Slave-Boson Functional-Integral Approach to

the Hubbard Model with Orbital Degeneracy

Hideo Hasegawa†

Department of Physics, Tokyo Gakugei University
Koganei, Tokyo 184, Japan

(Received December 13, 1996)

Abstract

A slave-boson functional-integral method has been developed for the Hubbard model with arbitrary, orbital degeneracy \( D \). Its saddle-point mean-field theory is equivalent to the Gutzwiller approximation, as in the case of single-band Hubbard model. Our theory is applied to the doubly degenerate \( (D = 2) \) model, whose paramagnetic state has been studied by numerical calculations. The effect of the exchange interaction on the metal-insulator (MI) transition is discussed. The critical interaction for the MI transition is analytically calculated as functions of orbital degeneracy and electron occupancy.

Keywords: slave boson, Gutzwiller approximation, metal-insulator transition

† e-mail address: hasegawa@u-gakugei.ac.jp
§1. Introduction

The Hubbard model has been accepted as a model for a study of the strongly correlated systems such as transition metals, valence-mixing and high-$T_c$ materials. The single-band Hubbard has been extensively investigated by using various methods.$^{1-3}$ Gutzwiller$^1$ adopted a variational approach, employing the variational wave function. Since the exact evaluation of the ground-state energy is difficult, he used an additional approximation which is now called the Gutzwiller approximation (GA). A validity of the GA was investigated by Monte-Carlo technique for finite-size clusters.$^{4,5}$ It is realized that the GA becomes a better approximation for the higher-dimensional system.$^{6,7}$ The GA has been widely employed for various studies including magnetism and the metal-insulator (MI) transition.$^8$

Kotliar and Ruckenstein (KR)$^9$ proposed the slave-boson functional-integral method, whose saddle-point approximation is shown to be equivalent to the GA. The KR method has a wider applicability than the GA as follows:

(1) within the saddle-point theory, we can deal with the complicated magnetic systems such as antiferromagnetic state besides paramagnetic and ferromagnetic states.$^{10,11}$
(2) we can go beyond the saddle-point approximation, by including fluctuations around the saddle points.$^{12-16}$
(3) we can extend the theory to finite temperatures.$^{11,17}$

In contrast with the single-band Hubbard model, little studies based on the GA had been reported on the degenerate-band Hubbard model since its first application was made by Gutzwiller and Chao.$^{18}$ In the last few years, however, several attempts$^{19-21}$ were reported of re-formulating and applying the GA to degenerate-band Hubbard model. Lu$^{19}$
obtained the analytical expression of the critical interaction for the MI transition. Okabe$^{20}$ proposed a sophisticated method in calculating the band-narrowing factor, $q$, which is the most difficult part in applying the GA. Quite recently Bünemann and Weber$^{21}$ discussed the first-order MI transition in the half-filled doubly degenerate Hubbard model when the exchange interaction is included.

It is desirable to develop the slave-boson functional-integral theory for the degenerate-band Hubbard model, which is the purpose of the present paper. We have developed such a theory, adopting the slave-boson method of Dorin and Schlottman$^{22}$ which was originally employed for the Anderson lattice model. As in the single-band Hubbard model, the saddle-point approximation to our slave-boson theory is equivalent to the GA in the degenerate-band Hubbard model, and our slave-boson theory has the above-mentioned advantages with the wider applicability than the GA.

The paper is organized as follows: In the next §2, we present a slave-boson functional-integral formulation for the Hubbard model with the $D$-fold orbital degeneracy. Our formalism is applied to the doubly degenerate ($D = 2$) model, for which numerical calculations are performed and reported in §3. Section 4 is devoted to conclusion and supplementary discussion. In the Appendix we analytically calculate the critical interaction strength for the MI transition, in order to demonstrate the feasibility of our theory.

§2. Formulation

§2.1 Basic Equations

We adopt the Hubbard model with $D$-fold orbital degeneracy whose Hamiltonian is
given by

\[ H = \sum_{\sigma} \sum_{ij} \sum_{mm'} t_{ij}^{mm'} c_{im\sigma}^\dagger c_{jm'\sigma} + \frac{1}{2} \sum_i \sum_{(m,\sigma) \neq (m',\sigma')} U_{mm'}^{\sigma\sigma'} c_{im\sigma}^\dagger c_{im\sigma'}^\dagger c_{im'\sigma'} c_{im'\sigma}, \]  

(1)

where \( c_{im\sigma} \) is an annihilation operator of an electron with an orbital index \( m \) and spin \( \sigma (=\uparrow, \downarrow) \) on the lattice site \( i \) and \( t_{ij}^{mm'} \) is the hopping integrals. As for the on-site interaction, \( U_{mm'}^{\sigma\sigma'} \), we introduce three parameters: \( U_0 \) for \( m = m', \sigma \neq \sigma' \), \( U_1 \) for \( m \neq m', \sigma \neq \sigma' \), and \( U_2 \) for \( m \neq m', \sigma = \sigma' \). We assume that the spin and orbital degrees of freedom are not coupled for simplicity.

