相関電子系における運動量依存局所変分理論の研究

Form 3

論 文 要 旨
Abstract

論文題目

Title Theoretical Study of Momentum Dependent Local-Ansatz Variational Approach to Correlated Electron System. (相関電子系における運動量依存局所変分理論の研究)

We propose in this thesis a local-ansatz wavefunction approach with momentum dependent variational parameters (momentum-dependent local-ansatz = MLA) in order to describe correlated electrons in the ground state. The idea is to choose the best local basis set obtained from the two-particle excited states in the momentum representation by projecting out those states onto the local subspace and by controlling the amplitudes of the excited states in the momentum space. Within a single-site approximation we calculate the ground-state energy and derive a self-consistent equation for the variational parameters by minimizing the energy. We obtain an approximate solution which interpolates between the weak Coulomb interaction limit and the atomic limit. We further developed the theory to obtain the best value of the variational parameter self-consistently.

In order to verify the validity of the MLA, we perform the numerical calculations for the non-half-filled band as well as half-filled band in the Hubbard model on the hypercubic lattice in infinite dimensions. We confirm that the self-consistent scheme significantly improves the correlation energy, the momentum distribution and quasiparticle weight. We also demonstrate that the theory improves the standard variational methods such as the local-ansatz approach (LA) and the Gutzwiller wavefunction approach (GW); the ground-state energy in the MLA is lower than those of the LA and the GW in the weak and intermediate Coulomb interaction regimes. The double occupation number is shown to be suppressed as compared with the LA. Calculated momentum distribution functions show a clear momentum dependence, which is qualitatively different from those of the LA and the GW. We also obtained the critical Coulomb interaction $U_{c2} = 3.40$ at which effective mass of electrons diverges. The value is comparable to the best value $U_{c2} = 4.10$ based on the numerical renormalization group method.

We propose an improved MLA wavefunction which can describe the strong Coulomb interaction regime by modifying the starting wavefunction from the Hartree-Fock (HF) type to an alloy-analogy (AA) type wavefunction. Numerical results based on the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions show that the MLA-AA wavefunction yields the ground-state energy lower than the GW in the strong Coulomb interaction regime. The MLA-AA yields the metal-insulator transition at $U_c = 3.26$. Calculated double occupation number is smaller than the result of the GW in the metallic regime, and is finite in the insulator regime as it should be, while the GW gives the Brinkman-Rice atom. Furthermore, the momentum distribution of MLA-AA shows a momentum-dependence in both the metallic and insulator regions, on the other hand the GW as well as the LA gives the constant value below and above the Fermi level.

Finally, we generalize the variational theory of the MLA by introducing a hybrid (HB) wavefunction as a starting wavefunction, whose potential can flexibly change from the HF type to the AA type by varying a weighting factor from zero to one. The MLA-HB scheme yields the ground-state energy lower than that of the GW in the whole Coulomb interaction regime, and shows the first-order transition at $U_c = 2.81$ from the Fermi liquid to the non-Fermi liquid, indicating the metal-insulator transition. The MLA-HB reduces the double occupancy more effectively than the GW and the LA in the weak U region. The resulting double occupancy jumps at the transition point $U_c = 2.81$, and again monotonically decreases with increasing U. Finally the momentum distribution of MLA-HB shows a distinct momentum dependence, which is qualitatively different from that of the GW.

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