Momentum Dependent Local-Ansatz with Hybrid Wavefunction from Weak to Strong Electron Correlations

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The variational theory of momentum dependent local-ansatz (MLA) has been generalized by introducing a hybrid (HB) wavefunction as a starting wavefunction, whose potential can flexibly change from the Hartree-Fock type to the alloy-analogy type by varying a weighting factor from zero to one. Numerical results based on the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions show up that the new wavefunction yields the ground-state energy lower than that of the Gutzwiller wavefunction (GW) in the whole Coulomb interaction regime. Calculated double occupation number is smaller than the result of the GW in the weak Coulomb interaction regime, and remains finite in the strong regime. Furthermore, the momentum distribution shows a distinct momentum dependence, which is qualitatively different from that of the GW.

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

1. Introduction

It is well recognized that electron correlations are essential for understanding the electronic structure, the magnetism, the metal-insulator transition, and the high-temperature superconductivity in solids.1, 2) To describe the correlations at the ground-state, various methods have been developed. The variational approach is one of the simplest methods among them and has been applied to many systems as a practical tool.3–16) A minimum basis set is constructed in the approach by applying one-particle, two-particle, and higher-order particle operators onto the Hartree-Fock (HF) wavefun-
tion, and their amplitudes are chosen to be best.

For the Hubbard-type Hamiltonian, the Gutzwiller wavefunction (GW) is one of useful wavefunctions, because of its simplicity and applicability to realistic systems.\(^3\) When the intra-atomic Coulomb repulsion \(U\) is large, the double occupancy on the same orbital should be suppressed to avoid the energy loss due to the Coulomb repulsion \(U\).\(^{17-19}\) The HF wavefunction does not describe such correlations because it consists of a single Slater determinant. Taking into account these facts, Gutzwiller proposed a trial wavefunction which controls the probability amplitudes of doubly occupied states in the HF wavefunction by making use of a projection operator \(\Pi_i(1 - g\hat{n}_i\hat{n}_i)\). Here \(\hat{n}_i\sigma\) is the number operator for an electron on site \(i\) with spin \(\sigma\), variational parameter \(g\) reduces the amplitudes of doubly occupied states on local orbitals. Stollhoff and Fulde\(^6\) proposed a method called the local-ansatz approach (LA), which is simpler than the GW in treatment. The LA wavefunction takes into account the states created by local two-particle operators such as the residual Coulomb interactions \(\{O_i\} = \{\delta\hat{n}_i\delta\hat{n}_i\}\). Here \(\delta\hat{n}_i\sigma = \hat{n}_i\sigma - \langle \hat{n}_i\sigma \rangle_{HF}\), \(\langle \hat{n}_i\sigma \rangle_{HF}\) being the average electron number on site \(i\) with spin \(\sigma\) in the HF approximation.

Though the GW and the LA are applicable for various correlated electron systems, they are not sufficient for the description of correlations from the weak to the strong interaction regimes. Indeed, the Hilbert space expanded 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. The same difficulty also arises for the GW even in infinite dimensions. Moreover, in the strong Coulomb interaction regime, the GW yields the Brinkman-Rice atom (i.e., no charge fluctuation on an atom) instead of the insulator solid in infinite dimensions.\(^{20}\) To overcome the difficulty in the weak Coulomb interaction regime and to improve the behaviors in the intermediate Coulomb interaction regime, we have recently proposed the momentum dependent local-ansatz wavefunction (MLA),\(^{21-23}\) and demonstrated that the MLA approach much improves both the GW and the LA in these regimes. In the MLA, we consider two-particle operators in the momentum space with momentum dependent parameters and project them onto the local orbitals. With use of such local operators \(\{\hat{O}_i\}\), we construct the MLA wavefunction as \(|\Psi_{MLA}\rangle = \prod_i(1 - \hat{O}_i)|\phi_{HF}\rangle\). Here \(|\phi_{HF}\rangle\) is the HF wavefunction and \(i\) denotes sites of atoms. The best local basis set is chosen by controlling the variational parameters in the momentum space.

Baeriswyl, on the other hand, proposed a wavefunction called Baeriswyl wavefunc-
tion (BW) which accurately describes electron correlations in the strong Coulomb interaction regime.\(^9\text{--}^{12}\) It is constructed by applying a hopping operator \(\hat{T}\) onto the atomic wavefunction \(|\Psi_\infty\rangle\); \(|\Psi_{\text{BW}}\rangle = e^{-\eta\hat{T}}|\Psi_\infty\rangle\). Here \(\hat{T} = -\sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}\) is the kinetic energy operator, \(t_{ij}\) denotes the transfer integral between sites \(i\) and \(j\), \(a_{i\sigma}^\dagger\) \((a_{i\sigma})\) being the creation \((\text{annihilation})\) operator for an electron on site \(i\) with spin \(\sigma\). The operator \(e^{-\eta\hat{T}}\) with a variational parameter \(\eta\) describes electron hopping from the atomic state and suppresses the configurations with high kinetic energy. The BW describes well the insulator state in the strong correlation regime. However, it is not easy to describe the metallic state from this viewpoint.

In order to describe the correlations in the strong Coulomb interaction regime, we have recently proposed an improved MLA wavefunction,\(^{24}\) which starts from the alloy-analogy (AA) wavefunction instead of the HF one. The concept of the AA approximation can be traced back to Hubbard’s original work on electron correlations.\(^{19}\) He considered that electrons move slowly from site to site in the strong Coulomb interaction regime, so that an electron on a site with (without) opposite spin electron on the same site feels a potential \(\epsilon_0 + U\) \((\epsilon_0)\), where \(\epsilon_0\) and \(U\) denote the atomic level and the on-site Coulomb interaction parameter, respectively. The AA wavefunction is the ground-state wavefunction for the independent-particle Hamiltonian with such two kind of random potentials. We found numerically that the MLA theory with the AA wavefunction describes the strongly correlated regime reasonably, and can go beyond the GW in both the weak and the strong Coulomb interaction regimes.

From the above discussions it is recognized that the MLA wavefunction can describe reasonably electron correlations from the weak to the intermediate Coulomb interaction regime and to the strong Coulomb interaction regime by choosing the starting wavefunction. In order to describe the whole Coulomb interaction regime on the same footing, we propose in this paper a new MLA wavefunction which starts from a hybrid (HB) wavefunction, and clarify the validity of our theory on the basis of the results of numerical calculations for the half-filled band Hubbard model. The HB wavefunction is defined by the ground-state of the independent-particle Hamiltonian with a HB potential consisting of the HF potential with a weight \(1 - w\) and the AA potential with a weight \(w\), and can vary from the HF wavefunction to the AA one via the new variational parameter \(w\). Hereafter we call the new wavefunction the MLA-HB. We will demonstrate that the MLA-HB much improves both the GW and the LA, and describes electron correlations from the weak to the strong Coulomb interaction regime.
The outline of the paper is as follows. In the following section we adopt the Hubbard model and introduce the HB Hamiltonian as well as the HB wavefunction. We will clarify the properties of the HB wavefunction, calculating the ground-state energy, the double occupation number and the momentum distribution in infinite dimensions. In §3, we present the correlated MLA-HB wavefunction which starts from the HB wavefunction. We obtain the ground-state energy within the single-site approximation (SSA), and derive the self-consistent equation for the momentum dependent variational parameters. We also obtain the double occupation number as well as the momentum distribution. In §4, we present our results of numerical calculations for the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions. We discuss the ground-state energy, the double occupation number, the momentum distribution, and the quasiparticle weight as a function of the Coulomb interaction energy parameter, and verify that the present approach improves both the GW and the LA in the whole Coulomb interaction regime. We summarize our results in the last section and discuss the remaining problems.