We employ the slave boson formulation of Dorin and Schlottman,\(^{22}\) introducing \( 2^{2D} \) bose annihilation operators:

\[ b_{i;m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}}^{(\ell)} \]  

(2)

which project to the configuration of \( \ell \) electrons with pairs of orbital and spin indices \( \{m\sigma\} \). In eq. (2) all the index pairs are different because of the Pauli principles.

We introduce the following product operations:\(^{22}\)

(1) A full contraction is defined as

\[ \left( b_{i}^{(\ell)\dagger} \cdot b_{i}^{(\ell)} \right) \equiv \sum_{m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}} b_{i;m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}}^{(\ell)\dagger} b_{i;m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}}^{(\ell)} \]  

(3)

(2) A partial contraction with a fixed pair of \( (m_n\sigma_n) \) for \( \ell \geq 1 \) is defined as

\[ \left( b_{i}^{(\ell)\dagger} \cdot b_{i}^{(\ell)} \right)_{m_n\sigma_n} \equiv \sum_{m_1\sigma_1,m_2\sigma_2,...,m_{n-1}\sigma_{n-1},m_{n+1}\sigma_{n+1},...,m_{\ell}\sigma_{\ell}} b_{i;m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}}^{(\ell)\dagger} b_{i;m_1\sigma_1,m_2\sigma_2,...,m_{\ell}\sigma_{\ell}}^{(\ell)} \]  

(4)

With the use of these operations the completeness of the slave boson operators is given by

\[ \sum_{\ell=0}^{2D} \left( b_{i}^{(\ell)\dagger} \cdot b_{i}^{(\ell)} \right) = 1, \]  

(5)
while the correspondence between bosons and fermions is expressed by
\[ c_{im\sigma}^\dagger c_{im'\sigma} = \sum_{\ell=1}^{2D} (b_{i}^{(\ell)}\dagger \cdot L_{i}^{(\ell)})_{m\sigma} = n_{im\sigma}. \]  

(6)

The partition function of the model given by eq. (1) is expressed as a functional
integral over coherent states of Fermi and Bose fields. The constraints given by eqs. (5)
and (6) are incorporated with Lagrange multipliers, \( \lambda^{(1)} \) and \( \lambda^{(2)}_{\sigma} \), to get
\[ Z = \int \prod_{\ell=0}^{2D} Db^{(\ell)} \int D\lambda^{(1)} \int D\lambda^{(2)}_{\sigma} \exp[- \int_{0}^{\beta} d\tau \left( L_{f}(\tau) + L_{b}(\tau) \right)] \],

where the actions, \( L_{f} \) and \( L_{b} \), are given by
\[ L_{f}(\tau) = \sum_{i} \sum_{m\sigma} \left[ c_{i}^{\dagger} (\partial/\partial \tau + \lambda^{(2)}_{im\sigma}) c_{im\sigma} \right] + \sum_{\ell} \sum_{ij} \sum_{m'n'} t^{m'n'}_{ij} z_{im\sigma}^{\dagger} c_{im\sigma}^{\dagger} c_{jm'\sigma} z_{jm'\sigma}, \]
\[ L_{b}(\tau) = \sum_{i} \left[ \sum_{\ell=0}^{2D} b_{i}^{\dagger} (\partial/\partial \tau + \lambda^{(1)}_{i}) b_{i} - \sum_{m\sigma} \lambda^{(2)}_{im\sigma} (b_{i}^{(\ell)}\dagger \cdot b_{i}^{(\ell)})_{m\sigma} - \lambda^{(1)}_{i} \right] + \Phi_{0}, \]

\[ \Phi_{0} = \sum_{i} \sum_{\ell=2}^{2D} \sum_{m_{1}m_{2}m_{3}...m_{\ell}} U_{m_{1}m_{2}m_{3}...m_{\ell}} b_{i;im_{1}m_{2}m_{3}...m_{\ell}}^{(\ell)} \]
\[ \times b_{i;im_{1}m_{2}m_{3}...m_{\ell}}^{(\ell)} \]
\[ \times \sum_{m'=m'} U_{m'm'}^{*}, \]

