Momentum Dependent Local-Ansatz Approach to Correlated Electron Systems: Non Half-Filled Case

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Momentum dependent local-ansatz wavefunction approach (MLA) to the correlated electron systems in solids has been further developed to solve best a self-consistent equation for variational parameters at non half-filling. With use of the improved variational scheme we performed the numerical calculations for the non-half-filled band Hubbard model on the hypercubic lattice in infinite dimensions. We verified that the self-consistent scheme significantly improves the correlation energy and the momentum distribution as compared with the original scheme in the MLA. We also demonstrate that the theory improves the standard variational methods such as the Local-Ansatz approach (LA) and the Gutzwiller wavefunction approach (GA); the ground-state energy in the MLA is lower than those of the LA and the GA in the weak and intermediate Coulomb interaction regimes. The double occupation number is shown to be suppressed as compared with the LA. Calculated momentum distribution functions show a distinct momentum dependence, which is qualitatively different from those of the LA and the GA.

KEYWORDS: variational method, electron correlations, Gutzwiller wavefunction, local ansatz, Hubbard model, critical Coulomb interaction, infinite dimensions

1. Introduction

Electron correlations play an important role for understanding the electronic structure, metal-insulator transition, and the high-temperature superconductivity in the solid-state physics. Thus many theories have been proposed so far to describe correlated electron system1,2) on the basis of the variational method,3–5) the Green function techniques, as well as many numerical techniques such as the Monte-Carlo method.6–8) The variational theory among various methods has been developed as a practical method for understanding the ground-state properties of correlated electrons from molecules to solids over 50 years. A minimum basis set to describe correlated electrons is constructed in this approach by applying one-particle, two-particle, and higher-order particle operators onto the Hartree-Fock wavefunction, and their amplitudes are chosen to be best on the basis of the variational principle. The Gutzwiller wavefunction is one of the popular trial wavefunction in solids because of its simple and intuitive structure. This approach was first introduced by Gutzwiller to clarify the role of electron correlations in metallic ferromagnetism,9–11) There, one reduces the amplitudes of doubly occupied states on the local orbitals in the Hartree-Fock wavefunction by making use of a projection operator \( \Pi_i(1 - gn_i^\uparrow n_i^\downarrow) \). Here \( n_i^\sigma \) is the number operator for electrons on site \( i \) with spin \( \sigma \). The variational parameter \( g \) is determined by minimization of the ground-state energy. Brinkman and Rice recognized that the Gutzwiller approximation describes the metal-insulator transition.12) Because the Gutzwiller method is a nonperturbative approach, it has extensively been applied to the strongly correlated electron systems.13)

The Gutzwiller wavefunction in the Gutzwiller ansatz approach (GA) yields a physical picture of electron correlations and is useful for correlation problems, but it was not so easy to apply the method to realistic Hamiltonians. The approach was successfully generalized by Stollhoff and Fulde14–16) by using an alternative method called the local-ansatz approach.

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(LA), which is simpler in treatment and applicable to realistic Hamiltonians. The LA takes into account the excited states created by local two-particle operators such as \( \{O_i\} = \{\delta n_i \uparrow \delta n_i \downarrow\} \), and determines their amplitudes variationally. Here \( \delta n_i \sigma = n_i \sigma - \langle n_i \sigma \rangle_0 \), \( \langle n_i \sigma \rangle_0 \) being the average electron number on site \( i \) with spin \( \sigma \) in the Hartree-Fock approximation. The theory has been applied to many systems such as molecules, transition metals, polyacetylene, transition metal oxides and semiconductors.\(^{1,17}\)

Although the LA is able to explain fruitfully the correlation effects in actual materials, the application has been limited to the weakly correlated region because of the difficulty in evaluation of the higher-order terms in average quantities. The expansion of the Hilbert space by the local operators is not sufficient to characterize precisely the weakly correlated states; the LA does not reduce to the second-order perturbation theory in the weak correlation limit. For the Gutzwiller wavefunction, the same difficulty also arises even in infinite dimensions. To overcome the difficulty, Kakehashi \textit{et. al.}\(^{18}\) proposed a variational wavefunction theory called the momentum-dependent local ansatz approach (MLA).

When we expand the local operators \( \{O_i\} \) in the LA by means of the two particle operators in the momentum space, we find that each coefficient of the expansion is momentum independent. In the MLA wavefunction,\(^{18}\) we replace the constant coefficients in the LA with the momentum-dependent variational parameters in order to obtain the best local operators. It results in a new set of local operators \( \{\tilde{O}_i\} \). We then construct the MLA wavefunction with use of the local operators \( \{\tilde{O}_i\} \) as \( |\Psi_{\text{MLA}}\rangle = \prod_i (1 - \tilde{O}_i)|\phi_0\rangle \). Here \( |\phi_0\rangle \) is the Hartree-Fock wavefunction and \( i \) denotes site of atoms. The best local basis set is chosen by controlling the variational parameters in the momentum space. We calculate the ground-state energy using the MLA wavefunction within a single-site approximation (SSA). Minimizing the energy, we obtain a self-consistent equation with variational parameters. It is however difficult to solve the self-consistent equation directly. Because of this, we obtained in the previous paper, which we refer to I, an approximate solution which interpolates between the weak Coulomb interaction limit and the atomic limit.

In this paper we point out that it is indispensable toward quantitative calculations to choose the variational parameters best, though in our paper \(^{18}\) we applied approximate variational parameters, and improve the variational parameters on the basis of the variational principle. We investigate the validity of our theory for the non half-filled case performing numerical calculations of various physical quantities. Especially for non half-filled case we observe that the best choice of variational parameters gives reasonable results for the momentum distribution, while the previous version of the variational parameters yields unphysical results near the Fermi level. Moreover, we demonstrate that the improved variational parameters much improve the LA in the weak and intermediate correlation regimes.

The outline of the paper is as follows. In the following section we write down our wavefunction for the single-band Hubbard model. We obtain the ground-state energy within the SSA and derive the self-consistent equation for the momentum dependent variational parameters on the basis of the variational principle. We develop the theory to obtain the best value of variational parameters to solve the self-consistent equation. In §3, we present our results of numerical calculations. We will clarify the role of the best choice of variational parameters on various quantities. Furthermore, we discuss the correlation energy, the double occupation number, the momentum distribution function, and the quasiparticle weight as a function of the Coulomb interaction energy parameter, and verify that the present approach improves the LA in the weak and intermediate Coulomb interaction regimes for non half-filled band. We summarize our results in the last section and discuss the remaining problems.

2. Momentum-Dependent Local Ansatz with the best Variational Parameters

We adopt in this paper the single-band Hubbard model\(^{18–22}\) as follows.

\[
H = \sum_{i\sigma} (\epsilon_0 - \sigma \hbar) n_i \sigma + \sum_{ij\sigma} t_{ij} a_{ij\uparrow}^\dagger a_{ij\downarrow} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{1}
\]
Here $\epsilon_0$ ($h$) is the atomic level (magnetic field), $t_{ij}$ is the transfer integral between sites $i$ and $j$. $U$ is the intra-atomic Coulomb energy parameter. $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) denotes the creation (annihilation) operator for an electron on site $i$ with spin $\sigma$, and $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ is the electron density operator on site $i$ for spin $\sigma$.

