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Validity of the Gutzwiller Scheme for Electron Correlation in Narrow Bands

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The Gutzwiller variational method for narrow energy bands has been re-examined near the metal-insulator transition. We found that in this case the peak-term approximation breaks down. The correct treatment is pointed out for future analysis.

I. INTRODUCTION

THE electron correction effect has been extensively studied since the early stage of the modern solid state physics. The short range correlation of electrons in narrow energy bands has been generally investigated in terms of the Hubbard model[1]. In 1963 Gutzwiller[2] proposed a variational method to treat the Hubbard model, which provided a reasonable interporation between the exact solutions of the atomic limit and the band limit. The basic idea of the Gutzwiller scheme is that the amplitudes of doubly occupied states in an unperturbed single-Slater-determinant state are reduced via a single variational parameter. For a half-filled band, the amplitudes of doubly occupied states become zero when the intra-atomic correlation energy exceedes a critical value. Accoıding to Brinkman and Rice[3], such vanishing amplitudes mark a metal to insulator transition. However, simple second order perturbation calculation indicates that such amplitudes can never be zero, though may be very small(*). Therefore, the validity of the Gutzwiller scheme in the vicinity of the metal-insulator transition needs further examination. In this paper we will show that one of the three approximations in the Gutzwiller scheme, namely, the peak-term approximation breaks down when the metal-insulator transition is approached from the metallic side.

II. GUTZWILLER SCHEME

Let us write the Hubbard Hamiltonian[1] as

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + U \sum_{l} n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

where $a_{i\sigma}^{+}$ and $a_{i\sigma}$ are respectively, the creation and the annihilation operators associated to the d-spin Wannier function localized around the ith lattice site. $n_{i\sigma} = a_{i\sigma}^{+} a_{i\sigma}$ is the number operator and U is the intra-atomic Coulomb energy for doubly occupied site. Via the transformation between the Bloch and the Wannier representations, the first term in (1) yields the ordinary energy band picture where

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(1) J. Hubbard, Proc. Roy. Soc. A276, 238 (1963).
(2) M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963): Phys. Rev. 137, Al726 (1965).
(3) W. F. Brinkman and T. M. Rice, Phys. Rev. B2, 4302 (1970).
(4) J. Florencio Jr. and K. A. Chao, Phys. Rev. Lett. 35, 741 (1975); Phys. Rev. B14, 3121 (1976).

the band energy E(k) can be obtained from the electron transfer energy t_{ij}.

Since the metal-insulator transition occurs only in half-filled bands, we will consider only the case that both the number of electrons and the number of lattice sites are N. We further restrict ourselves to the case of nonmagnetic state such that $N(\uparrow)=N(\downarrow)=N/2$, where $N(\sigma)$ is the number of u-spin electrons. We first consider a particular configuration containing μ doubly occupied sites. If $G(\updownarrow;\mu)$ is a set of μ lattice sites and $G(\uparrow;\mu)$ and $G(\downarrow;\mu)$ are two sets containing $N/2-\mu$ lattice sites each, then a localized many-electron wave function can be written as

$$\Phi(G_\mu)=\prod_{g\in G(\uparrow\downarrow;\mu)} a_{g\uparrow}^{+}a_{g\downarrow}^{+}\prod_{g\in G(\uparrow;\mu)} a_{g\uparrow}^{+}\prod_{g\in G(\downarrow;\mu)} a_{g\downarrow}^{+}\mid 0> \tag{2}$$

where $\mid 0>$ is the vacum. For convenience, we define the linear combination

$$\Psi_{c\mu}=\sum_{G_\mu} A(G_\mu)\Phi(G_\mu). \tag{3}$$

Then the eigenfunctions of the Hubbard Hamiltonian have the general form

$$\Psi_c=\sum_{\mu=0}^{N/4} F_\mu\Psi_{c\mu}=\sum_{\mu=0}^{N/4}\sum_{G_\mu} F_\mu A(G_\mu)\Phi(G_\mu) \tag{4}$$

with proper choices of the coefficients $A(G_\mu)$'s and F_μ's.