(10)

the fourth summation in eq. (10) being made over a pair of indices \((m\sigma, m'\sigma')\) with
\((m\sigma) \neq (m'\sigma')\) in the configuration: \( \{m_{1}m_{1}, m_{2}m_{2}, ..., m_{\ell}m_{\ell}\} \) occupied by \( \ell \) electrons. It
is noted that when \( U_{0} = U_{1} = U_{2} = U \), we get \( \Phi_{0} = U \sum_{i} \sum_{\ell=2}^{2D} C_{2}^{\ell} (b_{i}^{(\ell)}\dagger \cdot b_{i}^{(\ell)}) \) where
\( C_{k}^{\ell} = \ell! / k! (\ell - k)! \). Although a choice of the factor, \( z_{im\sigma} \), is not unique, the expression
given by
\[ z_{im\sigma} = (1 - n_{im\sigma})^{-1/2} \sum_{\ell=1}^{2D} \left( b_{i}^{(\ell-1)}\dagger \cdot b_{i}^{(\ell)} \right)_{m\sigma} n_{im\sigma}^{-1/2}, \]
\[ \text{is shown to yield the correct result in the limit of vanishing interactions.}^{22)} \]

We employ the static approximation for boson fields. Furthermore we adopt the
following change of variables:
\[ \nu_{im} = (\lambda_{iim\uparrow}^{(2)} + \lambda_{iim\downarrow}^{(2)}) / 2, \quad \xi_{im} = - (\lambda_{iim\uparrow}^{(2)} - \lambda_{iim\downarrow}^{(2)}) / 2, \]
\[ \text{with} \quad \lambda^{(2)}_{im\sigma} = \nu_{im} - \xi_{im}, \]

(12)
\[ \langle n \rangle = \langle n \rangle_{\uparrow} + \langle n \rangle_{\downarrow}, \quad \langle m \rangle = \langle n \rangle_{\uparrow} - \langle n \rangle_{\downarrow}, \tag{13} \]

where the brackets, \(< >\), stand for the average. Thus the expression of the partition function becomes

\[ Z = \int \Pi_{\ell=2}^{2D} D b^{(\ell)} \int D\nu \int D\zeta \int Dn \int Dm \exp(\beta \Phi), \tag{14} \]

where

\[ e^{-\beta \Phi} = \exp\left(-\beta \left[ \sum_i \sum_m (\xi_{im} m - \nu_{im} n_{im}) + \Phi_0 \right] \right) Tr \exp(-\beta H_{\text{eff}}). \tag{15} \]

The effective one-electron Hamiltonian, \( H_{\text{eff}} \), is given by

\[ H_{\text{eff}} = \sum_{ij} \sum_{mm'} z_{im\sigma} z_{jm'\sigma} t_{ij}^{mm'} c_{im\sigma}^\dagger c_{jm'\sigma} + \sum_{\sigma} \sum_i \sum_m (\nu_{im} - \sigma \xi_{im}) c_{im\sigma}^\dagger c_{im\sigma}, \tag{16} \]

\[ z_{im\sigma} = 2(2 - n_{im})^{-1/2} n_{im}^{-1/2} \left[ \sqrt{e_i p_{im\sigma}} + \sqrt{p_{im\sigma}} b_i^{(2)}(\ell) + \sum_{\ell=3}^{2D} (b_i^{(\ell-1)} \cdot b_i^{(\ell)})_{m\sigma} \right], \tag{17} \]

where \( e_i \) and \( p_{im\sigma} \) are given by

\[ e_i = (b_i^{(0)} \cdot b_i^{(0)}) = 1 - \sum_m n_{im} + \sum_{m\sigma} \sum_{\ell=2}^{2D} \left[ (\ell - 1)/\ell \right] (b_i^{(\ell)} \cdot b_i^{(\ell)})_{m\sigma}, \tag{18} \]

\[ p_{im\sigma} = (b_i^{(1)} \cdot b_i^{(1)})_{m\sigma} = (n_{im} + \sigma m_{im})/2 - \sum_{\ell=2}^{2D} (b_i^{(\ell)} \cdot b_i^{(\ell)})_{m\sigma}. \tag{19} \]

It should be noted that the functional integral given by eqs. (14)-(19) is performed over variables of \( \xi, \nu, n, m, \) and \( b^{(\ell)} \) with \( \ell \geq 2 \). Our expression has physically more transparent meaning than an original static approximation in which the functional integral is carried out over the variables of \( \lambda^{(1)}, \lambda^{(2)}_0 \) and \( b^{(\ell)} \) with \( \ell \geq 0 \), although both the approaches are equivalent. The expression for the functional integral given by eqs. (14)-(19) is a simple generalization of the single-band model to the degenerated-band model.\(^{11}\) When
all the integration variables are replaced by their saddle-point values, we get the mean-field approximation, which is expected to be equivalent with the GA theory,\textsuperscript{19-21} related discussions being given in §4.