2. Hybrid wavefunction

We adopt in this paper the single-band Hubbard model\textsuperscript{(17-19)} as follows.

\[ H = \sum_{i\sigma} (\epsilon_0 - \mu) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} . \]  

Here \( \epsilon_0 \) (\( \mu \)) is the atomic level (chemical potential), \( t_{ij} \) 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 \( \hat{n}_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma} \) is the electron density operator on site \( i \) for spin \( \sigma \).

In the HF approximation, we neglect the fluctuations \( \delta \hat{n}_{i\uparrow} \delta \hat{n}_{i\downarrow} \) and replace the many-body Hamiltonian (1) with an effective Hamiltonian \( H_{HF} \) for independent-particle system.

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

Here \( \langle \sim \rangle_{HF} \) denotes the HF average \( \langle \phi_{HF}|(\sim)|\phi_{HF} \rangle \), and \( \langle n_{i\sigma} \rangle_{HF} \) is the average electron number on site \( i \) with spin \( \sigma \). \( |\phi_{HF} \rangle \) denotes the ground-state wavefunction for the HF Hamiltonian \( H_{HF} \).

In the AA approximation, we consider the strong Coulomb interaction regime, where electrons with spin \( \sigma \) move slowly from site to site due to electron correlations. Instead
of the HF average potential \( U\langle \hat{n}_{i-\sigma}\rangle_{\text{HF}} \), electrons should feel there a potential \( U(0) \), when the opposite spin electron is occupied (unoccupied) on the same site. Hubbard regarded this system as an alloy with different random potentials \( \varepsilon_0 + U \) and \( \varepsilon_0 \). The AA Hamiltonian is then defined by

\[
H_{\AA} = \sum_{i\sigma}(\varepsilon_0 - \mu + U n_{i-\sigma})\hat{n}_{i\sigma} + \sum_{ij\sigma}t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - U \sum_i (n_{i\uparrow}\langle n_{i\downarrow}\rangle_{\AA} + n_{i\downarrow}\langle n_{i\uparrow}\rangle_{\AA}) \\
+ U \sum_i \langle n_{i\uparrow}\rangle_{\AA}\langle n_{i\downarrow}\rangle_{\AA}.
\]

(3)

Here \( \langle \sim \rangle_{\AA} \) denotes the AA average \( \langle \phi_{\AA} | (\sim) | \phi_{\AA} \rangle \) with respect to the ground-state wavefunction \( | \phi_{\AA} \rangle \) of the AA Hamiltonian \( H_{\AA} \). Since the electrons with opposite spin are treated to be static in the AA approximation, related operators \( \{ \hat{n}_{i-\sigma} \} \) are regarded as a random static \( C \) number \( n_{i-\sigma} (0 \text{ or } 1) \). Each configuration \( \{ n_{i\sigma} \} \) is considered as a snapshot in time development.

The HF Hamiltonian works best in the weakly correlated regime, while the AA Hamiltonian works better in the strongly correlated regime. In order to obtain a good starting wavefunction for any interaction strength \( U \), we introduce the HB Hamiltonian which is a linear combination of both the HF and the AA Hamiltonian as follows.

\[
H_{\text{HB}} = \sum_{i\sigma}(\varepsilon_0 - \mu + U n_{i-\sigma})\hat{n}_{i\sigma} + \sum_{ij\sigma}t_{ij} a_{i\sigma}^\dagger a_{j\sigma} \\
- (U - \tilde{U}) \sum_i \langle n_{i\uparrow}\rangle_0 \langle n_{i\downarrow}\rangle_0 - \tilde{U} \sum_i (n_{i\uparrow}\langle n_{i\downarrow}\rangle_0 + n_{i\downarrow}\langle n_{i\uparrow}\rangle_0).
\]

(4)

Here \( \langle \sim \rangle_0 \) denotes the HB average \( \langle \phi_0 | (\sim) | \phi_0 \rangle \) with respect to the ground-state \( | \phi_0 \rangle \) of the HB Hamiltonian, \( \tilde{U} = (1 - w)U \) and \( \tilde{U} = wU \). We introduced a variational parameter \( w \). Note that \( H_{\text{HB}} \) reduces to the HF Hamiltonian when \( w = 0 \), while \( H_{\text{HB}} \) reduces to the AA when \( w = 1.0 \).

The ground-state energy \( E \) satisfies the following inequality for a normalized wavefunction \( | \phi_0 \rangle \).

\[
E \leq \langle \phi_0 | H | \phi_0 \rangle = \langle H_{\text{HB}} \rangle_0.
\]

(5)

The HB ground-state energy per atom is obtained by taking the configurational average.

\[
\langle H \rangle_{\text{HB}} = n\mu + 2 \int_{-\infty}^0 \varepsilon \rho_{i\sigma}(\varepsilon) d\varepsilon - (U - \tilde{U}) \langle n_{i\uparrow}\rangle_0 \langle n_{i\downarrow}\rangle_0 - \tilde{U} \langle n_{i\uparrow}\langle n_{i\downarrow}\rangle_0 + n_{i\downarrow}\langle n_{i\uparrow}\rangle_0 \rangle .
\]

(6)

Here we assumed the system with one atom per unit cell. \( \langle H \rangle_{\text{HB}} \) denotes the HB average \( \langle \phi_0 | H | \phi_0 \rangle \). The upper bar denotes the configurational average and \( n \) is the electron number per atom. \( \rho_{i\sigma}(\varepsilon) \) is the local density of states (DOS) and is obtained from the
one-electron Green function.

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

(7)

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

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

(8)

Note that \( z = \epsilon + i\delta \), \( \delta \) being the infinitesimal positive number. \((H_\sigma)_{ij}\) is the one-electron Hamiltonian matrix for the HB Hamiltonian (4), which is defined by

\[ (H_\sigma)_{ij} = (\epsilon_0 - \mu + U\langle n_{i-\sigma}\rangle_0 + \tilde{U} n_{i-\sigma})\delta_{ij} + t_{ij}(1 - \delta_{ij}) . \]  

(9)

The average electron number \( \langle n_{i\sigma}\rangle_0 \) with respect to the HB Hamiltonian (4) is given as

\[ \langle n_{i\sigma}\rangle_0 = \int f(\epsilon)\rho_{i\sigma}(\epsilon) \, d\epsilon , \]  

(10)

\( f(\epsilon) \) being the Fermi distribution function.

To obtain the local DOS, we make use of the coherent potential approximation (CPA).

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

\[ G_{i\sigma}(z) = \frac{1}{F_{\sigma}(z)^{-1} - \epsilon_0 + \mu - U\langle n_{i-\sigma}\rangle_0 + \tilde{U} n_{i-\sigma} + \Sigma_{\sigma}(z)} . \]  

(11)

Here \( F_{\sigma}(z) \) is the on-site Green function for the coherent system in which all the random potentials have been replaced by the coherent ones. It is given by

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

(12)

Here \( \rho(\epsilon) \) is the DOS per site for the noninteracting system.