Gutzwiller[2] proposed the following variational method to find from (4) the ground state of H. At the band limit $U=0$, we know that the ground state is simply the Fermi sea

$$\Psi_0=\prod_\sigma\prod_{k\in K(\sigma)} a_{k\sigma}^{+}\mid 0> \tag{5}$$

where $a_{k\sigma}^{+}$ is the creation operator for the $k\sigma$-Bloch state and $K(\uparrow)$ and $K(\downarrow)$ are two state of k-vectors in the reciprocal space. Using the transformation

$$a_{k\sigma}^{+}=\frac{1}{\sqrt{N}}\sum_g e^{ikg}\,a_{g\sigma}^{+} \tag{6}$$

we can rewrite (5) as

$$\Psi_0=\sum_{\mu,G_\mu} A_0(K,\ G_\mu)\Phi(G_\mu) \tag{7}$$

where K represents both $K(\uparrow)$ and $K(\downarrow)$. Since we know the explicit expression (6), the coefficients $A_0(K,G_\mu)$'s are known quantities. For finite intra-atomic Coulomb energy $U\neq 0$, Gutzwiller proposed the trial function for the ground state

$$\Psi_c(K)=\prod_i\{1-(1-\eta)n_{i\uparrow}n_{i\downarrow}\}\Psi_0=\sum_{\mu=0}^{N/4}\sum_{G_\mu}\eta^\mu A_0(K,\ G_\mu)\Phi(G_\mu) \tag{8}$$

where η is a variational parameter to minimize the total energy $E(\eta)=\langle\Psi_c(K)\mid H\mid\Psi_c(K)\rangle/\langle\Psi_c(K)\mid\Psi_c(K)\rangle$.

Comparing (4) and (8), we see that Gutzwiller made the following approximations: (1) The phase factor in $A(K,\ G_\mu)$ for $U\neq 0$ is approximated by the phase factor in $A_0(K,\ G_\mu)$ for $U=0$, and (2) The coefficients F_μ's satisfy the condition $F_{\mu+1}/F_\mu=\eta$.

With the single-site approximation for the Kikuchi cluster variational method"[5], Gutzwiller calculated all the mateix elements appeared in $\langle\Psi_c(K_l)\mid\Psi_c(K)\rangle$ and $(K,(K)\mid H\mid\Psi_c(K)\rangle$. In particular, $\langle\Psi_c(K)\mid V',(K)\rangle$ turns out to be a hypergeometric function of η, which is sharply peaked at $\mu=\nu$. For given value of η, we have

$$\nu=N\eta/2(1+\eta). \tag{9}$$

Therefore, in calculating $\langle\Psi_c(K)\mid H\mid\Psi_c(K)\rangle/\langle\Psi_c(K)\mid\Psi_c(K_l)\rangle$ Gutzwiller retained only the contribution from the term with $\mu=\nu$. We call this third approximation the peak-term approximation. In this approximation, the total energy is found to be

(5) R. Kikuchi, Phys. **81,** 988 (1951).

$$E=(1-U/8|\bar{\varepsilon}|)^2\bar{\varepsilon} \tag{10}$$

and (9) becomes

$$\nu=0.25(1\text{ -U/8 }|\bar{\varepsilon}|,$$

where $\bar{\varepsilon}<0$ is the mean energy per electron when $U=0$. We note that ν approaches zero as U approaches the critical value $U_c=8|\bar{\varepsilon}|$.

III. VALIDITY OF THE PERK-TERM APPROXIMATION

Brinkman and Rice[3] pointed out that for the metallic state we must have $\nu\neq 0$, and $\nu=0$ corresponds to the insulating state. Since $\nu\geq 0$, we then have $\nu=0$ as the criterion for the metal-insulator transition in the Gutzwiller scheme. We can describe the Brinkman-Rice result in an alternative manner: In the metallic state ν is of order N, while in the very near vicinity of the metal-insulator transition ν is of order 1.

Let us recall that the peak-term approximation is based on the fact that the hypergeometric series of <K,(K) $|\Psi_c(K)\rangle$ can be approximated by a single term. In such approximation we have neglected terms of order 1. Therefore, since ν is of order 1 near the metal-insulator transition, in this region the peak-term approximation most likely breaks down. If so, as the metal-insulator transition is approached from the metallic side, ν should not approach zero continuously as predicted by the Gutzwiller result[2,3]. Rather, ν may be finite in agreement with the prediction of the second order perturbation theory.