\section*{§2.2 Doubly degenerate band}

We apply our theory developed so far to the doubly degenerate Hubbard model. After a simple calculation, the expressions for the functional integral given by eqs. (14)-(19) become

\begin{equation}
Z = \int Dd_0 \int Dd_1 \int Dd_\sigma \int Dt_\sigma \int Df \int D\xi \int Dm \int D\nu \int Dn \ \exp[-\beta(\Phi_0 + \Phi_1 + \Phi_2)],
\end{equation}

\begin{equation}
\Phi_0 = \sum_i [2U_0d_{i0} + 2U_1d_{i1} + U_2(d_{i\uparrow} + d_{i\downarrow}) + 2(U_0 + U_1 + U_2)(t_{i\uparrow} + t_{i\downarrow} + f_i)],
\end{equation}

\begin{equation}
\Phi_1 = \sum_{im} [\xi_{im}m_{im} + (\mu - \nu_{im})n_{im}],
\end{equation}

\begin{equation}
\Phi_2 = \int d\varepsilon f(\varepsilon)(-1/\pi)Im \ Tr \ ln G(\varepsilon).
\end{equation}

where \(f(\varepsilon)\) is the Fermi distribution function and \(\mu\) Fermi level. The one-particle Green function, \(G(\varepsilon)\), is expressed in terms of the effective Hamiltonian, \(H_{\text{eff}}\), for the system under the charge \(\nu_{im}\) and exchange \(\xi_{im}\) fields, as

\begin{equation}
G(\varepsilon) = (\varepsilon - H_{\text{eff}})^{-1},
\end{equation}

with

\begin{equation}
H_{\text{eff}} = \sum_{\sigma} \sum_{ij} \sum_{mm'} z_{im\sigma} t_{ij}^{mm'} z_{jm'\sigma} c_{im\sigma}^\dagger c_{jm'\sigma} + \sum_{\sigma} \sum_i \sum_m (\nu_{im} - \sigma\xi_{im}) c_{im\sigma}^\dagger c_{im\sigma},
\end{equation}

\begin{equation}
z_{im\sigma} = \frac{2\left[\sqrt{p_{i\sigma}}(\sqrt{e_i} + \sqrt{d_{i\sigma}}) + (\sqrt{d_{i0}} + \sqrt{d_{i1}})(\sqrt{m_{i-\sigma}} + \sqrt{t_{i\sigma}}) + \sqrt{t_{i-\sigma}}(\sqrt{d_{i-\sigma}} + \sqrt{f_i})\right]}{(n_{im} + \sigma m_{im})^{1/2} (2 - n_{im} - \sigma m_{im})^{1/2}},
\end{equation}
\[ e_i = 1 - 2n_{im} + 2d_{i0} + 2d_{i1} + d_{i\uparrow} + d_{i\downarrow} + 4(t_{i\uparrow} + t_{i\downarrow}) + 3f_i, \]  
\[ p_{i\sigma} = (n_{im} + \sigma m_{im})/2 - (d_{i0} + d_{i1} + d_{i\sigma}) - (2t_{i\sigma} + t_{i-\sigma}) - f_i, \]

where \( t_{i\sigma} \) and \( f_i \) stand for the \( \ell = 3 \) and \( 4 \) components of \( (b_i^{(\ell)} \cdot b_i^{(\ell)})_{m\sigma} \), respectively. As for \( \ell = 2 \), we take into account the three kinds of configurations: \( d_{i0} \) for a pair of electrons on the same orbital with opposite spin, \( d_{i1} \) on the different orbital with opposite spin, and \( d_{i\sigma} \) on the different orbital with same spin \( \sigma \).

The explicit form of the Green function, \( G(\varepsilon) \), depends on the electronic and magnetic structures of a system to be investigated. Since the effective transfer integrals in eq. (25) is expressed as a product form: \( z_{ima} t_{ij}^{mm' \sigma} z_{jm' \sigma} \), we can express the one-electron Green function in terms of the locators defined by

\[ X_{ima} = (\varepsilon - \nu_{im} + \sigma \xi_{im})/r_{ima}, \]

where \( r_{ima} = (z_{ima})^2 \), with which the band-narrowing factor, \( q_{ij}^{mm'} \), is expressed as

\[ q_{ij}^{mm'} \equiv z_{ima} z_{jm' \sigma} = \sqrt{r_{ima} r_{jm' \sigma}}, \]

