|R_i - R_j|$ only and hence the first term of $(2\cdot1)$ can be diagonalized by a set of the Bloch function with a spectrum $\varepsilon_p = L^{-1} \sum_{ij} \varepsilon_{ij} \exp[ip(R_i - R_j)]$. Sometimes we call electrons with up spin a-electrons and with down spin b-electrons for convenience.

We adopt the site state representation in which 4^L bases are chosen to describe the possible configurations of the system: Each site can take four states. They are (1) doubly occupied, (2) only a-electron occupied, (3) only b-electron occupied and (4) empty states. In order to pick up these four states, four kinds of projection operators are introduced:

$$P_{1i} = D_i = a_i^+ a_i b_i^+ b_i , \qquad D = \sum_i D_i ,$$

$$P_{2i} = A_i = a_i^+ a_i b_i b_i^+ , \qquad A = \sum_i A_i ,$$

$$P_{3i} = B_i = a_i a_i^+ b_i^+ b_i , \qquad B = \sum_i B_i , \qquad (2\cdot2)$$

$$P_{4i} = E_i = a_i a_i^+ b_i b_i^+ , \qquad E = \sum_i E_i .$$

These projection operators have the following properties:

$$P_{\lambda i} P_{\mu i} = \delta_{\lambda \mu} P_{\lambda i} , \qquad P_{\lambda i} P_{\mu j} = P_{\mu j} P_{\lambda i} , \qquad (\lambda, \mu = 1, 2, 3, 4)$$

$$\sum_{\lambda=1}^{4} P_{\lambda i} = 1 . \qquad (2\cdot3)$$

It turns out convenient to define the following operators:

$$M_i = A_i + D_i = a_i^+ a_i, \qquad M = \sum_i M_i,$$

$$N_i = B_i + D_i = b_i^+ b_i, \qquad N = \sum_i N_i,$$

$$\bar{M}_1 = B_i + E_i = a_i a_i^+, \qquad \bar{M} = \sum_i \bar{M}_i, \qquad (2\cdot4)$$

$$\bar{N}_i = A_i + E_i = b_i b_i^+, \qquad \bar{N} = \sum_i \bar{N}_i.$$

$M(N)$ is the number operator of $a(b)$-electron. Now let us define the Gutzwiller operators for a site and the whole system by

$$G_i(g) = g D_i + A_i + B_i + E_i = g^{D_i}, \qquad (2\cdot5)$$

$$G(g) = \prod_i G_i(g) = g^D, \qquad (2\cdot6)$$

where g is the Gutzwiller parameter taking a non-negative value. The Gutzwiller operators satisfy the following relations:

$$G_i(g) G_j(g) = G_j(g) G_i(g), \qquad [G_i(g)]^n = G_i(g^n), \qquad (2\cdot7)$$

$$[G(g)]^n = G(g^n). \qquad (2\cdot8)$$

In the second quantized form, a single Slater determinant state is generally expressed as

$$|\Phi_0\rangle = \prod_{p \in \mathscr{P}} \alpha_p^+ \prod_{q \in Q} \beta_q^+ |0\rangle, \qquad (2\cdot9)$$

where $|0\rangle$ is the vacuum state and $\alpha_p^+ (\beta_q^+)$ are creation operators defined by the use of some complete set of the single-particle wave function $\xi_p(R) (\eta_q(R))$ such as

$$\alpha_p^+ = \sum_i \xi_p(R_i) a_i^+, \qquad \beta_q^+ = \sum_i \eta_q(R_i) b_i^+. \qquad (2\cdot10)$$

$\mathscr{P}(Q)$ is a certain set of quantum number $p(q)$ representing the occupied states. In the Gutzwiller variation, a trial function is chosen as

$$|\Psi_g\rangle = G(g) |\Phi_0\rangle / [\langle \Phi_0 | G(g^2) | \Phi_0 \rangle]^{1/2} \qquad (2\cdot11)$$

and two steps of variation procedure are taken: One is related with the best choice of a set of the single-particle wave functions $\{\xi_p(R)\}$, $\{\eta_q(R)\}$, $\mathscr{P}$ and Q. The second is to minimize the energy with respect to g. It should be noted that Gutzwiller variation includes the Hartree-Fock approximation because the trial functions of the latter belong to those of the former as a special case of $g=1$. Therefore the Gutzwiller variation does not give a ground state energy larger than the Hartree-Fock approximation:

$$E_{\text{Gutzwiller}} = \underset{(g)}{\text{Min}} \, E_g \leqq E_{g=1} \equiv E_{\text{HF}},$$

$$E_g = \underset{(\xi, \eta, \mathscr{P}, Q)}{\text{Min}} \langle \Phi_0 | G(g) H G(g) | \Phi_0 \rangle / \langle \Phi_0 | G(g^2) | \Phi_0 \rangle. \qquad (2\cdot12)$$

It is shown that this variation leads to the exact ground state for a two-site Hubbard model.

In order to facilitate the evaluation of E_g, we first summarize the relations useful for evaluating the expectation values which appear in Eq. (2·12). Let $|\varPhi_a\rangle$ and $|\varPhi_b\rangle$ be defined respectively by

$$|\varPhi_a\rangle = \prod_{p\in\mathcal{P}} \boldsymbol{\alpha}_p^+ |0\rangle , \qquad |\varPhi_b\rangle = \prod_{q\in Q} \boldsymbol{\beta}_q^+ |0\rangle , \qquad (2\cdot13)$$

and introduce the following functions:

$$u(ij) = \langle\varPhi_a|\boldsymbol{a}_i^+\boldsymbol{a}_j|\varPhi_a\rangle = \sum_{p\in\mathcal{P}} \xi_p^*(R_i)\xi_p(R_j),$$

$$v(ij) = \langle\varPhi_b|\boldsymbol{b}_i^+\boldsymbol{b}_j|\varPhi_b\rangle = \sum_{q\in Q} \eta_q^*(R_i)\eta_q(R_j). \qquad (2\cdot14)$$

Then it is not hard to show that

$$\langle\varPhi_a| \prod_{k\in\mathcal{M}} \boldsymbol{M}_k \prod_{l\in\bar{\mathcal{M}}} \bar{\boldsymbol{M}}_l |\varPhi_a\rangle = \begin{cases} \det U_{\mathcal{M}} & \text{when } \nu(\mathcal{M})=\nu(\mathcal{P}), \\ 0 & \text{when } \nu(\mathcal{M})\neq\nu(\mathcal{P}), \end{cases} \qquad (2\cdot15)$$

where $\mathcal{M}$ is a set of sites occupied by a-electrons, and $\mathcal{M}$ and $\bar{\mathcal{M}}$ are complementary in the sense that

$$\mathcal{M}\cup\bar{\mathcal{M}}=\mathcal{L}, \qquad \mathcal{M}\cap\bar{\mathcal{M}}=0 .$$

$\nu(\mathcal{M})$ is the number of elements of the set $\mathcal{M}$, and $\nu(\mathcal{P})$ is the number of states occupied in the configuration $|\varPhi_a\rangle$. $U_{\mathcal{M}}$ is a $L\times L$ matrix whose (ij) element is

$$[U_{\mathcal{M}}]_{ij} = \begin{cases} u(ij) & \text{when } i\in\mathcal{M}, \\ \bar{u}(ij)=\delta_{ij}-u(ij) & \text{when } i\in\bar{\mathcal{M}}. \end{cases} \qquad (2\cdot16)$$

Similarly we can prove that

$$\langle\varPhi_a|\boldsymbol{a}_i^+\boldsymbol{a}_j \prod_{k\in\mathcal{M}} \boldsymbol{M}_k \prod_{l\in\bar{\mathcal{M}}} \bar{\boldsymbol{M}}_l |\varPhi_a\rangle = \begin{cases} \det U_{\mathcal{M}}^{(ij)} & \text{when } \begin{matrix} i\in\bar{\mathcal{M}}, \, j\in\mathcal{M}, \\ \nu(\mathcal{M})=\nu(\mathcal{P}), \end{matrix} \\ 0 & \text{otherwise}, \end{cases} \qquad (2\cdot17)$$

where $U_{\mathcal{M}}^{(ij)}$ is a $(L-1)\times(L-1)$ matrix derived from $U_{\mathcal{M}}$ by first exchanging the i-th column with the j-th column in $U_{\mathcal{M}}$ and then by removing the j-th row and the j-th column to produce a $(L-1)\times(L-1)$ matrix.