In the Hartree-Fock approximation, we neglect the fluctuation term and replace the many-body Hamiltonian (1) with an effective Hamiltonian for independent particle system,

$$H_0 = \sum_{i,j,\sigma} t_{ij\sigma} a_{i\sigma}^\dagger a_{j\sigma} - U \sum_i \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0,$$

and approximate the ground-state wavefunction $|\Psi\rangle$ with that of the Hartree-Fock Hamiltonian $H_0$, i.e., $|\phi_0\rangle$. Here $t_{ij\sigma} = (\epsilon_0 + U(n_{i-\sigma})_0 - \sigma h)\delta_{ij} + t_{ij}(1 - \delta_{ij})$. $\langle \cdots \rangle_0$ denotes the Hartree-Fock average $\langle \phi_0 | \langle \cdots | \phi_0 \rangle$, and $\langle n_{i\sigma} \rangle_0$ is the average electron number on site $i$ with spin $\sigma$. The original Hamiltonian (1) is then expressed as a sum of the Hartree-Fock Hamiltonian (2) and the residual interactions as follows.

$$H = H_0 + U \sum_i O_i.$$

Here $O_i = \delta n_{i\uparrow} \delta n_{i\downarrow}$ and $\delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma} \rangle_0$.

In the LA, the Hilbert space expanded by the local operators such as the residual Coulomb interactions $\{O_i\} = \delta n_{i\uparrow} \delta n_{i\downarrow}$ is taken into account in order to describe the weak Coulomb interaction regime. The ansatz for the Hubbard model is written as

$$|\Psi_{\text{LA}}\rangle = \prod_i \left( 1 - \eta_{\text{LA}} O_i \right) |\phi_0\rangle.$$

Here $\eta_{\text{LA}}$ is the variational parameter as the amplitudes of the basis set expanded by $\{O_i\}$.

The LA is different from the Gutzwiller ansatz wavefunction $|\Psi_{\text{GA}}\rangle = \prod_i \left( 1 - g n_{i\uparrow} n_{i\downarrow} \right) |\phi_0\rangle$ in which the doubly occupied states are explicitly controlled by a variational parameter $g$ ($0 \leq g \leq 1$), and simplify the evaluation of the physical quantities in the weakly correlated region.

As we have emphasized in our previous paper I, though the LA is useful for understanding correlation effects in real system, the Hilbert space expanded by the local operators $\{O_i\}$ is not sufficient to characterize exactly the weakly correlated region; it does not reduce to the second-order perturbation theory. In order to describe the weak Coulomb interaction regime correctly we introduced a new set of local operator

$$\hat{O}_i = \sum_{k_1 k_2 k_1' k_2'} \langle \eta_{k_2 k_1 k_1' k_2'} \rangle_{A_{i\downarrow}} \delta(n_{k_1' k_1} a_{k_2 k_2}^\dagger) \delta(n_{k_1' k_1} a_{k_2 k_2}^\dagger) \delta(n_{k_1' k_1} a_{k_2 k_2}^\dagger),$$

and proposed the following new wavefunction with momentum dependent variational parameters $\{\eta_{k_2 k_1' k_1} \}$.

$$|\Psi\rangle = \prod_i \left( 1 - \hat{O}_i \right) |\phi_0\rangle.$$

Here $\langle i|k\rangle = \exp(-i \mathbf{k} \cdot \mathbf{R}_i)/\sqrt{N}$ is an overlap integral between the localized orbital and the Bloch state with momentum $\mathbf{k}$, $\mathbf{R}_i$ denotes the atomic position, and $N$ is the number of sites. $a_{k\sigma}^\dagger$ ($a_{k\sigma}$) denotes the creation (annihilation) operator for an electron with momentum $\mathbf{k}$ and spin $\sigma$, and $\delta(n_{k\sigma} a_{k\sigma}) = a_{k\sigma}^\dagger a_{k\sigma} - \langle n_{k\sigma} a_{k\sigma} \rangle_0$.

The operator $\hat{O}_i$ is still localized on site $i$ because of the projection $\langle k_1' | i \rangle \langle i | k_1 \rangle \langle k_2' | i \rangle \langle i | k_2 \rangle$. It should be noted that $\hat{O}_i^\dagger \neq \hat{O}_i$ and $\hat{O}_i \hat{O}_j \neq \hat{O}_j \hat{O}_i$ ($i \neq j$) in general. The wavefunction $|\Psi\rangle$ reduces to $|\Psi_{\text{LA}}\rangle$ when $\{\eta_{k_2 k_1' k_1} \}$ become momentum-independent because $\hat{O}_i \rightarrow \eta_{\text{LA}} O_i$. 

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when \( \eta_{k'k_1} \rightarrow \eta_{LA} \).

The variational parameters are determined by minimizing the ground-state correlation energy \( E_c \).

\[
E_c = \langle H \rangle - \langle H \rangle_0 = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.
\]

(7)

Here \( \hat{H} = H - \langle H \rangle_0 \).

Although it is not easy to calculate the correlation energy with use of the wavefunction (6), one can obtain the energy within the single-site approximation (SSA). In the SSA, the average of \( \langle \hat{A} \rangle \) of an operator \( \hat{A} = A - \langle A \rangle_0 \) with respect to the wavefunction (6) is given as follows:

\[
\langle \hat{A} \rangle = \sum_i \frac{\langle (1 - \hat{O}_i^\dagger) \hat{A} (1 - \hat{O}_i) \rangle_0}{\langle (1 - \hat{O}_i^\dagger) (1 - \hat{O}_i) \rangle_0}.
\]

(8)

The derivation of the above formula has been given in Appendix A of our paper I.\(^{18}\)

By making use of the above formula, one can obtain the correlation energy per atom as follows.

\[
\epsilon_c = \frac{-\langle \hat{O}_i^\dagger \hat{H} \rangle_0 - \langle \hat{H} \hat{O}_i \rangle_0 + \langle \hat{O}_i^\dagger \hat{H} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0}.
\]

(9)

Here we assumed that all the sites are equivalent to each other for simplicity and we made use of the fact \( \langle \hat{O}_i^\dagger \rangle_0 = \langle \hat{O}_i \rangle_0 = 0 \).

Each term in the correlation energy (9) can be calculated by making use of Wick’s theorem as follows.

\[
\langle \hat{H} \hat{O}_i \rangle_0 = U \sum_{k_1 k_2 k' k_1'} \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \sum_j \langle k_1 | j \rangle \langle j | k'_1 \rangle \langle k_2 | j \rangle \langle j | k'_2 \rangle \times \eta_{k'k_2 k' k_1} f(\bar{\epsilon}_{k_1 \uparrow}) (1 - f(\bar{\epsilon}_{k'_1 \uparrow})) f(\bar{\epsilon}_{k_2 \downarrow}) (1 - f(\bar{\epsilon}_{k'_2 \downarrow})) ,
\]

(10)

\[
\langle \hat{O}_i^\dagger \hat{H} \rangle_0 = \langle \hat{H} \hat{O}_i \rangle_0^* ,
\]

(11)

\[
\langle \hat{O}_i^\dagger \hat{H} \hat{O}_i \rangle_0 = \sum_{k_1 k_2 k' k_1'} \langle i | k'_1 \rangle \langle k_1 | i \rangle \langle k'_2 | i \rangle \langle k_2 | i \rangle \eta_{k'k_2 k' k_1} \times f(\bar{\epsilon}_{k_1 \uparrow}) (1 - f(\bar{\epsilon}_{k'_1 \uparrow})) f(\bar{\epsilon}_{k_2 \downarrow}) (1 - f(\bar{\epsilon}_{k'_2 \downarrow})) \sum_{k_3 k_4 k_3' k_4'} \langle k_3' | i \rangle \langle i | k_3 \rangle \langle k_4' | i \rangle \langle i | k_4 \rangle \times \left( \Delta E_{k_3' k_2 k_3 k_4' k_3'} \delta_{k_1 k_3} \delta_{k_2 k_3'} \delta_{k_3 k_4} \delta_{k_2 k_4'} + U_{k_3 k_2 k_3 k_4} \right) \eta_{k_3' k_2 k_3'} ,
\]