The mean-field free energy can be obtained from the saddle-point values of the integration variables for which the variational conditions yield the following simultaneous equations:

\[ n_{im} = \sum_{\sigma} <c_{ima}^{\dagger} c_{ima}>; \]
\[ m_{im} = \sum_{\sigma} \sigma <c_{ima}^{\dagger} c_{ima}>; \]
\[ \mu - \nu_{im} + \sum_{\sigma} R_{ima} (\partial r_{ima}/\partial n_{im}) = 0, \]
\[ \xi_{im} + \sum_{\sigma} R_{ima} (\partial r_{ima}/\partial m_{im}) = 0, \]
\[ 2U_0 + \sum_{m\sigma} R_{im\sigma}(\partial r_{im\sigma}/\partial d_{i0}) = 0, \] (35)

\[ 2U_1 + \sum_{m\sigma} R_{im\sigma}(\partial r_{im\sigma}/\partial d_{i1}) = 0, \] (36)

\[ U_2 + \sum_{m\sigma'} R_{im\sigma'}(\partial r_{im\sigma'}/\partial d_{i\sigma}) = 0, \] (37)

\[ 2(U_0 + U_1 + U_2) + \sum_{m\sigma} R_{im\sigma}(\partial r_{im\sigma}/\partial t_{i\sigma}) = 0, \] (38)

\[ 2(U_0 + U_1 + U_2) + \sum_{m\sigma} R_{im\sigma}(\partial r_{im\sigma}/\partial f_i) = 0, \] (39)

where \( R_{im\sigma} = \partial \Phi_2/\partial r_{im\sigma} \).

In the remainder of this paper we consider only the paramagnetic states at \( T = 0 \) K, for which we get

\[ \Phi_2 = \int^{\epsilon} d\epsilon \ (\epsilon - \mu) (-1/\pi) \text{Im} \text{Tr} G(\epsilon), \] (40)

\[ \text{Tr} G(\epsilon) = \sum_{\sigma} \sum_{m} \frac{1}{(\epsilon - \nu - q\xi_k)}, \] (41)

\[ \xi_0(n) = \sum_{\sigma} R_\sigma, \] (42)

\[ q = r = 4 \frac{[(\sqrt{d_0} + \sqrt{d_1} + \sqrt{d_2})(\sqrt{p} + \sqrt{t}) + \sqrt{ep} + \sqrt{tf})]^2}{n(2 - n)}, \] (43)

with

\[ e = 1 - 2n + 2(d_0 + d_1 + d_2) + 8t + 3f, \] (44)

\[ p = n/2 - (d_0 + d_1 + d_2) - 3t - f. \] (45)

Here \( d_2 = d_\sigma, \ t = t_\sigma \) and \( R_\sigma = R_{im\sigma} \text{ et al.} \), subscripts \( i \) and \( m \) being omitted; \( \xi_k \) is the Fourier transform of the transfer integrals and \( \xi_0(n) \) is the ground-state energy per sub-band for \( U_0 = U_1 = U_2 = 0 \) as a function of \( n \), the number of electrons per sub-band.

The ground-state energy per site is then given by

\[ E = 2q\xi_0(n) + 2U_0d_0 + 2U_1d_1 + 2U_2d_2 + 2(U_0 + U_1 + U_2)(2t + f), \] (46)
which is identical with that obtained by Blümenann and Weber.\(^{21}\) Employing the Gutzwiller-type wave function, they obtained the ground-state energy given by eq. (46), from which the optimum values of the occupancies are determined by the variational conditions for \(E\) given by

\[
U_0 + \varepsilon_0(\partial q/\partial d_0) = 0, \tag{47}
\]

\[
U_1 + \varepsilon_0(\partial q/\partial d_1) = 0, \tag{48}
\]

\[
U_2 + \varepsilon_0(\partial q/\partial d_2) = 0, \tag{49}
\]

\[
2(U_0 + U_1 + U_2) + \varepsilon_0(\partial q/\partial t) = 0, \tag{50}
\]

\[
(U_0 + U_1 + U_2) + \varepsilon_0(\partial q/\partial f) = 0. \tag{51}
\]

It is easy to see that eqs. (35)-(39) reduce to eqs. (47)-(51) in the paramagnetic states.

\section{3. Numerical Calculations}

Numerical calculations have been performed for \(D = 2\) model with the quarter-filled \((n = 0.5)\) and half-filled \((n = 1)\) bands, which are considered to be most interesting.

We firstly show the calculated results by taking \(U_0 = U_1 = U_2 = U\), for which \(d_0, d_1\) and \(d_2\) are equivalent: \(d_0 = d_1 = d_2 = d\). The \(U\)-dependence of the occupancies for \(n = 0.5\) is shown in Fig. 1. At \(U = 0\) we get \(e = 0.3164, p = 0.1055, d = 0.0352, t = 0.0117\) and \(f = 0.0039\). When \(U\) value is increased, \(e, t\) and \(f\) decrease while \(p\) increases. In particular, \(t\) and \(f\) become at least ten times smaller than \(e, p\) or \(d\) at \(U/|\varepsilon_0(n)| > 3\). The \(q\) factor also decreases and vanishes above \(U_c\) which stands for the critical interaction for the metal-insulator (MI) transition. Near the MI transition, \(q\) behaves as \(q \propto (U_c - U)\) as in the single-band model.\(^{8}\) We get \(U_c = 13.2 \, |\varepsilon_0(n)|\), which agrees with the previous
results.\cite{19,21} Above $U_c$ only $p$ remains finite with a value of 0.25. The $U$ dependence of the ground-state energy is shown in Fig. 2, where the energy calculated by the Hartree-Fock approximation (HFA):

$$E_{\text{HF}} = 2\varepsilon_0(n) + (1/2)(U_0 + U_1 + U_2) n^2,$$

is also plotted for a comparison. The ground-state energy in the GA is always lower than $E_{\text{HF}}$ as expected.