The coherent potential \( \Sigma_{\sigma}(z) \) is determined from a self-consistent condition.

\[ \overline{G_{00\sigma}(z)} = F_{\sigma}(z) . \]  

(13)

The configurational average of the impurity Green function is now given as

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

(14)

Here \( \alpha = 00, 10, 01, 11 \) denotes the on-site electron configuration \((n_{0\uparrow}, n_{0\downarrow})\). Alternative notation \( \nu = 0 \) (empty on a site), \( 1 \uparrow \) (occupied by an electron with spin \( \uparrow \)), \( 1 \downarrow \) (occupied by an electron with spin \( \downarrow \)) and \( 2 \) (occupied by 2 electrons) is also useful. In this case, the probability \( P_{\alpha} \) for the configuration \( \alpha \) is expressed as \( P_0, P_{1\uparrow}, P_{1\downarrow} \) and \( P_2 \).
The impurity Green functions in eq. (14) for each configuration are given as follows.

\[
G_{00\sigma}^{00}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{-\sigma} \rangle_{00} + \Sigma_\sigma(z)},
\]

\[
G_{00\uparrow}^{10}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{\downarrow} \rangle_{10} + \Sigma_\sigma(z)},
\]

\[
G_{00\downarrow}^{10}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{\uparrow} \rangle_{10} - \overline{U} + \Sigma_\sigma(z)},
\]

\[
G_{00\uparrow}^{10}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{\downarrow} \rangle_{01} - \overline{U} + \Sigma_\sigma(z)},
\]

\[
G_{00\downarrow}^{10}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{\uparrow} \rangle_{01} + \Sigma_\sigma(z)},
\]

\[
G_{00\sigma}^{11}(z) = \frac{1}{F_\sigma(z)^{-1} - \epsilon_0 + \mu - \overline{U} \langle n_{-\sigma} \rangle_{11} - \overline{U} + \Sigma_\sigma(z)}.
\]

Here the electron number in the denominator is given by

\[
\langle n_\sigma \rangle_\alpha = \int f(\epsilon)\rho_\sigma^\alpha(\epsilon) \, d\epsilon,
\]

\[
\rho_\sigma^\alpha(\epsilon) = -\frac{1}{\pi} \text{Im} \ G_{00\sigma}^\alpha(z).
\]

Furthermore, the average DOS in the second term at the right hand side (rhs) of eq. (6) is given by

\[
\rho_{\sigma\alpha}(\epsilon) = -\frac{1}{\pi} \text{Im} \ G_{00\sigma}^{\alpha}(z).
\]

It should be noted that \( P_0 + P_{\uparrow\uparrow} + P_{\downarrow\downarrow} + P_2 = 1 \), and the probability of finding an electron with spin \( \uparrow \) (\( \downarrow \)) on a site is given by \( P_{\uparrow(\downarrow)} = P_{\uparrow(\downarrow,\downarrow)} + P_2 \). Three statistical probabilities \( P_0, P_{\uparrow\uparrow}, \) and \( P_{\downarrow\downarrow} \) therefore depend on the probability \( P_2 \). The expression of \( P_2 \) is given as follows as shown in Appendix A.

\[
P_2 = \frac{(1 - w)\langle n_{\uparrow\downarrow} \rangle_{00}^2 + (P_\uparrow + P_\downarrow)\{1/2w \langle n_{\uparrow\downarrow} \rangle_{01} + (1 - w)\langle n_{\uparrow\downarrow} \rangle_{10} \langle n_{\uparrow\downarrow} \rangle_{01} - \langle n_{\uparrow\downarrow} \rangle_{00}^2\}}{1 - w(\langle n_{\uparrow\downarrow} \rangle_{11} - \langle n_{\uparrow\downarrow} \rangle_{01}) - (1 - w)(\langle n_{\uparrow\downarrow} \rangle_{00}^2 - 2\langle n_{\uparrow\downarrow} \rangle_{10} \langle n_{\uparrow\downarrow} \rangle_{01} + \langle n_{\uparrow\downarrow} \rangle_{11}^2)}.
\]

The double occupation numbers at the rhs of eq. (6) are obtained in the SSA as follows.

\[
\overline{n_{\uparrow\uparrow}n_{\downarrow\downarrow}} = \overline{n_{\uparrow\downarrow}n_{\downarrow\uparrow}} = \sum_\alpha P_\alpha \langle n_{\uparrow\downarrow} \rangle_\alpha \langle n_{\uparrow\downarrow} \rangle_\alpha,
\]

\[
\overline{n_{\uparrow\uparrow}n_{\downarrow\downarrow}} + \overline{n_{\downarrow\uparrow}n_{\uparrow\downarrow}} = (P_\uparrow + P_\downarrow)\langle n_{\uparrow\downarrow} \rangle_{01} + 2P_2(\langle n_{\uparrow\downarrow} \rangle_{11} - \langle n_{\uparrow\downarrow} \rangle_{01}).
\]
The momentum distribution in the HB scheme is given by
\[
\langle n_{k\sigma} \rangle_0 = \int f(\epsilon) \rho_{k\sigma}(\epsilon) d\epsilon ,
\]
(27)

\[
\rho_{k\sigma}(\epsilon) = -\frac{1}{\pi} \text{Im} F_{k\sigma} ,
\]
(28)

\[
F_{k\sigma} = \frac{1}{z - \Sigma_{\sigma}(z) - \epsilon_k} .
\]
(29)

Here \(\epsilon_k\) is the eigen value of \(t_{ij}\) with momentum \(k\).

3. Local-_ansatz + Hybrid Wavefunction Approach with Momentum Dependent Variational Parameters

The momentum dependent local-ansatz (MLA) wavefunction is based on the local-ansatz (LA) proposed by Stollhoff and Fulde: \(|\Psi_{LA}\rangle = \left[ \prod_i (1 - \eta_{LA} O_i) \right] |\phi_{HF}\rangle\)\(^{6,8}\). Here \(O_i = \delta n_{i\uparrow} \delta n_{i\downarrow}\) are the residual interaction, the amplitude \(\eta_{LA}\) is determined variationally. The operators \(\{O_i\}\) expand the Hilbert space to describe the weak Coulomb interaction regime. The LA however does not yield the exact result in the weak interaction limit. The MLA wavefunction is constructed to describe exactly the weak limit as follows\(^{21,22}\):

\[
|\Psi_{MLA}\rangle = \prod_i (1 - \tilde{O}_i) |\phi_{HF}\rangle ,
\]
(30)

\[
\tilde{O}_i = \sum_{k_1'k_2'k_1k_2} \langle k_1'|i|k_1\rangle \langle k_2'|i|k_2\rangle \eta_{k_1'k_2'k_1k_2} \delta(a_{k_2'\sigma}^\dagger a_{k_1\sigma}) \delta(a_{k_1'\sigma}^\dagger a_{k_2\sigma}) .
\]
(31)

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 atomic position, and \(N\) is the number of sites. \(\eta_{k_1'k_2'k_1k_2}\) is a momentum dependent variational parameter. \(a_{k\sigma}^\dagger\) (\(a_{k\sigma}\)) denotes a creation (annihilation) operator for an electron with momentum \(\mathbf{k}\) and spin \(\sigma\), and \(\delta(a_{k'\sigma}^\dagger a_{k\sigma}) = a_{k'\sigma}^\dagger a_{k\sigma} - \langle a_{k'\sigma}^\dagger a_{k\sigma}\rangle\)\(_{HF}\). Note that the local operator \(\tilde{O}_i\) reduces to \(\eta_{LA} O_i\) when \(\eta_{k_1'k_2'k_1k_2} \rightarrow \eta_{LA}\). The best wavefunction is chosen by minimizing the energy with respect to the variational parameters in the momentum space.