(12)

\[
U_{k'k_2 k' k_1 k_3 k_4} = U \sum_j \langle j | k_1 \rangle \langle k_3 | j \rangle f(\bar{\epsilon}_{k_3 \uparrow}) \delta_{k_1 k_3} - \langle k'_1 | j \rangle \langle j | k'_3 \rangle (1 - f(\bar{\epsilon}_{k'_3 \uparrow})) \delta_{k_1 k_3} \times \langle j | k_2 \rangle \langle k_4 | j \rangle f(\bar{\epsilon}_{k_4 \downarrow}) \delta_{k_2 k_4} - \langle k'_2 | j \rangle \langle j | k'_4 \rangle (1 - f(\bar{\epsilon}_{k'_4 \downarrow})) \delta_{k_2 k_4} ,
\]

(13)

\[
\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 = \frac{1}{N^2} \sum_{k_1 k_2 k_1' k_2'} |\eta_{k'k_2 k_1' k_2'}|^2 f(\bar{\epsilon}_{k_1 \uparrow}) (1 - f(\bar{\epsilon}_{k'_1 \uparrow})) f(\bar{\epsilon}_{k_2 \downarrow}) (1 - f(\bar{\epsilon}_{k'_2 \downarrow})) .
\]

(14)

Here \( \bar{\epsilon}_{k \sigma} = \epsilon_{k \sigma} - \mu, \epsilon_{k \sigma} = \epsilon_0 + U \langle n_{i-\sigma} \rangle_0 + \epsilon_k - \sigma \hbar \) and \( \Delta E_{k'k_2 k' k_1} = \epsilon_{k_2 \downarrow} - \epsilon_{k_1 \uparrow} + \epsilon_{k'_1 \uparrow} - \epsilon_{k'_2 \downarrow} \) is a two-particle excitation energy. \( \epsilon_k \) is the the Fourier transform of \( t_{ij} \).

The above expressions (10) and (13) contain nonlocal terms via summation over \( j \) (i.e., \( \sum_j \)). We thus make additional SSA called the \( R = 0 \) approximation.\(^{23,24}\) For example, we
have in eq. (10)
\[ \sum_j \langle k'_1| j| k_1 \rangle \langle k'_2| j| k_2 \rangle \langle j| k'_1 \rangle \langle j| k'_2 \rangle = \frac{1}{N^4} \sum_j \delta^{4}(k_1+k_2-k'_1-k'_2)(R_j-R_i), \] but we only take into account the local term \((j = i)\). In the \(R = 0\) approximation, \(\langle \tilde{H} \tilde{O}_i \rangle_0 = \langle \tilde{O}_i \tilde{H} \rangle_0 \), and \(\langle \tilde{O}_i \tilde{H} \rangle_0 \) reduce as follows.
\[
\langle \tilde{H} \tilde{O}_i \rangle_0 = \frac{U}{N^4} \sum_{k_1k_2k'_1k'_2} f(\tilde{\epsilon}_{k_1}) (1 - f(\tilde{\epsilon}_{k'_1})) f(\tilde{\epsilon}_{k_2}) (1 - f(\tilde{\epsilon}_{k'_2})) \eta_{k'_2k_2k'_1k_1},
\]
\[
\langle \tilde{O}_i \tilde{H} \rangle_0 = \frac{1}{N^4} \sum_{k_1k_2k'_1k'_2} f(\tilde{\epsilon}_{k_1}) (1 - f(\tilde{\epsilon}_{k'_1})) f(\tilde{\epsilon}_{k_2}) (1 - f(\tilde{\epsilon}_{k'_2})) \eta^*_{k_2k_1k'_1k'_2}
\times \left[ \Delta E_{k'_2k_2k'_1k_1} \eta_{k'_2k_2k'_1k_1} + \frac{U}{N^2} \left\{ \sum_{k_3k_4} f(\tilde{\epsilon}_{k_3}) f(\tilde{\epsilon}_{k_4}) \eta_{k'_2k_4k'_3k_3} - \sum_{k_3k'_4} f(\tilde{\epsilon}_{k_3}) (1 - f(\tilde{\epsilon}_{k'_4})) \eta_{k'_2k_4k'_3k_3} - \sum_{k_3k'_4} (1 - f(\tilde{\epsilon}_{k'_3})) f(\tilde{\epsilon}_{k_4}) \eta_{k_2k_4k'_3k_3} + \sum_{k_3k'_4} (1 - f(\tilde{\epsilon}_{k'_3})) (1 - f(\tilde{\epsilon}_{k'_4})) \eta_{k_2k_4k'_3k_3} \right\} \right].
\]
Variational parameters \(\{\eta_{k'_2k_2k'_1k_1}\}\) are obtained by minimizing the correlation energy \(\epsilon_c\), i.e., eq. (9) with eqs. (14), (16), and (17). The self-consistent equations for \(\{\eta_{k'_2k_2k'_1k_1}\}\) in the SSA are given as follows.
\[
(\Delta E_{k'_2k_2k'_1k_1} - \epsilon_c) \eta_{k'_2k_2k'_1k_1}
+ \frac{U}{N^2} \left[ \sum_{k_3k_4} f(\tilde{\epsilon}_{k_3}) f(\tilde{\epsilon}_{k_4}) \eta_{k'_2k_4k'_3k_3} - \sum_{k_3k'_4} f(\tilde{\epsilon}_{k_3}) (1 - f(\tilde{\epsilon}_{k'_4})) \eta_{k'_2k_4k'_3k_3} - \sum_{k_3k'_4} (1 - f(\tilde{\epsilon}_{k'_3})) f(\tilde{\epsilon}_{k_4}) \eta_{k_2k_4k'_3k_3} + \sum_{k_3k'_4} (1 - f(\tilde{\epsilon}_{k'_3})) (1 - f(\tilde{\epsilon}_{k'_4})) \eta_{k_2k_4k'_3k_3} \right] = U.
\]
It should be noted that the variational parameters \(\{\eta_{k'_2k_2k'_1k_1}\}\) in eq. (18) vanish when \(U \to 0\), i.e., \(\eta_{k'_2k_2k'_1k_1} \sim O(U)\). Thus in the weak \(U\) limit, one can omit the second term at the l.h.s. (left-hand-side). We then obtain the solution in the weak \(U\) limit as
\[
\eta_{k'_2k_2k'_1k_1} = \frac{U}{\Delta E_{k'_2k_2k'_1k_1}}.
\]
In the atomic limit the transfer integrals \(t_{ij}\) disappear, and one electron energy eigen value \(\epsilon_k\) becomes \(k\)-independent, \(\epsilon_0\). Thus, \(\Delta E_{k'_2k_2k'_1k_1}\) vanishes. In this limit we can drop the \(k\) dependence of \(\eta_{k'_2k_2k'_1k_1}\), i.e., \(\eta_{k'_2k_2k'_1k_1} \to \eta\). Then, we find a \(k\)-independent solution being identical with the LA.
\[
\eta_{LA} = \frac{-(O_{i}\tilde{H}O_{i})_0 + \sqrt{(O_{i}\tilde{H}O_{i})_0^2 + 4(O_{i}\tilde{H})_0^2(O_{i})_0^2}}{2(O_{i}\tilde{H})_0(O_{i})_0}.
\]
It is not easy to find the solution of eq. (18) for the intermediate strength of Coulomb interaction \(U\). We therefore proposed in our paper I an approximate solution which interpolates between the weak and the atomic limits; we approximate \(\{\eta_{k'_2k_2k'_1k_1}\}\) in the second term with the momentum-independent parameter \(\eta\) which is suitable for the atomic region. We have
then
\[ \eta_{k'_2k'_1k_1} = \frac{U[1 - \eta(1 - 2\langle n_i \rangle_0)(1 - 2\langle n_i \rangle_0)]}{\Delta E_{k'_2k_2k'_1k_1} - \epsilon_c}. \] (21)

In the previous paper \(^{18}\) we made use of that in the LA for \( \eta \), and adopted the correlation energy in the LA for \( \epsilon_c \) in the denominator. We call this the non-self-consistent MLA in the followings.

