Non-Local Dynamical CPA in Itinerant Electron System

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Quantitative explanation of the finite-temperature properties of 3d transition metals such as the Curie (Néel) temperatures and susceptibilities has been a long standing problem in the theory of magnetism because their Coulomb interactions are comparable to the band widths and simple perturbation approach is not applicable to such systems. According to the recent calculations of Fe and Co based on the first-principles dynamical CPA theory their Curie temperatures are reported to be 1.8 times higher than the experimental values [1]. One needs to take into account the long-range electron correlations characteristic of the metallic magnetism. Therefore, we formulated the non-local dynamical CPA by taking into account the long-range non-local electron correlations on the basis of incremental cluster expansion. In this theory we introduce the non-local off-diagonal effective medium $\Sigma_{ij}(i\omega)$ as shown in Fig.1, and calculate the effective potential $E^{(c)}_{\text{eff}}(\xi)$ in effective medium. We expand the residual self-energy into single-site clusters, two-sites clusters, three-sites ones, and so on. Next we calculate cluster matrices $\langle T^{(c)} \rangle$ by making use of functional derivative, and obtain the cluster self-energy. We finally calculate crystalline self-energy $\Lambda_{ij}$. In this way we can self-consistently determine the non-local effective medium as well as non-local self-energy. We present some numerical results for the 3D Hubbard model on the fcc lattice within the static approximation, and discuss non-local effects on the Curie temperature.

![Figure 1: Self-consistent loop of non-local dynamical CPA theory.](image)

[1] Y. Kakehashi et.al., JPSJ 77, 094706 (’08); 78, 093705 (’09); PRB 81 245133 (’10); JPSJ 80 034706 (’11); PRB 83 144409 (’11).