Figure 3 shows the $U$ dependence of the occupancies for half-filled ($n = 1.0$) case, in which the relation:

$$e = f, \ p = t,$$

holds by the electron-hole symmetry. When $U$ value is increased, only $d$ increases while other occupancies decrease. The band-narrowing factor, $q$, vanishes above $U_c$, which is $12.0 \mid \varepsilon_0(n) \mid$ in agreement with the result of refs. 19 and 21. The double occupancy $d$ persists even above $U_c$ with a value of 0.167, which is in contrast with the quarter-filled case where only single occupancy $p$ survives. We might expect that in the limit of infinite $U$, any states with more than doubly occupied state vanish. This seems not the case for the half-filled $D = 2$ degenerate band, where doubly occupied state may survive by making a compromise with the constraints given by the completeness of bosons (eq. (5)) and the electron-hole symmetry (eq. (53)). This situation is changed when the exchange interaction is introduced, as will be discussed shortly. Fig. 4 shows the ground-state energy of the half-filled case as a function of $U$. Again the energy obtained in our theory is lower than that in the HFA.

Next we take into account the exchange interaction, $J$, with which our three interaction
parameters are expressed as

\[ U_0 = U, \quad U_1 = U' - J = U - 2J, \quad U_2 = U' - J = U - 3J, \quad (54) \]

where we employ the relation: \( U - U' = 2J \) required for the rotational symmetry,\(^{24}\) \( U \) and \( U' \) being the intra- and inter-band Coulomb interactions, respectively.

Figures 5 and 6 show the \( U \) dependence of the occupancies and the ground-state energy, respectively, for the quarter-filled band with \( J/U = 0.1 \). The general behavior shown in Figs. 5 and 6 is similar to that in Figs. 1 and 2, respectively, except the fact that the degeneracy among doubly occupied states is removed with an inclusion of the exchange interaction, \( J \). Because \( U_0 > U_1 > U_2 \) for finite \( J \), we get \( d_0 < d_1 < d_2 \). We realize that an inclusion of the exchange interaction also enhances the value of \( U_c \): \( U_c/|\varepsilon(n)| = 13.2, 16.4, \) and \( 24.8 \) for \( J/U = 0.0, 0.1 \) and \( 0.2 \), respectively. The MI transition is of the second order in all the quarter-filled cases investigated.

On the contrary, the effect of exchange interaction is quite different in the case of half-filled band. The MI transition becomes the first-order transition as is shown in Fig. 7, where the \( U \) dependence of the occupancies with \( J/U = 0.1 \) for \( n = 1.0 \) is plotted. This first-order MI transition has been recently pointed out by B"unemann an Weber.\(^{21}\) A change from the second-order to first-order MI transition is induced with an infinitesimally small inclusion of \( J \). When \( J = 0 \), all doubly occupies states are equivalent and remain finite even at \( U > U_c \), as was shown in Fig. 3. For a finite \( J \), however, \( d_2 \) is the most favorable state among the three doubly occupied states, and only \( d_2 \) survives above \( U = 6.0 \), where neither \( d_0 \) nor \( d_1 \) remain finite. This first-order transition is realized in the \( U \) dependence of the ground-state energy shown in Fig. 8, where the \( E - U \) curve
of the metallic state does not tangentially intersect that of the insulating state at the MI transition, in contrast with the case of the second-order transition shown in Fig. 2, 4 and 6.

§4. Conclusion and Discussion

To summarize, we have developed the slave-boson functional-integral theory for the Hubbard model with the orbital degeneracy $D$, employing the slave-boson method of Dorin and Schllotman$^{22}$ who originally applied it to the Anderson model. Our slave-boson mean-field theory has been used for a study of the doubly degenerate model, for which numerical calculations have been performed. We have shown that our slave-boson mean-field theory is equivalent with the GA for $D = 2$. It is shown in the Appendix that our mean-field theory and Lu’s$^{19}$ yield the identical critical interaction of the MI transition for arbitrary $D$. This suggests that the equivalence between the slave-boson mean-field theory and the GA$^{19-21}$ generally holds for any degeneracy $D$, although it has not been rigorously proved yet.