The best value of \( \eta \), however, should be determined variationally in general. In this paper we further develop the theory in which \( \eta \) is determined best. According to the variational principle, the ground-state energy \( E_0 \) satisfies the following inequality:

\[ E_0 \leq E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \] (22)

Here \( \Psi \) is a trial wavefunction.

In the MLA, we choose the wavefunction \( \Psi = \Psi(\{\eta_{k'_2k_2k'_1k_1}\}) \) and the corresponding energy \( E(\{\eta_{k'_2k_2k'_1k_1}\}) \) satisfies the inequality \( E_0 \leq E(\{\eta_{k'_2k_2k'_1k_1}\}) \).

For the stationary values \( \eta^*_{k'_2k_2k'_1k_1} \), we have

\[ E_0 \leq E(\{\eta^*_{k'_2k_2k'_1k_1}\}) \leq E(\{\eta_{k'_2k_2k'_1k_1}\}). \] (23)

In the previous calculations, \(^{18}\) we obtained an approximate \( \eta^*_{k'_2k_2k'_1k_1} \) (21):

\[ \eta_{k'_2k_2k'_1k_1}(\tilde{\eta}, \epsilon_c) = \frac{U \tilde{\eta}}{\Delta E_{k'_2k_2k'_1k_1} - \epsilon_c}, \] (24)

which is determined by the correlation energy \( \epsilon_c \) and a momentum independent parameter \( \tilde{\eta} \). Here

\[ \tilde{\eta} = [1 - \eta(1 - 2\langle n_i \rangle_0)(1 - 2\langle n_i \rangle_0)]. \] (25)

When we adopt the form (24) as a trial set of amplitudes, we have an inequality as

\[ \langle E_0 \rangle \leq E(\{\eta^*_{k'_2k_2k'_1k_1}\}) \leq E(\{\eta_{k'_2k_2k'_1k_1}(\tilde{\eta}, \epsilon_c)\}). \] (26)

The above relation implies that the best \( \tilde{\eta} \) is again determined from the stationary condition of the trial energy \( E(\{\eta^*_{k'_2k_2k'_1k_1}(\tilde{\eta}, \epsilon_c)\}) \). Because \( \epsilon_c \) should satisfy the stationary condition \( \delta \epsilon_c = 0 \) for the value \( \tilde{\eta}^* \), \( \tilde{\eta}^* \) is determined by the following condition

\[ \left[ \frac{\partial \epsilon(\{\eta^*_{k'_2k_2k'_1k_1}(\tilde{\eta}, \epsilon_c)\})}{\partial \tilde{\eta}} \right]_{\epsilon_c} = 0. \] (27)

The self-consistent equation is obtained from eq.(27) in the same way as in eq. (18)

\[ \frac{1}{N^4} \sum_{k_1k'_1k_2k'_2} f(\tilde{\epsilon}_{k_1 \uparrow})[1 - f(\tilde{\epsilon}_{k'_1 \uparrow})] f(\tilde{\epsilon}_{k_2 \downarrow})[1 - f(\tilde{\epsilon}_{k'_2 \downarrow})] \frac{\partial \eta_{k'_2k_2k'_1k_1}}{\partial \tilde{\eta}} \] 

\[ + \frac{U}{N^6} \sum_{k_1k'_1k_2k'_2} f(\tilde{\epsilon}_{k_1 \uparrow})[1 - f(\tilde{\epsilon}_{k'_1 \uparrow})] f(\tilde{\epsilon}_{k_2 \downarrow})[1 - f(\tilde{\epsilon}_{k'_2 \downarrow})] \frac{\partial \eta_{k'_2k_2k'_1k_1}}{\partial \tilde{\eta}} \] 

\[ \times \left[ \sum_{k_3k_4} f(\tilde{\epsilon}_{k_3 \uparrow})f(\tilde{\epsilon}_{k_4 \downarrow})\eta_{k'_2k_2k'_1k_3} - \sum_{k'_3k_4} [1 - f(\tilde{\epsilon}_{k_3 \uparrow})] f(\tilde{\epsilon}_{k_4 \downarrow})\eta_{k'_2k_2k'_1k_3} \right] \] 

\[ - \sum_{k_3k'_3} f(\tilde{\epsilon}_{k_3 \uparrow})[1 - f(\tilde{\epsilon}_{k'_3 \uparrow})] \eta_{k'_2k_2k'_1k_3} + \sum_{k'_3k'_3} [1 - f(\tilde{\epsilon}_{k'_3 \uparrow})][1 - f(\tilde{\epsilon}_{k'_3 \uparrow})] \eta_{k'_2k_2k'_1k_3} \]
\[ \frac{U}{N^4} \sum_{k_1'k_2'k_2} f(\tilde{\epsilon}_{k_1}) [1 - f(\tilde{\epsilon}^{\uparrow}_{k_1})] f(\tilde{\epsilon}_{k_2}) [1 - f(\tilde{\epsilon}^{\downarrow}_{k_2})] \frac{\partial \eta_{k_1'k_2k'_1}}{\partial \tilde{\eta}}. \] (28)

Here \( \partial \eta_{k_1'k_2k'_1}/\partial \tilde{\eta} \) is obtained from eq. (24) as

\[ \frac{\partial \eta_{k_1'k_2k'_1}}{\partial \tilde{\eta}} = \frac{U}{\Delta E_{k_1'k_2k'_1k_1} - \epsilon_c}. \] (29)

Substituting the above expression into the self-consistent equation (28) we obtain

\[ \tilde{\eta} = \frac{1}{1 + \frac{UC}{D}}. \] (30)

Here

\[ C = \frac{1}{N^6} \sum_{k_1'k_2'k_2'} f(\tilde{\epsilon}_{k_1'}) [1 - f(\tilde{\epsilon}^{\uparrow}_{k_1'})] f(\tilde{\epsilon}_{k_2}) [1 - f(\tilde{\epsilon}^{\downarrow}_{k_2})] \frac{\Delta E_{k_1'k_2k'_1k_1} - \epsilon_c}{(\Delta E_{k_1'k_2k'_1k_1} - \epsilon_c)} \]

\[ \times \left\{ \sum_{k_3k_4} \frac{f(\tilde{\epsilon}_{k_3}) f(\tilde{\epsilon}_{k_4})}{(\Delta E_{k_1'k_4k'_1k_3} - \epsilon_c)} \right\} \]

\[ - \sum_{k_3k_4} \frac{f(\tilde{\epsilon}_{k_3}) [1 - f(\tilde{\epsilon}_{k_4'})]}{(\Delta E_{k_1'k_4k'_1k_3} - \epsilon_c)} \] (31)

and

\[ D = \frac{1}{N^4} \sum_{k_1'k_2'k_2'} f(\tilde{\epsilon}_{k_1'}) [1 - f(\tilde{\epsilon}^{\uparrow}_{k_1'})] f(\tilde{\epsilon}_{k_2}) [1 - f(\tilde{\epsilon}^{\downarrow}_{k_2})] \frac{\Delta E_{k_1'k_2k'_1k_1} - \epsilon_c}{(\Delta E_{k_1'k_2k'_1k_1} - \epsilon_c)} \] (32)

