The combination method of the dynamical mean field theory with the first principle electronic structure theory

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1. INTRODUCTION

Beyond LDA (Local Density Approximation)

Combination of LDA and Ligand field theory by DMFT

LDA
One electron spectrum

DMFT (Dynamical mean field theory)
Treatment for on site electron correlation

\[ \left[ \xi(\omega) \right] \sim \xi(\omega) \]

Ligand field theory
Many particle spectrum,
Treatment for arbitrary electron occupation

2. FORMULATION

LDA

\[ g_{0}(\omega) = \frac{1}{\pi} \int \frac{\omega d\omega}{E_{F}(\omega)} \]

DMFT

\[ g_{0}(\omega) = \frac{1}{\pi} \int \frac{\omega d\omega}{E_{F}(\omega)} \]

Ligand field theory

\[ g_{0}(\omega) = \frac{1}{\pi} \int \frac{\omega d\omega}{E_{F}(\omega)} \]

3. NUMERICAL RESULTS

\[ U=1.0 : \text{Peaks at the Fermi energy strongly depend on } k \text{ and the spectrum becomes sharper rapidly near the Fermi energy.} \]

\[ U=2.0 : \text{Peaks at the Fermi energy hardly depend on } k \text{. Coherent peaks appear.} \]

\[ U=3.0 : \text{The spectrum splits into upper and lower Hubbard bands.} \]

Fig.1 (up): The imaginary part of the k-dependent Green's function G(k,\omega) (shaded regions) of d-bands on a simple cubic lattice. The energy bands (\epsilon(k)) shifted by \pm U/2 at high symmetry lines are also shown. The high symmetry k-points are \( M(\pi/2,\pi/2,0), X(\pi/2,0,0), \Gamma(0,0,0), R(\pi/2,\pi/2,\pi/2) \). The inverse temperature \( \beta=30 \). Red and green shades represent \( g_{0}(\omega) \) and \( g_{2}(\omega) \) of the diagonalized k-dependent Green's function matrix, respectively.

\[ g_{0}(\omega) = \frac{1}{\pi} \int \frac{\omega d\omega}{E_{F}(\omega)} \]

The spectra simultaneously show the electron ionization and affinity levels of different electron occupations, coherent peaks at the Fermi energy in the metallic phase and a gap at an integer filling of electrons for sufficiently large Coulomb U.

Fig.3 (up): The electron occupation dependence of the imaginary part of the local Green's functions for \( t_{2g} \) bands on a simple cubic lattice of the half band width \( \Delta = 1 \) and the inverse temperature \( \beta = 30 \). The numbers in the figure denote the electron occupation per each orbital.

In the metallic side of the critical region one can observe a sharp coherent peak at \( \omega = 0 \). The critical \( U/D \) ratio is different between \( t_{2g} \) and \( e_{g} \) bands. In the insulating case, the band width is shrinking more at the same \( U/D \) ratio for \( t_{2g} \) bands than that is for \( e_{g} \) bands. This is because that the self-energy is much larger for \( t_{2g} \) bands than for \( e_{g} \) bands for the same \( U/D \) value due to the degree of the degeneracy with respect to spins and orbitals. On the contrary, the critical \( U/D \) ratio for \( t_{2g} \) bands on bcc is larger than that for \( e_{g} \) bands. This is because that the off-diagonal elements of Hamiltonian are non-zero for \( t_{2g} \) bands on bcc and this makes more hopping between different orbitals. On the other hand, those are always zero for \( e_{g} \) bands on sc.

Fig.2 (up): The imaginary part of the local Green's functions in a half-filled case \( n = 0.5 \).
(a) \( t_{2g} \) bands on a simple cubic lattice of half band width \( \Delta = 7/6 \).
(b) \( e_{g} \) bands on a simple cubic lattice of the half band width \( \Delta = 1 \). The inverse temperature \( \beta = 30 \).

4. CONCLUSION

We have generalized the combination method of LDA and ligand field theory by DMFT. We have had success of spectrum calculation in arbitrary electron occupation cases and the spectrum simultaneously shows the effects of ligand field structure and DMFT. The effects of exchange interaction \( J \) is important in the sense that \( J \) extends the spectral region and mixes many configurations.

Fig.4 (up): The imaginary part of the local Green's functions for paramagnetic bcc Fe. The inverse temperature \( \beta = 30 \).