The corresponding relations hold for b-electron system if we make appropriate change of notations:

$$\boldsymbol{M}_k\to\boldsymbol{N}_k, \qquad U_{\mathcal{M}}\to V_{\mathcal{N}}, \qquad U_{\mathcal{M}}^{(ij)}\to V_{\mathcal{N}}^{(ij)}, \qquad \varPhi_a\to\varPhi_b,$$

$$\bar{\boldsymbol{M}}_k\to\bar{\boldsymbol{N}}_k, \qquad u(ij)\to v(ij), \qquad \boldsymbol{a}_i\to\boldsymbol{b}_i, \qquad \nu(\mathcal{P})\to\nu(Q). \qquad (2\cdot18)$$

It should be noted that the state $|\varPhi_0\rangle$ defined by (2·9) is a direct product of $|\varPhi_a\rangle$ and $|\varPhi_b\rangle$ and therefore the expectation values in which both electrons concern can be expressed as a product of two determinants. For instance,

$$\langle \varPhi_0 | \prod_{i \in \mathcal{M}} M_i \prod_{j \in \bar{\mathcal{M}}} \bar{M}_j \prod_{k \in \mathcal{N}} N_k \prod_{l \in \bar{\mathcal{N}}} \bar{N}_l | \varPhi_0 \rangle = \det U_{\mathcal{M}} \det V_{\mathcal{N}} . \qquad (2\cdot19)$$

The expectation values of energy with respect to the trial state (2·11) are expressed by the use of the computation rules given above. First we consider the normalization factor which is written as

$$\langle \varPhi_0 | G(g^2) | \varPhi_0 \rangle = \langle \varPhi_0 | \prod_i (g^2 D_i + A_i + B_i + E_i) | \varPhi_0 \rangle$$
$$= \sum \langle \varPhi_0 | \prod_{i \in \mathcal{D}} g^2 D_i \prod_{j \in \mathcal{A}} A_j \prod_{k \in \mathcal{B}} B_k \prod_{l \in \mathcal{E}} E_l | \varPhi_0 \rangle . \qquad (2\cdot20)$$

$\mathcal{D}$ is a set of sites which are doubly occupied and $\mathcal{A}, \mathcal{B}, \mathcal{E}$ have similar meaning. Hereafter we abbreviate the number of elements in a set as $M = \nu(\mathcal{M})$, $N = \nu(\mathcal{N})$ and so on. Then among 4^L terms in (2·20) only

$$T_0 = \frac{L!}{M!(L-M)!} \frac{L!}{N!(L-N)!} \qquad (2\cdot21)$$

terms have non-zero contribution for given M and N. Each non-zero contribution has the same form as (2·19), where

$$\mathcal{M} = \mathcal{D} \cup \mathcal{A} , \qquad \mathcal{N} = \mathcal{D} \cup \mathcal{B} ,$$
$$\bar{\mathcal{M}} = \mathcal{B} \cup \mathcal{E} , \qquad \bar{\mathcal{N}} = \mathcal{A} \cup \mathcal{E} . \qquad (2\cdot22)$$

Therefore the normalization factor can be written as

$$\langle \varPhi_0 | G(g^2) | \varPhi_0 \rangle = \sum_D \sum_{(\mathcal{M}, \mathcal{N})}^{D} g^{2D} \det U_{\mathcal{M}} \det V_{\mathcal{N}} . \qquad (2\cdot23)$$

In this expression $\sum_{(\mathcal{M}, \mathcal{N})}^{D}$ is the sum over all the possible configurations of $(\mathcal{M}, \mathcal{N})$ such that $\mathcal{M}$ and $\mathcal{N}$ have common D sites.

Now we turn to the expectation value of the kinetic energy. It is enough to consider a-electron system, because the result for b-electron system is easily derived from that of a-electron by suitable change of notation. First we observe an identity

$$G_i(g) G_j(g) a_i^+ a_j G_i(g) G_j(g) = a_i^+ a_j (b_i b_i^+ + g b_i^+ b_i)(b_j b_j^+ + g b_j^+ b_j) . \qquad (2\cdot24)$$

In virtue of this relation

$$\langle \varPhi_0 | G(g) a_i^+ a_j G(g) | \varPhi_0 \rangle$$
$$= \langle \varPhi_0 | a_i^+ a_j (b_i b_i^+ + g b_i^+ b_i)(b_j b_j^+ + g b_j^+ b_j) \prod_{k \neq i, j} G_k(g^2) | \varPhi_0 \rangle \qquad (2\cdot25)$$

which can be expressed as a sum of products, each consisting of two factors, one with the form similar to (2·17) and the other similar to (2·16). Thus we have

$$\langle \varPhi_0 | G(g) a_i^+ a_j G(g) | \varPhi_0 \rangle = \sum_D [\sum_{\mathcal{M} : \mathcal{N}}^{(1)} g^{2D} \det U_{\mathcal{M}}^{(ij)} \det V_{\mathcal{N}}$$

Table I.

sum	i-th site	j-th site	total number of terms
$\sum^{(1)}$	empty	a-electron	$(L-2)!/D!(A-1)!\,B!(E-1)!$
$\sum^{(2)}$	empty	a- and b-electron	$(L-2)!/D!(A-1)!(B-1)!\,E!$
$\sum^{(3)}$	b-electron	a-electron	$(L-2)!/D!(A-1)!(B-1)!\,E!$
$\sum^{(4)}$	b-electron	a- and b-electron	$(L-2)!/D!(A-1)!(B-2)!(E+1)!$

$$+\sum_{\mathcal{M}\mathcal{N}}^{(2)} g^{2D+1} \det U_{\mathcal{M}}^{(ij)} \det V_{\mathcal{N}} + \sum_{\mathcal{M}\mathcal{N}}^{(3)} g^{2D+1} \det U_{\mathcal{M}}^{(ij)} \det V_{\mathcal{N}}$$

$$+\sum_{\mathcal{M}\mathcal{N}}^{(4)} g^{2D+2} \det U_{\mathcal{M}}^{(ij)} \det V_{\mathcal{N}}], \qquad (2\cdot26)$$

where summation over $(\mathcal{M}, \mathcal{N})$ is extended to all the possible configurations of L sites except for the i-th and the j-th sites such that $\mathcal{M}$ and $\mathcal{N}$ have common D sites doubly occupied. The restriction imposed on the i- and the j-th sites are different for each summation $\sum^{(s)}$ $(s=1, \cdots 4)$. In Table I we summarize the configurations of the i- and the j-th sites and the total number of terms under each summation. The expectation value of the interaction energy $U\sum_i a_i^+ a_i b_i^+ b_i$ can be obtained if we know $\langle \Phi_0 | G(g) D_i G(g) | \Phi_0 \rangle$. It is not difficult to show that

