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Momentum-dependent local ansatz approach to correlated electrons YOSHIRO KAKEHASHI, SUMAL CHANDRA, Dept of Physics and Earth Sciences, University of the Ryukyus, M. ATIQUR R. PATOARY, Department of Physics, University of Rajshahi — Variational approach has been a simple and useful tool to describe the ground state of correlated electrons in solids, and many methods as well as wavefunctions for electron correlations have been proposed. Although the numerical methods such as the variational Monte-Carlo can quantitatively describe the correlations in the low dimensional system, the description of the real 3D system based on the wavefunction method has not yet been established well. We present here the momentum-dependent local ansatz approach (MLA) to the correlated electron system. The wavefunction consists of the two-particle excitation operators with momentum-dependent variational parameters, which are projected onto local orbitals, and a hybrid wavefunction which interpolates between the Hartree-Fock and the Hubbard alloy-analogy wavefunctions. On the basis of the numerical calculations in infinite dimensions, we demonstrate that the analytic MLA improves the Gutzwiller method in both the weak and strong interaction regimes, and that the MLA is applicable to the realistic systems with use of the 1st-principles LDA+U Hamiltonian.

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