MOMENTUM-DEPENDENT LOCAL ANSATZ APPROACH TO CORRELATED ELECTRONS

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The wavefunction method provides us with a useful tool to describe electron correlations in solids at the ground state. In this paper we review the recent development of the momentum-dependent local ansatz wavefunction (MLA). It is constructed by taking into account two-particle excited states projected onto the local orbitals, and the momentum-dependent amplitudes of these states are chosen as variational parameters. The MLA describes accurately correlated electron states from the weak to the intermediate Coulomb interaction regime in infinite dimensions, and works well even in the strongly correlated region by introducing a new starting wavefunction called the hybrid (HB) wavefunction. The MLA-HB is therefore shown to overcome the limitation of the original local ansatz (LA) wavefunction as well as the Gutzwiller wavefunction. In particular, the calculated quasiparticle weight vs Coulomb interaction curve is shown to be close to that obtained by the numerical renormalization group approach. It is also shown that the MLA is applicable to the first-principles Hamiltonian.

Keywords: Momentum-dependent local ansatz; electron correlations; variational method; wavefunction method; Gutzwiller wavefunction.

1. Introduction

Properties of solids are well-known to be determined by the quantum mechanical motion of electrons. The electrons move there in the periodic potential and hence form energy bands, but they are also influenced by the electron-electron interactions. The latter effects are usually taken into account as an effective mean-field
potential. The Hartree-Fock approximation is an approximate method to describe the interactions with an effective potential. The band theory based on the effective potential explains many aspects of solids such as the cohesive properties, the Fermi surface in metals, and optical properties of many metallic systems, especially when the electron-electron interaction energy is small as compared with the kinetic energy of band electrons.

When electron-electron interactions become comparable to the kinetic energy of electrons, various effects which cannot be explained by the simple band picture appear. These effects are called electron-correlation effects. Correlation effects originate in the quantum charge and spin fluctuations neglected in the mean field approximation.

Correlated motion of electrons, for example, suppresses the electron hopping in a solid, and yields the reduction of cohesive energy in 3d transition metals, the band narrowing, and the formation of a satellite peak in the X-ray photoemission spectroscopy (XPS) data of Ni. Strong mass enhancement of quasiparticle states is also a consequence of the localization of electrons. Further electron localization is known to cause the Mott-type metal-insulator transition.

In the magnetic materials, the quantum spin fluctuations are well known to make the ferromagnetism at the ground state unstable, create the magnetic entropy at finite temperatures, and consequently much reduce the Curie temperatures. The long-range quantum spin fluctuations are known to cause the spin wave excitations. The high-temperature superconductivity in cuprates is also believed to be caused by the antiferromagnetic spin fluctuations in the vicinity of the Mott transition, which is missing in the band theory.

The density functional theory for band structure calculations has overcome some of these difficulties at the ground state using the effective potentials based on the local density approximation (LDA) or the generalized gradient approximation (GGA). Most of the problems mentioned above, however, cannot be understood without taking into account the correlated motion of electrons, and we need to develop the many-body theory of electron correlations.

Theoretical approaches to interacting electrons have been developed since quantum mechanics was established. The diagram technique is the standard method to calculate the Green function and the free energy for correlated electrons starting from non-interacting electrons. The equation of motion method and projection technique are alternative approaches to obtain the Green functions for interacting electrons. The renormalization-group (RG) approach considers successive transformations to effective Hamiltonians, leading to the same low-energy eigenvalues. Numerical methods which directly treat the many-body system on computers have also been much developed. In the exact diagonalization method (ED), one directly solves the eigen-value problem for a small cluster with use of the Lanczos method. In the quantum Monte-Carlo method (QMC), we reduce the quantum mechanical average into a classical one with use of the Suzuki-Trotter theorem, and apply the Monte-Carlo technique.
In the past two decades, effective medium approaches such as the dynamical coherent potential approximation (CPA)\textsuperscript{23,24} and the dynamical mean field theory (DMFT)\textsuperscript{25,26} have been developed. There we replace the surrounding interactions with a momentum-independent effective medium in the Green function and determine the medium self-consistently solving an impurity problem with use of many-body techniques.

Among various methods to treat interacting electrons, the variational wavefunction method is the simplest and oldest method\textsuperscript{3,4,27}. We assume there a trial wavefunction consisting of the minimum basis set with variational parameters and determine the parameters on the basis of the variational principle at the ground-state. The wavefunction method has a merit of efficiency to best determine the wavefunction, though one has to find a physically suitable trial wave function or the minimum basis set for correlated electrons. It also allows us to calculate any static quantities such as the double occupation number and correlation functions.

The Gutzwiller wavefunction (GW)\textsuperscript{28,29,30} is the first which described the correlated electrons in a narrow band. In the GW, one varies the amplitudes of doubly-occupied sites which appear in the Hartree-Fock wavefunction in order to reduce the loss of Coulomb interaction energy. The local ansatz (LA) wavefunction\textsuperscript{31,32,33,34,35,4} is an approach from the weakly correlated limit. It makes use of the Hilbert space expanded by the two-particle operators which appear in the residual Coulomb interactions. The Baeriswyl wavefunction\textsuperscript{34,35,36} expands the Hilbert space with use of the hopping operators onto the atomic wavefunctions aiming at an accurate description of electron correlations in the strong interaction regime. There are various trial wavefunctions which describe the nonlocal electron correlations\textsuperscript{37,38,39,40}. These wavefunctions are usually treated by means of numerical techniques such as the variational Monte-Carlo method\textsuperscript{41,42}.

Most of the wavefunctions mentioned above, however, do not reduce to the exact result of the Rayleigh-Schrödinger perturbation theory in the weak Coulomb interaction limit, because they are designed mainly to describe the electrons in the strong Coulomb interaction regime. It is indispensable for a quantitative description to construct the wavefunction leading to the exact result in the weak Coulomb interaction limit. In particular, the Fermi liquid state of the strongly correlated electrons should be connected to that of the weakly correlated system according to the adiabatic principle for interacting electrons\textsuperscript{43}, and thus associated Fermi liquid parameters such as the quasiparticle weight should be obtained by a suitable renormalization of their parameters in the weakly correlated interaction limit.

In this brief review article, we elucidate the momentum-dependent local ansatz wavefunction (MLA)\textsuperscript{44,45,46,47} which reproduces exactly the weak Coulomb interaction limit and interpolates between the weak and strong Coulomb interaction limits. The MLA is an extension of the LA. In the MLA, we first expand the Hilbert space by means of the two-particle excited operators in the momentum representation, introduce momentum-dependent variational parameters as the amplitudes of the excited states, and project these states onto the local orbitals again. In this way,
we can obtain more flexible correlated electron states as compared with the LA. Furthermore we can improve the MLA by introducing a hybrid (HB) wavefunction as a starting wavefunction, so that the MLA improves upon both the GW and the LA in infinite dimensions. The MLA wavefunction is a counterpart of the DMFT because it leads to an accurate description of the Fermi liquid state in infinite dimensions.

In the following section, we briefly review the wavefunction method and various wavefunctions including the Gutzwiller and LA wavefunctions, as well as their results for calculations of physical quantities. In Sec. 3, we introduce the MLA wavefunction. We argue the validity on the basis of the numerical results in infinite dimensions. The MLA does describe well the weak and intermediate Coulomb interaction regimes, but it does not explain the insulating state in the strong Coulomb interaction regime. In Sec. 4, we present the MLA with hybrid (HB) wavefunction, which allows us to describe both the metallic and insulator states. The idea is to start from the best wavefunction of a hybrid Hamiltonian obtained by superposing the Hartree-Fock (HF) and the alloy-analogy (AA) Hamiltonians. In the strong Coulomb interaction region, the AA wavefunction is a good starting wavefunction, while the HF one is the best in the weakly correlated regime. Since the first-principles GW method does not describe correctly the weak interaction regime, one needs an alternative first-principles wavefunction method which describes quantitatively the correlated electrons in the weak and intermediate interaction regimes. We present an extension of the MLA to the realistic system in Sec. 5. Finally, we summarize the MLA and discuss future problems in Sec. 6.

2. Wavefunction Method and Various Wavefunctions

The ground-state properties of a system are completely determined by the wavefunction. The wavefunction method is based on the variational principle for the wavefunction. It states that the expectation value $E$ of the Hamiltonian $H$ for any trial wavefunction $|\Psi\rangle$ is equal to or larger than the ground-state energy $E_0$.

$$E_0 \leq E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$  \hspace{1cm} (1)

The variational principle allows us to find an approximate but best wavefunction for a given ansatz, and its energy expectation value gives us the upper limit of the exact ground-state energy. In the actual application of Eq. (1), it is important that we adopt a size-consistent wavefunction close to the exact one and calculate the energy expectation value as accurate as we can in order to avoid uncertainty.

We consider hereafter the tight-binding model Hamiltonian with intra-atomic Coulomb interaction called the Hubbard model \cite{Hubbard1,Hubbard2}, for simplicity.

$$H = \sum_{i\sigma} \epsilon_0 n_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$ \hspace{1cm} (2)
Here \( \epsilon_0 \) is the atomic level, \( t_{ij} \) is the transfer integral between sites \( i \) and \( j \). \( U \) is the intra-atomic Coulomb energy parameter. \( a^\dagger_{i\sigma} \) (\( a_{i\sigma} \)) denotes the creation (annihilation) operator for an electron on site \( i \) with spin \( \sigma \), and \( n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma} \) denotes the electron density operator on site \( i \) for spin \( \sigma \).

The Hamiltonian can be separated into the Hartree-Fock mean-field Hamiltonian \( H_0 \) and the residual interaction part as follows.

\[
H = H_0 + U \sum_i O_i ,
\]

\[
H_0 = \sum_i (\epsilon_0 + U \langle n_{i-\sigma} \rangle_0) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij\sigma} a^\dagger_{i\sigma} a_{j\sigma} - U \sum_i \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0 ,
\]

Here \( \langle \sim \rangle_0 \) denotes the Hartree-Fock average at the ground state. The operator \( O_i \) in the residual interaction is defined by

\[
O_i = \delta n_{i\uparrow} \delta n_{i\downarrow} \quad \text{and} \quad \delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma} \rangle_0 .
\]

The Hartree-Fock ground-state wavefunction \( |\phi \rangle \) is given by

\[
|\phi \rangle = \prod_{k\sigma}^{occ} a^\dagger_{k\sigma} |0 \rangle .
\]

Here \( \prod_{k\sigma}^{occ} \) means taking the products over the momentum \( k \) and spin \( \sigma \) of electrons below the Fermi level. \( |0 \rangle \) denotes the vacuum state. \( a^\dagger_{k\sigma} \) is the creation operator for an electron with momentum \( k \) and spin \( \sigma \); \( a^\dagger_{i\sigma} = \sum_k a^\dagger_{k\sigma} \langle i | k \rangle \). \( \langle i | k \rangle (= \exp(-ik \cdot R_i)/\sqrt{N}) \) is an overlap integral between the localized orbital on site \( i \) and the Bloch state \( k \). \( R_i \) denotes atomic position of site \( i \), and \( N \) is the number of sites.