In this work, we generalize the wavefunction (30) to be suitable in both the strong and the weak Coulomb interaction regime; we adopt the HB ground-state wavefunction \(|\phi_0\rangle\) for the Hamiltonian \(H_{HB}\) (4), and apply a new correlator \(\prod_i (1 - \tilde{O}_i)\) as follows.

\[
|\Psi_{MLA-HB}\rangle = \prod_i (1 - \tilde{O}_i) |\phi_0\rangle .
\]
(32)
Note that the local operators \{\tilde{O}_i\} have been modified as follows.

\[
\tilde{O}_i = \sum_{\kappa_2' \kappa_2 \kappa_1} \langle \kappa'_2 | i | \kappa_1 \rangle \langle \kappa'_2 | i | \kappa_2 \rangle \eta_{\kappa_2' \kappa_2 \kappa'_1 \kappa_1} \delta(a_{\kappa'_2}^{\dagger} a_{\kappa_2}) \delta(a_{\kappa'_1}^{\dagger} a_{\kappa_1}) \quad (33)
\]

Here \(\eta_{\kappa_2' \kappa_2 \kappa'_1 \kappa_1}\) is a variational parameter, \(a_{\kappa}^{\dagger}\) and \(a_{\kappa}\) are the creation and annihilation operators which diagonalize the Hamiltonian \(H_{\text{HB}}\) \((4)\), and \(\delta(a_{\kappa}^{\dagger} a_{\kappa}) = a_{\kappa}^{\dagger} a_{\kappa} - \langle a_{\kappa}^{\dagger} a_{\kappa} \rangle_0\). It should be noted that the MLA-HB wavefunction \((32)\) reduces to the MLA-HF with the uniform potential \(U\langle n_{i-} \rangle_{\text{HF}}\) when the variational parameter \(w = 0\), and reduces to the MLA-AA with the random potential \(U n_{i-}\) when \(w = 1\). The MLA-HB wavefunction interpolates between the two wavefunctions.

The ground-state energy \(E\) satisfies the following inequality for any wavefunction \(|\Psi\rangle\).

\[
E \leq \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \langle H \rangle_{\text{HB}} + N \epsilon_c \quad (34)
\]

Here \(\langle H \rangle_{\text{HB}}\) denotes the energy for the HB wavefunction. \(\epsilon_c\) is the correlation energy per atom defined by

\[
N \epsilon_c = \frac{\langle \Psi | \tilde{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (35)
\]

with \(\tilde{H} = H - \langle H \rangle_{\text{HB}}\). Since it depends on the electron configuration \(\{n_{i\sigma}\}\) via the AA potential, we have to take into account the configurational average at the end. To determine the variational parameters, we minimize the ground-state energy.

It is not easy to calculate exactly the correlation energy with use of the HB wavefunction \((32)\). Therefore, we adopt here the single-site approximation (SSA). The average of \(\langle \tilde{A} \rangle\) of an operator \(\tilde{A} = A - \langle A \rangle_0\) with respect to the wavefunction \((32)\) is then given as follows.

\[
\langle \tilde{A} \rangle = \sum_i \frac{\langle (1 - \tilde{O}_i^{\dagger}) \tilde{A} (1 - \tilde{O}_i) \rangle_0}{\langle (1 - \tilde{O}_i^{\dagger}) (1 - \tilde{O}_i) \rangle_0} \quad (36)
\]

The detailed derivation of the above formula has been given in Appendix A of our paper.\(^{21}\) Making use of the above formula, the correlation energy per atom is obtained as follows.

\[
\epsilon_c = \frac{-\langle \tilde{O}_i^{\dagger} \tilde{H} \rangle_0 - \langle \tilde{H} \tilde{O}_i \rangle_0 + \langle \tilde{O}_i^{\dagger} \tilde{H} \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0} \quad (37)
\]

Each term in the correlation energy \((37)\) can be calculated by making use of Wick’s
Here $\tilde{f}$ is a fermi factor of two-particle excitations which is defined by $\tilde{f} = f(\epsilon_{\alpha\sigma})(1 - f(\epsilon_{\alpha\sigma}))(1 - f(\epsilon_{\alpha\sigma}^\dagger))$, $f(\epsilon)$ is the Fermi distribution function at zero temperature, $\epsilon_{\alpha\sigma} = \epsilon_{\alpha\sigma} - \mu$, and $\epsilon_{\alpha\sigma}^\dagger$ is the one-electron energy eigen value for the HB Hamiltonian. Moreover, $\Delta E_{\kappa_2'\kappa_4'\kappa_1} = \epsilon_{\kappa_2'} - \epsilon_{\kappa_4'} + \epsilon_{\kappa_1'} - \epsilon_{\kappa_1}$ is a two-particle excitation energy.

The above expressions (38) and (41) contain nonlocal terms via summation over $j$ ($i.e., \sum_j$). We thus make additional SSA that we only take into account the local term ($j = i$), so that $\langle \tilde{H}\tilde{O}_i \rangle_0 ( = \langle \tilde{O}_i^\dagger \tilde{H} \rangle_0^*$ and $\langle \tilde{O}_i^\dagger \tilde{H}\tilde{O}_i \rangle_0$ reduce as follows.

$$\langle \tilde{H}\tilde{O}_i \rangle_0 = U \sum_{\kappa'_2\kappa_2'\kappa_1} |\langle \kappa'_1|i \rangle|^2 |\langle \kappa_1|i \rangle|^2 |\langle \kappa'_2|i \rangle|^2 |\langle \kappa_2|i \rangle|^2 \eta_{\kappa'_2\kappa_4\kappa'_1} \tilde{f}_{\kappa_2\kappa_2'\kappa_1}$$ (43)

$$\langle \tilde{O}_i^\dagger \tilde{H}\tilde{O}_i \rangle_0 = \sum_{\kappa'_2\kappa_2'\kappa_1} |\langle \kappa'_1|i \rangle|^2 |\langle \kappa_1|i \rangle|^2 |\langle \kappa'_2|i \rangle|^2 |\langle \kappa_2|i \rangle|^2 \eta_{\kappa'_2\kappa_4\kappa'_1} \tilde{f}_{\kappa_2\kappa_2'\kappa_1} \left[ \Delta E_{\kappa_2'\kappa_4'\kappa_1} \eta_{\kappa_2'\kappa_4\kappa_1} + U \sum_{\kappa_3\kappa_4} |\langle \kappa_3|i \rangle|^2 |\langle \kappa_4|i \rangle|^2 f(\epsilon_{\kappa_3}) f(\epsilon_{\kappa_4}) \eta_{\kappa_2'\kappa_4'\kappa_1} \right]$$ (44)
In order to obtain the variational parameters \( \{ \eta_{n_2}^{\prime} \} \), we minimize the correlation energy \( \epsilon_c \), i.e., eq. (37) with eqs. (42), (43), and (44). The self-consistent equations for \( \{ \eta_{n_2}^{\prime} \} \) in the SSA are given as follows.

\[
(\Delta E_{n_2} - \epsilon_c) \eta_{n_2} + U \left[ \sum_{k_3, n_1} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 f(\bar{\epsilon}_{n_3}^{\prime}) f(\bar{\epsilon}_{n_1}^{\prime}) \eta_{n_2, n_1, n_1} \right.
\]
\[
- \sum_{k_3, n_1} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 (1 - f(\bar{\epsilon}_{n_3}^{\prime})) f(\bar{\epsilon}_{n_1}^{\prime}) \eta_{n_2, n_1, n_1} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \]
\[
- \sum_{k_3, n_1} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 f(\bar{\epsilon}_{n_3}^{\prime}) (1 - f(\bar{\epsilon}_{n_1}^{\prime})) \eta_{n_2, n_1, n_1} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \]
\[
+ \sum_{k_3, n_1} |\langle \kappa_3 | i \rangle|^2 |\langle \kappa_4 | i \rangle|^2 (1 - f(\bar{\epsilon}_{n_3}^{\prime})) (1 - f(\bar{\epsilon}_{n_1}^{\prime})) \eta_{n_2, n_1, n_1} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \eta_{n_2, n_1, n_1}^{\prime} \]
\[
] = U . \quad (45)
\]