$$\langle \Phi_0 | G(g) D_i G(g) | \Phi_0 \rangle = \sum_D \sum_{\mathcal{M}\mathcal{N}}^{(i)} g^{2D+2} \det U_{\mathcal{M}} \det V_{\mathcal{N}}, \qquad (2\cdot27)$$

where the summation over $(\mathcal{M}, \mathcal{N})$ is the same as before with one exception that the i-th site is always kept as doubly occupied. The number of terms under summation is therefore estimated as

$$(L-1)!/D!(A-1)!(B-1)!(E+1)!.$$

The great difficulty in the estimation of the energy expectation values lies in the evaluation of the determinants $\det U_{\mathcal{M}}$, $\det V_{\mathcal{N}}$ etc. These determinants generally depend on the structure of configurations in $(\mathcal{M}, \mathcal{N})$, and this fact makes it hard to perform the summation over $\mathcal{M}$ and $\mathcal{N}$. To avoid this situation, Gutzwiller has introduced a simplifying assumption which is equivalent to neglecting the configuration dependence of all the determinants. To be more specific, consider $\det U_{\mathcal{M}}$ for example. If we could neglect its dependence on $\mathcal{M}$, $\det U_{\mathcal{M}}$ should be a function only of M, the number of a-electron on L sites. Thus we assume

$$\det U_{\mathcal{M}} = \langle \Phi_0 | \prod_{k \in \mathcal{M}} M_k \prod_{l \in \mathcal{M}} \bar{M}_l | \Phi_0 \rangle$$

$$\simeq \{\langle \Phi_0 | M_k | \Phi_0 \rangle\}^M \{\langle \Phi_0 | \bar{M}_l | \Phi_0 \rangle\}^{L-M} = m^M (1-m)^{L-M}, \qquad (2\cdot28)$$

where we have put

$$\langle \Phi_0 | M_k | \Phi_0 \rangle = L^{-1} \langle \Phi_0 | M | \Phi_0 \rangle = M/L = m. \qquad (2\cdot29)$$

Similarly we assume

$$\det V_{\mathfrak{N}} \simeq n^N (1-n)^{L-N},$$

$$\det U_{\mathfrak{M}}^{(ij)} \simeq m^{M-1} (1-m)^{L-M-1} u(ij), \qquad (2\cdot30)$$

$$\det V_{\mathfrak{N}}^{(ij)} \simeq n^{N-1} (1-n)^{L-N-1} v(ij)$$

with n defined by

$$\langle \Phi_0 | N_k | \Phi_0 \rangle = L^{-1} \langle \Phi_0 | N | \Phi_0 \rangle = N/L = n . \qquad (2\cdot31)$$

In this approximation, all the expressions for the expectation values of energy are much simplified, leading to the results

$$\langle \Phi_0 | G(g^2) | \Phi_0 \rangle = \sum_D g^{2D} (L!/D! \, A! \, B! \, E!) \, m^M (1-m)^{L-M} n^N (1-n)^{L-N},$$

$$\langle \Phi_0 | G(g) \sum_{ij} \varepsilon_{ij} a_i^+ a_j G(g) | \Phi_0 \rangle$$

$$= \sum_D g^{2D} (L!/D! \, A! \, B! \, E!) \, [AE + 2gAB + g^2 AB (B-1) (E+1)^{-1}]$$

$$\times m^{M-1} (1-m)^{L-M-1} n^N (1-n)^{L-N} L^{-1} (L-1)^{-1} \sum_{ij} \varepsilon_{ij} \langle \Phi_0 | a_i^+ a_j | \Phi_0 \rangle,$$

$$\langle \Phi_0 | G(g) \sum_{ij} \varepsilon_{ij} b_i^+ b_j G(g) | \Phi_0 \rangle$$

$$= \sum_D g^{2D} (L!/D! \, A! \, B! \, E!) \, [BE + 2gAB + g^2 BA (A-1) (E+1)^{-1}]$$

$$\times m^M (1-m)^{L-M} n^{N-1} (1-n)^{L-N-1} L^{-1} (L-1)^{-1} \sum_{ij} \varepsilon_{ij} \langle \Phi_0 | b_i^+ b_j | \Phi_0 \rangle,$$

$$\langle \Phi_0 | G(g) UDG(g) | \Phi_0 \rangle$$

$$= U \sum_D g^{2D+2} (L!/D! \, A! \, B! \, E!) \, AB (E+1)^{-1} m^M (1-m)^{L-M} n^N (1-n)^{L-N}.$$

$$(2\cdot32)$$

Now we are interested only in the limit of an infinitely large system $(L \gg 1)$. Then it is allowed to replace the sum over D by its largest term. For instance the normalization factor is given by one term

$$\langle \Phi_0 | G(g^2) | \Phi_0 \rangle \simeq g^{2D} (L!/D! \, A! \, B! \, E!) \, m^M (1-m)^{L-M} n^N (1-n)^{L-N}, \quad (2\cdot33)$$

where D is determined through a condition

$$\frac{\partial}{\partial D} (g^{2D}/D! \, A! \, B! \, E!) = 0 \qquad (2\cdot34)$$

which, upon using the relations

$$D+A=M, \qquad D+B=N, \qquad D+A+B+E=L, \qquad (2\cdot35)$$

turns out to give

$$g^2 = \frac{D(L-M-N+D)}{(M-D)(N-D)} = \frac{d(1-2c+d)}{(m-d)(n-d)} \qquad (2\cdot36)$$

with $D/L = d$ and $2c = m + n$. Performing the similar procedure for all other

expressions, we arrive at the final result

$$\langle \varPsi_g | H | \varPsi_g \rangle = \gamma_a \sum_{ij} \varepsilon_{ij} \langle \varPhi_0 | a_i^+ a_j | \varPhi_0 \rangle + \gamma_b \sum_{ij} \varepsilon_{ij} \langle \varPhi_0 | b_i^+ b_j | \varPhi_0 \rangle + UD , \quad (2\cdot37)$$

where

$$\gamma_a = [\sqrt{(m-d)(1-2c+d)} + \sqrt{(n-d)d}\,]^2 / m(1-m) ,$$
$$\gamma_b = [\sqrt{(n-d)(1-2c+d)} + \sqrt{(m-d)d}\,]^2 / n(1-n) . \quad (2\cdot38)$$

In deriving the last expressions $(2\cdot37)$ and $(2\cdot38)$, use has been made of the relation $(2\cdot36)$ and all the quantities of the order $1/L$ are ignored. γ_a and γ_b may be called the loss factor of the hopping energy, because they express the enhancement of the hopping energy which compensates the gain of the interaction energy due to the reduction of doubly occupied states. The expression $(2\cdot37)$ is essentially the same as that obtained by Gutzwiller in his original paper.

By making the expression $(2\cdot37)$ minimum, Gutzwiller derived a condition in which the energy of the saturated ferromagnetic state is lower than that of the paramagnetic state. Brinkman and Rice calculated the susceptibility for the case of one electron per atom $(c=1/2)$ and regarded the disappearance of the doubly occupied states as a metal-insulator transition.[5] Some discussion has been given for the case with band degeneracy.[6] In spite of the general believing that the ground state of this model is antiferromagnetic at least for sufficiently large U, the extention of the Gutzwiller method to the antiferromagnetic case has not been performed so far until recently.[7] In the following sections we extend the Gutzwiller approximation so as to include antiferromagnetism.

§ 3. Extension of the Gutzwiller approximation for antiferromagnetism

Hereafter we consider only the lattice which can be divided into two equivalent sublattices I and II in such a way that the nearest neighbours of a site on I always belong to II and vice versa. We shall not consider the case of ferrimagnetism explicitly for the sake of simplicity.