The energy difference between the ground state for the correlated electrons and the Hartree-Fock one is given by

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

Here \( \hat{H} = H - \langle H \rangle_0 \). It is the energy gain due to correlated motion of electrons, and is called the correlation energy.

### 2.1. Gutzwiller wavefunction

The Hartree-Fock mean-field wavefunction overestimates the ground-state energy because independent motion of electrons produces excessively many doubly-occupied sites with loss of energy due to Coulomb repulsion. The wavefunction proposed by Gutzwiller \cite{282930} reduces the amplitudes of doubly occupied states in the Hartree-Fock ground state. It is given by

\[
|\Psi_G \rangle = \left[ \prod_i (1 - (1 - g)n_{i\uparrow} n_{i\downarrow}) \right] |\phi \rangle .
\]

The projection operator \( n_{i\uparrow} n_{i\downarrow} \) picks up the doubly occupied state on site \( i \). The parameter \( 1 - g \) denotes the amplitude of the doubly occupied states. The variational
parameter $g = 1$ corresponds to the Hartree-Fock state, while $g = 0$ corresponds to the atomic state with no doubly occupied state. Varying the variational parameter $g$ from 1 to 0, one can choose the best amplitude of doubly occupied states for correlated electrons on the basis of the variational principle (1).

Gutzwiller obtained approximately the ground-state energy by making use of a quasichemical method [30]. The Gutzwiller approximation was proved to be exact in infinite dimensions [50]. In the nonmagnetic state at half-filling, we obtain a simple result for the ground-state energy per atom in infinite dimensions as [3012]

$$
\epsilon_G = -\frac{1}{8} U_c \left(1 - \frac{U}{U_c}\right)^2.
$$

(8)

Here we assumed $\epsilon_0 = 0$. $U_c = 16\int_{-\infty}^{0} \epsilon \rho(\epsilon) d\epsilon$ and $\rho(\epsilon)$ is the noninteracting density of states per atom per spin. The ground-state energy increases with increasing $U$ and becomes zero at $U = U_c$. For $U > U_c$, we have a solution $\epsilon_G$ with $g = 0$. Therefore the metal-insulator transition occurs at $U = U_c$.

Similarly the double occupation number per atom linearly decreases with increasing $U$ at half-filling as

$$
d_G = \langle n_{i\uparrow} n_{i\downarrow} \rangle = \frac{1}{4} \left(1 - \frac{U}{U_c}\right),
$$

(9)

and $d_G = 0$ beyond $U_c$. We call the state $d_G = 0$ the Brinkman-Rice atomic state [51]. It is therefore realized for $U > U_c$, i.e., in the insulating state. The Brinkman-Rice atomic state is not consistent with the super-exchange state with charge fluctuations in the strongly correlated region.

The momentum distribution for the GW is known to be flat below and above the Fermi level, and shows a jump at the Fermi level [30]. The latter is the quasiparticle weight according to the Fermi liquid theory. For half-filling it is given by

$$
Z_G = 1 - \frac{U^2}{U_c^2}.
$$

(10)

Beyond $U_c$, the jump disappears and the distribution becomes completely flat. The flat behavior in infinite dimensions is not consistent with the result of the second-order perturbation theory for the Green function [52].

2.2. Local-ansatz wavefunction

The Hartree-Fock Hamiltonian neglects the charge (or spin) fluctuations $\{O_i\} = \{\delta n_{i\uparrow} \delta n_{i\downarrow}\}$ which appear in the residual interactions. An alternative way to take into account electron correlations is therefore to include the Hilbert space expanded by the fluctuations $\{O_i\}$. Such a wavefunction is called the local ansatz (LA) [3113283]. It is given by

$$
|\Psi_{\text{LA}}\rangle = \prod_i (1 - \eta_{i\text{LA}} O_i) |\phi\rangle.
$$

(11)
Here $\eta_{\text{LA}}$ is a variational parameter.

In the single-site approximation, the correlation energy per atom is given as follows\cite{5,3,54}.

$$\epsilon_c(\text{LA}) = \frac{-2\eta_{\text{LA}} \langle O_i \hat{H} \rangle_0 + \eta_{\text{LA}}^2 \langle O_i \hat{H} O_i \rangle_0}{1 + \eta_{\text{LA}}^2 \langle O_i^2 \rangle_0}.$$  \hspace{1cm} (12)

Each element of $\langle O_i \hat{H} \rangle_0$, $\langle O_i \hat{H} O_i \rangle_0$, and $\langle O_i^2 \rangle_0$ are expressed by the electron number $\langle n_{i\sigma} \rangle_0$ and the Hartree-Fock local density of states $\rho_{i\sigma}(\epsilon)$. Minimizing the energy $\epsilon_c(\text{LA})$ with respect to the variational parameter $\eta_{\text{LA}}$, we obtain

$$\eta_{\text{LA}} = \frac{-\langle O_i \hat{H} O_i \rangle_0 + \sqrt{\langle O_i \hat{H} O_i \rangle_0^2 + 4 \langle O_i \hat{H} \rangle_0^2 \langle O_i^2 \rangle_0}}{2 \langle O_i \hat{H} \rangle_0 \langle O_i^2 \rangle_0}.$$  \hspace{1cm} (13)

In the nonmagnetic state at half-filling, the double occupation number in the LA has a simple form,

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle_{\text{LA}} = \frac{1}{4} \left(1 - \frac{\eta_{\text{LA}}^2/4}{1 + \eta_{\text{LA}}^2/16}\right).$$  \hspace{1cm} (14)

The momentum distribution function in the LA also shows a flat behavior as a function of $\epsilon_k$ below and above the Fermi level. Here $\epsilon_k$ is the Fourier transform of $t_{ij}$. The quasiparticle weight as the jump in the momentum distribution on the Fermi surface is obtained analytically for half-filling as follows.

$$Z_{\text{LA}} = 1 - \frac{\eta_{\text{LA}}^2/4}{1 + \eta_{\text{LA}}^2/16}.$$  \hspace{1cm} (15)

Therefore the effective mass diverges at $\eta_{\text{LA}}^* = \sqrt{16/3}$ in the LA.

Note that the space expanded by $\{O_i\}$ is not sufficient to describe the atomic states. In order to describe the strongly correlated regime, one has to extend the LA as follows.

$$|\Psi_{\text{LA}}\rangle = \prod_i (1 - \zeta_{\text{LA}} \delta n_i - \xi_{\text{LA}} \delta m_i - \eta_{\text{LA}} O_i) |\phi\rangle.$$  \hspace{1cm} (16)

Here $\zeta_{\text{LA}}$ and $\xi_{\text{LA}}$ are additional parameters controlling the charge and spin fluctuations, respectively.

The LA is suitable for the description of correlated-electron systems with a weak or intermediate Coulomb interaction strength, while the Gutzwiller wavefunction is more suitable in the strongly correlated region. More details on the LA and the GW and their applications to various topics are found in the books by Fulde\cite{3} and by Fazekas\cite{55}, respectively.

2.3. Other wavefunctions

There are many other wavefunctions which have been proposed. Both the Gutzwiller and the LA wavefunctions do not explicitly include the inter-site correlation oper-
The wavefunction proposed by Jastrow describes the inter-site density-density correlations and has the form
\[ |\Psi_J\rangle = \exp \left( -\sum_{(i,j)} f_{ij} n_i n_j \right) |\phi\rangle. \] (17)

Here \( n_i \equiv n_{i\uparrow} + n_{i\downarrow} \) is the density operator on site \( i \) and \( f_{ij} \) are variational parameters. Note that the Gutzwiller wavefunction is expressed as
\[ |\Psi_G\rangle = e^{\eta_G \sum_i n_{i\uparrow} n_{i\downarrow}} |\phi\rangle \propto e^{\frac{1}{2} \eta_G \sum_i n_i n_i} |\phi\rangle, \] (18)

where the variational parameters \( \eta_G \) and \( g \) are related through \( \eta_G = \ln g \). Therefore the on-site Jastrow wavefunction is equivalent to the Gutzwiller wavefunction.

A wavefunction being suitable in the strong correlation regime is the Baeriswyl wavefunction \[ |\Psi_B\rangle = e^{-\eta_B \hat{T}} |\Psi_\infty\rangle. \] (19)

The operator \( \exp(-\eta_B \hat{T}) \) creates the electron hopping states from the atomic one and the variational parameter \( \eta_B \) controls the hopping rate to minimize the energy.

In order to describe the doublon (doubly occupied state)-holon (empty state) bound state, which appears in the super-exchange process in the strong Coulomb interaction regime, one can consider the wavefunction \[ |\Psi_{dh}\rangle = e^{-\alpha \hat{Q}} |\Psi_G\rangle. \] (20)

Here \( \hat{Q} = \sum_i [\hat{d}_i \prod_{\tau} (1-\hat{h}_{i+\tau}) + \hat{h}_i \prod_{\tau} (1-\hat{d}_{i+\tau})], \hat{d}_i = n_{i\uparrow} n_{i\downarrow} \) is the doublon (holon) operator, and \( \tau \) is taken over the nearest-neighbor sites. The variational parameter \( \alpha \) controls the amplitudes of the nearest-neighbor doublon-holon bound states. The ground-state of the non-local wavefunctions are usually calculated by means of the numerical technique called the variational Monte-Carlo method (VMC).

### 3. Momentum-Dependent Local Ansatz Wavefunction

Most of the wavefunctions mentioned in the last section aim to describe correlated electrons in the intermediate and strong Coulomb interaction regimes. The behavior of these wavefunctions in the weak Coulomb interaction regime was not discussed seriously. Kakehashi et al. have recently pointed out that the wavefunctions mentioned above do not yield the exact results in the weak Coulomb interaction limit according to the Rayleigh-Schrödinger perturbation theory of the wavefunction. They proposed a new wavefunction called the momentum-dependent local ansatz (MLA) which is consistent with the perturbation theory. The MLA is a new wavefunction which reproduces well-known results in infinite dimensions.

In the following subsection, we introduce the MLA that describes exactly the correlated electrons in the weak Coulomb interaction limit, and elucidate the results obtained by the MLA wavefunction in infinite dimensions.
3.1. Momentum-dependent local ansatz based on the Hartree-Fock wavefunction

The momentum-dependent local ansatz wavefunction (MLA) is constructed from the local-ansatz (LA) wavefunction \( \psi_{\text{LA}} \) so as to reproduce the result of the Rayleigh-Schrödinger perturbation theory. We expand the LA wavefunction \( \psi_{\text{LA}} \) in the weak Coulomb interaction limit as

\[
|\psi_{\text{LA}}\rangle = |\phi\rangle + |\phi_1\rangle_{\text{LA}} + \cdots,
\]

\[
|\phi_1\rangle_{\text{LA}} = -\sum_{i} \sum_{k_1 k_2 k_1' k_2'} \langle k_1' | i \rangle \langle i | k_1 \rangle \langle k_2' | i \rangle \langle i | k_2 \rangle \eta_{\text{LA}} \delta(a_{k_1} d a_{k_2}) \delta(a_{k_1'} d a_{k_1}) |\phi\rangle.
\]

Here \( \langle i | k \rangle = \exp(-ik \cdot R_i)/\sqrt{N} \) is an overlap integral between the localized orbital on site \( i \) and the Bloch state with momentum \( k \), and \( \delta(a_{k,\sigma} \cdot a_{k,\sigma}) = a_{k,\sigma} \cdot a_{k,\sigma} - \langle a_{k,\sigma} \cdot a_{k,\sigma} \rangle \).

