Theory of Momentum-Dependent Variational Ansatz to Correlated Electron Systems

Univ. of the Ryukyus        Md. Atiquur Rahman Patoary, Y. Kakehashi

We have recently proposed a Momentum dependent Local-Ansatz wavefunction approach (MLA) [1, 2] to describe the correlated electron system in the weak and intermediate Coulomb interaction regime $U$. Since we started from the Hartree-Fock (HF) wavefunction there, the theory did not work best in the strong $U$ regime. In order to overcome the difficulty, we propose here a new hybrid wavefunction in which the starting wavefunction can vary via a new variational parameter $w$ from the HF wavefunction ($w=0$) suitable for the weak interaction regime to the alloy-analogy (AA) wavefunction ($w=1$) suitable in the strong interaction regime. The present method overcomes the Gutzwiller wavefunction approach (GA) irrespective of $U$. In fact, figure 1 shows the result of the total energy vs $U$ curves for the MLA-HF ($w=0$), MLA-AA ($w=1$) for the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions. We observe that the energy for the MLA-AA ($w=1$) is lower than those of the MLA-HF ($w=0$) in the strong $U$ region. Moreover, the energy of the MLA ($w=0$ and 1) is always lower than the GA. We also discuss the double occupation number, quasi-particle weight and momentum distribution function in comparison with the LA and GA.

![Figure 1: The energy vs. Coulomb interaction energy parameter $U$ curves in the MLA-AA (solid curve), the MLA-HF (dashed curve), and the GA (thin solid curve).](image)