(PS1)

Analysis of photoemission spectrum of Pr skutterudite by non-crossing approximation

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The resonant photoemission spectrum of f-electron in filled Pr skutterudite shows three peaks structure. In $PrFe_4P_{12}$ the intensity of the low energy excitation below 1eV from Fermi level becomes large in comparison with other Pr compounds [1, 2], however, the origin of this large intensity is not clear. We calculate the single particle excitation spectrum of impurity Anderson model for filled Pr skutterudite by using the non-crossing approximation (NCA). The multiplet states of Pr^{3+} ion ($^3H_4$,$^3H_5$ and $^3H_6$) and Pr^{4+} ion ($^2F_{5/2}$ and $^2F_{7/2}$) are taken into account. We find the resonance peak at the Fermi level with satellite structures from the excited states of multiplet in Pr^{3+}. Note that the final state of the satellite is $f^2\underline{v}^1$, where $\underline{v}^1$ means a hole in the valence band. The mechanism that the satellite appears is the same as that for spin-orbit partner of the Kondo resonance in CeB_6. The characteristic energy of the resonance peak depends on the strength of p-f hybridization and the energy difference between f^2 and f^1 states. It is expected that the intensity of the peak just below the Fermi level becomes large, if the characteristic energy of the resonance and the energy split of the multiplets in Pr^{3+} have the same order. We also find that the intensity of the resonant peak becomes large, when the partial DOS of p-band has a gap-like structure just above the Fermi level which is given by the band calculation for the filled skutterudite [3]. These two mechanisms become important in the analysis of photoemission spectrum in the filled Pr skutterudite.

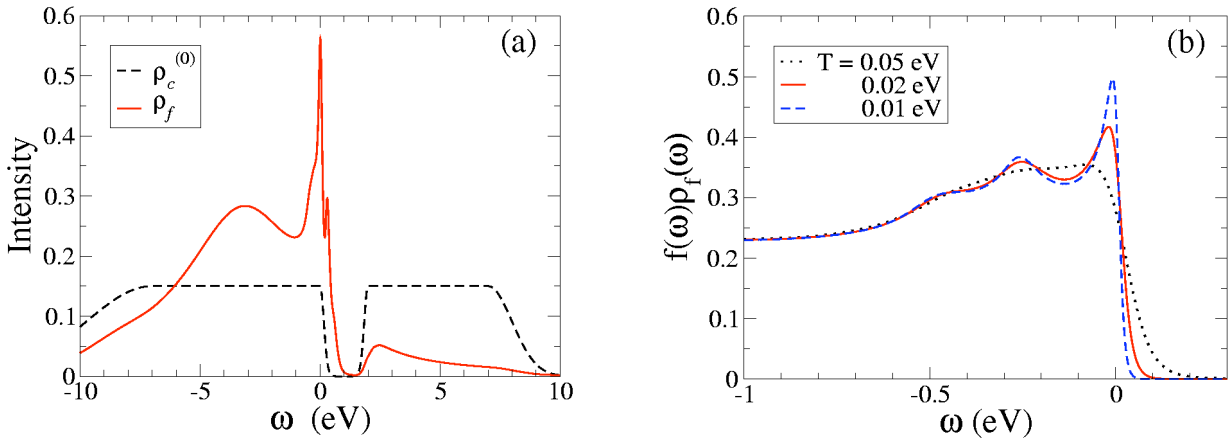

Figure 1: (a) Single particle excitation spectrum of f-electron (solid line) and the partial DOS of p-band (dashed line) which is employed by the NCA calculation. (b) The multiplet satellite structure of the resonance peak for various temperatures.

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