The Rayleigh-Schrödinger perturbation theory for the exact ground-state wavefunction, on the other hand, yields the following form

\[
|\Psi\rangle = |\phi\rangle + |\phi_1\rangle + \cdots,
\]

\[
|\phi_1\rangle = -\sum_{i} \sum_{k_1 k_2 k_1' k_2'} \langle k_1' | i \rangle \langle i | k_1 \rangle \langle k_2' | i \rangle \langle i | k_2 \rangle \eta_{0} \delta(a_{k_1} d a_{k_2}) \delta(a_{k_1'} d a_{k_1}) |\phi\rangle.
\]

The amplitude \( \eta_{0} \) is given by

\[
\eta_{0} = -U \lim_{z \rightarrow 0} f(\epsilon_{k_{1}}) (1 - f(\epsilon_{k_{1}})) \frac{f(\epsilon_{k_{2}}) (1 - f(\epsilon_{k_{2}}))}{z - \epsilon_{k_{1}} - \epsilon_{k_{2}} + \epsilon_{k_{2}} - \epsilon_{k_{1}} + \epsilon_{k_{2}} + \epsilon_{k_{2}}}. \tag{25}
\]

Here \( f(\epsilon) \) is the Fermi distribution function at zero temperature, and \( \epsilon_{k,\sigma} = \epsilon_{k,\sigma} - \mu \). \( \mu \) is the Fermi level. \( \epsilon_{k,\sigma} \) is the Hartree-Fock one-electron energy eigen value given by \( \epsilon_{k,\sigma} = \epsilon_0 + U \langle n_{i,\sigma} \rangle_0 + \epsilon_k \), \( \epsilon_k \) being the Fourier transform of \( t_{ij} \).

Comparing Eq. (24) with Eq. (22) indicates that one has to take into account the momentum dependence of the variational parameters in order to improve the LA so as to be consistent with the perturbation theory in the weak Coulomb interaction limit.

In the MLA, we introduce a new local ansatz operator \( \hat{O}_1 \) such that

\[
\hat{O}_1 = \sum_{k_1 k_2 k_1' k_2'} \langle k_1' | i \rangle \langle i | k_1 \rangle \langle k_2' | i \rangle \langle i | k_2 \rangle \eta_{k_1 k_2 k_1' k_2'} \delta(a_{k_1} d a_{k_2}) \delta(a_{k_1'} d a_{k_1}) , \tag{26}
\]

and construct a new wavefunction with momentum-dependent variational parameters \( \eta_{k_1 k_2 k_1' k_2'} \) as follows

\[
|\Psi\rangle = \left[ \prod_{i} (1 - \hat{O}_1) \right] |\phi\rangle . \tag{27}
\]
The operator $\hat{O}_i$ is still localized on site $i$ because of the projection $\langle k'_i|i\rangle\langle i|k_1\rangle(k'_2|i\rangle\langle i|k_2\rangle$. Note 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. These properties however do not cause any problem when we make a single-site approximation. In order that we treat the nonlocal correlations, we have to adopt symmetrized operators in general. Needless to say, the wavefunction $|\Psi\rangle$ reduces to the LA $|\Psi_{LA}\rangle$ when the variational parameters $\{\eta_{k'_2k_2k'_1k_1}\}$ are taken to be momentum-independent.

The energy expectation values for the MLA wavefunction can be obtained analytically within the single-site approximation [44]. Let us consider the numerator $A_N = \langle \Psi|H|\Psi\rangle$ and the denominator $B_N$ in the correlation energy $\langle H \rangle = A_N/B_N$.

\[
A_N = \left\langle \left[ \prod_i (1 - \hat{O}_i^\dagger) \right] \hat{H} \left[ \prod_i (1 - \hat{O}_i) \right] \right\rangle_0 ,
\]

\[
B_N = \left\langle \left[ \prod_i (1 - \hat{O}_i^\dagger) \right] \left[ \prod_i (1 - \hat{O}_i) \right] \right\rangle_0 .
\]

Expanding $B_N$ with respect to site 1, we obtain

\[
B_N = B_{N-1}^{(1)} - \left\langle \hat{O}_1^\dagger \left[ \prod_i^{(1)} (1 - \hat{O}_i^\dagger) \right] \left[ \prod_i^{(1)} (1 - \hat{O}_i) \right] \right\rangle_0 \\
- \left\langle \left[ \prod_i^{(1)} (1 - \hat{O}_i^\dagger) \right] \hat{O}_1 \left[ \prod_i^{(1)} (1 - \hat{O}_i) \right] \right\rangle_0 \\
+ \left\langle \hat{O}_1 \left[ \prod_i^{(1)} (1 - \hat{O}_i^\dagger) \right] \hat{O}_1 \left[ \prod_i^{(1)} (1 - \hat{O}_i) \right] \right\rangle_0 ,
\]

and

\[
B_{N-1}^{(1)} = \left\langle \left[ \prod_i^{(1)} (1 - \hat{O}_i^\dagger) \right] \left[ \prod_i^{(1)} (1 - \hat{O}_i) \right] \right\rangle_0 .
\]

Here the product $\prod_i^{(1)}$ means the products with respect to all the sites except site 1.

When we apply Wick’s theorem for the calculation of $B_N$, we neglect the contractions between different sites. This is a single-site approximation and then Eq. (30) is expressed as

\[
B_N = \left\langle (1 - \hat{O}_1^\dagger)(1 - \hat{O}_1) \right\rangle_0 B_{N-1}^{(1)} .
\]

In the case of $A_N$, we take into account the two types of terms after application of Wick’s theorem, the terms in which the operator $\hat{O}_1$ is contracted to $\hat{H}$ and the other terms with $\hat{O}_1$ contracted to the operators $\hat{O}_i$ ($i \neq 1$). We have then in the single-site approximation

\[
A_N = \left\langle (1 - \hat{O}_1^\dagger)\hat{H}(1 - \hat{O}_1) \right\rangle_0 B_{N-1}^{(1)} + \left\langle (1 - \hat{O}_1^\dagger)(1 - \hat{O}_1) \right\rangle_0 A_{N-1}^{(1)} .
\]

Here $A_{N-1}^{(1)}$ is defined by $A_N^{(1)}$ in which the correlator $(1 - \hat{O}_1^\dagger)(1 - \hat{O}_1)$ on site 1 has been removed.
Successive application of the recursive relations (32) and (33) yields

\[ A_N = \sum_{i} \langle (1 - \tilde{O}_i^{\dagger}) \tilde{H} (1 - \tilde{O}_i) \rangle_{0} B_{N-1}^{(i)} , \]  

(34)

\[ B_N = \prod_{i} \langle (1 - \tilde{O}_i^{\dagger}) (1 - \tilde{O}_i) \rangle_{0} = \langle (1 - \tilde{O}_i^{\dagger}) (1 - \tilde{O}_i) \rangle_{0} B_{N-1}^{(i)} . \]  

(35)

Thus we obtain the expression for the correlation energy \( E_c \) as follows.

\[ E_c = \langle \tilde{H} \rangle = \sum_{i} \langle (1 - \tilde{O}_i^{\dagger}) \tilde{H} (1 - \tilde{O}_i) \rangle_{0} . \]  

(36)

Assuming a site per unit cell and using the relation \( \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_{0} = \langle \tilde{O}_i \tilde{O}_i \rangle_{0} = 0 \), we obtain the correlation energy per site as follows.

\[ \epsilon_c = -\langle \tilde{O}_i^{\dagger} \tilde{H} \rangle_{0} - \langle \tilde{H} \tilde{O}_i \rangle_{0} + \langle \tilde{O}_i^{\dagger} \tilde{H} \tilde{O}_i \rangle_{0} . \]  

(37)

By making use of Wick’s theorem and the \( R = 0 \) approximation, we obtain \( \langle \tilde{H} \tilde{O}_i \rangle_{0} = \langle \tilde{O}_i^{\dagger} \tilde{H} \rangle_{0} \), \( \langle \tilde{O}_i^{\dagger} \tilde{H} \tilde{O}_i \rangle_{0} \), and \( \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_{0} \) as follows.

\[ \langle \tilde{H} \tilde{O}_i \rangle_{0} = \frac{U}{N^4} \sum_{k_1,k_2,k'_1,k'_2} \tilde{f}_{k_1,k_2,k'_1,k'_2} \eta_{k_1,k_2,k'_1,k'_2} \langle \Delta E_{k_2,k_1,k'_2,k'_1} \eta_{k_2,k_1,k'_2,k'_1} \rangle_{1} \]

(38)

\[ \langle \tilde{O}_i^{\dagger} \tilde{H} \tilde{O}_i \rangle_{0} = \frac{1}{N^4} \sum_{k_1,k_2,k'_1,k'_2} \tilde{f}_{k_1,k_2,k'_1,k'_2} \eta_{k_1,k_2,k'_1,k'_2} \eta_{k_2,k_1,k'_2,k'_1} \]

(39)

Here \( \Delta E_{k_2,k_1,k'_2,k'_1} = \epsilon_{k_2,k_1} - \epsilon_{k_2,k'_1} + \epsilon_{k_1,k'_2} - \epsilon_{k_1,k_2} \) is a two-particle excitation energy. \( \tilde{f}_{k_1,k_2,k'_1,k'_2} \) is a Fermi factor of two-particle excitations defined by \( \tilde{f}_{k_1,k_2,k'_1,k'_2} = f(\tilde{\epsilon}_{k_1})(1-f(\tilde{\epsilon}_{k_2}))(1-f(\tilde{\epsilon}_{k'_1}))(1-f(\tilde{\epsilon}_{k'_2})) \).

Minimizing the correlation energy (37), we obtain the self-consistent equations for \( \{ \eta_{k_2,k_1,k'_2,k'_1} \} \) in the single-site approximation as follows.

\[ (\Delta E_{k_2,k_1,k'_2,k'_1} - \epsilon_c) \eta_{k_2,k_1,k'_2,k'_1} + \frac{U}{N^4} \left[ \sum_{k_3,k'_3} f(\tilde{\epsilon}_{k_3}) f(\tilde{\epsilon}_{k'_3}) \eta_{k_3,k'_3,k_2,k_1} - \sum_{k_3,k'_3} f(\tilde{\epsilon}_{k_3}) (1-f(\tilde{\epsilon}_{k'_3})) \eta_{k_3,k'_3,k_2,k_1} \right. \]

(40)

\[ - \sum_{k_4,k'_4} (1-f(\tilde{\epsilon}_{k_4})) f(\tilde{\epsilon}_{k'_4}) \eta_{k_4,k'_4,k_2,k_1} + \sum_{k_4,k'_4} (1-f(\tilde{\epsilon}_{k_4})) (1-f(\tilde{\epsilon}_{k'_4})) \eta_{k_4,k'_4,k_2,k_1} \]

(41)
It is possible to solve approximately the above equation for \( \eta_{k'k_1k_2k_1} \) for a given \( \epsilon_c \). We first note that \( \eta_{k'k_2k_1k_1} \) should vanish in the weak \( U \) limit. Thus, we can omit the second term at the l.h.s. of Eq. (41) in the weak interaction limit. Then we obtain the solution as \( \eta_{k'k_2k_1k_1} = U/\Delta E_{k_2k_1k_1} \). In the atomic limit, on the other hand, we have \( \Delta E_{k_2k_1k_1} = 0 \), and find a \( k \)-independent solution \( \eta \). Therefore we approximate \( \{ \eta_{k'k_2k_1k_1} \} \) in the second term with a \( k \)-independent solution \( \eta \), so that we obtain an approximate solution which interpolates between the weak and strong interaction regimes.

\[
\eta_{k'k_2k_1k_1}(\tilde{\eta}, \epsilon_c) = \frac{U\tilde{\eta}}{\Delta E_{k_2k_1k_1} - \epsilon_c}.
\]

(42)

Here \( \tilde{\eta} = 1 - \eta(1 - 2\langle n_{i\uparrow}\rangle)(1 - 2\langle n_{i\downarrow}\rangle) \).