In the energy representation, each term is expressed as follows:

\[ C = \int \left[ \prod_{n=1}^{6} \rho(\epsilon_n) \right] \left[ \prod_{n=1}^{6} f(\tilde{\epsilon}_{n}) [1 - f(\tilde{\epsilon}_{2n})] f(\tilde{\epsilon}_{3n}) [1 - f(\tilde{\epsilon}_{4n})] f(\tilde{\epsilon}_{5n}) f(\tilde{\epsilon}_{6n}) \right] \]

\[ \frac{\partial \eta_{n_1n_2n_3}}{\partial \tilde{\eta}_{n_1n_2n_3}} \] (33)

Here \( \tilde{\epsilon}_{n\sigma} = \epsilon_n + \tilde{\sigma} \) and \( \tilde{\sigma} = \epsilon_0 + U \langle n_{-\sigma} \rangle - \mu \) is the atomic level measured from the chemical potential, and \( \rho(\epsilon) \) is the density of states for the one-electron energy eigen values for the non-interacting system \( t_{ij} \).
It should be noted that the self-consistent solution (30) is also obtained by solving approximately the original self-consistent eq. (18). In order to do this, first we divide the both sides of eq. (18) by \((\Delta E_{k_1'k_2'k_1} - \epsilon_c)\), substitute the form (24), and we obtain eq. (30) after taking the average with respect to \(k_1k_2k'_1k'_2\) with a weight \(f(\epsilon_{k_1})[1 - f(\epsilon_{k_1'})][1 - f(\epsilon_{k_2})][1 - f(\epsilon_{k_2'})]\). The variational principles on \(\tilde{\eta}\) tells us that such a solution should be the best among possible approximate solutions. We also note that an approximate form (25), which was obtained in paper I, is derived from the solution (30). In fact, we rewrite eq. (30) as \(\tilde{\eta}\) approximate solutions. We also note that an approximate form (25), which was obtained in paper I, is derived from the solution (30). In fact, we rewrite eq. (30) as \(\tilde{\eta} = 1 - U\tilde{\eta}C/D\). By replacing the approximate form (24) in the expression of \(U\tilde{\eta}C\) with the momentum independent value \(\tilde{\eta}\), we reach eq. (25).

The ground-state correlation energy is obtained by substituting the variational parameters (24) into eq. (9). The each element in the energy is given as follows.

\[
\langle \tilde{H}\tilde{O}_i\rangle_0 = \langle \tilde{O}_i^\dagger \tilde{H} \rangle_0^* \\
= U^2\tilde{\eta} \int \left[ \prod_{n=1}^{4} d\epsilon_n \right] \left[ \prod_{n=1}^{4} \rho(\epsilon_n) \right] \frac{f(\epsilon_1')f(\epsilon_2')f(\epsilon_3')f(\epsilon_4')}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)} ,
\]

\[
\langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i\rangle_0 = \langle \tilde{O}_i^\dagger \tilde{H}_0 \tilde{O}_i\rangle_0 + U \langle \tilde{O}_i^\dagger O_i \tilde{O}_i\rangle_0 ,
\]

\[
\langle \tilde{O}_i^\dagger \tilde{O}_i^\dagger O_i \tilde{O}_i\rangle_0 = U^2\tilde{\eta} \int \left[ \prod_{n=1}^{4} d\epsilon_n \right] \left[ \prod_{n=1}^{4} \rho(\epsilon_n) \right] \frac{f(\epsilon_1')f(\epsilon_2')f(\epsilon_3')f(\epsilon_4')}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2}\]

\[
\times \left[ \int \left[ \prod_{n=5}^{6} d\epsilon_n \right] \left[ \prod_{n=5}^{6} \rho(\epsilon_n) \right] \frac{f(\epsilon_5')f(\epsilon_6')}{(\epsilon_4 - \epsilon_6 + \epsilon_2 - \epsilon_5 - \epsilon_c)} - \int \left[ \prod_{n=5}^{6} d\epsilon_n \right] \left[ \prod_{n=5}^{6} \rho(\epsilon_n) \right] \frac{f(\epsilon_5')f(\epsilon_6')}{(\epsilon_6 - \epsilon_3 + \epsilon_2 - \epsilon_5 - \epsilon_c)} - \int \left[ \prod_{n=5}^{6} d\epsilon_n \right] \left[ \prod_{n=5}^{6} \rho(\epsilon_n) \right] \frac{f(\epsilon_5')f(\epsilon_6')}{(\epsilon_4 - \epsilon_6 + \epsilon_5 - \epsilon_1 - \epsilon_c)} + \int \left[ \prod_{n=5}^{6} d\epsilon_n \right] \left[ \prod_{n=5}^{6} \rho(\epsilon_n) \right] \frac{f(\epsilon_5')f(\epsilon_6')}{(\epsilon_6 - \epsilon_3 + \epsilon_5 - \epsilon_1 - \epsilon_c)} \right] \right) .
\]

\[
\langle \tilde{O}_i^\dagger \tilde{O}_i\rangle_0 = U^2\tilde{\eta} \int \left[ \prod_{n=1}^{4} d\epsilon_n \right] \left[ \prod_{n=1}^{4} \rho(\epsilon_n) \right] \frac{f(\epsilon_1')f(\epsilon_2')f(\epsilon_3')f(\epsilon_4')}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2} .
\]

It should be noted that \(\tilde{\eta}\) in eq. (30) is given as a function of \(\epsilon_c\), and \(\epsilon_c\) in eq. (9) depends
on $\tilde{\eta}$ and $\epsilon_c$. Therefore, both equations have to be solved self-consistently. To determine the best value of $\tilde{\eta}$, we start from $\epsilon_c$ in the LA for example, and calculate $\tilde{\eta}$ according to eq. (30). Next we calculate various elements $\langle \hat{H} \hat{O}_i \rangle_0$ ($\langle \hat{O}_i \hat{H} \rangle_0$, $\langle \hat{O}_i \hat{H} \hat{O}_i \rangle_0$, and $\langle \hat{O}_i \hat{O}_i \rangle_0$) which are given by eqs. (35), (36), and (39), respectively. Using these values we calculate $\epsilon_c$ according to eq. (9). We repeat this cycle until the self-consistency of $\epsilon_c$ and $\tilde{\eta}$ is satisfied. We call this scheme the self-consistent MLA.

Electron number $\langle n_i \rangle = \sum_\sigma \langle n_{i\sigma} \rangle$, the momentum distribution $\langle n_{k\sigma} \rangle$, and the double occupation number $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ are obtained from $\partial \langle H \rangle / \partial \epsilon_0$, $\partial \langle H \rangle / \partial \epsilon_{k\sigma}$, and $\partial \langle H \rangle / \partial U_i$, respectively. Here $\hat{\epsilon}_{k\sigma} = \epsilon_k - \sigma \hbar$. Making use of the single-site energy (9) and the Feynman-Hellmann theorem,25 we obtain the following expressions:

$$\langle n_i \rangle = \langle n_i \rangle_0 + \frac{\langle \hat{O}_i \hat{n}_i \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i \hat{O}_i \rangle_0}, \quad (40)$$

$$\langle n_{k\sigma} \rangle = \langle n_{k\sigma} \rangle_0 + \frac{N \langle \hat{O}_i \hat{n}_{k\sigma} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i \hat{O}_i \rangle_0}, \quad (41)$$

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0 + \frac{-\langle \hat{O}_i \hat{O}_i \rangle_0 - \langle \hat{O}_i \hat{O}_i \rangle_0 + \langle \hat{O}_i \hat{O}_i \rangle_0 + \sum_\sigma \langle n_{i\sigma} \rangle_0 \langle \hat{O}_i \hat{n}_{i\sigma} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i \hat{O}_i \rangle_0}. \quad (42)$$

