# First-Principles Momentum Dependent Local-Ansatz Approach to Correlated Electrons: Case of Iron

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Many methods have been proposed to describe electron correlations in transitions metals. Among them variational approach has been a simple and useful tool to describe the ground state properties. Although the numerical methods such as the variational Monte-Carlo can quantitatively explain the correlations in the low dimensional system, the first-principles method based on the real wavefunction has not been established well for the 3 dimensional system. The momentum dependent local ansatz approach (MLA) improves the Gutzwiller method in both the weak and strong interaction regimes [1]. In this work, we present a first-principles theory of the MLA combined with the tight-binding LDA+U Hamiltonian, and report numerical results of correlation energy, charge fluctuations, amplitude of magnetic moments, as well as quasipartical weight of bcc Fe in the lowest order [2]. Electron correlations increase the correlation energy in magnitude, suppress the charge fluctuations for d electrons, and enhance the amplitude of local moment. Figure 1 shows the charge fluctuations vs Coulomb interaction strength curve for bcc Fe. The Hartree-Fock value is $2.2$. With increasing Coulomb interaction strength the intra-orbital correlations suppress the fluctuations and yields $\langle(\delta n_{id})^2\rangle = 1.6$ for $\alpha U_0 = 0.27$ Ry. The inter-orbital correlations decrease further the fluctuations. We find $\langle(\delta n_{id})^2\rangle \approx 1.2$ for $\alpha U_0 = 0.27$ Ry, showing strong suppression of the charge fluctuations in bcc Fe.

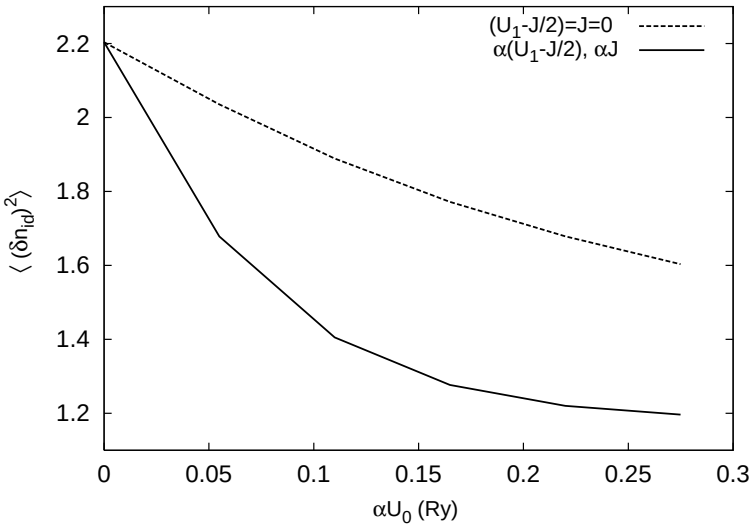


Figure 1: The charge fluctuations $\langle(\delta n_{id})^2\rangle$ vs Coulomb interaction strength $\alpha U_0$ curve for the bcc Fe. Dashed curve: with the intra-orbital correlations, solid curve: with both the intra- and inter-orbital correlations.

## References

[1] Y. Kakehashi, S. Chandra, D. Rowlands, and M. Atiqur R. Patoary, Mod. Phys. Lett. B Vol. 28 (2014) 1430007.

[2] S. Chandra and Y. Kakehashi, arXiv:1508.01998 [cond-mat.str-el] (2015).