When we adopt the approximate form (42), we have the following inequality.

\[
E_0 \leq E(\{\eta_{k'k_2k_1k_1}^*\}) \leq E(\{\eta_{k'k_2k_1k_1}(\tilde{\eta}, \epsilon_c)\}),
\]

(43)

where \( \eta_{k'k_2k_1k_1}^* \) is the exact stationary value. Therefore \( \tilde{\eta} \) is again determined from the stationary condition of the correlation energy \( \epsilon_c \).

\[
\tilde{\eta} = \frac{1}{1 + \frac{U\epsilon_c}{D}}.
\]

(44)

Here

\[
C = \frac{1}{N^v} \sum_{k_1k_2k_1k_2} \frac{\hat{f}_{k'k_2k_1k_1}}{(\Delta E_{k_2k_1k_1} - \epsilon_c)} \times \left\{ \frac{f(\tilde{e}_{k_2\uparrow})f(\tilde{e}_{k_1\downarrow})}{(\Delta E_{k_2k_1k_1} - \epsilon_c)} - \frac{1 - f(\tilde{e}_{k_2\uparrow})f(\tilde{e}_{k_1\downarrow})}{(\Delta E_{k_2k_1k_1} - \epsilon_c)} \right\},
\]

(45)

and

\[
D = \frac{1}{N^v} \sum_{k_1k_2k_1k_2} \frac{\hat{f}_{k'k_2k_1k_1}}{(\Delta E_{k_2k_1k_1} - \epsilon_c)}.
\]

(46)

Note that \( \tilde{\eta} \) in Eq. (44) is given as a function of \( \epsilon_c \), and \( \epsilon_c \) in Eq. (45) depends on \( \tilde{\eta} \) and \( \epsilon_c \). Thus both equations are solved self-consistently. This is the self-consistent MLA which starts from the Hartree-Fock wavefunction. The self-consistency is significant when the average electron number deviates from half-filling.

In the numerical calculations of \( C, D, \langle \hat{H}\hat{O}_i \rangle_0, \langle \hat{O}_i^\dagger \hat{H}\hat{O}_i \rangle_0 \), and \( \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 \), the six-fold \( k \) sums appear. This means that one has to perform the six-fold integrals in the energy representation. One can reduce the six-fold integrals into two-fold ones by using a Laplace transformation:

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

(47)
Here \( z = \omega + i\delta \), and \( \delta \) is an infinitesimal positive number.

Electron number \( \langle n_i \rangle \), momentum distribution \( \langle n_{k\sigma} \rangle \), and double occupation number \( \langle n_{i\uparrow} n_{i\downarrow} \rangle \) are obtained from \( \langle H \rangle \) by taking the derivative with respect to \( \epsilon_0 \) on site \( i \), \( \epsilon_k - \sigma h \), and \( U_i \), respectively. Here we added the external magnetic field \( h \) in the atomic level, and the site index \( i \) in the Coulomb energy parameter \( U \) for convenience.

\[
\langle n_i \rangle = \langle n_i \rangle_0 + \frac{\sum_{\sigma} \langle \hat{O}_i^\dagger \hat{n}_{i\sigma} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0},
\]
(48)

\[
\langle n_{k\sigma} \rangle = \langle n_{k\sigma} \rangle_0 + \frac{N \langle \hat{O}_i^\dagger \hat{n}_{k\sigma} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0},
\]
(49)

\[
\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle_0 \langle n_{i\downarrow} \rangle_0 + \langle n_{i\uparrow} n_{i\downarrow} \rangle_c,
\]
(50)

\[
\langle n_{i\uparrow} n_{i\downarrow} \rangle_c = -\frac{\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 - \langle \hat{O}_i \hat{O}_i^\dagger \rangle_0 + \langle \hat{O}_i^\dagger \hat{O}_i \hat{O}_i \rangle_0 + \sum_{\sigma} \langle n_{i\sigma} \rangle_0 \langle \hat{O}_i^\dagger \hat{n}_{i\sigma} \hat{O}_i \rangle_0}{1 + \langle \hat{O}_i^\dagger \hat{O}_i \rangle_0}.
\]
(51)

The second terms at the r.h.s. of the above expressions (48), (49), and (50) are correlation corrections and they are again calculated by using the Laplace transformation.

### 3.2. MLA in infinite dimensions

The MLA improves upon the LA irrespective of the Coulomb interaction strength and the electron number. One can demonstrate this fact by means of numerical calculations in infinite dimensions. We adopt hereafter the Hubbard model on the hypercubic lattice in infinite dimensions. In this case, the density of states (DOS) for the noninteracting system is given by \( \rho(\epsilon) = (1/\sqrt{\pi}) \exp(-\epsilon^2) \).

Figure 1 shows the correlation energy per atom as a function of \( U \) for various electron numbers. We verify that the ground-state energy in the MLA is lower than that of the LA over all Coulomb interactions \( U \) and electron numbers \( n \). In particular, the small \( U \) behavior of \( \epsilon_c \) in the MLA is exact. For a given \( U \), the difference between the LA and the MLA increases with increasing \( n \) and becomes maximum at half-filling because the number of doubly occupied sites in the Hartree-Fock ground state increases with increasing electron number.

The double occupation number decreases with increasing interaction \( U \) irrespective of electron number \( n \) so as to suppress the loss of Coulomb interaction energy as seen in Fig. 2. We find that the MLA wavefunction gives greater reduction in the double occupancy as compared with that of the LA.

The momentum dependence of the variational parameters causes qualitative change in the momentum distribution as shown in Fig. 3. The momentum distribution in the LA and the GW are constant below and above the Fermi level as
Fig. 1. The correlation energies $\epsilon_c$ per atom vs. Coulomb interaction energy parameter $U$ in the MLA (solid curve) and the LA (dashed curve) for various electron number $n$ on the hypercubic lattice in infinite dimensions (Ref. 45). The energy unit is chosen so that the band width of noninteracting system be 2.

Fig. 2. 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) (Ref. 45).

mentioned in the last section, while the distribution in the MLA monotonically decreases with increasing energy $\epsilon_{k\sigma}$ below and above the Fermi level, as it should.[22]

The quasi-particle weight obtained from the jump in the momentum distribution
at the Fermi level is also much improved by taking into account the momentum dependence of variational parameters. Figure 4 shows the quasiparticle weight $Z_{\text{LA}}$ as a function of the Coulomb interaction strength $U$ in various methods at half filling. The quasiparticle weight in the LA changes as $Z_{\text{LA}} = (1 - 3\eta_{\text{LA}}^2/16)/(1 + \eta_{\text{LA}}^2/16)$ (see Eq. (15)) and vanishes at $U_{c2}(\text{LA}) = 24/\sqrt{3\pi} (= 7.82)$. In the GW [51], the quasiparticle weight decreases as $Z_{\text{GW}} = 1 - (U/U_{c2})^2$ (see Eq. (10)), and vanishes at $U_{c2}(\text{GW}) = 8/\sqrt{\pi} (= 4.51)$. These curves deviate strongly from the curve obtained by the numerical renormalization group method (NRG) [60] which is considered to be the best. The curve in the MLA on the other hand is close to the that of the NRG, and significantly improves upon the LA, though calculated $U_{c2}(\text{MLA}) = 3.40$ is somewhat smaller than the value $U_{c2}(\text{NRG}) = 4.10$.

The numerical results mentioned above indicate that the momentum dependence of the variational parameters much improves upon the LA as well as the GW in the metallic region. In particular, this is significant in order to describe the properties associated with the low-energy excitations.

4. Momentum Dependent Local Ansatz with Hybrid Wavefunction

The MLA describes the electron correlations in the weak Coulomb interaction limit exactly, and much improves the LA wavefunction, as we have seen in the last section. It cannot, however, suppress sufficiently the loss of Coulomb interaction energy in the strongly correlated region. The usual way to take into account more correlations is to expand the Hilbert space applying additional correlators with variational parameters onto the Hartree-Fock wavefunction. In particular, the correlator which
suppresses the double occupancy is required in the strongly correlated regime. Such an extension, however, would make it more difficult to treat the wavefunction analytically. An alternative way to overcome the difficulty is to start from a wavefunction which is more suitable for the strongly correlated electrons. In this section we present an improvement of the MLA from the latter point of view.

### 4.1. Alloy analogy wavefunction

The Hartree-Fock approximation is exact in energy up to the first order with respect to the Coulomb interaction energy, therefore the wavefunction is suitable as a starting state for describing correlations in the weak and intermediate Coulomb interaction regime. However, the wavefunction is not suitable in the strongly correlated region because it allows for the double occupation of electrons at each site.

Hubbard proposed an alternative one-electron picture in the strong Coulomb interaction regime. Let us consider the atomic limit. There each electron number $\hat{n}_{i\sigma}$ is a good quantum number taking a value $n_{i\sigma} = 0$ or 1. Here and in the following we distinguish the number operator $\hat{n}_{i\sigma}$ with the c-number $n_{i\sigma}(= 0$ or 1). When the electron hopping is switched on in the strongly correlated region, an electron with spin $\sigma$ should move slowly from site to site, and feel a different potential $U\hat{n}_{i-\sigma} = U$ or 0, instead of the Hartree-Fock average potential $U \langle \hat{n}_{i-\sigma} \rangle_0$, depending on whether the opposite-spin electron is occupied or unoccupied on the same site. Hubbard regarded the system as an alloy with different random potentials $\epsilon_0 + U$ and $\epsilon_0$ having the concentration $\langle \hat{n}_{i-\sigma} \rangle$ (occupied) and $1 - \langle \hat{n}_{i-\sigma} \rangle$ (unoccupied), respectively. This is the alloy-analogy (AA) picture for strongly correlated electrons.