Here $n_i = \langle n_i \rangle_0$, $n_{k\sigma} = \langle n_{k\sigma} \rangle_0$, and $n_{i\uparrow} n_{i\downarrow} = \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0$, and

$$\langle \hat{O}_i \hat{n}_{i\sigma} \hat{O}_i \rangle_0 = U^2 \eta^2 \int \prod_{n=1}^{5} \text{d} \epsilon_n \left[ \left( \frac{\prod_{n=1}^{5} \rho(\epsilon_n) f(\epsilon_{1-\sigma}) [1 - f(\epsilon_{2-\sigma})] f(\epsilon_{3\sigma}) [1 - f(\epsilon_{4\sigma})]}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2} \right) \right. \times \left[ \frac{1 - f(\epsilon_{5\sigma})}{(\epsilon_5 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)} - \frac{f(\epsilon_{5\sigma})}{(\epsilon_4 - \epsilon_5 + \epsilon_2 - \epsilon_1 - \epsilon_c)} \right]. \quad (43)$$

$$N \langle \hat{O}_i \hat{n}_{k\sigma} \hat{O}_i \rangle_0 = U^2 \eta^2 \left[ 1 - f(\epsilon_{k\sigma}) \right] \int \prod_{n=1}^{3} \text{d} \epsilon_n \left[ \left( \frac{\prod_{n=1}^{3} \rho(\epsilon_n) f(\epsilon_{1-\sigma}) [1 - f(\epsilon_{2-\sigma})] f(\epsilon_{3\sigma})}{(\epsilon_{k\sigma} - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2} \right) - f(\epsilon_{k\sigma}) \right] \left[ \left( \frac{3}{\epsilon_3 - \epsilon_{k\sigma} + \epsilon_2 - \epsilon_1 - \epsilon_c} \right) \right]. \quad (44)$$

$$\langle \hat{O}_i \hat{O}_i \rangle_0 + \langle \hat{O}_i \hat{O}_i \rangle_0 = 2U \tilde{\eta} \int \prod_{n=1}^{4} \text{d} \epsilon_n \left[ \left( \frac{4}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)} \right) \right]. \quad (45)$$

Note that $\langle \hat{O}_i \hat{O}_i \rangle_0$ has been given by eq. (38). The expressions of these physical quantities consist of the multiple integrals up to the 6-folds. One can reduce these integrals up to the 2-folds using the Laplace transform.26 Their expressions are given in Appendix.

3. Numerical Results

We have performed the numerical calculations for the non-half-filled as well as half-filled bands of the Hubbard model in order to examine the validity of the improved scheme of the
Fig. 1. The correlation energy $E_c$ vs. Coulomb interaction energy curve for $n = 0.8$. The thick solid curve: the MLA with self-consistent $\tilde{\eta}$, the thin curve: the MLA with non self-consistent $\tilde{\eta}$, and the dashed curve: the LA.

3.1 Role of the best choice of $\tilde{\eta}$

To calculate various quantities in the MLA, we solved the self-consistent equations (9) and (30) with use of the Laplace transforms of elements, which are given in Appendix. In this sub-section, we compare the self-consistent results with the non self-consistent ones to clarify the role of the best $\tilde{\eta}$.

Figure 1 shows the calculated correlation energy as a function of Coulomb interaction. The correlation energy for the MLA without best choice of $\tilde{\eta}$ gives the lower correlation energy compared with the LA. The correlation energy for the MLA with the best choice of $\tilde{\eta}$ is lower than that of the non-self-consistent MLA. The results indicate that the self-consistency of $\tilde{\eta}$ is significant for finding the best energy.

In Fig. 2 we show an example of the momentum distribution as a function of energy $\epsilon_{k\sigma}$ when electron number is deviated from 1. The MLA with non self-consistent $\tilde{\eta}$ (25) shows a bump in the vicinity of the Fermi level, leading to an unphysical result. The MLA with self-consistent $\tilde{\eta}$ yields a significant momentum dependence which shows monotonical decrease of the distribution with increasing $\epsilon_{k\sigma}$.

We have also calculated the quasiparticle weight $Z$ vs. Coulomb interaction energy curves at half-filling. As shown in Fig. 3, we find that the best choice of $\tilde{\eta}$ increases $Z$ (i.e., decreases the inverse effective mass), so that the critical Coulomb interaction of the divergence of the effective mass, $U_{c2}$ changes from 3.21 to 3.40. The latter is closer to the NRG value $U_{c2} = 4.10$, which is believed to be the best at present.

From the above discussions on the results with and without self-consistent $\tilde{\eta}$, it is obvious that the best choice of $\tilde{\eta}$ improves the results of the MLA. In the following discussions we adopt the best choice of $\tilde{\eta}$. 

MLA and the effect of electron correlations in the local ansatz. To calculate various physical quantities, we have adopted the hypercubic lattice in infinite dimensions, where the single-site approximation works best. The density of states (DOS) for non-interacting system is given by $\rho(\epsilon) = (1/\sqrt{\pi})\exp(-\epsilon^2)$ in this case.$^{18}$ The energy unit is chosen to be $\int d\epsilon \rho(\epsilon)\epsilon^2 = 1/2$. The external magnetic field $h$ is assumed to be zero.

The external magnetic field $h$ is assumed to be zero.
Fig. 2. The momentum distribution as a function of energy $\epsilon_k$ for various theories with $n = 0.6$ and $U = 2.0$. The solid curve: the MLA with the best choice of $\tilde{\eta}$, the dashed curve: the MLA without the best choice of $\tilde{\eta}$, and the dotted curve: the LA.

Fig. 3. Quasiparticle-weight $Z$ vs. Coulomb interaction curves in the MLA with self-consistent $\tilde{\eta}$ (solid curve), and without (dashed curve).

3.2 MLA vs LA in various physical quantities

In this section, we present the numerical results on various physical quantities, and discuss the new aspects of the MLA and related electron correlation effects by comparing the MLA with the LA.

In Fig. 4, we represent the calculated correlation energy per atom as a function of Coulomb interaction $U$. The energy in the MLA is lower than that of the LA over all Coulomb interaction
energy parameters $U$ and electron numbers $n$. These results imply that the MLA improves the LA. The magnitude of the correlation energy $|\epsilon_c|$ tends to increase with increasing $U$, because with increasing $U$ the correlation corrections increase as $U^2$ for small $U$ and cancel the Hartree-Fock energy loss being linear in $U$ for large $U$. For a fixed value of the Coulomb interaction $U$, the gain of the correlation energy $|\epsilon_c|$ increases with increasing $n$, because there is a correlation energy gain at each doubly-occupied site and the number of such sites increases with increasing $n$.

Fig. 4. The correlation energies $E_c$ vs. Coulomb interaction energy parameter $U$ in the MLA (solid curve) and the LA (dashed curve) for various electron number $n$.

Fig. 5. The double occupation number $\langle n^+_\uparrow n^\downarrow \rangle$ vs. Coulomb interaction energy $U$ curves in the MLA (solid curve) and the LA (dotted curve).
Figure 5 depicts the double occupation number $\langle n_\uparrow n_\downarrow \rangle$ vs. Coulomb interaction curves for the non-half-filled case. In the uncorrelated limit, the double occupancy is the same for both LA and MLA and it decreases with increasing Coulomb interaction $U$ because electrons move on the lattice so as to suppress the loss of Coulomb energy due to double occupation. We find that the MLA wavefunction reduces the double occupancy as compared with that of the LA in the range $0 < U \lesssim 5$, while in the range $5 \lesssim U$ the double occupancy in the MLA is larger than that of the LA. It implies that the LA with momentum-independent $\eta_{LA}$ overestimates the itinerant character for weak and intermediate $U$ regions, while it overestimates the atomic character for large $U$ region.