It is not easy to find the solution of eq. (45) for the intermediate strength of Coulomb interaction \( U \). To solve the equation approximately, we make use of an interpolate solution which is valid in both the weak Coulomb interaction limit and the atomic limit. Note that the first term at the left hand side (lhs) of eq. (45) is dominant and the second term is negligible in the weak Coulomb interaction limit. In the atomic limit, the momentum dependence of \( \eta_{n_2}^{\prime} \) is negligible. Thus, we approximate \( \{ \eta_{n_2}^{\prime} \} \) in the second term at the lhs of eq. (45) with a momentum independent parameter \( \eta \) which is suitable for the atomic region. Solving the equation, we obtain

\[
\eta_{n_2} = \frac{U \tilde{\eta}}{\Delta E_{n_2} - \epsilon_c} . \quad (46)
\]

Here \( \tilde{\eta} = [1 - \eta (1 - 2 \langle n_{i\uparrow} \rangle_0) (1 - 2 \langle n_{i\downarrow} \rangle_0)] . \)

The ground-state correlation energy is obtained by substituting the variational parameters (46) into eq. (37). Each element in the energy is given as follows.

\[
\langle \tilde{H} \tilde{O}_i \rangle_0 = \langle \tilde{O}_i^{\dagger} \tilde{H} \rangle_0 = AU^2 \tilde{\eta} , \quad (47)
\]
\[
\langle \tilde{O}_i^{\dagger} \tilde{H} \tilde{O}_i \rangle_0 = BU^2 \eta^2 = \langle \tilde{O}_i^{\dagger} \tilde{H}_0 \tilde{O}_i \rangle_0 + U \langle \tilde{O}_i^{\dagger} \tilde{O}_i \rangle_0 \tilde{\eta} , \quad (48)
\]
\[
\langle \tilde{O}_i^{\dagger} \tilde{H}_0 \tilde{O}_i \rangle_0 = B_1 U^2 \tilde{\eta}^2 , \quad (49)
\]
\begin{equation}
\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 = B_2 U^2 \eta^2 ,
\end{equation}
\begin{equation}
\langle \hat{O}_i^\dagger \hat{O}_i \rangle_0 = C U^2 \eta^2 .
\end{equation}

Here
\begin{equation}
A = \int \left[ \prod_{n=1}^{4} \frac{d\epsilon_n}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_C} \rho^\dagger_1(\epsilon_1)\rho_2(\epsilon_2)\rho_3(\epsilon_3)\rho_4(\epsilon_4) f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4)) \right],
\end{equation}
\begin{equation}
B = B_1 + U B_2 ,
\end{equation}
\begin{equation}
B_1 = \int \left[ \prod_{n=1}^{4} \frac{d\epsilon_n}{(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_C)^{-1}(\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_C)^2} \rho^\dagger_1(\epsilon_1)\rho_2(\epsilon_2)\rho_3(\epsilon_3)\rho_4(\epsilon_4) f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4)) \right],
\end{equation}
\begin{equation}
B_2 = \int \left[ \prod_{n=1}^{4} \frac{d\epsilon_n}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_C} \rho^\dagger_1(\epsilon_1)\rho_2(\epsilon_2)\rho_3(\epsilon_3)\rho_4(\epsilon_4) f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4)) \right] \times \left[ \int \frac{d\epsilon_5 d\epsilon_6 \rho^\dagger_1(\epsilon_5)\rho_3(\epsilon_6)f(\epsilon_5)f(\epsilon_6)}{\epsilon_4 - \epsilon_6 + \epsilon_2 - \epsilon_5 - \epsilon_C} - \int \frac{d\epsilon_5 d\epsilon_6 \rho^\dagger_1(\epsilon_5)\rho_3(\epsilon_6)f(\epsilon_5)(1 - f(\epsilon_6))}{\epsilon_6 - \epsilon_3 + \epsilon_2 - \epsilon_5 - \epsilon_C} \\
- \int \frac{d\epsilon_5 d\epsilon_6 \rho^\dagger_1(\epsilon_5)\rho_3(\epsilon_6)(1 - f(\epsilon_5))f(\epsilon_6)}{\epsilon_4 - \epsilon_6 + \epsilon_5 - \epsilon_1 - \epsilon_C} + \int \frac{d\epsilon_5 d\epsilon_6 \rho^\dagger_1(\epsilon_5)\rho_3(\epsilon_6)(1 - f(\epsilon_5))(1 - f(\epsilon_6))}{\epsilon_6 - \epsilon_3 + \epsilon_5 - \epsilon_1 - \epsilon_C} \right],
\end{equation}
\begin{equation}
C = \int \left[ \prod_{n=1}^{4} \frac{d\epsilon_n}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_C^2} \rho^\dagger_1(\epsilon_1)\rho_2(\epsilon_2)\rho_3(\epsilon_3)\rho_4(\epsilon_4) f(\epsilon_1)(1 - f(\epsilon_2))f(\epsilon_3)(1 - f(\epsilon_4)) \right].
\end{equation}

Here \( \rho_\sigma(\epsilon) \) is the local DOS for the one-electron energy eigen values of the HB Hamiltonian matrix (9).

The best value of \( \tilde{\eta} \) should be determined variationally. Indeed, when we adopt the approximate form (46) as a trial set of amplitudes, we have a following inequality
\begin{equation}
E \leq \langle H \rangle \langle w \{ \eta_{\kappa}\kappa^\prime_{\kappa} \} \rangle \leq \langle H \rangle \langle w \{ \eta_{\kappa}\kappa^\prime_{\kappa} \rangle \tilde{\eta}, \epsilon_c \} \rangle .
\end{equation}

Here \( \{ \eta_{\kappa}\kappa^\prime_{\kappa} \} \) are the exact solution for the eq. (45). The above relation implies that the best value of \( \tilde{\eta} \) is again determined from the stationary condition \( i.e., \delta \epsilon_c = 0 \), so that we obtain
\begin{equation}
\tilde{\eta} = -\frac{B + \sqrt{B^2 + 4A^2CU^2}}{2ACU^2} .
\end{equation}

The total energy per atom should be obtained by taking the configurational average.
\begin{equation}
\langle H \rangle = \langle H \rangle_{HB} + \epsilon_c .
\end{equation}
The HB contribution $\langle H \rangle_{\text{HB}}$ has been given by eq. (6). The correlation energy can be obtained as follows.

$$\bar{\epsilon}_c = \sum_\alpha P_\alpha \epsilon_{ca},$$

(60)

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

$$\epsilon_{ca} = \frac{[\langle \tilde{O}_i \tilde{H} \rangle_0 - \langle \tilde{H} \tilde{O}_i \rangle_0 + \langle \tilde{O}_i \tilde{H} \tilde{O}_i \rangle_0]}{1 + \langle \tilde{O}_i \tilde{O}_i \rangle_0}.$$

(61)

The quantities $\langle \tilde{H} \tilde{O}_i \rangle_0$, $\langle \tilde{O}_i \tilde{H} \tilde{O}_i \rangle_0$, and $\langle \tilde{O}_i \tilde{O}_i \rangle_0$ are given by eqs. (47), (48), and (51), respectively, in which the local DOS have been replaced by those of the single-site CPA, i.e., eq. (22).

The double occupation number $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ is obtained from $\partial \langle H \rangle / \partial U_i$. Making use of the single-site energy (37), the Feynman-Hellmann theorem$^{27}$ and taking the configurational average, we obtain the following expression.

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} + \langle n_{i\uparrow} n_{i\downarrow} \rangle_c,$$

(62)

Here the HB contribution of the double occupancy $\langle n_{i\uparrow} n_{i\downarrow} \rangle_c$ has been given by eq. (25). The second term is the correlation contribution given as follows.

