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First-principles momentum-dependent local ansatz approach to correlated electron system YOSHIRO KAKEHASHI, SUMAL CHANDRA, Dept. of Physics and Earth Sciences, University of the Ryukyus — In spite of a great success of the density functional theory (DFT), quantitative description of correlated electron systems has not yet been achieved because of the difficulty in improvement of exchange-correlation potential. Toward the quantitative description of correlated electrons, we recently proposed the momentum-dependent local ansatz approach (MLA) based on the wavefunction method [1]. The theory describes exactly the weak Coulomb interaction regime, and goes beyond the Gutzwiller wavefunction method in both the weak and strong interaction regimes. We present here the first principles version of the MLA, which is obtained by combining the LDA+U Hamiltonian with the MLA. We demonstrate that the theory describes quantitatively the Hund-rule correlation energies, the charge fluctuations, the amplitudes of local moments, the momentum distribution functions, as well as the mass enhancement factors in iron-group transition metals. The DFT does not describe these quantities because it is based on the Hohenberg-Kohn theorem and the Kohn-Sham independent-electron scheme. [1] Y. Kakehashi et. al., JPSJ 82, 084710 (2013); 85, 064714 (2016).

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