In the antiferromagnetic phase, the single-particle wave function can be chosen as

$$\xi_p(R_i) = (2L)^{-1/2}\left[\left\{1 - \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \varDelta^2}}\right\}^{1/2} + \exp(iKR_i)\left\{1 + \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \varDelta^2}}\right\}^{1/2}\right]\exp(ipR_i) ,$$

$$\eta_p(R_i) = (2L)^{-1/2}\left[\left\{1 - \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \varDelta^2}}\right\}^{1/2} - \exp(iKR_i)\left\{1 + \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \varDelta^2}}\right\}^{1/2}\right]\exp(ipR_i) ,$$

$$(3\cdot1)$$

where K is a reciprocal lattice vector having property

$$\exp(iKR_i) = \begin{cases} 1 & \text{for } i \epsilon \text{I} , \\ -1 & \text{for } i \epsilon \text{II} . \end{cases} \quad (3\cdot2)$$

The sets of single-particle wave functions $\{\xi_p(R)\}$ and $\{\eta_p(R)\}$ are specified by one parameter Δ, and in the Hartree-Fock approximation Δ is determined by an equation,[8]

$$\left(\frac{U}{L}\sum_{p\in\mathcal{P}}\frac{\text{sign}(\varepsilon_p)}{\sqrt{\varepsilon_p^2+\Delta^2}}+1\right)\Delta=0,\tag{3.3}$$

which is derived from the variation with respect to Δ as will be seen later. The functions $u(ij)$ $(v(ij))$ defined in (2.14) now become

$$\begin{matrix}u(ij)\\(v(ij))\end{matrix}=\begin{cases}\dfrac{1}{L}\sum_{p\in\mathcal{P}}\left(1-\dfrac{\text{sign}(\varepsilon_p)\Delta}{\sqrt{\varepsilon_p^2+\Delta^2}}\right)\exp[ip(R_i-R_j)] & \text{for } \begin{matrix}i\epsilon\mathrm{I},\ j\epsilon\mathrm{I}\\(i\epsilon\mathrm{II},\ j\epsilon\mathrm{II}),\end{matrix}\\[3mm]-\dfrac{1}{L}\sum_{p\in\mathcal{P}}\dfrac{\varepsilon_p}{\sqrt{\varepsilon_p^2+\Delta^2}}\exp[ip(R_i-R_j)] & \text{for }\begin{matrix}i\epsilon\mathrm{I},\ j\epsilon\mathrm{II}\\ \text{or } i\epsilon\mathrm{II}\ j\epsilon\mathrm{I},\end{matrix}\\[3mm]\dfrac{1}{L}\sum_{p\in\mathcal{P}}\left(1+\dfrac{\text{sign}(\varepsilon_p)\Delta}{\sqrt{\varepsilon_p^2+\Delta^2}}\right)\exp[ip(R_i-R_j)] & \text{for }\begin{matrix}i\epsilon\mathrm{II},\ j\epsilon\mathrm{II}\\(i\epsilon\mathrm{I},\ j\epsilon\mathrm{I}).\end{matrix}\end{cases}\tag{3.4}$$

If we call

$$r=\frac{1}{L}\sum_{p\in\mathcal{P}}\left(1-\frac{\text{sign}(\varepsilon_p)\Delta}{\sqrt{\varepsilon_p^2+\Delta^2}}\right),\qquad w=\frac{1}{L}\sum_{p\in\mathcal{P}}\left(1+\frac{\text{sign}(\varepsilon_p)\Delta}{\sqrt{\varepsilon_p^2+\Delta^2}}\right),\tag{3.5}$$

then $r(w)$ may be interpreted as the site probability of the right (wrong) particle which is either $a(b)$-electron on I(II) sublattice or $b(a)$-electron on I(II) sublattice.

The variation problem can be formulated through almost the same argument as in §2 even in the present case except that there is an additional freedom concerning the allotment of particles into two sublattices. The normalization factor for instance can be evaluated in the following way. We adopt the same approximation as stated in §2. The configurations of the sublattice I are specified by the number of sites in each four states, i.e., $(D_1A_1B_1E_1)$ and those of II by $(D_2A_2B_2E_2)$. Since we are considering the antiferromagnetic case, we can assume a symmetry between a- and b-electrons so that

$$D_1=D_2=D/2,\qquad A_1=B_2,\qquad A_2=B_1,$$
$$D_1+A_1=M_1=D_2+B_2=N_2,$$
$$D_2+A_2=M_2=D_1+B_1=N_1.\tag{3.6}$$

It is convenient to introduce the number of right (wrong) particle $X(Y)$ by

$$X=M_1+N_2,\qquad Y=M_2+N_1.\tag{3.7}$$

By the symmetry mentioned above

$$M_1=N_2=X/2,\qquad M_2=N_1=Y/2$$

and

$$M+N=M_1+M_2+N_1+N_2=X+Y=2C.\tag{3.8}$$

Then it is straightforward to find that

$$\langle \Phi_0 | G(g^2) | \Phi_0 \rangle$$
$$= \sum_D \sum_X g^{2D} [(L/2)!/(D/2)!\{(X-D)/2\}!\{(Y-D)/2\}!\{(L+D-2C)/2\}!]^2$$
$$\times r^X (1-r)^{L-X} w^Y (1-w)^{L-Y}. \tag{3.9}$$

Now we make the approximation to replace the sum over D and X with the largest term. The maximum term condition with respect to D gives a relation

$$g^2 = \frac{d(1-2c+d)}{(x-d)(y-d)} \tag{3.10}$$

and with respect to X gives

$$(y-d)/(x-d) = w(1-r)/r(1-w), \tag{3.11}$$

where $x=X/L$, $y=Y/L$, $c=C/L$. From the definitions (3.5), (3.7) and (3.8), it follows that

$$x+y = r+w = 2c. \tag{3.12}$$

The evaluation of the expectation values of energy in the antiferromagnetic case goes almost parallel with the argument given in § 2. We can easily show that

$$\langle \Phi_0 | G(g) a_i^+ a_j G(g) | \Phi_0 \rangle$$
$$= g^{2D} [(L/2)!/(D/2)!\{(X-D)/2\}!\{(Y-D)/2\}!\{(L+D-2C)/2\}!]^2$$
$$\times r^X (1-r)^{L-X-1} w^{Y-1} (1-w)^{L-Y}$$
$$\times u(ij) [(1-2c+d)(y-d) + g(y-d)(x+y-2d)$$
$$+ g^2(y-d)^2(x-d)/(1-2c+d)] \quad \text{when } i\epsilon\text{I}, \, j\epsilon\text{II}.$$

Upon dividing this expression by the normalization factor and eliminating g with (3.10), we have

$$\frac{\langle \Phi_0 | G(g) a_i^+ a_j G(g) | \Phi_0 \rangle}{\langle \Phi_0 | G(g^2) | \Phi_0 \rangle}$$
$$= \frac{(c-d)}{(c-rw)} \left[\sqrt{\frac{(1-w)(1-2c+d)}{(1-r)}} + \sqrt{\frac{w}{r}} d \right]$$
$$\times \left[\sqrt{\frac{(1-r)(1-2c+d)}{(1-w)}} + \sqrt{\frac{r}{w}} d \right] u(ij) \tag{3.13}$$

when $i\epsilon\text{I}$ and $j\epsilon\text{II}$. Quite similarly the same result is obtained for $i\epsilon\text{II}$ and $j\epsilon\text{I}$. All other quantities are similarly derived. For instance,

$$\langle \Phi_0 | G(g) D_i G(g) | \Phi_0 \rangle / \langle \Phi_0 | G(g^2) | \Phi_0 \rangle = d. \tag{3.14}$$