We expect that our slave-boson mean-field theory is a convenient and useful method in studying strongly correlated systems described by the degenerate-band Hubbard model. With the use of the Green function method, we can deal with the complicated magnetic states within the mean-field approximation. It would be indispensable to investigate the antiferromagnetic states$^{25}$ for a deeper understanding of the MI transition of the $D = 2$ Hubbard model. Our slave-boson mean-field theory enables us to investigate the occupation versus interaction phase diagram of the degenerate Hubbard model, which was previously studied within the Hartree-Fock approximation. Furthermore, we can take account
of fluctuations around the saddle points, going beyond the mean-field approximation. It is interesting to extend our theory such as to include the effect of spin fluctuations at finite temperatures in order to discuss the finite-temperature magnetism of transition metals.

**Acknowledgment**

This work is partly supported by a Grant-in-Aid for Scientific Research from the Japanese Ministry of Education, Science and Culture.
§ Appendix

As one of applications of our formalism, we calculate the critical interaction, $U_c$, for the MI transition of the Hubbard with the orbital degeneracy, $D$, in the paramagnetic states. We assume that near the second-order MI transition point, fluctuations of the electron occupancy around its average $N$ (integer) are small. Then we take into only three possible states: $N-1$, $N$ and $N+1$ states, whose occupancies are expressed by $e$, $p$ and $d$, respectively, after Lu.\(^{19}\)

The constraints given by eqs. (5) and (6) become

\[
C_{N-1}^{2D} e + C_N^{2D} p + C_{N+1}^{2D} d = 1, \quad (A·1)
\]
\[
C_{N-2}^{2D} e + C_{N-1}^{2D} p + C_N^{2D} d = n/2, \quad (A·2)
\]

where $n \,(=N/D)$ is the number of electrons per sub-band and $C_{k}^{\ell} \,[= \ell!/k! (\ell-k)!]$ is zero when either $\ell$, $k$, or $(\ell-k)$ is negative as convention. The ground-state energy when $U_0 = U_1 = U_2 = U$ in eq. (1) is given by

\[
E = q D \varepsilon_0(n) + U \left[ C_{N-1}^{2D} C_2^{N-1} e + C_N^{2D} C_2^{N} p + C_{N+1}^{2D} C_2^{N+1} d \right], \quad (A·3)
\]

where $q$, $e$ and $p$ are given as a function of $d$ as

\[
q = \left[4/n(2-n)\right] \left[ C_{N-1}^{2D-1} \sqrt{e p} + C_N^{2D-1} \sqrt{p d} \right]^2. \quad (A·4)
\]
\[
e = (\Delta_1/\Delta) \, d, \quad (A·5)
\]
\[
p = (\Delta_2/\Delta) - (\Delta_3/\Delta) \, d, \quad (A·6)
\]
with

\[ \Delta = C_{N-1}^{2D-1}C_{N-1}^{2D} - C_{N-2}^{2D-1}C_{N}^{2D}, \quad \text{(A-7)} \]

\[ \Delta_1 = C_{N}^{2D-1}C_{N}^{2D} - C_{N-1}^{2D-1}C_{N+1}^{2D}, \quad \text{(A-8)} \]

\[ \Delta_2 = (n/2)C_{N-1}^{2D} - C_{N-2}^{2D-1}, \quad \text{(A-9)} \]

\[ \Delta_3 = C_{N}^{2D-1}C_{N-1}^{2D} - C_{N-2}^{2D-1}C_{N+1}^{2D}. \quad \text{(A-10)} \]

Taking the variational condition for \( E \) with respect to \( d \), we obtain the critical interaction, \( U_c \), given by

\[
\frac{U_c}{|\varepsilon_0(n)|} = \frac{D}{N(2D - N)} \left[ \sqrt{N(2D - N + 1)} + \sqrt{(2D - N)(N + 1)} \right]^2, \quad \text{(A-11)}
\]

which is identical with the result obtained by Lu.\(^{19}\) Equation (A-11) is symmetric with respect to the interchange of the variable: \( N \leftrightarrow (2D - N) \) as it should be. In the limit of infinite \( D \) and finite \( N \), eq. (A-11) becomes

\[
\lim_{D \to \infty} \left[ \frac{U_c}{D |\varepsilon_0(n)|} \right] = \frac{1}{N} \left[ \sqrt{N} + \sqrt{N + 1} \right]^2. \quad \text{(A-12)}
\]

Equation (A-12) is in agreement with the result of ref. 26, in which the fermion problem is treated as the boson problem using the GA. Some calculations using Eq. (A-11) are shown in Fig. 9.
References

[1] M. C. Gutzwiller: Phys. Rev. Lett. 10 (1963) 159; Phys. Rev. 137 (1965) A1726.

[2] J. Kanamori: Prog. Theor. Phys. 30 (1963) 235.

