Momentum-Dependent Variational Approach to Correlated Electron System

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Abstract. We present here the momentum dependent local-ansatz wavefunction approach (MLA) with the best choice of the self-consistent variational parameters to describe the ground-state properties of the correlated electron systems in solids. With use of the self-consistent variational scheme, we performed the numerical calculations for the half-filled band as well as non-half-filled band Hubbard model on the hypercubic lattice in infinite dimensions. The ground-state energy in the MLA is lower than those of the local-ansatz approach (LA) and the Gutzwiller approach (GA) in weak and intermediate Coulomb interaction regimes. The double occupation number is suppressed as compared with the LA. We observe the distinct momentum dependence of the momentum distribution functions which is qualitatively different from those of the LA and the GA.

The variational theory has been developed to describe the ground state properties of correlated electron system in solids [1]. To characterize the correlated electrons in the variational approach a minimum basis set is constructed by applying one-particle, two-particle, and higher-order particle operators onto the Hartree-Fock wavefunction. In principle, their amplitudes are chosen to be best. Gutzwiller [2, 3, 4] described a simple trial wavefunction to clarify the role of electron correlations in metallic ferromagnetism. It reduces the amplitudes of doubly occupied states on the local orbitals by making use of a projection operator \( \Pi_i(1 - \delta n_i^{\uparrow} \delta n_i^{\downarrow}) \) onto the Hartree-Fock wavefunction \( |\phi_0\rangle \); \( |\Psi_{GA}\rangle = \prod_i(1 - \delta n_i^{\uparrow} \delta n_i^{\downarrow}) |\phi_0\rangle \). Here \( n_{i\sigma} \) is the number operator for electrons on site \( i \) with spin \( \sigma \), variational parameter \( g \) controls the double occupations on sites.

Stollhoff and Fulde [5, 6, 7] proposed a method called the local-ansatz approach (LA), which is simpler than the GA in treatment. The LA wavefunction takes into account the states created by local two-particle operators such as the residual Coulomb interactions \( \{O_i\} = \{ \delta n_i^{\uparrow} \delta n_i^{\downarrow} \} \); \( |\Psi_{LA}\rangle = \prod_i(1 - \eta_{LA}(O_i)) |\phi_0\rangle \). Here \( \delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma}\rangle_0 \), \( \langle n_{i\sigma}\rangle_0 \) being the average electron number on site \( i \) with spin \( \sigma \) in the Hartree-Fock approximation. The amplitudes \( \eta_{LA} \) is determined variationally.

The Hilbert space of the LA expanded by the local operators \( \{O_i\} \) is not sufficient to characterize exactly the weakly correlated region; it does not reduce to the second-order perturbation theory in the weak Coulomb interaction limit. The same difficulty arises also in the GA. To overcome the difficulty in the weak Coulomb interaction regime and to improve the correlated states in the intermediate Coulomb interaction regime, we introduce in this paper a wavefunction with momentum-dependent variational parameters, and demonstrate that the
new approach much improves the LA as well as the GA in those regimes. We call our new scheme the momentum-dependent local ansatz approach (MLA).

To introduce the MLA wavefunction, we expand the wavefunction with respect to the Coulomb interaction strength. We find that each coefficient of the two-particle excited states is momentum independent. In order to obtain the best local operators, we replace the momentum-dependent variational parameters with the momentum dependent variational parameters resulting in a new set of local operators \( \{ O_i \} \). That is, we define the local operators \( O_i \) with the momentum-dependent variational parameter \( \eta_{k_1'k_2'k_1k_2} \) as follows:

\[
\tilde{O}_i = \sum_{k_1k_1'k_2k_2'} \langle k_1' | i \rangle \langle i | k_1 \rangle \langle k_2' | i \rangle \langle i | k_2 \rangle \eta_{k_2'k_2k_1'k_1} \delta (a_{k_2}^\dagger a_{k_2'}) \delta (a_{k_1'}^\dagger a_{k_1}) .
\] (1)

Here \( \langle i | k \rangle = \exp(-ik \cdot R_i) / \sqrt{N} \) is an overlap integral between the localized orbital and the Bloch state with momentum \( k \), \( R_i \) denotes the atomic position, and \( N \) is the number of sites. \( a_{k\sigma}^\dagger \) (\( a_{k\sigma} \)) denotes the creation (annihilation) operator for an electron with momentum \( k \) and spin \( \sigma \), and \( \delta (a_{k\sigma}^\dagger a_{k\sigma}) = a_{k\sigma}^\dagger a_{k\sigma} - \delta (a_{k\sigma}^\dagger a_{k\sigma}) \). We then construct the MLA wavefunction from the flexible set of local operators \( \{ \tilde{O}_i \} \) as

\[
| \Psi_{MLA} \rangle = \prod_i (1 - \tilde{O}_i) | \phi_0 \rangle .
\] (2)

The best local basis set is chosen by controlling the variational parameters in the momentum space, which leads to the best wavefunction.