It is an easy task to sum up these results to find out the final result

$$\varepsilon_g = E_g/L = 2\gamma \frac{1}{L} \sum_{p \in \mathcal{P}} \frac{\mathrm{sign}(\varepsilon_p)\varepsilon_p{}^2}{\sqrt{\varepsilon_p{}^2 + \varDelta^2}} + Ud, \qquad (3 \cdot 15)$$

where

$$\gamma = \left(\frac{c-d}{c-rw}\right)\left[\sqrt{\frac{(1-w)(1-2c+d)}{(1-r)}} + \sqrt{\frac{w}{r}d}\right]$$

$$\times \left[\sqrt{\frac{(1-r)(1-2c+d)}{(1-w)}} + \sqrt{\frac{r}{w}d}\right]. \qquad (3 \cdot 16)$$

Since d is a function of g, we may take d as the variation parameter instead of g. Then the variation function ε_g has to be minimized as the function of d and $\varDelta$. When we fix $g=1$, the variation problem should reduce to the Hartree-Fock theory of antiferromagnetism, and if we put $\varDelta=0$, it should go back to the Gutzwiller approximation in the paramagnetic case, i.e., the case $m=n=c$ in § 2. To check these points, first we assume $g=1$ in (3·10). Then it immediately follows from (3·10) and (3·11) that $d=rw$. Hence we obtain $\gamma=1$ from (3·16) and the variation function is reduced to

$$\varepsilon_A = \frac{2}{L} \sum_{p \in \mathcal{P}} \frac{\mathrm{sign}(\varepsilon_p)\varepsilon_p{}^2}{\sqrt{\varepsilon_p{}^2 + \varDelta^2}} + Urw. \qquad (3 \cdot 17)$$

It is not hard to show that $\partial \varepsilon_A / \partial \varDelta = 0$ leads to Eq. (3·3). In the next place we assume $\varDelta = 0$. For this case from (3·5)

$$r = w = c$$

and (3·11) gives us $x = y$. Thus the loss factor (3·16) now becomes

$$\gamma = [(c-d)/c(1-c)][\sqrt{1-2c+d} + \sqrt{d}]^2 \qquad (3 \cdot 18)$$

which is precisely the same as (2·38) when $m=n=c$.

§ 4. Numerical calculation

In the preceeding section, we have derived a prescription for the energy to be used as the variation function. This section is devoted to the numerical calculation for actual variation procedure.

For simplicity, we assume that the state density function is of the form

$$\rho(\varepsilon) = \begin{cases} \dfrac{1}{2W} & \text{if } |\varepsilon| < W, \\ \\ 0 & \text{otherwise}. \end{cases} \qquad (4 \cdot 1)$$

$2W$ is the full band width and the center of gravity of the state density is chosen at $\varepsilon = 0$ in accord with the present model Hamiltonian (2·1). (Note that $L^{-1}\sum_p \varepsilon_p = \varepsilon_{ii} = 0$.) Since $\rho(\varepsilon)$ is normalized to unity, the Fermi energy ε_F is related to the number of electron per site c by

$$\int_{-W}^{\varepsilon_F} \rho(\varepsilon)\, d\varepsilon = (W + \varepsilon_F)/2W = c\,. \tag{4.2}$$

In what follows, it is convenient to use W as a unit of energy so that all the quantities may become dimensionless. Then (4.2) reads

$$\varepsilon_F = 2c - 1\,. \tag{4.2'}$$

With (4.1), the expectation value of energy (3.15) is, after short manipulation, given as

$$\varepsilon_g = (\gamma/2)\left[|2c-1|\sqrt{(2c-1)^2 + \varDelta^2} - \sqrt{1+\varDelta^2}\right.$$
$$\left. + \varDelta^2 \log\left[\{1 + \sqrt{1+\varDelta^2}\}/\{|2c-1| + \sqrt{(2c-1)^2 + \varDelta^2}\}\right]\right] + Ud\,. \tag{4.3}$$

In this expression γ is still a function of $\varDelta$ through the definition (3.16) in which r and w are given by $r + w = 2c$ and

$$r - w = \varDelta \log\left[(1 + \sqrt{1+\varDelta^2})/\{|2c-1| + \sqrt{(2c-1)^2 + \varDelta^2}\}\right]. \tag{4.4}$$

The problem is now to find out the minimum of ε_g as a function of g (or d) and $\varDelta$ for given values of c and U. It is not easy, however, to carry out this variation analytically for general value of c except for a special case $c = 1/2$. Therefore, inserting various values of g and $\varDelta$ into Eq. (4.3), we calculate ε_g numerically for given c and U, and look for the values of g and $\varDelta$ for which ε_g becomes minimum. (As a check, in the Appendix we discuss the case of $c = 1/2$ somewhat in detail by an analytical method.) As an example, in Figs. 1(a) $\sim$ (c) the contour maps of ε_g for various values of the parameters are shown. It turns out (more or less unexpectedly) that, for any values of c and U, ε_g never takes the minimum value so long as $\varDelta > 0$ and $0 < g < 1$. From a reason we shall give in §5, the value of g may be restricted to $g \leq 1$. Thus the minimum of ε_g can occur only on the boundaries of the variable range of g and $\varDelta$, i.e., $g = 1$ or $\varDelta = 0$. This means that it is enough to compare the energy of the antiferromagnetic state in the Hartree-Fock approximation ($g = 1$, $\varDelta \neq 0$) and that of the paramagnetic state in the Gutwiller approximation ($g \neq 1$, $\varDelta = 0$).

First we examine the case $g = 1$. Using (4.1) we can easily set up the gap equation (3.3) which is in the present model put in a form

$$\varDelta\{1 - (U/2)\log[(1 + \sqrt{1+\varDelta^2})/(|2c-1| + \sqrt{(2c-1)^2 + \varDelta^2})]\} = 0\,, \tag{4.5}$$

the relevant solution of which is given by

$$\varDelta = \frac{[\{|2c-1| - \exp(2/U)\}\{|2c-1| - \exp(-2/U)\}]^{1/2}}{\sinh(2/U)}\,. \tag{4.6}$$

The minimized energy in this case denoted by ε_A is written as

$$\varepsilon_A = \tfrac{1}{2}\left[|2c-1|\sqrt{(2c-1)^2 + \varDelta^2} - \sqrt{1+\varDelta^2}\right] + Uc^2$$
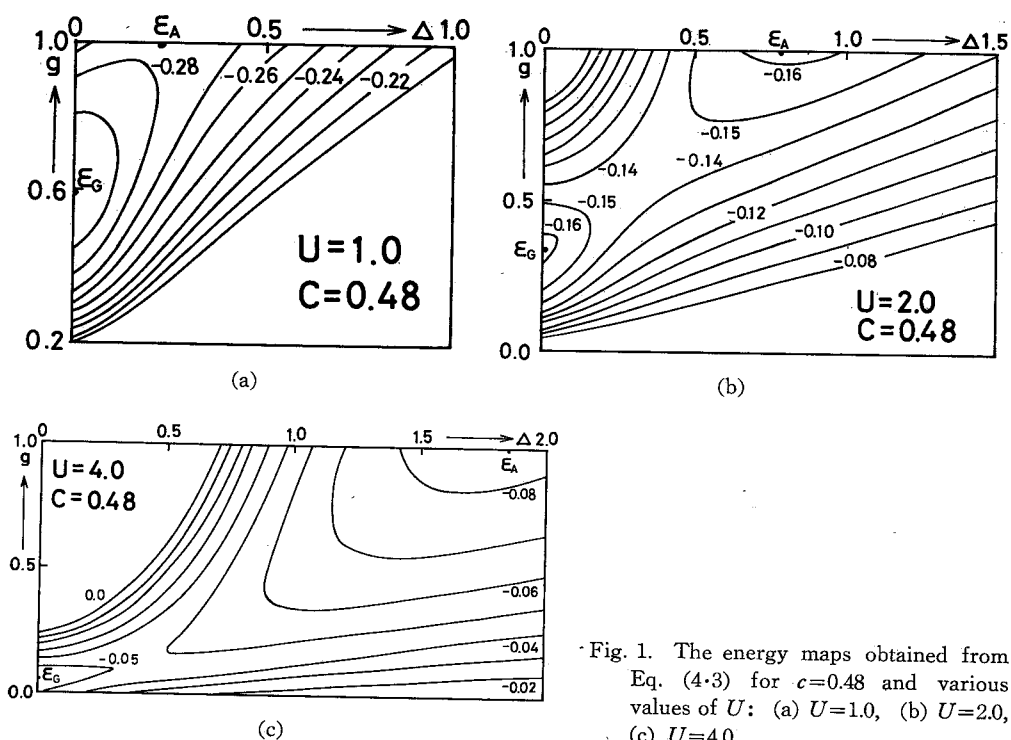$$= -\{1 + 2c(c-1)\}\coth(2/U) + |1-2c|/\sinh(2/U) + Uc^2. \tag{4.7}$$