Fig. 4. Quasiparticle-weight vs. Coulomb interaction curves in various theories (Ref. 45). The RPT (Renormalized Perturbation Theory)-1: dashed curve (Ref. 52), the NRG: thin solid curve (Ref. 60), the LA: dotted curve, the MLA: solid curve, and the GW: dot-dashed curve.
The AA Hamiltonian is given by

\[ H_{AA} = \sum_{i\sigma} (\epsilon_0 + U n_{i-\sigma}) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - U \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle_{AA} + U \sum_i \langle \hat{n}_{i\uparrow} \rangle_{AA} \langle \hat{n}_{i\downarrow} \rangle_{AA} \]  

(52)

Here \( \langle \sim \rangle_{AA} \) denotes the AA average \( \langle \phi_{AA} | \langle \sim \rangle | \phi_{AA} \rangle \) with respect to the ground-state wavefunction \( |\phi_{AA}\rangle \) of the AA Hamiltonian \( H_{AA} \). \( n_{i\sigma} \) is a c-number taking a value 0 or 1. Each configuration \( \{n_{i\sigma}\} \) is considered as a snapshot in time development.

The ground-state energy \( E_0 \) satisfies the following inequality for any configuration of \( \{n_{i\sigma}\} \).

\[ E_0 \leq \langle H \rangle_{AA} = \langle H_{AA} \rangle_{AA} \]  

(53)

Thus, when we take the configurational average on \( \{n_{i\sigma}\} \), we have

\[ E_0 \leq \langle H \rangle_{AA} \]  

(54)

Here the upper bar denotes the configurational average.

The configurational averages of various quantities can be obtained with use of the single-site approximation (SSA) called the coherent potential approximation (CPA) \(^{61,62,63}\). Note that the averaged electron number is obtained from the local density of state (LDOS) for an electron with spin \( \sigma \), i.e., \( \rho_{i\sigma}(\epsilon) \), as follows.

\[ \langle \hat{n}_{i\sigma} \rangle_{AA} = \int f(\epsilon) \rho_{i\sigma}(\epsilon) d\epsilon \]  

(55)

and the LDOS is obtained from the one-electron Green function as

\[ \rho_{i\sigma}(\epsilon) = -\frac{1}{\pi} \text{Im} G_{i\sigma}(z) \]  

(56)

The Green function \( G_{i\sigma}(z) \) is defined by

\[ G_{i\sigma}(z) = [ (z - H_\sigma)^{-1} ]_{ii} \]  

(57)

Here \( (H_\sigma)_{ij} \) is the one-electron Hamiltonian matrix for the AA Hamiltonian minus chemical potential \( \mu \).

In the CPA, we replace the random potential at the surrounding sites with the energy-dependent coherent potential \( \Sigma_\sigma(z) \). The on-site impurity Green function \( G_{i\sigma}(z) \) is then obtained as follows.

\[ G_{i\sigma}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_{i\sigma} + \Sigma_\sigma(z)} \]  

(58)

Here \( \epsilon_{i\sigma} = \epsilon_0 - \mu + U n_{i-\sigma} \). \( F_\sigma(z) \) is the on-site Green function for the coherent system in which all the random potentials have been replaced by the coherent potentials.

\[ F_\sigma(z) = \int \frac{\rho(\epsilon) d\epsilon}{z - \Sigma_\sigma(z) - \epsilon} \]  

(59)
Note that $\rho(\epsilon)$ is the DOS per site per spin for the noninteracting system. The coherent potential $\Sigma_\sigma(z)$ is determined from the self-consistent condition.

$$G_{00\sigma}(z) = F_\sigma(z).$$  \hfill (60)

The configurational average of the impurity Green function is given as

$$G_{00\sigma}(z) = \frac{\langle \hat{n}_{i-\sigma}\rangle_{AA}}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - U + \Sigma_\sigma(z)} + \frac{1 - \langle \hat{n}_{i-\sigma}\rangle_{AA}}{F_\sigma(z)^{-1} - \epsilon_0 + \mu + \Sigma_\sigma(z)} \hfill (61)$$

The ground-state wavefunction $\phi_{AA}$ for the alloy-analogy Hamiltonian [52] provides us with a good starting wave function for the strongly correlated electrons, though such a wavefunction depends on electron configuration $\{n_{i\sigma}\}$ via atomic potentials.

### 4.2. MLA with hybrid wavefunction

We can improve the MLA correlated wavefunction using the best starting wavefunction. The Hartree-Fock (HF) wavefunction $|\phi_{HF}\rangle$ works best in the weakly correlated region. In the strongly correlated region the alloy-analogy (AA) wavefunction $|\phi_{AA}\rangle$ works better. Therefore we introduce a hybrid (HB) wavefunction $|\phi_{HB}\rangle$ which is the ground state of a hybrid Hamiltonian $H_{HB}$. The Hamiltonian is defined by a linear combination of the HF and AA Hamiltonians [47].

$$H_{HB} = \sum_{i\sigma} (\epsilon_0 + U \langle n_{i-\sigma}\rangle_{HB} + \bar{U} n_{i-\sigma}) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}$$

$$- (U - \bar{U}) \sum_i \langle \hat{n}_{i\uparrow}\rangle_{HB} \langle \hat{n}_{i\downarrow}\rangle_{HB} - \bar{U} \sum_i (n_{i\uparrow} \langle \hat{n}_{i\downarrow}\rangle_{HB} + n_{i\downarrow} \langle \hat{n}_{i\uparrow}\rangle_{HB}). \hfill (62)$$

Here $\langle \sim \rangle_{HB}$ denotes the HB average $\langle \phi_{HB}\rangle\langle \sim | \phi_{HB}\rangle$, $U = (1 - w)U$, and $\bar{U} = wU$. $w$ is a weight in the linear combination; $H_{HB} = (1 - w)H_{HF} + wH_{AA}$, where $H_{HF}$ denotes the HF Hamiltonian. $H_{HB}$ reduces to the HF $\langle AA \rangle$ Hamiltonian when $w = 0$ ($w = 1$).

The new MLA with the HB wavefunction is given by

$$|\Psi\rangle = \left[ \prod_i (1 - \hat{O}_i) \right] |\phi_{HB}\rangle. \hfill (63)$$

The local operators $\{\hat{O}_i\}$ have been modified as follows.

$$\hat{O}_i = \sum_{\kappa'_1,\kappa'_2,\kappa_1,\kappa_2} \langle \kappa'_1 | i | \kappa_1 \rangle \langle \kappa'_2 | i | \kappa_2 \rangle \eta_{\kappa_1\kappa_2\kappa'_1\kappa'_2} \delta(a_{\kappa'_1\kappa_2}^\dagger a_{\kappa_1\kappa_2}) \delta(a_{\kappa'_1\kappa_2}^\dagger a_{\kappa'_2\kappa_1}) \hfill (64)$$

Here $\eta_{\kappa_1\kappa_2\kappa'_1\kappa'_2}$ is a variational parameter, $a_{\kappa_\sigma}^\dagger$ and $a_{\kappa_\sigma}$ are the creation and annihilation operators which diagonalize the Hamiltonian $H_{HB}$ [52], and $\langle \kappa | i \rangle$ are overlap integrals defined by $a_{\kappa_\sigma} = \sum_i a_{i\sigma} \langle \kappa | i \rangle$. Furthermore $\delta(a_{\kappa'_1\kappa_2}^\dagger a_{\kappa_1\kappa_2}) = a_{\kappa_1\kappa_2}^\dagger a_{\kappa_2\kappa_1} - \langle a_{\kappa'_1\kappa_2} a_{\kappa_1\kappa_2} \rangle_{HB}$. 

The ground-state energy $E_0$ again satisfies the following inequality for any wavefunction $|\Psi\rangle$:

$$E_0 \leq \langle H \rangle_{\text{HB}} + N\epsilon_c \ .$$

(65)

The correlation energy per atom $\epsilon_c$ in the single-site approximation (SSA) is given as follows (see Eq. (37)).

$$\epsilon_c = -\frac{(\hat{O}_i^\dagger \hat{H})_{\text{HB}} - \langle \hat{H} \hat{O}_i \rangle_{\text{HB}} + \langle \hat{O}_i^\dagger \hat{H} \hat{O}_i \rangle_{\text{HB}}}{1 + \langle \hat{O}_i^\dagger \hat{O}_i \rangle_{\text{HB}}} \ .$$

(66)

Here $\hat{H} = H - \langle H \rangle_{\text{HB}}$.

The energy elements $\langle \hat{H} \hat{O}_i \rangle_{\text{HB}}$, $\langle \hat{O}_i^\dagger \hat{H} \hat{O}_i \rangle_{\text{HB}}$, and $\langle \hat{O}_i^\dagger \hat{O}_i \rangle_{\text{HB}}$ are given by

$$\langle \hat{H} \hat{O}_i \rangle_{\text{HB}} = U \sum_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} |\langle \kappa_1^{\prime} | i \rangle|^2 |\langle \kappa_1 | i \rangle|^2 |\langle \kappa_2^{\prime} | i \rangle|^2 |\langle \kappa_2 | i \rangle|^2 \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} f_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \ .$$

(67)

$$\langle \hat{O}_i^\dagger \hat{H} \hat{O}_i \rangle_{\text{HB}} = \sum_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} |\langle \kappa_1^{\prime} | i \rangle|^2 |\langle \kappa_1 | i \rangle|^2 |\langle \kappa_2^{\prime} | i \rangle|^2 |\langle \kappa_2 | i \rangle|^2 \times \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} f_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \left[ \Delta E_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} + U \left\{ \sum_{\kappa_3\kappa_4} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 \tilde{f}(\tilde{e}_{\kappa_3^{\prime} \downarrow}) \tilde{f}(\tilde{e}_{\kappa_4} \downarrow) \eta_{\kappa_3^{\prime}\kappa_4} \right. \right.

\left. - \sum_{\kappa_3\kappa_4} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 \left(1 - \tilde{f}(\tilde{e}_{\kappa_3^{\prime} \uparrow}) \tilde{f}(\tilde{e}_{\kappa_3^{\prime} \downarrow}) \right) \eta_{\kappa_3^{\prime}\kappa_4} \right]

+ \sum_{\kappa_3\kappa_4} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 \left(1 - \tilde{f}(\tilde{e}_{\kappa_3^{\prime} \uparrow}) \right) \eta_{\kappa_3^{\prime}\kappa_4} \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \right\} \right] \ .$$

(68)

$$\langle \hat{O}_i^\dagger \hat{O}_i \rangle_{\text{HB}} = \sum_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} |\langle \kappa_1^{\prime} | i \rangle|^2 |\langle \kappa_1 | i \rangle|^2 |\langle \kappa_2^{\prime} | i \rangle|^2 |\langle \kappa_2 | i \rangle|^2 \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} \ .$$

(69)

Here $f_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4}$ is the Fermi factor; $f_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} = \tilde{f}(\tilde{e}_{\kappa_1^{\prime} \downarrow})(1 - \tilde{f}(\tilde{e}_{\kappa_1^{\prime} \uparrow}))\tilde{f}(\tilde{e}_{\kappa_2} \downarrow)(1 - \tilde{f}(\tilde{e}_{\kappa_2} \uparrow)) \tilde{f}(\tilde{e}_{\kappa_3} \downarrow)(1 - \tilde{f}(\tilde{e}_{\kappa_3} \uparrow)) \tilde{f}(\tilde{e}_{\kappa_4} \downarrow)$ and $\Delta E_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4}$ is the one-electron energy eigenvalue for $H_{\text{HB}}$. For the ground state $|\phi_{\text{HB}}\rangle$, $\tilde{f}(\tilde{e}_{\kappa_1^{\prime} \downarrow}) \tilde{f}(\tilde{e}_{\kappa_1^{\prime} \uparrow}) \tilde{f}(\tilde{e}_{\kappa_2} \downarrow) \tilde{f}(\tilde{e}_{\kappa_2} \uparrow) \tilde{f}(\tilde{e}_{\kappa_3} \downarrow) \tilde{f}(\tilde{e}_{\kappa_3} \uparrow) \tilde{f}(\tilde{e}_{\kappa_4} \downarrow)$ denotes the two-particle excitation energy from the ground state $|\phi_{\text{HB}}\rangle$. Note that the above expressions reduce to Eqs. (83), (39), and (40), therefore the correlation energy (66) reduces to Eq. (37) when $w \to 0$.