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle_c = \sum_\alpha P_\alpha \langle n_{i\uparrow} n_{i\downarrow} \rangle_{ca},$$

(63)

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle_{ca} = \frac{[\langle \tilde{O}_i O_i \rangle_0 - \langle O_i \tilde{O}_i \rangle_0 + \langle \tilde{O}_i O_i \tilde{O}_i \rangle_0 + \sum_\sigma \langle n_{i-\sigma} \rangle_0 \langle \tilde{O}_i \tilde{n}_{i\sigma} \tilde{O}_i \rangle_0]}{1 + \langle \tilde{O}_i \tilde{O}_i \rangle_0},$$

(64)

$$\langle \tilde{O}_i O_i \rangle_0 + \langle O_i \tilde{O}_i \rangle_0 = 2U \tilde{\eta} \int \left[ \prod_{n=1}^4 d\epsilon_n \right] \rho_\uparrow(\epsilon_1) \rho_\uparrow(\epsilon_2) \rho_\downarrow(\epsilon_3) \rho_\downarrow(\epsilon_4) \times f(\epsilon_1)(1 - f(\epsilon_2)) f(\epsilon_3)(1 - f(\epsilon_4))$$

$$\times \frac{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c},$$

(65)

$$\langle \tilde{O}_i \tilde{n}_{i\sigma} \tilde{O}_i \rangle_0 = U^2 \tilde{\eta}^2 \int \left[ \prod_{n=1}^5 d\epsilon_n \right] \rho_{-\sigma}(\epsilon_1) \rho_{-\sigma}(\epsilon_2) \rho_\sigma(\epsilon_3) \rho_\sigma(\epsilon_4) \rho_\sigma(\epsilon_5) \times f(\epsilon_1)(1 - f(\epsilon_2)) f(\epsilon_3)(1 - f(\epsilon_4))$$

$$\times \frac{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c}{\epsilon_4 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c} \times \left[ \frac{1 - f(\epsilon_5)}{\epsilon_5 - \epsilon_3 + \epsilon_2 - \epsilon_1 - \epsilon_c} - \frac{f(\epsilon_5)}{\epsilon_4 - \epsilon_5 + \epsilon_2 - \epsilon_1 - \epsilon_c} \right].$$

(66)

The quantities $\langle \tilde{O}_i O_i \tilde{O}_i \rangle_0$ and $\langle \tilde{O}_i \tilde{O}_i \rangle_0$ are defined by eqs. (50) and (51), respectively.
Similarly, the momentum distribution $\langle n_{k\sigma} \rangle$ is obtained from $\partial \langle H \rangle / \partial \epsilon_k$ as follows.

$$\langle n_{k\sigma} \rangle = \langle n_{k\sigma} \rangle_0 + \langle n_{k\sigma} \rangle_c.$$  \hfill (67)

The HB contribution of the momentum distribution $\langle n_{k\sigma} \rangle_0$ has been given by eq. (27). The correlation contribution $\langle n_{k\sigma} \rangle_c$ is expressed as follows.

$$\langle n_{k\sigma} \rangle_c = \sum_\alpha P_\alpha \langle n_{k\sigma} \rangle_{c\alpha},$$  \hfill (68)

$$N\langle \tilde{\mathcal{O}}^\dagger_i \tilde{n}_{k\sigma} \tilde{O}_i \rangle_0 = U^2 \eta^2 \int \prod_{n=1}^4 d\epsilon_n \rho_\sigma(\epsilon_1)\rho_{-\sigma}(\epsilon_2)\rho_{-\sigma}(\epsilon_3)\rho_{k\sigma}(\epsilon_4)f(\epsilon_2)(1-f(\epsilon_3))$$

$$\times \left\{ \frac{f(\epsilon_1)(1-f(\epsilon_4))}{(\epsilon_3-\epsilon_2+\epsilon_4-\epsilon_1-\epsilon_c)^2} - \frac{(1-f(\epsilon_1))f(\epsilon_4)}{(\epsilon_3-\epsilon_2+\epsilon_1-\epsilon_4-\epsilon_c)^2} \right\}. \hfill (70)$$

Here $\tilde{n}_{k\sigma} = n_{k\sigma} - \langle n_{k\sigma} \rangle_0$. The DOS in the momentum representation $\rho_{k\sigma}(\epsilon)$ has been given by eq. (28) in the SSA. The correlation contribution quantity $\langle \tilde{\mathcal{O}}^\dagger_i \tilde{\mathcal{O}}_i \rangle_0$ is given by eq. (51).

The expressions of these physical quantities are given by the multiple integrals up to the 6-folds. One can reduce these integrals up to the 2-folds using the Laplace transform.\textsuperscript{28) Their expressions are given in Appendix B.}

In summary, we calculate the correlation energy $\epsilon_{c\alpha}$ (eq. (61)) self-consistently with use of eqs. (47), (48), (51), and (58) for a given weight $w$, and calculate the average correlation energy $\bar{\epsilon}_c$ (eq. (60)) as well as the average HB energy $\langle H \rangle_{HB}$ (eq. (6)). Then we obtain the total energy $\langle H \rangle(w)$ (eq. (59)) for a given $w$. Varying $w$ from 0 to 1 numerically, we obtain the ground-state energy $\langle H \rangle$. We call this scheme the MLA-HB, while the simplified scheme in §2 the HB.

4. **Numerical Results: Half-filled band Hubbard Model**

We have performed the numerical calculations to investigate the validity of momentum dependent local-ansatz approach (MLA) with hybrid (HB) variational wavefunction (i.e., MLA-HB). We adopted here the half-filled band Hubbard model on the hyper-cubic lattice in infinite dimensions, where the SSA works best,\textsuperscript{29,30} and considered the non-magnetic case. In this case, the density of states (DOS) for non-interacting system is given by $\rho(\epsilon) = (1/\sqrt{\pi}) \exp(-\epsilon^2)$.\textsuperscript{29} The energy unit is chosen to be $\int d\epsilon \rho(\epsilon) \epsilon^2 = 1/2$. The characteristic band width $W$ is given by $W = 2$ in this unit.
We calculated the energy for given variational parameter $w$ by minimizing it with respect to the variational parameter $\tilde{\eta}$ self-consistently. Figure 1 shows the calculated energy vs $w$ curves for various Coulomb interactions, $U = 1, 2, \text{ and } 3$. In the HB scheme (without correlator) for $U = 1$, the energy increases monotonically with increasing $w$. Therefore the Fermi liquid HF state ($w = 0$) is stabilized as the ground state. When we increase the $U$ value, the HF energy continues to increase, while the random-potential states with $w \neq 0$, which is driven by the AA potential, are relatively stabilized. Such a random-potential state remains even at $w = \varepsilon$ as shown in the dashed curve $U = 2$, where $\varepsilon$ is the infinitesimal positive number. It is caused by the HF-type self-consistent random potentials and is accompanied by the disordered local moments.\textsuperscript{31,32} When we further increase $U$, the AA state ($w = 1$) is more stabilized (see the dashed curve $U = 3$), so that we find the first-order transition at $U = 2.31$, and the insulating state is realized. We also find the similar behavior for the MLA-HB, in which the transition takes place at $U = 2.81$. However it should be noted that the transition occurs between the Fermi liquid state ($w = 0$) and the disordered local moment state ($w = \varepsilon$) in the case of the MLA-HB; we found numerically that the latter ($w = \varepsilon$) remains stable as compared with the AA state ($w = 1$) even if we increase further the Coulomb interaction strength $U$.