The momentum-distribution function shown in Fig. 6 indicates more distinct difference between the LA and the MLA. The distributions in the LA are constant below and above the Fermi level irrespective of $U$. The same behavior is also found in the GA.$^{9-11}$ The MLA curves show a monotonical decrease of the distribution with increasing $\epsilon_{k\sigma}$, indicating a distinct momentum dependence of $\langle n_{k\sigma} \rangle$ via energy $\epsilon_{k\sigma}$, which is qualitatively different from both the LA and the GA.

The quasiparticle weight $Z$ (i.e. the inverse effective mass) is obtained from the jump at the Fermi level in the momentum distribution according to the Fermi liquid theory.$^{28, 29}$ Calculated quasiparticle weight vs Coulomb interaction energy parameters $U = 3$. The MLA: solid curves, the LA: dashed curves.

Fig. 6. The momentum distribution as a function of energy $\epsilon_k$ for various electron number with constant Coulomb interaction energy parameters $U = 3$. The MLA: solid curves, the LA: dashed curves.

The quasiparticle weight $Z$ (i.e. the inverse effective mass) is obtained from the jump at the Fermi level in the momentum distribution according to the Fermi liquid theory.$^{28, 29}$ Calculated quasiparticle weight vs Coulomb interaction curves are shown in Fig. 7 for the half-filled case. The quasiparticle weight in the LA changes as $Z = (1 - 3\eta_{LA}^2/16)/(1 + \eta_{LA}^2/16)$ and vanishes at $U_{c2}(LA) = 24/\sqrt{3\pi} (= 7.82)$. In the GA,$^{12}$ the quasiparticle weight changes as $Z = 1 - (U/U_{c2})^2$. The curve in the GA agrees with the LA curve for small $U$. But it deviates from the LA when $U$ becomes larger, and vanishes at $U_{c2}(GA) = 8/\sqrt{\pi} (= 4.51)$. It should be noted that the GA curve strongly deviates from the curve in the NRG$^{27}$ which is considered to be the best. We observe that the critical Coulomb interaction $U_{c2}$ for the self-consistent $\tilde{\eta}$ is 3.40 in the MLA while $U_{c2}$ in the non-self-consistent $\tilde{\eta}$ yields 3.21. The quasiparticle weight in the MLA much improves the LA as seen in Fig. 7. We note that the wavefunction itself does not show the metal-insulator transition at $U_{c2}$ in the present approximation because the approximate expression of variational parameters (21) has no singularity at finite value.
Fig. 7. Quasiparticle-weight vs. Coulomb interaction curves in various theories. The RPT-1: dashed curve,\textsuperscript{30} the NRG: thin solid curve,\textsuperscript{27} the LA: dotted curve, the MLA: solid curve, and the GA: dot-dashed curve.

of $U$. In this sense, the calculated $Z$ and wavefunction are not self-consistent in the present approximation. The values of $Z$ obtained by the LA and the MLA should be regarded as an estimate from the metallic side.

Fig. 8. Quasiparticle-weight $Z$ vs. Coulomb interaction curves. The MLA: solid curve, the LA: dashed curve.

Figure 8 also shows the quasiparticle weight as a function of Coulomb interaction energy $U$ for the non-half-filled case and the half-filled case. In the uncorrelated limit, the quasiparticle
weight is 1 as it should be. It decreases with increasing Coulomb interaction \( U \) for both the MLA and the LA. In general, the curves in the MLA are lower than those in the LA as expected from the fact \( U_{c2}(\text{MLA}) < U_{c2}(\text{LA}) \) at half-filling. This means that the electron effective mass is enhanced by the self-consistent treatment of \( \tilde{\eta} \) irrespective of \( U \) and \( n \).

4. Summary and Discussions

In the present paper, we improved the variational scheme of the MLA which self-consistently determines both the variational amplitude \( \tilde{\eta} \) and the correlation energy \( \epsilon_c \) making use of variational principles. To examine the improvement and validity of the theory, we performed the numerical calculations on the basis of the Hubbard model on the hypercubic lattice in infinite dimensions. We verified for both the half-filled and the non-half-filled bands that the self-consistent scheme of the MLA improves the correlation energy, the momentum distribution function as well as the quasiparticle weight. Therefore, the self-consistency of \( \tilde{\eta} \) is significant for quantitative understanding of electron correlations.

Within the self-consistent MLA, we have clarified the role of the momentum dependence of variational parameters in comparison with the original LA. We demonstrated that the self-consistent MLA improves the LA irrespective of the Coulomb interaction energy parameter \( U \) and electron number \( n \). The correlation energy in the MLA is lower than those of the LA and the GA in the weak and intermediate Coulomb interaction regimes. Thus the MLA wavefunction should be better than both the LA and the GA in these regimes. The double occupation number is suppressed as compared with the LA both in the same interaction regimes. We found that the calculated momentum distribution functions show a distinct momentum dependence. This is qualitatively different from the LA and the GA because both of them lead to the momentum-independence of the distributions below and above the Fermi level. We also found that the quasiparticle weight in the MLA is lower than that of the LA irrespective of \( U \) and \( n \), and is close to the result of the NRG. Accordingly the critical Coulomb interaction \( U_{c2} \) of the MLA becomes closer to that obtained in the NRG.

The variational theories discussed in the present paper construct the correlated ground state by applying the two-particle operators to the Hartree-Fock ground state. The wavefunctions of both the LA and the GA are expressed by the momentum dependent two-particle excited states in addition to the Hartree-Fock one. Each amplitude of the excited states is momentum independent in these methods. The MLA wavefunction, on the other hand, each amplitude of the two-particle excited states is momentum dependent. By choosing the momentum-dependent amplitudes \( \eta_{k_1'k_2k_1k_2} \) best on the basis of the variational principle, we improved the LA and the GA in the weak and intermediate Coulomb interaction regimes. Note that this procedure does not depend on dimensions of the system within the SSA because of the local projection \( \langle k_1' | \tilde{i} | k_1 \rangle \langle k_2' | \tilde{i} | k_2 \rangle \) in the operator \( \tilde{O}_i \) and thus the improvement remains unchanged even in infinite dimensions.

Needless to say, many methods to solve the correlation problems in infinite dimensions have been developed.\(^2\,3^1\) The NRG is one of the best approaches to calculate the excitations at zero temperature as well as related ground-state properties. The accuracy of MLA is on the level of the iterative perturbation theory\(^3^2\) at the present stage. Furthermore excitation properties cannot directly be calculated by the variational approach. It is also true, however, that the high-quality methods such as the NRG\(^2^7\) are not applicable to the realistic systems because of their complexity. The present approach is applicable to more complex systems. Moreover the wavefunction method arrows us to calculate any static averages as we have demonstrated in paper I.\(^1^8\) We therefore believe that further developments of the MLA wavefunction approach will provide us with a useful tool for understanding correlated electrons in the realistic systems and their physics. Developments of the theory towards the strongly correlated system and its extension to the realistic systems are our current problems in progress.

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Appendix: Laplace transform for the correlation calculations

The Laplace transform can significantly reduce the number of integrals in the physical quantities which appear in our variational theory. It is written as follows:

\[
\frac{1}{z - \epsilon_4 + \epsilon_3 - \epsilon_2 + \epsilon_1 + \epsilon_c} = -i \int_0^\infty dt e^{i(z - \epsilon_4 + \epsilon_3 - \epsilon_2 + \epsilon_1 + \epsilon_c) t} .
\]  (A-1)

Here \( z = \omega + i \delta \), and \( \delta \) is an infinitesimal positive number.