[3] J. Hubbard: Proc. Roy. Soc. London A281 (1964) 401.

[4] T. A. Kaplan, P. Horsch and P. Fulde: Phys. Rev. Lett. 49 (1982) 889.

[5] H. Yokoyama and H. Shiba: J. Phys. Soc. Jpn. 56 (1987) 1490; ibid. 3582.

[6] W. Metzner and D. Vohlhardt: Phys. Rev. Letter 59 (1987) 121; Phys. Rev. B 37 (1988) 7382.

[7] F. Gebhard: Phys. Rev. B 41 (1990) 253.

[8] W. F. Brinkman and T. M. Rice: Phys. Rev. B 2 (1970) 4302.

[9] G. Kotliar and A. E. Ruckenstein: Phys. Rev. Lett. 57 (1986) 1362.

[10] W. Metzner: Z. Phys. B 77 (1989) 253.

[11] H. Hasegawa: J. Phys. Cond. Matter. 1 (1989) 9325; Phys. Rev. 41 (1990) 9168.

[12] J. W. Rasul and T. Li: J. Phys. C 21 (1988) 5119.

[13] M. Lavagna: Phys. Rev. B 41 (1990) 142; R. Raimondi and M. Lavagna: J. Low Temp. Phys. 99 (1995) 355.

[14] A. Sudbø and A. Houhton: Phys. Rev. B 42 (1990) 4105.

[15] P. Wölfle and T. Li: Z. Phys. B 78 (1990) 45.
[16] Th. Jolicour and J. C. Le Guillou: Phys. Rev. B 44 (1991) 2403.

[17] H. Hasegawa: Prog. Theor. Phys. Suppl. 101 (1990) 463.

[18] K. A. Chao and M. C. Gutzwiller: Phys. Rev. B 4 (1971) 4034; K. A. Chao: J. Appl. Phys. 42 (1971) 1420.

[19] J. P. Lu: Phys. Rev. 49 (1994) 5687; preprint (SISSA: cond-mat/9601133).

[20] T. Okabe: J. Phys. Soc. Jpn. 65 (1996) 1056.

[21] J. Bünemann and W. Weber: preprint (SISSA: cond-mat/9611031 and 9611032).

[22] V. Dorin and P. Schlottmann: Phys. Rev. 47 (1993) 5095.

[23] H. Shiba: Prog. Theor. Phys. 46 (1971) 77.

[24] C. Lacroix-Lyon-Caen and M. Cyrot: Solid State Commun. 21 (1977) 837.

[25] H. Hasegawa: preprint (SISSA: cond-mat/9702034).

[26] W. Krauth, M. Caffarel and J. Bouchaud: Phys. Rev. B 45 (1992) 3137.
Figure Captions

**Fig. 1** The occupancies, \( e, p, d, t \) and \( f \), and the band narrowing factor, \( q \), as a function of \( U \) for the quarter-filled \((n = 0.5)\) case with \( J = 0 \), the results of \( t \) and \( f \) being multiplied by a factor of ten.

**Fig. 2** The ground-state energy for \( n = 0.5 \) and \( J = 0 \) in the GA (solid curve) and the HFA (dashed curve), the arrow denoting the MI transition.

**Fig. 3** The occupancies, \( e, p, d, t \) and \( f \), and the band narrowing factor, \( q \), as a function of \( U \) for the half-filled \((n = 1.0)\) case with \( J = 0 \).

**Fig. 4** The ground-state energy for \( n = 1.0 \) and \( J = 0 \) in the GA (solid curve) and the HFA (dashed curve), the arrow denoting the MI transition.

**Fig. 5** The occupancies and the band narrowing factor, \( q \), as a function of \( U \) for the quarter-filled \((n = 1/2)\) case with \( J/U = 0.1 \), the results of \( t \) and \( f \) being multiplied by a factor of ten.

**Fig. 6** The ground-state energy for \( n = 0.5 \) and \( J/U = 0.1 \) in the GA (solid curve) and the HFA (dashed curve), the arrow denoting the MI transition.

**Fig. 7** The occupancies and the band narrowing factor, \( q \), as a function of \( U \) for the half-filled \((n = 1.0)\) case with \( J/U = 0.1 \).
Fig. 8 The ground-state energy for \( n = 1.0 \) with \( J/U = 0.1 \) in the GA (solid curve) and the HFA (dashed curve), the dotted curve showing the energy of the insulating state \( (q = 0) \) and the arrow denoting the MI transition.

Fig. 9 The critical interaction for the MI transition, \( U_c/\mid \varepsilon_0(n) \mid \), against the electron occupancy per sub-band \( (n = N/D) \) of the Hubbard model with \( N \) electrons and \( D \)-fold orbital degeneracy. Only points shown by filled circles are meaningful, dashed curves being drawn using eq. (A.11).