The results of the ground-state energy vs Coulomb interaction energy curves are
Fig. 2. The energy vs Coulomb interaction energy $U$ curves in the HB (dashed curve), the MLA-HB (solid curve), the GW (dot-dashed curve) and the LA (dotted curve) for the electron number $n = 1.0$. The energy of the HB wavefunction linearly increases with increasing Coulomb interaction strength $U$ in the weak $U$ regime. At $U_{c0} = 1.43$, the system shows a transition from the Fermi liquid (FL) state ($w = 0$) to a non-Fermi liquid (NFL) state ($w \neq 0$), and shows a kink at the critical Coulomb interaction $U_c = 2.31$, indicating the metal-insulator transition. The transition is of the first order in the present approach. The HB wavefunction gives lower energy in comparison with the GW and the LA in the strong Coulomb interaction regime ($U/W \gtrsim 1.5$). The MLA-HB wavefunction further lowers the energy. In the weak Coulomb interaction regime, the ground-state energy of the MLA-HB is the lowest among the HB, LA, GW, and the MLA-HB. The MLA-HB shows the first-order transition at $U_c = 2.81$ from the FL to the NFL, indicating the metal-insulator transition. The MLA-HB scheme gives lower energy for overall Coulomb interaction and therefore overcomes the GW.

Figure 3 shows the double occupation number $\langle n_\uparrow n_\downarrow \rangle$ as a function of Coulomb interaction energy $U$ at half-filling. In the case of the HB, the double occupancy is constant (1/4) up to $U_{c0} = 1.43$, and decreases rapidly up to the critical point $U_c = 2.31$, at which it jumps from 0.110 to 0.060. In the strong Coulomb interaction regime the double occupancy decreases with increasing $U$ and vanishes in the atomic limit. In the case of the MLA-HB, the double occupation number decreases smoothly from 1/4 with increasing Coulomb interaction so as to reduce the loss of Coulomb energy $U$. Note
Fig. 3. The double occupation number $\langle n_\uparrow n_\downarrow \rangle$ vs Coulomb interaction energy $U$ curves at half-filling ($n = 1.0$) in the HB (dashed curve), the MLA-HB (solid curve), the GW (dot-dashed curve), and the LA (dotted curve).

that the MLA-HB reduces more the double occupancy as compared with that of the HB, GW and the LA in the weak $U$ region. The double occupancy in the MLA-HB jumps from 0.106 to 0.045 at the transition point $U_c = 2.81$, and 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.

The momentum distribution for the MLA-HB is shown in Fig. 4. It decreases monotonically with increasing $\epsilon_{k\sigma} (= \epsilon_0 - \mu + \epsilon_k)$ and shows a jump at the Fermi energy in the metallic regime. The jump decreases with increasing $U$, and disappears beyond $U_c$. When we further increase the Coulomb interaction $U$ the curve becomes flatter. Note that the momentum distributions for the GW are constant below and above the Fermi level.\textsuperscript{3-5} These results indicate that the MLA-HB improves the GW.

The quasiparticle weight $Z$ (\textit{i.e.}, inverse effective mass) is obtained from the jump at the Fermi level in the momentum distribution according to the Fermi liquid theory.\textsuperscript{33,34} Calculated quasiparticle weight vs Coulomb interaction curves are shown in Fig. 5. The GW and the LA curves strongly deviate from the curve of the NRG\textsuperscript{35} which is considered to be the best. The MLA-HB is close to the NRG in the metallic regime, and vanishes beyond $U_c = 2.81$. It should be noted that the NRG\textsuperscript{35} also shows the first-
Fig. 4. 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.

Fig. 5. Quasiparticle-weight vs. Coulomb interaction curves in various theories. The MLA-HB: solid curve, the GW: dot-dashed, the LA: dotted curve, and the NRG: dashed curve.\textsuperscript{35)}

order transition at a critical Coulomb interaction $U_c$ before $Z$ vanishes at $U_{c2} = 4.1$. The values of $U_c$ in the NRG, however, has not yet been published.
5. Summary and Discussions

We have proposed a new hybrid (HB) wavefunction and combined it with the momentum dependent local-ansatz approach MLA \(i.e.,\) the MLA-HB) to describe the correlated electron system from the weak to the strong Coulomb interaction regime. The HB wavefunction as a starting wavefunction is the ground-state for the HB Hamiltonian. The latter was constructed as a superposition of the Hartree-Fock (HF) Hamiltonian and the alloy-analogy (AA) one. The weight \(w\) of superposition is regarded as a variational parameter. When we adopt \(w = 0\), the HB wavefunction reduces to the HF (AA) state. In the MLA-HB, the best wavefunction is chosen by controlling the momentum dependent variational parameters for the two-particle excited states as well as the HB parameter \(w\). We obtained the ground-state energy of the MLA-HB within a single-site approximation, and derived an approximate solution for the self-consistent equations of the variational parameters which interpolates between the weak Coulomb interaction limit and the atomic limit.

To examine the improvement and validity of the theory, we have performed the numerical calculations for the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions. In case of the HB wavefunction we clarified that the ground-state energy increases linearly in the weak \(U\) regime and it shows a lower energy as compared with the GW and the LA in the strong \(U\) regime. The double occupation number is constant up to the \(U = 1.43\) \(i.e.,\) \(\langle n_1 n_\uparrow \rangle_{\text{HB}} = 0.25\) and then decreases rapidly to the critical value \(U_c = 2.31\) where the first-order metal-insulator transition occurs. In the strong \(U\) regime the \(\langle n_1 n_\uparrow \rangle_{\text{HB}}\) remains finite.

We have demonstrated that the ground-state energy of the MLA-HB is lower than that of the HB, GW and the LA in the whole Coulomb interaction regime. In the weak and intermediate Coulomb interaction regimes, the double occupation number is suppressed as compared with the others. It jumps at \(U_c = 2.81\) and remains finite in the strongly correlated regime as it should be. The momentum distribution functions show a distinct momentum dependence in both the weak and the strong \(U\) regimes. Moreover, we found that the behavior of the quasiparticle weight is close to the NRG one. The above mentioned results indicate that the MLA-HB approach overcomes the limitations of the original MLA,\(^{21,22}\) and describes reasonably correlated electrons from the weak to the strong Coulomb interaction regime, so that it goes beyond the GW in the whole Coulomb interaction \(U\) regime. Although advanced theories based on the QMC and the...
NRG have been developed, the MLA-HB approach presented in this work is applicable to more complex systems and allows us to calculate any static averages with use of the wavefunction. Further developments of the MLA wavefunction approach should provide us with a useful tool for understanding the properties of correlated electrons and their physics in the realistic systems.

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Appendix A: Derivation of $P_2$

In the derivation of the hybrid (HB) Hamiltonian we made the following approximations for the alloy-analogy (AA) and the Hartree-Fock (HF) Hamiltonians, respectively.

\[ \hat{n}_\uparrow \hat{n}_\downarrow \approx \hat{n}_\uparrow \hat{n}_\downarrow + \hat{n}_\downarrow \hat{n}_\uparrow + n_\downarrow \bar{n}_\uparrow - n_\uparrow \bar{n}_\downarrow \quad \text{(AA)}, \]

\[ \hat{n}_\uparrow \hat{n}_\downarrow \approx \hat{n}_\uparrow \langle \hat{n}_\downarrow \rangle + \hat{n}_\downarrow \langle \hat{n}_\uparrow \rangle - \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle \quad \text{(HF)}. \]

In the HB scheme, we approximate the averages $\langle \sim \rangle$ at the rhs of the above expressions with those of the HB Hamiltonian (4), and superpose them with the weight $w$ and $(1 - w)$, respectively. Taking the the quantum mechanical average of the superposed double occupation number as well as the configurational average, we obtain the probability of the double occupation $P_2 \ (= \langle n_\uparrow n_\downarrow \rangle)$ in the HB approximation as follows.

\[ P_2 = \frac{1}{2} \left[ (w n_\uparrow + (1 - w) \langle n_\uparrow \rangle) \langle n_\downarrow \rangle + (w n_\downarrow + (1 - w) \langle n_\downarrow \rangle) \langle n_\uparrow \rangle \right] \]

\[ = \frac{1}{2} w \langle n_\uparrow \rangle \langle n_\downarrow \rangle + \frac{1}{2} w \langle n_\downarrow \rangle \langle n_\uparrow \rangle + (1 - w) \langle n_\uparrow \rangle \langle n_\downarrow \rangle. \quad \text{(A\cdot3)} \]