To check this point, we must analyze the expression <K,(K) $|\Psi_c(K)\rangle$ in more details. Our purpose is to see whether the hypergeometric series of $\langle\Psi_c(K)|\Psi_c(K)\rangle$ is really sharply peaked at $\mu=\nu$ when ν is of order 1. Therefore, we should rewrite (8) as

$$\Psi_c(K)=\sum_{\mu=0}^{N/4}\Psi_\mu(K) \tag{12}$$

and calculate $\langle K,(K)|\Psi_\mu(K)\rangle$ for small values of ν, where

$$\Psi_\mu(K)=\sum_{G_\mu}\eta^\mu A_0(K,G_\mu)\Phi(G_\mu). \tag{13}$$

For given value of η, let us define

$$P(\mu)=\langle\Psi_\mu(K)|\Psi_\mu(K)\rangle/\langle\Psi_\nu(K)|\Psi_\nu(K)\rangle \tag{14}$$

where ν is determined by (9). It is straight forward to show

$$\begin{aligned} P(\mu)&=\eta^{2(\mu-\nu)}\prod_{j=1}^{\mu-\nu}(N-2\nu-2j)^2/4(\nu+j)^2 && \text{if } \mu>\nu,\\ 1&= && \text{if } \mu=\nu,\\ &=\eta^{2(\mu-\nu)}\prod_{j=1}^{\nu-\mu}4(\nu-j)^2/(N-2\nu+2j)^2 && \text{if } 0\leq\mu<\nu. \end{aligned} \tag{15}$$

Since the crucial range of μ is of order ν, using the relation (9) we obtain

$$\begin{aligned} P(\mu)&\simeq\prod_{j=1}^{\mu-\nu}\nu^2/(\nu+j)^2 && \text{if } \mu>\nu,\\ &=1 && \text{if } \mu=\nu,\\ &\simeq\prod_{j=1}^{\nu-\mu}(\nu-j)^2/\nu^2 && \text{if } 0\leq\mu<\nu. \end{aligned} \tag{16}$$

For given value of ν, $P(\mu)$ as a function of μ is shown in Fig. 1. If we follow the peak-term approximation, we should set $P(\mu)=\delta_{\mu,\nu}$. However, Fig. 1 clearly indicates that the peak-term approximation breaks down for small finite values of ν. Only when $\nu=0$ the peak-term approximation holds, i. *e.*, $P(\mu)=0$ if $\mu>0$. Consequently, the result that $\nu=0$ for $U\geq U_c$ is incorrect since

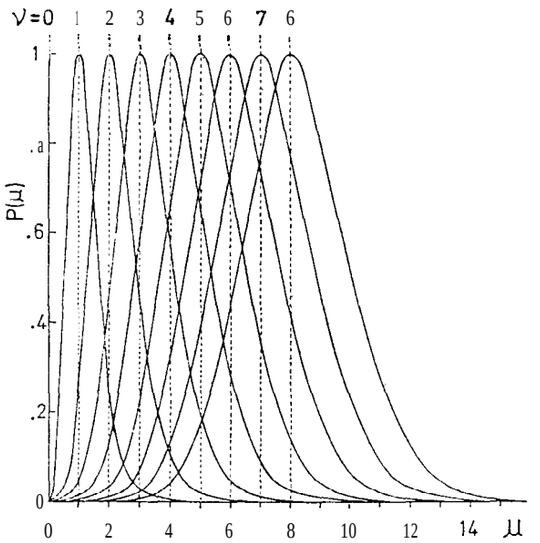

Fig. 1. The probability $P(\mu)$ given by (16) as a function of the number of double occupancies μ. Number at the top mark curves corresponding to different peak-term values υ of the number of double occupancies.

this result is based on the peak-term approximation which already breaks down before JJ reaches the limiting value 0.

Nevertheless, it is easy to prove that the energy E given by (10) derived with the peak-term approximation is still correct if ν is of order or greater than $\sqrt{N}$. We will not discuss this point further because it is outside the interest of the present paper.

IV. DISCUSSION

We have proved that in the Gutzwiller scheme the condition $\nu=0$ can not be taken as the criterion of metal-insulator transition. However, since the peak-term approximation is valid for $\nu\geq\sqrt{N}$ and ν is of order N in the metallic state, we can consider the condition $\nu=0$ as a rough estimate of the metal-insulator transition. In order to derive the correct behavior of $\langle n_{i\uparrow}n_{i\downarrow}\rangle$ near the metal-insulator transition, one must abandon the peak-term approximation in calculating the energy of the ground state. In this respect, one should also drop the approximation No. 2 stated below (8). Such energy calculation will be reported in the near future.

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