The term \( \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 \) in eq. (39) can be written in the energy as follows:

\[
\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 = U^2 \eta^2 \lim_{z \to 0} \int \frac{\left[ \prod_{n=1}^4 d\epsilon_n \right] \left[ \prod_{n=1}^4 \rho(\epsilon_n) \right] f(\tilde{\epsilon}_{1\uparrow})[1 - f(\tilde{\epsilon}_{2\uparrow})]f(\tilde{\epsilon}_{3\downarrow})[1 - f(\tilde{\epsilon}_{4\downarrow})]}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2} .
\]  (A-2)

\[
= U^2 \eta^2 \lim_{z \to 0} \int \frac{\left[ \prod_{n=1}^4 d\epsilon_n \right] \left[ \prod_{n=1}^4 \rho(\epsilon_n) \right] f(\tilde{\epsilon}_{1\uparrow})[1 - f(\tilde{\epsilon}_{2\uparrow})]f(\tilde{\epsilon}_{3\downarrow})[1 - f(\tilde{\epsilon}_{4\downarrow})]}{(z - \epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c)^2} .
\]  (A-3)

Here, \( \tilde{\epsilon}_{n\sigma} = \epsilon_n + \epsilon_c \), and \( \tilde{\epsilon}_\sigma = \epsilon_0 + U \langle n_{1-\sigma} \rangle - \mu \) is the Hartree-Fock level measured from the Fermi level \( \mu \). \( \rho(\epsilon) \) in the above expressions denotes the density of states for \( \epsilon_k \), i.e., the Fourier transform of \( t_{ij} \). Now using the relation of Laplace transform (A-1), we obtain

\[
\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 = -U^2 \eta^2 \lim_{z \to 0} \int_0^\infty dt dt' e^{i(\epsilon + \epsilon_c)(t + t')} \int d\epsilon_1 e^{i\epsilon_1(t + t')} \rho(\epsilon_1) f(\tilde{\epsilon}_{1\uparrow})
\times \int d\epsilon_2 e^{-i\epsilon_2(t + t')} \rho(\epsilon_2)[1 - f(\tilde{\epsilon}_{2\uparrow})] \int d\epsilon_3 e^{i\epsilon_3(t + t')} \rho(\epsilon_3)f(\tilde{\epsilon}_{3\downarrow})
\times \int d\epsilon_4 e^{-i\epsilon_4(t + t')} \rho(\epsilon_4)[1 - f(\tilde{\epsilon}_{4\downarrow})]
= -U^2 \eta^2 \int_0^\infty dt dt' e^{i\epsilon_c(t + t')} a_{\uparrow}(t) a_{\downarrow}(t + t') b_{\uparrow}(t + t') a_{\downarrow}(t) b_{\downarrow}(t + t') .
\]  (A-4)

Here

\[
a_\sigma(t) = \int d\epsilon \rho(\epsilon) f(\epsilon + \tilde{\epsilon}_\sigma) e^{-i\epsilon t} ,
\]  (A-6)

\[
b_\sigma(t) = \int d\epsilon \rho(\epsilon)[1 - f(\epsilon + \tilde{\epsilon}_\sigma)] e^{-i\epsilon t} .
\]  (A-7)

The 4-fold integrals of \( \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 \) in eq. (A-2) reduce to the 2-fold integrals in eq. (A-5).

In the same way, we can perform the Laplace transform of various elements in the physical quantities as follows:

\[
\langle \hat{H} \hat{O}_i \rangle_0 = \langle \hat{O}_i^\dagger \hat{H} \rangle_0^* = iU^2 \eta \int_0^\infty dt e^{i\epsilon t} a_{\uparrow}(t) a_{\downarrow}(t) b_{\uparrow}(t) b_{\downarrow}(t) ,
\]  (A-8)

\[
\langle \hat{O}_i^\dagger \hat{H}_0 \hat{O}_i \rangle_0 = -U^2 \eta^2 \int_0^\infty dt dt' e^{i\epsilon(t + t')} \left[ a_{\uparrow}(t) a_{\downarrow}(t + t') b_{\uparrow}(t + t') a_{\downarrow}(t) b_{\downarrow}(t) - a_{\uparrow}(t) b_{\uparrow}(t + t') a_{\downarrow}(t) b_{\downarrow}(t + t') + a_{\uparrow}(t) a_{\downarrow}(t + t') b_{\uparrow}(t + t') a_{\downarrow}(t) + a_{\uparrow}(t) a_{\downarrow}(t) b_{\uparrow}(t) a_{\downarrow}(t) b_{\uparrow}(t) a_{\downarrow}(t) b_{\downarrow}(t + t') \right] .
\]  (A-9)
Here

\[ a_{1\sigma}(t) = \int d\epsilon \rho(\epsilon) f(\epsilon + \epsilon_\sigma) \epsilon e^{-i\epsilon t}, \]  

\[ b_{1\sigma}(t) = \int d\epsilon \rho(\epsilon) [(1 - f(\epsilon + \epsilon_\sigma)) \epsilon e^{-i\epsilon t}]. \]

The element (34) and (33) for the calculation of the best choice of \( \tilde{\eta} \) are expressed as

\[ C = -\int_0^\infty dt dt' e^{i\epsilon(t+t')} [a_{\uparrow}(t)b_{\downarrow}(t+t')a_{\downarrow}(t)t'] \\
- a_{\uparrow}(-t-t')b_{\downarrow}(t)a_{\downarrow}(t+t')b_{\downarrow}(t')a_{\downarrow}(t+t') \\
- a_{\uparrow}(-t-t')b_{\downarrow}(t)a_{\downarrow}(t+t')b_{\downarrow}(t')a_{\downarrow}(t+t') \\
+ a_{\uparrow}(-t-t')b_{\downarrow}(t)a_{\downarrow}(t+t')b_{\downarrow}(t')b_{\downarrow}(t')]. \]  

(\text{A-10})

and

\[ D = i \int_0^\infty dt e^{i\epsilon t} a_{\uparrow}(t)b_{\downarrow}(t)b_{\downarrow}(t). \]  

(\text{A-11})

The correlation contribution to the momentum distribution function (44) is given by

\[ N(\tilde{O}_{\eta_{k\sigma}}\tilde{O}_{\eta})_0 = U^2 \eta^2 \int_0^\infty dt dt' e^{i\epsilon(t+t')} a_{-\sigma}(-t-t')b_{-\sigma}(t+t') \]
\[ \times \left[ f(\epsilon_{k\sigma})b_{\sigma}(t+t') - 1 - f(\epsilon_{k\sigma}) \epsilon(t+t') \right]. \]  

(\text{A-12})

The correlation contribution to the electron number (43) which appears in the calculation of the double occupancy number is expressed as

\[ \langle \tilde{O}_{\eta_{k\sigma}}\tilde{O}_{\eta} \rangle_0 = -U^2 \eta^2 \int_0^\infty dt dt' e^{i\epsilon(t+t')} [a_{-\sigma}(-t-t')b_{-\sigma}(t+t')a_{\sigma}(-t-t')b_{\sigma}(t+t')] \]
\[ - a_{-\sigma}(-t-t')b_{-\sigma}(t+t')a_{\sigma}(-t-t')b_{\sigma}(t+t')]. \]  

(\text{A-13})

The element (45) for the calculation of the double occupancy is expressed as

\[ \langle \tilde{O}_{\eta_{k\sigma}}\tilde{O}_{\eta} \rangle_0 + \langle O_{\eta}O_{\eta} \rangle_0 = 2i U \eta \int_0^\infty dt e^{i\epsilon t} a_{\uparrow}(t)b_{\uparrow}(t)b_{\downarrow}(t). \]

(\text{A-14})
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