Fig. 1. The energy maps obtained from Eq. (4·3) for $c=0.48$ and various values of U: (a) $U=1.0$, (b) $U=2.0$, (c) $U=4.0$.

If we put $\varDelta=0$ in this expression, we have the energy of the paramagnetic state in the Hartree-Fock approximation

$$\varepsilon_p = 2c(c-1) + Uc^2. \tag{4·8}$$

For the case that $\varDelta=0$ and $g \neq 1$ (Gutzwiller case), the energy which is denoted by ε_G becomes, upon using (3·18) and (4·3) with $\varDelta=0$,

$$\varepsilon_G = -2(c-d) \left[\sqrt{1-2c+d} + \sqrt{d}\right]^2 + Ud. \tag{4·9}$$

The condition to minimize ε_G yields an equation

$$U = 2[\sqrt{1-2c+d} + \sqrt{d}]^2 [(c-d) \{d(1-2c+d)\}^{-1/2} - 1]. \tag{4·10}$$

It is hard to express the minimum value of ε_G in terms of U in a simple form.

In Fig. 2 the minimum energy per electron ε_A/c, ε_p/c and ε_G/c are plotted as a function of U for the case $c=0.45$, 0.48 and 0.5. From these figures we can draw important conclusions:

(1) There exists a threshold value of c, say c_s, only above which the antiferromagnetic phase can appear. In other words, the system is always paramagnetic if $c < c_s$ regardless of the magnitude of U.

(2) When $c_s < c < 1/2$, where we confine ourselves to the case $c < 1/2$ for a moment, three cases can be discriminated according to the magnitude of U:
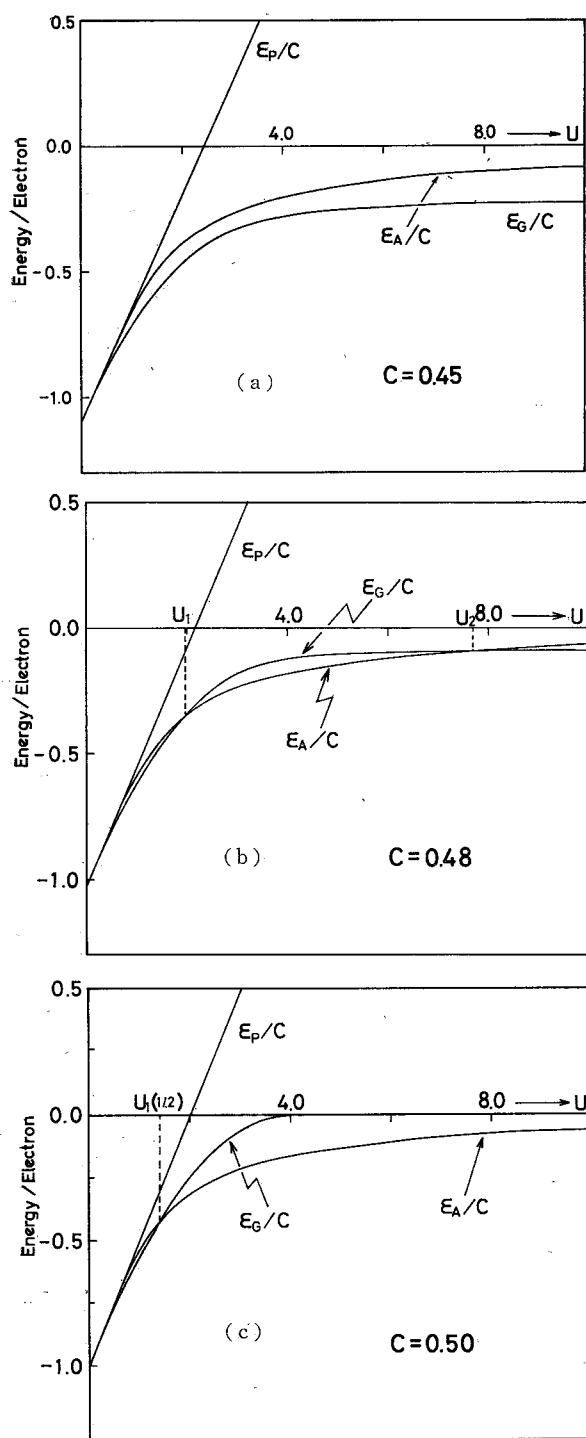
(a) For $U < U_1(c)$, the energy of the antiferromagnetic phase is higher than that of the paramagnetic phase in the Gutzwiller approximation.

(b) For $U_1(c) < U < U_2(c)$, the paramagnetic state is stable, but the antiferromagnetic state is more stable than the Gutzwiller paramagnetic state. (See also Fig. 1(c).)

(c) For $U > U_2(c)$, the energy of the paramagnetic state becomes again lower than that of the antiferromagnetic state.

As obvious from the above results, the antiferro-paramagnetic transition is of first order.

Figure 3 shows the phase diagram calculated in the U-c plane. Due to the particle-hole symmetry inherent to the model Hamiltonian (2·1), the phase diagram itself becomes symmetric with respect to the line $c = 1/2$. The solid line shows the phase boundary $\varepsilon_A = \varepsilon_G$ and the dotted line that of $\Delta = 0$