From the stationary condition $\delta \epsilon_c = 0$, we obtain the self-consistent equations for $\{\eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4}\}$, and again obtain an approximate form (see Eq. (12)) such as

$$\eta_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4}(\tilde{\eta}, \epsilon_c) = \frac{U \tilde{\eta}}{\Delta E_{\kappa_1^{\prime}\kappa_2\kappa_3\kappa_4} - \epsilon_c} \ .$$

(70)
Substituting the above expression into \( \langle H \tilde{O}_i \rangle_{\text{HB}} \), \( \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_{\text{HB}} \), and \( \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_{\text{HB}} \), we have the forms such as \( \langle H \tilde{O}_i \rangle_{\text{HB}} = \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_{\text{HB}} = \tilde{A} U^2 \eta_{\tilde{c}}, \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_{\text{HB}} = \tilde{B} U^2 \eta_{\tilde{c}}^2 \), and \( \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_{\text{HB}} = \tilde{C} U^2 \eta_{\tilde{c}}^2 \). Minimizing the energy \( \epsilon_{c} \) with respect to \( \eta_{\tilde{c}} \), we obtain

\[
\eta_{\tilde{c}} = \frac{-\tilde{B} + \sqrt{\tilde{B}^2 + 4 \tilde{A} \tilde{C} U^2}}{2 \tilde{A} C U^2}.
\]  

(71)

The total energy should be obtained by taking the configurational average as

\[
\langle H \rangle = \langle \tilde{H} \rangle_{\text{HB}} + \eta_{\tilde{c}} \langle c \rangle.
\]  

(72)

The HB ground-state energy is given by

\[
\langle \tilde{H} \rangle_{\text{HB}} = n \mu + \sum_{\sigma} \int_{-\infty}^{0} \epsilon \rho_{c\sigma}(\epsilon) \, d\epsilon
\]

\[
- (\tilde{U} - \tilde{U}) \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} - \tilde{U} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}}.
\]  

(73)

Here \( \rho_{c\sigma}(\epsilon) \) is the local density of states (LDOS). It is obtained from the one-electron Green function,

\[
\rho_{c\sigma}(\epsilon) = -\frac{1}{\pi} \text{Im} G_{c\sigma}(\epsilon),
\]  

(74)

and the Green function \( G_{c\sigma}(\epsilon) \) is defined by Eq. (57), in which \( (H_{\sigma})_{ij} \) has been replaced by the one-electron Hamiltonian matrix for the HB Hamiltonian (62):

\[
(H_{\sigma})_{ij} = (\epsilon_0 - \mu + \tilde{U} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} + \tilde{U} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} + \delta_{ij}(1 - \delta_{ij}) + t_{ij}(1 - \delta_{ij}) - \delta_{ij}(1 - \delta_{ij}).
\]  

The average electron number \( \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} \) is given by the LDOS as

\[
\langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} = \int f(\epsilon) \rho_{c\sigma}(\epsilon) \, d\epsilon.
\]  

(75)

Since the HB Hamiltonian contains a random potential and the energy \( \langle \tilde{H} \rangle_{\text{HB}} \) is given by the LDOS, we can calculate the ground-state energy by means of the alloy-analogy approximation, (i.e., the CPA) as explained in the last subsection. In the CPA, we replace the random potentials at the surrounding sites with a coherent potential \( \Sigma_{\sigma}(z) \). The on-site impurity Green function is obtained as follows.

\[
G_{c\sigma}(\epsilon) = \frac{1}{F_{c}(\epsilon) \epsilon_0 - \mu + \tilde{U} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} - \tilde{U} \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} + \Sigma_{\sigma}(z)}.
\]  

(76)

Here \( F_{c}(\epsilon) \) is the coherent Green function given by Eq. (59).

The self-consistent condition to determine the coherent potential \( \Sigma_{\sigma}(z) \) is given by Eq. (60). However, \( G_{c\sigma}(\epsilon) \) for the HB potential fully depends on the 4 local configurations \( \alpha = (n_{i\uparrow}, n_{i\downarrow}) \) via the Hartree-Fock type potential \( U \langle \tilde{n}_{\tilde{c}\sigma} \rangle_{\text{HB}} \) in the denominator. Thus the configurational average of \( G_{00\sigma}(\epsilon) \) is given by

\[
G_{00\sigma}(\epsilon) = \sum_{\alpha} P_{\alpha} G_{00\sigma}^{\alpha}(\epsilon).
\]  

(77)

Here \( P_{\alpha} \) is the probability when taking a configuration \( \alpha \). Note that instead of the configurations \( \alpha = 00, 10, 01, 11 \), one can make use of an alternative notation.
Here the probability of finding an electron with spin $\uparrow$ can express $P^\uparrow$ and the electron number for a given configuration by

$$G^\sigma_{\alpha\sigma}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{-\sigma})_{00} + \Sigma^\sigma(z)}, \quad (78)$$

$$G^{10}_{\alpha\downarrow}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{\downarrow})_{10} + \Sigma^\sigma(z)}, \quad (79)$$

$$G^{00}_{\alpha\downarrow}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{\downarrow})_{10} - \mathcal{U} + \Sigma^\sigma(z)}, \quad (80)$$

$$G^{01}_{\alpha\downarrow}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{\downarrow})_{01} + \Sigma^\sigma(z)}, \quad (81)$$

$$G^{01}_{\alpha\uparrow}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{\downarrow})_{01} - \mathcal{U} + \Sigma^\sigma(z)}, \quad (82)$$

$$G^{11}_{\alpha\uparrow}(z) = \frac{1}{F^\sigma(z)^{-1} - \epsilon_0 + \mu - \mathcal{U}(\hat{n}_{-\sigma})_{11} - \mathcal{U} + \Sigma^\sigma(z)}, \quad (83)$$

and the electron number for a given configuration $\alpha$ in the denominators is given by

$$\langle \hat{n}_\sigma \rangle_\alpha = \int f(\epsilon) \rho^\sigma_\alpha(\epsilon) \, d\epsilon, \quad (84)$$

$$\rho^\sigma_\alpha(\epsilon) = -\frac{1}{\pi} \text{Im} \, G^\sigma_{00\sigma}(z). \quad (85)$$

The above expressions mean that the electron numbers $\langle \hat{n}_\sigma \rangle_\alpha$ have to be solved self-consistently for a given configuration with probabilities $\{P_\alpha\}$ and for an effective medium $\Sigma^\sigma(z)$. The latter is obtained from the CPA equation (60).

The third and last terms at the r.h.s. of Eq. (73) are calculated in the SSA as follows.

$$\langle \hat{n}_\alpha \rangle_{\text{HB}} = \sum_\sigma P_\alpha \langle \hat{n}_\uparrow \rangle_{\alpha} \langle \hat{n}_\downarrow \rangle_{\alpha}, \quad (86)$$

$$\sum_\sigma n_{-\sigma} \langle \hat{n}_{-\sigma} \rangle_{\text{HB}} = \sum_\sigma \sum_\alpha P_\alpha n^\alpha_{-\sigma} \langle \hat{n}_{-\sigma} \rangle_{\alpha}. \quad (87)$$

Here $n^\alpha_\uparrow = 0, 1, 0, 1$ and $n^\alpha_\downarrow = 0, 0, 1, 1$ for $\alpha = 00, 10, 01, 11$, respectively.

The on-site probability satisfies the sum rule $P_0 + P_{1\uparrow} + P_{1\downarrow} + P_2 = 1$, and the probability of finding an electron with spin $\uparrow$ (\downarrow) on a site is given by $P_{\uparrow(\downarrow)} = P_{1\uparrow(1\downarrow)} + P_2$. Therefore, $P_0, P_{1\uparrow}$, and $P_{1\downarrow}$ are given by the probability $P_2$ in the paramagnetic state.
An approximate form of $P_2$ for the hybrid wavefunction is derived as follows. We have two kinds of approximate expressions for the operator $\hat{n}_\uparrow \hat{n}_\downarrow$ according to the alloy-analogy (AA) and Hartree-Fock (HF) approximation.

$$\hat{n}_\uparrow \hat{n}_\downarrow \approx n_\uparrow n_\downarrow + n_\downarrow n_\uparrow - n_\uparrow n_\downarrow \quad \text{(AA)}, \quad (88)$$

$$\hat{n}_\uparrow \hat{n}_\downarrow \approx \hat{n}_\uparrow \langle \hat{n}_\downarrow \rangle_{\text{HB}} + \hat{n}_\downarrow \langle \hat{n}_\uparrow \rangle_{\text{HB}} - \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}} \quad \text{(HF)}. \quad (89)$$

In the HB scheme, we superpose the above expressions with the weights $w$ and $1 - w$, respectively. Taking the quantum mechanical and configurational average, we obtain an approximate form of $P_2 = \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}$. Then, we have the term $w n_\uparrow n_\downarrow + (1 - w)\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}$ at the r.h.s., which may be again regarded as the probability $P_2$ in the HB scheme. Thus we obtain an approximate form of $P_2$ as follows.

$$P_2 = \frac{1}{2} w \langle \hat{n}_\uparrow \langle \hat{n}_\downarrow \rangle_{\text{HB}} + \langle \hat{n}_\downarrow \rangle_{\text{HB}} \rangle_{\text{HB}} + (1 - w) \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}. \quad (90)$$

Since the r.h.s. of Eq. (90) is given by Eqs. (86) and (87), we can self-consistently obtain the probabilities $\{P_\alpha\}$.

Finally, the correlation energy $\epsilon_c$ in Eq. (72) is given as

$$\epsilon_c = \sum_\alpha P_\alpha \epsilon_{ca}. \quad (91)$$

Here $\epsilon_{ca}$ denotes the correlation energy for a given on-site configuration $\alpha$.

$$\epsilon_{ca} = \left[ -\langle \hat{O}_1^\dagger \hat{H} \rangle_{\text{HB}} - \langle \hat{H} \hat{O}_1 \rangle_{\text{HB}} + \langle \hat{O}_1^\dagger \hat{H} \hat{O}_1 \rangle_{\text{HB}} \right]_\alpha. \quad (92)$$

The quantities $\langle \hat{H} \hat{O}_1 \rangle_{\text{HB}}$, $\langle \hat{O}_1^\dagger \hat{H} \hat{O}_1 \rangle_{\text{HB}}$, and $\langle \hat{O}_1^\dagger \hat{O}_1 \rangle_{\text{HB}}$ are expressed by the LDOS for the HB Hamiltonian, therefore the correlation energy $\epsilon_{ca}$ is obtained from the LDOS $\rho_\alpha^h(\epsilon)$ in the single-site CPA.