We calculate the ground-state energy using the MLA wavefunction within a single-site approximation (SSA) \[8\]. The correlation energy per atom is then given by

\[
\epsilon_c = - \langle \tilde{O}_i^\dagger \hat{H} \rangle_0 - \langle \hat{H} \tilde{O}_i \rangle_0 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0 .
\] (3)

Here \( \hat{H} = H - \langle H \rangle_0 \). Minimizing the energy, we obtain a self-consistent equation with variational parameters. It is difficult to solve the self-consistent equation exactly. Because of this, we obtained an approximate solution as follows, which interpolates between the weak Coulomb interaction limit and the atomic limit.

\[
\eta_{k_2'k_2k_1'k_1} (\tilde{\eta}, \epsilon_c) = \frac{U \tilde{\eta}}{\Delta E_{k_2'k_2k_1'k_1} - \epsilon_c} .
\] (4)

Here \( \tilde{\eta} = [1 - \eta (1 - 2 \langle n_{i\uparrow} \rangle) / (1 - 2 \langle n_{i\uparrow} \rangle)] \), the two-particle excitation energy \( \Delta E_{k_2'k_2k_1'k_1} \) is given by :

\[
\Delta E_{k_2'k_2k_1'k_1} = \epsilon_{k_2'} - \epsilon_{k_2} + \epsilon_{k_1'} - \epsilon_{k_1} .
\] (5)

In the preliminary version of our theory \[8\], we made use of the variational parameter in the LA: \( \eta_{LA} = [1 - \eta_{LA} (1 - 2 \langle n_{i\uparrow} \rangle) / (1 - 2 \langle n_{i\uparrow} \rangle)] \) where \( \eta_{LA} \) is the variational parameter in the LA and for simplicity we might also adopt the correlation energy in the LA for \( \epsilon_c \) in Eq. (4). In this paper we determine \( \tilde{\eta} \) variationally. According to the variational principle, the ground-state energy \( E_0 \) satisfies the following inequality:

\[
| E_0 | \leq E(\{ \eta_{k_2'k_2k_1'k_1} \}) \leq E(\{ \eta_{k_2'k_2k_1'k_1} (\tilde{\eta}, \epsilon_c) \}) .
\] (6)

The above relation implies that the best \( \tilde{\eta} \) is again determined from the stationary condition of the trial energy \( E(\{ \eta_{k_2'k_2k_1'k_1} (\tilde{\eta}, \epsilon_c) \}) \). Because \( \epsilon_c \) should satisfy the stationary condition \( \delta \epsilon_c = 0 \) for the value \( \tilde{\eta}^* \), \( \tilde{\eta}^* \) is determined by the following condition

\[
\left[ \frac{\partial \epsilon_c (\{ \eta_{k_2'k_2k_1'k_1} (\tilde{\eta}, \epsilon_c) \})}{\partial \tilde{\eta}} \right]_{\epsilon_c} = 0 .
\] (7)
Therefore, we obtained the solution choosing the best variational parameter $\tilde{\eta}$ using the above variational scheme.

To verify the validity of the MLA, we have performed the numerical calculations for the half-filled band as well as non-half-filled band ($n = 0.6, 0.8$) in the Hubbard model [9, 10, 11] on the hypercubic lattice in infinite dimensions where the SSA works best [12]. In this case, the density of states (DOS) for non-interacting system is given by $\rho(\epsilon) = (1/\sqrt{\pi}) \exp(-\epsilon^2)$ [13]. The energy unit is chosen to be $\int d\epsilon \rho(\epsilon) \epsilon^2 = 1/2$.

We present in Fig. 1 the results of correlation energy per atom vs Coulomb interaction $U$. We observe that, the correlation energy for the MLA is lower than that of the LA over all Coulomb interaction energy parameters $U$ irrespective of electron number. Thus the MLA improves the LA. Note that, with increasing $U$ the correlation corrections increase as $U^2$ for small $U$ and cancel the Hartree-Fock energy loss being linear in $U$ for large $U$. Therefore, the magnitude

**Figure 1.** The correlation energies $E_c$ vs. Coulomb interaction energy parameter $U$ for electron number $n = 1.0, 0.8, 0.6$ in the MLA (solid curve) and the LA (dotted curve).

**Figure 2.** The energy vs. Coulomb interaction energy $U$ curves in the MLA (solid curve), LA (dotted curve), and the GA (thin solid curve) for electron number $n = 1.0$.

**Figure 3.** 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) for electron number $n = 1.0, 0.8, 0.6$.

**Figure 4.** The momentum distribution as a function of energy $\epsilon_k$ for various Coulomb interaction energy parameters $U$ with electron number $n = 0.8$. The MLA: solid curves, the LA: dotted curve.
of the correlation energy $|\epsilon_c|$ tends to increase with increasing $U$. The ground state energy vs Coulomb interaction energy $U$ curves for half-filling case are shown in Fig. 2. We observe that the energy for the MLA is lower than those of the LA and the GA in the weak and intermediate Coulomb interaction regimes $U$.

Figure 3 shows the double occupation number $\langle n_{\uparrow}n_{\downarrow} \rangle$ as a function of Coulomb interaction energy $U$ for the half-filled and the non-half-filled cases ($n = 0.8, 0.6$). The double occupancy is the same for both LA and MLA in the uncorrelated limit. In order to reduce the loss of Coulomb energy, the double occupancy decreases with increasing Coulomb interaction $U$. We find that the MLA wavefunction more reduces the double occupancy as compared with that of the LA.

We have also investigated the momentum-distribution functions which are shown in Fig 4. It shows a qualitative change between the LA and the MLA; the distribution functions in the LA are constant below and above the Fermi level irrespective of $U$, while the MLA curves show a monotonical decrease of the distribution with increasing $\epsilon_k$. It indicates a distinct momentum dependence of $\langle n_{k\sigma} \rangle$ via energy $\epsilon_k$, which is qualitatively different from both the LA and the GA.

In summary, we have presented the variational scheme of the MLA which self-consistently determines both the variational amplitude $\tilde{\eta}$ and the correlation energy $\epsilon_c$, making use of variational principles. We demonstrated that the theory much improves the standard variational methods such as the LA and the GA in the weak and intermediate regimes. The correlation energy as well as the ground-state energy in the MLA is lower than both the LA and the GA in those regimes. The double occupation number is suppressed as compared with the LA. Especially, we find that calculated momentum distribution functions show a distinct momentum dependence, which is qualitatively different from those of the LA and the GA.

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