Fig. 2. The dependence of energy per electron ε_A/c, ε_G/c and ε_p/c on the coupling constant U for various values of c: (a) $c = 0.45$ $\varepsilon_G < \varepsilon_A$ for all U, (b) $c = 0.48$ $\varepsilon_G < \varepsilon_A$ for $0 < U < U_1$ and $U_2 < U$, $\varepsilon_G > \varepsilon_A$ for $U_1 < U < U_2$, (c) $c = 0.5$ $\varepsilon_G < \varepsilon_A$ for $0 < U < U_c \equiv U_1(1/2)$, $\varepsilon_G > \varepsilon_A$ for $U > U_c$.
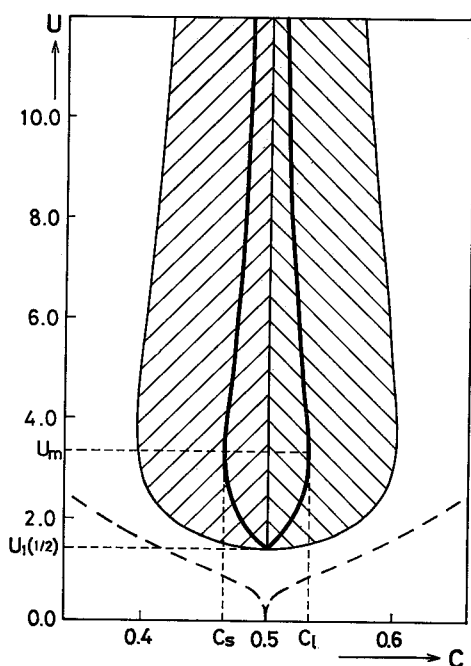
Fig. 3. The phase boundaries determined by $\varepsilon_A = \varepsilon_G$ and $\Delta = 0$ in Eq. (4·4). The thick solid line indicates $\varepsilon_A = \varepsilon_G$ and the dotted line indicates the critical line calculated by Penn's method at which the second order phase transition occurs. The hatched area shows the region where the antiferromagnetic phase with $c = 1/2$ and the paramagnetic phase ($c \neq 1/2$) coexist.
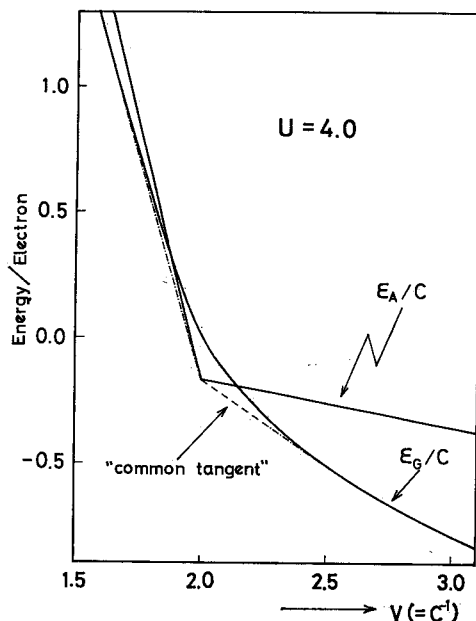
Fig. 4. The dependence of ε_A/c and ε_G/c on the volume $v = 1/c$.

in Eq. (4·6). As seen from this figure, it exhibits a striking contrast to Penn's diagram which was calculated on the basis of the Hartree-Fock approximation. Main differences between both diagrams are: In the present model

(i) as the coupling constant U becomes large, the region of c in which the antiferromagnetic phase appears becomes narrower.

(ii) In order that the antiferromagnetic phase may exist, a finite value of U or c is required. The critical values are: $c = 1/2$, $U_1(1/2) = 1.41$: $c_s = 0.467$, $c_1 = 1 - c_s = 0.533$, $U_m = 3.34$. The reason for this behaviour will be discussed in the following section.

So far we have assumed implicitly that the system is in a homogeneous state. However, in view of the fact that the antiferro-paramagnetic transition is of first order, it is necessary to consider a possibility that the system is in an inhomogenous state in which two phases with different magnetic order and c coexist.[9] For this purpose we plot the energy of each phase as a function of

volume $v = 1/c$ in Fig. 4. The curve for the antiferromagnetic phase has a cusp point at $v = 2$ because of the existence of the energy gap. In the present model, therefore, a common tangent line in the proper sense cannot be drawn between the antiferro- and paramagnetic phases. Nevertheless, by examining a condition where two phases have equal chemical potential, we find that a tangent line which touches the curve for the paramagnetic phase and passes through the cusp point gives the coexistence line. In Fig. 3 the coexistence region thus determined is also shown in the U-c diagram.

§ 5. Summary and discussion

We have extended the Gutzwiller variation method so as to include antiferromagnetism, and using a simplifying assumption corresponding to that adopted by Gutzwiller to discuss paramagnetic and ferromagnetic phases, we have tried to find out an antiferromagnetic ground state including electron correlation. Against our expectation, the final results are that the stable ground state is either the Gutzwiller paramagnetic state or the antiferromagnetic state in the Hartree-Fock approximation and we could not find out any antiferromagnetic state including electron correlation with lower energy than the above mentioned states. Inspecting the contour maps shown in Fig. 1, we observe that the Gutzwiller solution is locally stable against the variation of Δ. On the other hand the antiferromagnetic solution in the Hartree-Fock approximation is not stable against the variation of g, and for sufficiently large U, the larger is g than unity, the lower the energy is. At first sight this seems curious, because we are considering the effect of correlation due to repulsive force and hence the region where $g > 1$ should corresponds to the states energetically unfavourable. A careful calculation, however, reveals that when $g > 1$ the occupation number

$$\langle n_p \rangle = \sum_{ij} \langle \Psi_g | a_i^+ a_j | \Psi_g \rangle \exp[ip(R_i - R_j)] \tag{5.1}$$

becomes negative for certain region of momentum p within the present approximation. Thus the states with $g > 1$ should be rejected as unphysical.

Some of the situation mentioned above would have its origin in the too simplified approximation. The formation of the the antiferromagnetic superlattices with a long range order characterized by a finite Δ can reduce the repulsive interaction energy between electrons having opposite spin and at the same time keep the increase of hopping energy minimum. On the other hand in the Gutzwiller state under the simplified approximation, the increase of kinetic energy is not properly suppressed because of the neglection of configurational fluctuation, although the repulsive interaction energy is reduced by avoiding double occupation of sites. This is probably the reason why the Hartree-Fock antiferromagnetic state has lower energy than the Gutzwiller state for certain range of U. It is hoped to improve approximation in order to clarify these

points.

In spite of the involved problems arising from the nature of the adopted approximation, many of the results extracted from the present numerical calculation seems to remain valid. Let us discuss some of them.

A conspicuous result much different from Penn's calculation is that, with increasing U, the region of c where the antiferromagnetic state has lower energy than the paramagnetic state becomes narrower. We can easily show that in the limit $U \to \infty$ the energies ε_G and ε_A have asymptotic forms when $c < 1/2$:

$$\varepsilon_G \sim -2c(1-2c) - 4c^2(1-2c)/U , \tag{5.2}$$

$$\varepsilon_A \sim -(3-6c+4c^2)/3U . \tag{5.3}$$

The first term in the right-hand side of (5.2) corresponds to the hopping energy due to the presence of $(1-2c)L$ empty sites and is equal to the energy in the ferromagnetic state. This is in accord with the result obtained by Nagaoka[10] that the ground state for $U = \infty$, $c = 1/2 - \delta$ ($\delta \ll 1$) should be ferromagnetic. Thus Eq. (5.2) gives the correct limiting behaviour. For $c = 1/2$, Eqs. (5.2) and (5.3) give

$$\varepsilon_G - \varepsilon_A \sim 1/3U . \tag{5.4}$$

It can be shown that in the present approximation $\varepsilon_G - \varepsilon_A$ takes a maximum at a certain intermediate value of U and vanishes in proportion to the inverse of U as Eq. (5.4) for sufficiently large U. This limit corresponds to an insulating antiferromagnet with a superexchange $J \sim W^2/U$ (in the original energy unit) and leads to a correct result.

The next point to be dicussed is that in our calculation a finite value of U is needed for the appearance of antiferromagnetic phase. In a simple Hartree-Fock approximation, the staggered susceptibility is given by

$$\chi_{HF} = \chi_0 \Big/ \left(1 - \frac{U}{2}\chi_0\right), \tag{5.5}$$

where χ_0 is defined by

$$\chi_0 = -\sum_p (n_{p+K} - n_p)/(\varepsilon_{p+K} - \varepsilon_p) = -\log(1-2c) . \tag{5.6}$$

The last result of Eq. (5.6) is obtained when the use has been made of the state density (4.1). In virtue of Eq. (5.5) the paramagnetic state in the simple Hartree-Fock approximation makes a transition to the antiferromagnetic state when

$$U \geq 2/\chi_0 . \tag{5.7}$$

Since χ_0 diverges for $c = 1/2$, an infinitesimally small repulsion U is sufficient to realize the antiferromagnetic state. This is not the case, however, in the Gutzwiller state, for which the staggered susceptibility is calculated, when $c = 1/2$, as

$$\chi_{\mathrm{G}} = \chi_0 (4+U)/(4-U). \tag{5.8}$$

Although χ_0 diverges at $c=1/2$, χ_{G}^{-1} becomes negative only when

$$U > 4. \tag{5.9}$$

As seen from Figs. 2(c) and 3, actually ε_A becomes lower than ε_G when $U > 1.41$ for $c=1/2$. This behaviour will be discussed in the Appendix.