The double occupation number is obtained from $\partial \langle H \rangle / \partial U$. Making use of the SSA, we obtain

$$\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle = \langle \hat{n}_\uparrow \rangle_{\text{HB}} \langle \hat{n}_\downarrow \rangle_{\text{HB}} + \langle \hat{n}_\downarrow \rangle_{\text{HB}} + \langle \hat{n}_\uparrow \rangle_{\text{HB}} \langle \hat{n}_\downarrow \rangle_{\text{HB}}. \quad (93)$$

Here $\langle \hat{n}_\uparrow \rangle_{\text{HB}} \langle \hat{n}_\downarrow \rangle_{\text{HB}}$ has been obtained in Eq. (86), and the correlation correction $\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}$ is given by

$$\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}} = \sum_\alpha P_\alpha \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}. \quad (94)$$

Here $\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle_{\text{HB}}$ is the correlation correction for a given configuration $\alpha$, and is given by Eq. (51) in which the operator $\hat{O}_1$ has been replaced by Eq. (64) and the average $\langle \sim \rangle_0$ has been replaced by $\langle \sim \rangle_{\text{HB}}$.

The momentum distribution $\langle n_{k\sigma} \rangle$ is obtained from $\partial \langle H \rangle / \partial (\epsilon_k - \sigma \hbar)$ as follows.

$$\langle n_{k\sigma} \rangle = \langle n_{k\sigma} \rangle_{\text{HB}} + \langle n_{k\sigma} \rangle_{\text{HB}} \rangle_{\text{HB}}. \quad (95)$$
Here $\langle n_{k\sigma} \rangle_{HB}$ is the momentum distribution in the hybrid state.

$$\langle n_{k\sigma} \rangle_{HB} = \int f(\epsilon) \rho_{k\sigma}(\epsilon) \, d\epsilon ,$$  \hspace{1cm} (96)

$$\rho_{k\sigma}(\epsilon) = -\frac{1}{\pi} \text{Im} F_{k\sigma}.$$  \hspace{1cm} (97)

The Green function in the momentum representation is given in the CPA as follows.

$$F_{k\sigma} = \frac{1}{z - \Sigma_{\sigma}(z) - \epsilon_k}.$$  \hspace{1cm} (98)

Here $\epsilon_k$ is the eigenvalue of $t_{ij}$ with momentum $k$.

The correlation correction $\langle n_{k\sigma} \rangle_c$ is given as follows.

$$\langle n_{k\sigma} \rangle_c = \sum_{\alpha} P_\alpha \langle n_{k\sigma} \rangle_{c\alpha}.$$  \hspace{1cm} (99)

Here $\langle n_{k\sigma} \rangle_{c\alpha}$ is the correlation correction for the configuration $\alpha$, and is given by the second term at the r.h.s. of Eq. (49) in which $\tilde{O}_i$ has been replaced by Eq. (64) and $\langle \tilde{\sim} \rangle_0$ has been replaced by $\langle \tilde{\sim} \rangle_{HB}$.

### 4.3. MLA-HB in infinite dimensions

The MLA with HB wavefunction improves further the description of electron correlations in the strongly correlated region. One can verify the fact by means of some numerical calculations in infinite dimensions. The ground state energy in the MLA-HB was obtained by varying $w$ from 0 to 1 for each value of $U$. Figure 5 shows the ground-state energy obtained by various methods on the hypercubic lattice in infinite dimensions at half filling. The energy in the LA monotonically increases with increasing Coulomb interaction energy and becomes positive beyond $U = 3.4$ because it does not suppress sufficiently the double occupancy in the strongly correlated region.

The ground-state energy in the GW is lower than that of the LA, and approaches zero at $U_c(GW) = 4.51$ with increasing Coulomb interaction. The Brinkman-Rice atomic state is realized beyond $U_c(GW)$ (see Sec. 2.1). The ground-state energy of the MLA-HB is the lowest among three wavefunctions over all Coulomb interactions $U$. Note that there is a cusp in the energy vs $U$ curve at $U_c(MLA) = 2.81$. The Fermi-liquid ground state with $w = 0$ is obtained below $U_c(MLA)$, while the disordered local moment solution with infinitesimal $w$ is stabilized beyond $U_c(MLA)$.

As shown in Fig. 6, the double occupation number $\langle n_\uparrow n_\downarrow \rangle$ in the GW linearly decreases with increasing $U$ according to Eq. (9). In the case of the LA, it monotonically decreases according to Eq. (14). The double occupation number in the MLA-HB is lower than that in the LA and GW in the weak Coulomb interaction regime and jumps from 0.106 to 0.045 at $U_c(MLA) = 2.81$, indicating the metal-insulator transition. Beyond $U_c(MLA)$, it again monotonically decreases with increasing $U$. Note that the double occupancy in the MLA-HB remains finite in the
strong $U$ regime as it should be, while the GW gives the Brinkman-Rice atom, because the MLA takes into account the electron hopping from the atomic state.

The momentum distribution in the MLA-HB has the same behavior as the MLA-HF in the metallic region; it decreases monotonically with increasing energy $\epsilon_{k\sigma}$ and shows a jump at the Fermi level, while it disappears beyond $U_c$ (MLA) as shown in
Fig. 7. The momentum distribution as a function of energy $\epsilon_{k\sigma}$ for various Coulomb interaction energy parameters $U = 1.0, 2.0, 2.81, 3.0, 4.0$ and $5.0$ at half-filling. The MLA-HB: solid curves, the GW: dashed curves, and the HF: thin solid curve (Ref. 47).

With further increase of $U$, the curve becomes flatter. These results indicate that the MLA-HB improves upon the GW. Note that the distributions in the GW are constant below and above the Fermi level irrespective of $U$ as discussed in Sec. 2.1. The quasiparticle weight in the MLA-HB is the same as in the MLA-HF in the metallic region (see Fig. 4). With the metal-insulator transition at $U_c$ (MLA) = 2.81, it disappears. The existence of the first-order transition at $U = U_c$ is in agreement with the result of the NRG [64], though $U_c$ in the NRG has not yet been published.

5. Towards the First-Principles MLA

The momentum-dependent local ansatz (MLA) wavefunction yields a reasonable description of correlated electrons from the weak to strong Coulomb interaction regime, and overcomes the limitations of the LA and the GW wavefunction, in particular, for the description of physical quantities associated with the low-energy excitations near the Fermi surface. Therefore it is worthwhile to extend the MLA to the realistic system towards first-principles calculations.

Let us consider the first-principles LDA+U Hamiltonian which is based on the tight-binding linear muffin-tin orbital [65],

$$ H = H_0 + H_1, $$

$$ H_0 = \sum_{iL\sigma} \epsilon_{iL\sigma} n_{iL\sigma} + \sum_{iL,jL',\sigma} t_{iL,jL',\sigma} a^\dagger_{iL\sigma} a_{jL'\sigma}, $$

(100)
Here we assume a d metal system with an atom per unit cell for simplicity. \( H_0 \) and \( H_1 \) denote the non-interacting and interacting parts, respectively. \( \epsilon_0^L_i \) is an atomic level on site \( i \) and orbital \( L \), \( t_{iLJ^L'} \) is a transfer integral between orbitals \( iL \) and \( jL' \). \( L = (l, m) \) denotes s, p, and d orbitals. \( a^\dagger_{iL\sigma} \) (\( a_{iL\sigma} \)) is the creation (annihilation) operator for an electron with orbital \( L \) and spin \( \sigma \) on site \( i \), and \( \hat{n}_{iL\sigma} = a^\dagger_{iL\sigma} a_{iL\sigma} \) is a charge density operator for electrons with orbital \( L \) and spin \( \sigma \) on site \( i \).

The inter-site Coulomb interactions are considered to be well screened by the s and p band electrons, so that only the on-site Coulomb interactions between d \( (l = 2) \) electrons are taken into account in Eq. (102). \( U_{mm'} \) (\( U_{mm'} \)), and \( J_{mm'} \) denote the intra-orbital (inter-orbital) Coulomb and exchange interactions, respectively. \( \hat{n}_{ilm} \) (\( \hat{s}_{ilm} \)) with \( l = 2 \) is the charge (spin) density operator for d electrons on site \( i \) and orbital \( m \). The atomic level \( \epsilon_0^L_i \) in \( H_0 \) is calculated from the LDA atomic level \( \epsilon^L_i \) by subtracting the double counting potential; \( \epsilon_0^L_i = \epsilon^L_i - \partial E_{\text{LDA}} / \partial n_{iL\sigma} \). Here \( n_{iL\sigma} \) is the charge density at the ground state, \( E_{\text{LDA}} \) is a LDA functional for the intra-atomic Coulomb interactions \(^{65,66} \).

The Gutzwiller wavefunction (GW) has been extended to the case of a realistic Hamiltonian \(^{67,68,69} \). The wavefunction is constructed so as to reproduce the exact atomic states. We first solve the eigen value problem for the atomic Hamiltonian in \( H(= \sum_i H_A^i) \). The atomic Hamiltonian \( H_A^i \) on each site satisfies the eigen value equation as follows.

\[
H_A^i |\Gamma\rangle = E_{\Gamma} |\Gamma\rangle. \tag{103}
\]

Here we omitted the site index \( i \) for simplicity. \( E_{\Gamma} \) denotes the eigen value for the atomic eigen state \( |\Gamma\rangle \) which is obtained from the \( 2^M \) atomic configuration states \( \{I\} \) as \( |\Gamma\rangle = \sum_I |I\rangle T_{I\Gamma}, \) \( M \) being the number of orbitals in a site.

The atomic Hamiltonian is then expressed as

\[
H_A = \sum_{\Gamma} E_{\Gamma} \hat{m}_{\Gamma}, \tag{104}
\]

where \( \hat{m}_{\Gamma} \) are the projection operators such that \( \hat{m}_{\Gamma} = |\Gamma\rangle \langle \Gamma| \). The Gutzwiller wavefunction is constructed as

\[
|\Psi_G\rangle = P_G |\phi\rangle = \left[ \prod_i P_i \right] |\phi\rangle. \tag{105}
\]

Here \( |\phi\rangle \) is the Hartree-Fock wavefunction for the Hamiltonian \(^{100} \).

The local correlator \( P_i \) in the wavefunction \(^{105} \) is defined by

\[
P_i = 1 + \sum_{\Gamma} (\lambda_{i\Gamma} - 1) \hat{m}_{i\Gamma}. \tag{106}
\]
Here we recovered the site index \( i \). \( \lambda_{\Gamma} \) denotes the variational parameters. The Gutzwiller wavefunction for the multiband Hamiltonian has been applied to various correlated-electron systems such as Ni\[^{70}\] and Fe pnictides\[^{71\text{-}73}\].

