(PS1)

**Band calculation for f-electron compounds on the basis of DMFT method**

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We formulated the DMFT band calculation of the combination of the LMTO and the NCA methods. As a first step, it is applied to the $\gamma$- and $\alpha$- Ce. The calculation includes the spin orbit interaction, which is important in actual situation, but has not been included in the preceding studies. In the DMFT method, the local spectrum obtained by the band calculation including the self-energy and the spectrum obtained by the effective single site problem should agree as the self-consistency condition(SC condition).

At the starting, the usual LDA band calculation is carried out, then the trial c-f hybridization of f-state is calculated from it. We found that the electron self-energy originated from the f-f Coulomb interaction is usually about 100 times larger than the self-energy of the hybridization in the effective single impurity calculation, except the energy region very near the Fermi energy. In the $\gamma$-Ce case, the trial hybridization estimated from the LDA band calculation usually satisfy the SC condition when one imposes the accuracy of 20%. (The maximum difference of the both spectra occurs in the sharply increasing region of the peak at the Fermi energy, not in the peak region. The difference of 20% seem to be not so serious, and it is very hard to improve the accuracy further.) In the $\alpha$-Ce case, several iteration is needed to reach the SC condition. The effective c-f hybridization of $\alpha$-Ce is reduced near the Fermi energy from that of LDA band, but has small a small bump very near the Fermi energy. The effective Kondo temperature slightly decreases as the temperature decreases.

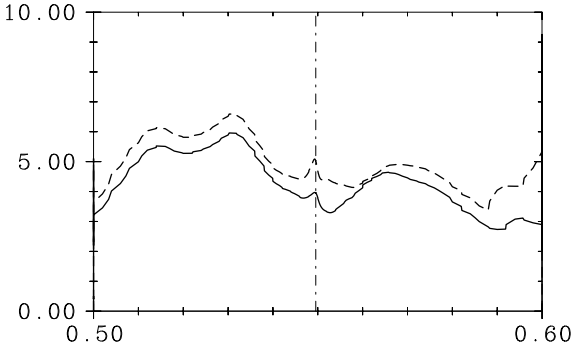


Figure 1: Effective hybridization very near the Fermi energy for $\alpha$-Ce at T=1.9D-3 Rydberg. The vertical dot-dashed line indicates the Fermi energy(0.5496Rydberg), and horizontal axis is the energy in Rydberg. The solid(dashed) line is the hybridization for j=5/2(j=7/2) component. Small bump appears at the Fermi energy in the SC process. The vertical axis is in $1\times10^{-3}$ Ryd

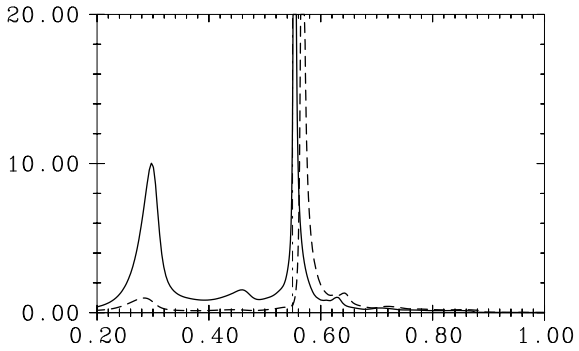


Figure 2: The single particle excitation spectra of $\alpha$-Ce. The horizontal axis is the energy in Rydberg, and other parameters are the same to those of Fig.1