So far we have paid little attention to the ferromagnetic state. This is because we have assumed a simplified model with Hamiltonian (2.1) and the state density function (4.1) and it is well known that the conditions for appearance of the ferromagnetic state depend heavily on state density and band degeneracy.[1] It should be stated, however, that in the present model the ferromagnetic state can appear only in the limit $U \to \infty$. It should be also remarked that the metal-insulator transition, which is expected at $U=4$ and $c=1/2$ according to Brinkman and Rice,[5] is eliminated in the present model, because before U exceeds 4 the ground state becomes antiferromagnetic where d always remains finite.

Acknowledgements

Appendix

Analytical Treatment of the Case c=1/2

In the special case $c=1/2$, the loss factor γ has a simple form

$$\gamma = d(1-2d)/rw(1-2rw). \tag{A.1}$$

Then, the variation function ε_g can be written as

$$\varepsilon_g = -\zeta(\varDelta)d(1-2d) + Ud, \tag{A.2}$$

where $\zeta(\varDelta)$ is a function of only $\varDelta$ defined by

$$\zeta(\varDelta) = \frac{2}{rw(1-2rw)} \frac{1}{L} \sum_{p \in \mathcal{P}} \frac{\varepsilon_p^2}{\sqrt{\varepsilon_p^2 + \varDelta^2}}. \tag{A.3}$$

For given $\varDelta$ or $\zeta(\varDelta)$, ε_g, as a function of d, takes a minimum

$$\varepsilon_g(\zeta) = -(\zeta/8)(1-U/\zeta)^2 \tag{A.4}$$

at

$$d(\zeta) = (1/4)(1-U/\zeta). \tag{A.5}$$

If $\zeta < U$, we should take $d = d(U) = 0$ instead of $d(\zeta)$, because d must be non-negative. Therefore we can consider as $\zeta \geq U$. Since $\varepsilon_g(\zeta)$ is a monotone decreasing function of ζ in the region $\zeta \geq U$, the maximum value of ζ as a function of $\varDelta$ corresponds to the minimum value of Eq. (A·4). As stated in §5, g is restricted to $g \leq 1$, and this restriction defines a boundary line $d \leq r(\varDelta) w(\varDelta)$. Combining this condition with (A·5), we have

$$\zeta(\varDelta)\{1 - 4r(\varDelta)w(\varDelta)\} \leq U. \quad (A\cdot 6)$$

Therefore the maximum of ζ satisfies either the equality of Eq. (A·6) or $d\zeta/d\varDelta = 0$. The function $\zeta(\varDelta)$ calculated

Fig. 5. $\zeta(\varDelta)$ as a function of $\varDelta$.

with the use of the state density function (4·1) is shown in Fig. 5. As seen from this figure $\varDelta = 0$ is the only local maximum of $\zeta(\varDelta)$, and hence for sufficiently small U the minimum value of $\varepsilon_g(\zeta)$ is provided by

$$\varepsilon_g = -(\zeta(0)/8)(1 - U/\zeta(0))^2 = \varepsilon_G(U), \quad (A\cdot 7)$$

which is nothing but the energy of the Gutzwiller state. This energy $\varepsilon_G(U)$ ceases to be the minimum when U exceeds a certain value U_0 determined from

$$\zeta(\varDelta_0)\{1 - 4r(\varDelta_0)w(\varDelta_0)\} = U_0, \quad (A\cdot 8)$$

where $\varDelta_0$ is such that $\zeta(0) = \zeta(\varDelta_0)$. (See Fig. 5) It is not excluded, however, that there exists a less energy state on the boundary line $d = rw$ at a point other than that given by (A·8). This is indeed the case and when $U > U_c$ (U_c has a value smaller than U_0) the true minimum of ε_g is taken over by $\varepsilon_A(U)$, which is the minimum value of $\varepsilon_{g=1}$ along the line $d = rw$ and corresponds to the anti-ferromagnetic solution of the Hartree-Fock approximation. Thus we have the behaviour depicted in Fig. 2(c).
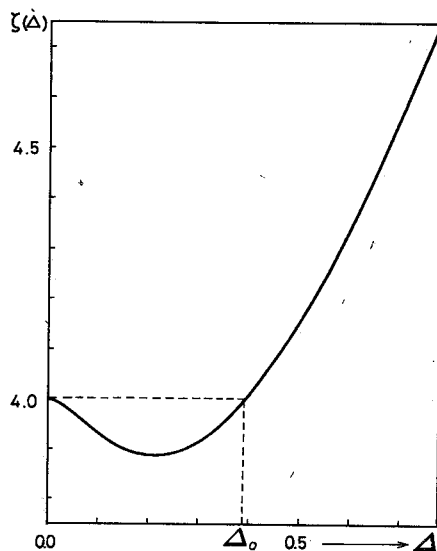
References

1) As a general reference see
   C. Herring, *Magnetism IV*, ed. G. T. Rado and H. Suhl (Academic Press, New York, 1966).
2) J. Hubbard, Proc. Roy. Soc. **A276** (1963), 236; **A277** (1964), 237; **A281** (1964), 401.
3) M. C. Gutzwiller, Phys. Rev. Letters **10** (1963), 159; Phys. Rev. **134** (1964), A923; **137** (1965), A1726.
4) D. R. Penn, Phys. Rev. **142** (1966), 350.
   Variational problem and instability in the Hartree-Fock approximation are discussed by many authors. For instance:

D. J. Thouless, Nucl. Phys. **21** (1960), 225.

K. Sawada and N. Fukuda, Prog. Theor. Phys. **25** (1961), 653.

N. Fukuda, Nucl. Phys. **44** (1963), 553.

F. Iwamoto and K. Sawada, Phys. Rev. **126** (1962), 882.

N. Fukuda, T. Ogawa and T. Soda, Prog. Theor. Phys. Suppl. Extra Number (1965), 492.

5) W. F. Brinkman and T. M. Rice, Phys. Rev. **B2** (1970), 4302.

See also K. A. Chao, Solid State Comm. **14** (1974), 525.

6) K. A. Chao and M. C. Gutzwiller, J. Appl. Phys. **42** (1971), 1420.

K. A. Chao, Phys. Rev. **B4** (1971), 4034; **B8** (1973), 1088; J. Phys. C: Solid State Phys. **7** (1974), 127.

7) J. Bernasconi, Phys. Kondens. Materie **14** (1972), 225.

F. Takano and M. Uchinami, Prog. Theor. Phys. **53** (1975), No. 5.

8) Gap equation of this sort for antiferromagnet has been first derived by one of the present authors:

T. Matsubara and T. Yokota, *Proceedings of the International Conference on Theoretical Physics, Kyoto* (1953), p. 693.

T. Matsubara, J. of the Faculty of Science, Hokkaido Univ. **4** (1954), 292.

9) A possibility of the coexistence of different phases is also remarked by Visscher:

P. B. Visscher, Phys. Rev. **B10** (1974), 932, 943.

10) Y. Nagaoka, Solid State Comm. **3** (1965), 409; Phys. Rev. **147** (1966), 397.