The last term at the rhs of eq. (A\cdot3) may be regarded as the probability $P_2$. Therefore, we obtain

\[ P_2 \approx \frac{1}{2} \left[ (w n_\uparrow + (1 - w) \langle n_\uparrow \rangle) \langle n_\downarrow \rangle + (w n_\downarrow + (1 - w) \langle n_\downarrow \rangle) \langle n_\uparrow \rangle \right] \]

\[ = \frac{1}{2} \left[ \sum_{\alpha} P_{\alpha} \langle n_\uparrow \rangle_{\alpha} \langle n_\downarrow \rangle_{\alpha} \right] = P_0 \langle n_\uparrow \rangle_{00} \langle n_\downarrow \rangle_{00} + P_{1\uparrow} \langle n_\uparrow \rangle_{10} \langle n_\downarrow \rangle_{10} + P_{1\downarrow} \langle n_\uparrow \rangle_{01} \langle n_\downarrow \rangle_{01} + P_2 \langle n_\uparrow \rangle_{11} \langle n_\downarrow \rangle_{11}. \quad \text{(A\cdot4)} \]

In the single-site approximation, the last term of the rhs is expressed as follows.

\[ \langle n_\uparrow \rangle \langle n_\downarrow \rangle = \sum_{\alpha} P_{\alpha} \langle n_\uparrow \rangle_{\alpha} \langle n_\downarrow \rangle_{\alpha} \]

\[ = P_0 \langle n_\uparrow \rangle_{00} \langle n_\downarrow \rangle_{00} + P_{1\uparrow} \langle n_\uparrow \rangle_{10} \langle n_\downarrow \rangle_{10} + P_{1\downarrow} \langle n_\uparrow \rangle_{01} \langle n_\downarrow \rangle_{01} + P_2 \langle n_\uparrow \rangle_{11} \langle n_\downarrow \rangle_{11}. \]
Appendix B: Laplace Transform for 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.

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

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

Laplace transforms of the physical quantities (47)-(51) are given as follows.

\[
A_\alpha = i \int_0^\infty dt \, e^{i\epsilon_\alpha t} a_\alpha^\dagger(-t)a_\alpha(-t)b_\alpha^\dagger(t)b_\alpha(t),
\] (B.2)

\[
B_{1\alpha} = -\int_0^\infty dt \, dt' \, e^{i\epsilon_\alpha (t+t')}
\times [a_\alpha^\dagger(-t-t')b_\alpha^\dagger(t+t')a_\alpha(-t-t')b_\alpha(t+t')
- a_\alpha^\dagger(-t-t')b_\alpha^\dagger(-t-t')a_\alpha(-t-t')b_\alpha(t+t')
+ a_\alpha^\dagger(-t-t')b_\alpha^\dagger(-t-t')a_\alpha(-t-t')b_\alpha(t+t')
- a_\alpha^\dagger(-t-t')b_\alpha^\dagger(t+t')a_\alpha(-t-t')b_\alpha(t+t')],
\] (B.3)

\[
B_{2\alpha} = -\int_0^\infty dt \, dt' \, e^{i\epsilon_\alpha (t+t')}
\times [a_\alpha^\dagger(-t)b_\alpha^\dagger(t+t')a_\alpha(-t)b_\alpha(t+t')a_\alpha^\dagger(-t-t')a_\alpha(-t')
- a_\alpha^\dagger(-t)b_\alpha^\dagger(t+t')a_\alpha(-t)b_\alpha(t)\alpha^\dagger(-t-t')b_\alpha(t')
- a_\alpha^\dagger(-t-t')b_\alpha^\dagger(t)a_\alpha(-t)b_\alpha(t)\alpha^\dagger(t')a_\alpha(-t')
+ a_\alpha^\dagger(-t-t')b_\alpha^\dagger(t)a_\alpha(-t)b_\alpha(t)\alpha^\dagger(t')b_\alpha(t')],
\] (B.4)
\[
C_\alpha = - \int_0^\infty dt dt' e^{i\epsilon_0 (t+t')} a_{\alpha \uparrow}(-t-t') b_{\alpha \uparrow}(t+t') a_{\alpha \downarrow}(-t-t') b_{\alpha \downarrow}(t+t').
\] (B.5)

Here \( \alpha \) denotes the local electron configuration (\( \alpha = 0, 1 \uparrow, 1 \downarrow, 2 \)), and

\[
a_{\alpha \sigma}(t) = \int d\epsilon \, \rho_\sigma^\alpha(\epsilon) f(\epsilon) e^{-i\epsilon t},
\] (B.6)

\[
b_{\alpha \sigma}(t) = \int d\epsilon \, \rho_\sigma^\alpha(\epsilon)[1 - f(\epsilon)] e^{-i\epsilon t},
\] (B.7)

\[
a_{1\alpha \sigma}(t) = \int d\epsilon \, \rho_\sigma^\alpha(\epsilon) f(\epsilon) e^{-i\epsilon t},
\] (B.8)

\[
b_{1\alpha \sigma}(t) = \int d\epsilon \, \rho_\sigma^\alpha(\epsilon)[1 - f(\epsilon)] e^{-i\epsilon t}.
\] (B.9)

The element (65) for the calculation of the double occupancy is expressed as

\[
\langle \tilde{O}^\dagger_i O_i \rangle_{0\alpha} + \langle O_i \tilde{O}^\dagger_i \rangle_{0\alpha} = 2iU\tilde{n}_\alpha \int_0^\infty dt \, e^{i\epsilon_0 t} a_{\alpha \uparrow}(-t)b_{\alpha \uparrow}(t)a_{\alpha \downarrow}(-t)b_{\alpha \downarrow}(t).
\] (B.10)

The correlation contribution to the electron number (66) which appears in the calculation of the double occupation number is expressed as

\[
\langle \tilde{O}^\dagger_i \tilde{n}_{i\sigma} \tilde{O}^\dagger_i \rangle_{0\alpha} = -U^2\tilde{n}_\alpha^2 \int_0^\infty dt dt' e^{i\epsilon_0 (t+t')}
\times \left[ a_{\alpha(-\sigma)}(-t-t')b_{\alpha(-\sigma)}(t+t') a_{\alpha\sigma}(-t-t')b_{\alpha\sigma}(t') \
- a_{\alpha(-\sigma)}(-t-t')b_{\alpha(-\sigma)}(t+t') a_{\alpha\sigma}(-t-t')b_{\alpha\sigma}(t') \right].
\] (B.11)

The correlation contribution to the momentum distribution function (70) is given by

\[
N\langle \tilde{O}^\dagger_i \tilde{\kappa}_{\sigma} \tilde{O}^\dagger_i \rangle_{0\alpha} = U^2\tilde{n}_\alpha^2 \int_0^\infty dt dt' e^{i\epsilon_0 (t+t')}
\times \left[ b_{\alpha\sigma}(t+t') a_{\kappa\sigma}(-t-t') - a_{\alpha\sigma}(-t-t')b_{\kappa\sigma}(t+t') \right].
\] (B.12)

Here

\[
a_{\kappa\sigma}(t) = \int d\epsilon \, \rho_{\kappa\sigma}(\epsilon) f(\epsilon) e^{-i\epsilon t},
\] (B.13)

\[
b_{\kappa\sigma}(t) = \int d\epsilon \, \rho_{\kappa\sigma}(\epsilon)[1 - f(\epsilon)] e^{-i\epsilon t}.
\] (B.14)
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