The Gutzwiller wavefunction is constructed to reproduce well the atomic regime. But it does not reproduce the correct wavefunction in the weak Coulomb interaction limit. The MLA wavefunction is constructed to reproduce the exact wavefunction in the weak interaction limit. We rewrite the Hamiltonian as the sum of the Hartree-Fock Hamiltonian \( H_{HF} \) and the residual interactions \( H_I \). The latter is given by

\[
H_I = \sum_i \left[ \sum_m U_{im} O_{imm}^{(0)} + \sum_{m > m'} (U_{mm'} - \frac{1}{2} J_{mm'}) O_{imm'}^{(1)} - \sum_{m > m'} J_{mm'} O_{imm'}^{(2)} \right].
\]

(107)

Here \( O_{imm}^{(0)} \), \( O_{imm'}^{(1)} \), and \( O_{imm'}^{(2)} \) are the two-particle intra-orbital operators, the charge-charge inter-orbital operators, and the spin-spin inter-orbital operators, respectively, which are defined as follows.

\[
O_{imm}^{(0)} = \delta \hat{n}_{i\lambda m\uparrow} \delta \hat{n}_{i\lambda m\downarrow},
\]

(108)

\[
O_{imm'}^{(1)} = \delta \hat{n}_{i\lambda m\uparrow} \delta \hat{n}_{i\lambda m'\downarrow},
\]

(109)

\[
O_{imm'}^{(2)} = \delta \hat{s}_{i\lambda m\uparrow} \cdot \delta \hat{s}_{i\lambda m'\downarrow}.
\]

(110)

Applying the Rayleigh-Schrödinger perturbation theory, we find that the first-order correction \(|\phi_1\rangle\) to the Hartree-Fock wavefunction \(|\phi\rangle\) is given by

\[
|\phi_1\rangle = -\sum_i \left( \sum_m O_{imm}^{(0)} + \sum_{m > m'} O_{imm'}^{(1)} + \sum_{m > m'} O_{imm'}^{(2)} \right) |\phi\rangle.
\]

(111)

The two-particle operators \( \tilde{O}_{iLL'}^{(n)} \), \((n = 0, 1, 2)\) are defined by

\[
\tilde{O}_{iLL'}^{(n)} = \sum_{\{kn\sigma\}} \langle k'2n'\sigma'1|L\rangle \langle L|k2n2\rangle \langle k'n'1|L'\rangle \langle L'|k1n1\rangle \times \lambda_{\{kn\sigma\}}^{(n)}(2')^{\delta(a_{k1n1\sigma1} a_{k2n2\sigma2})} \delta(a_{k1n1\sigma1} a_{k2n2\sigma2}) \cdot
\]

(112)

Here \( a_{k\sigma} \) (\( a_{k\sigma} \)) is the creation (annihilation) operator for an electron with momentum \( k \), band index \( n \), and spin \( \sigma \). They are related to those in the site representation by \( a_{knL} = \sum_{iL} a_{iL\sigma} (kn|iL) \). The momentum dependent coefficients \( \lambda_{\{kn\sigma\}}^{(n)}(2') \) are given by

\[
\lambda_{LL'}^{(0)}(2'21') = \eta_{LL'} k'2n'\sigma'1 k2n2\sigma2 k1n1 \delta_{LL'} \delta_{\sigma2\sigma2} \delta_{\sigma1\sigma1} \delta_{\sigma2\sigma1} \cdot
\]

\[
\lambda_{LL'}^{(1)}(2'21') = \xi_{LL'}(\sigma_{1\sigma2}) k'2n'\sigma'1 k2n2\sigma2 k1n1 \delta_{\sigma2\sigma2} \delta_{\sigma1\sigma1} \cdot
\]

\[
\lambda_{LL'}^{(2)}(2'21') = \sum_{\sigma} \xi_{LL'}(\sigma_{1\sigma2}) k'2n'\sigma'1 k2n2\sigma2 k1n1 \delta_{\sigma2\sigma2} \delta_{\sigma1\sigma1} \delta_{\sigma2\sigma1} \cdot
\]

\[
= \frac{1}{2} \sigma_{1\sigma2} \xi_{LL'}(\sigma_{1\sigma2}) k'2n'\sigma'1 k2n2\sigma2 k1n1 \delta_{\sigma2\sigma2} \delta_{\sigma1\sigma1} \cdot
\]

(113)
Finally, we obtain the MLA wavefunction for the realistic Hamiltonian (100) as follows.

\[ \Psi_{\text{MLA}} = \left[ \prod_i \left( 1 - \sum_m \tilde{O}_{imm}^{(0)} - \sum_{m>m'} \tilde{O}_{imm'}^{(1)} - \sum_{m>m'} \tilde{O}_{imm'}^{(2)} \right) \right] \phi . \]  

Here \( \tilde{O}_{imm}^{(0)} \), \( \tilde{O}_{imm'}^{(1)} \), and \( \tilde{O}_{imm'}^{(2)} \) are the intra-orbital charge-charge correlators, the inter-orbital charge-charge correlators, and the inter-orbital spin-spin correlators. \( \eta_{LL'}k'_2n'_2k'_1n'_1k'_1n_1, \xi^{(\sigma)}_{LL'k'_2n'_2k'_1n'_1k'_1n_1}, \xi^{(\sigma')}_{LL'k'_2n'_2k'_1n'_1k'_1n_1}, \) and \( \xi^{(\sigma \sigma')}_{LL'k'_2n'_2k'_1n'_1k'_1n_1} \) in these operators are the variational parameters. The correlation energy \( \epsilon_c \) is given by Eq. (47) with the operator \( \tilde{O}_i \) replaced by \( \sum_m \tilde{O}_{imm}^{(0)} + \sum_{m>m'} \tilde{O}_{imm'}^{(1)} + \sum_{m>m'} \tilde{O}_{imm'}^{(2)} \).

Solving the self-consistent equations obtained from the stationary condition \( \delta \epsilon_c = 0 \), we find approximate forms of the variational parameters (74) which correspond to Eq. (42).

\[ \eta_{LL'}k'_2n'_2k'_1n'_1n_1 = \frac{U_{mm} \tilde{\eta}_m}{\Delta E_{k'_2n'_2k'_1n'_1k'_1n_1} - \epsilon_c} , \]

\[ \xi^{(\sigma \sigma')}_{LL'k'_2n'_2k'_1n'_1n_1} = \frac{(U_{mm'} - J_{mm'})/2 \tilde{\chi}_{mm'}^{(\sigma \sigma')}}{\Delta E_{k'_2n'_2k'_1n'_1k'_1n_1} - \epsilon_c} , \]

\[ \xi^{(\sigma')}_{LL'k'_2n'_2k'_1n'_1n_1} = \frac{J_{mm'} \tilde{\chi}_{mm'}^{(\sigma')}}{\Delta E_{k'_2n'_2k'_1n'_1k'_1n_1 - \sigma} - \epsilon_c} , \]

\[ \xi^{(\sigma \sigma')}_{LL'k'_2n'_2k'_1n'_1n_1} = \frac{J_{mm'} \tilde{\chi}_{mm'}^{(\sigma \sigma')}}{\Delta E_{k'_2n'_2k'_1n'_1k'_1n_1 - \sigma} - \epsilon_c} . \]

Here \( \tilde{\eta}_m, \tilde{\chi}_{mm'}^{(\sigma \sigma')}, \tilde{\chi}_{mm'}^{(\sigma)}, \) and \( \tilde{\chi}_{mm'}^{(\sigma \sigma')} \) are new variational parameters. \( \Delta E_{k'_2n'_2k'_1n'_1k'_1n_1} \) is the two-particle excitation energy.

The realistic multi-band Hamiltonian and its wavefunction contains new physics: (1) orbital-dependent suppression of charge fluctuations, (2) formation of atomic magnetic moments due to Hund’s rule couplings, (3) intra-atomic instabilities such as the high-spin to the low-spin transition, (4) band-dependent quasiparticle weight (i.e., effective masses), (5) orbital selective metal-insulator transition. Implementation of the first-principles MLA calculations is left for future investigations (74).

6. Summary

We have presented recent progress in the development of the local ansatz wavefunction with momentum dependent variational parameters, i.e., the MLA. The MLA wavefunction takes into account the Hilbert space expanded by the two-particle operators of the residual Coulomb interactions, as in the local ansatz (LA).
function, but the amplitudes for the two-particle excited states in the momentum representation are assumed to be momentum dependent so as to be exact in the weak Coulomb interaction limit. Consequently, the two-particle operators \( \{ \eta_i O_i \} \) in the LA are replaced by a new set of operators \( \{ \tilde{O}_i \} \) with momentum-dependent variational parameters \( \{ \eta_{k,k',k_1} \} \) in the MLA. By making use of the variational principle, we determine the best amplitudes \( \eta_{k,k',k_1} \) for two-particle excited states and again project those states with the best amplitudes onto the local subspace.

We have demonstrated that the MLA improves upon the LA in terms of energy irrespective of the electron number and the Coulomb interaction energy, and more strongly suppresses the double occupation number as compared with the LA. In particular, the momentum distribution functions show a momentum dependence, while those in the LA and the Gutzwiller wavefunction (GW) show a flat behavior below and above the Fermi level. Furthermore, the quasiparticle weight vs Coulomb interaction curve is close to the NRG result, while those in the LA and the GW strongly deviates from the NRG curve.

One can improve the MLA by changing the starting wavefunction from the Hartree-Fock (HF) wavefunction to the hybrid (HB) one. The HB wavefunction is the ground state for the HB Hamiltonian which is a superposition of the Hartree-Fock Hamiltonian and the alloy-analogy (AA) one. The HF wavefunction is a good starting wavefunction in the weakly correlated regime, while the AA wavefunction is more suitable in the strongly correlated regime. One can choose the best HB wavefunction by controlling the weighting parameter in the HB Hamiltonian. The MLA with the HB wavefunction is applicable to both the weak and the strong Coulomb interaction systems.

The MLA-HB yields a lower ground-state energy than the LA and GW, and causes the first-order metal-insulator transition, at which point the double occupation number jumps as a function of the Coulomb interaction strength. The double occupation number in the insulating regime remains finite as it should be in infinite dimensions, while it vanishes in the GW because of the appearance of the Brinkman-Rice atomic state. The momentum distribution function shows a clear momentum dependence in both the metallic and the insulating regions. These facts indicate that the MLA-HB well describes correlated electrons in high dimensions.

We have also extended the MLA to the realistic system. The first principles MLA can describe the charge-charge correlations and the spin-spin correlations between electrons on the different orbitals, in addition to the intra-orbital correlations. It is useful for understanding the correlated electrons in real systems.

The MLA wavefunction method presented here is limited to the single-site approximation. Inclusion of nonlocal correlations is desired to describe magnetism, the metal-insulator transition, and the frustrated electrons in low dimensional systems. There one needs to introduce explicitly the nonlocal operators such as \( \tilde{O}_{ij} = \sum_{k_1,k_2,k_1',k_2'} (k_1|i\rangle\langle k_1|j\rangle (k_2|j\rangle\langle k_2|k_1) \eta_{k,k',k_1} \delta(a_{k_2\downarrow}^\dagger a_{k_1\downarrow}) \delta(a_{k_1\uparrow}^\dagger a_{k_2\uparrow}) \) with momentum-dependent variational parameters \( \eta_{k,k',k_1} \). Extension of the MLA to the nonlocal case is also left as future work.
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