(28b5)

Hybridization and Kondo effects in Pr skutterudites

J. Otsuki, Y. Kuramoto and H. Kusunose

Department of Physics, Tohoku University, Sendai, 980-8578

Some Pr skutterudites such as $PrFe_4P_{12}$ and $PrOs_4Sb_{12}$ show a large coefficient of electronic specific heat, and antiferroquadrupole (AFQ) orders at low temperatures. In the case of $PrOs_4Sb_{12}$, the AFQ order sets in after the exotic superconductivity is destroyed by magnetic field. In order to identify the origin of heavy mass and superconductivity, the structure of crystalline-electric-field (CEF) levels are highly relevant. We discuss the following topics:
(i) We propose that the actual CEF level scheme can be reproduced only by combining the point-charge energy and the p-f hybridization. Namely, the increasing energy according to the scheme $\Gamma_1 - \Gamma_4^{(2)} - \Gamma_4^{(1)} - \Gamma_{23}$ can be understood by the combination.
(ii) We derive the dynamics of a f^2 model system that describes the contrasting limits of strong and weak hybridization. With strong hybridization, Kondo effect should take place for individual f electrons, which then acquire itinerant character. In the opposite limit of weak hybridization, f^2 dynamics is controlled mostly by CEF levels.

We take a simplified model to study the competition between CEF and Kondo effects by simulating the CEF singlet by a pair singlet of spin 1/2, and the CEF triplet by a pair triplet. Then the CEF splitting is simulated by the exchange energy I. In order to allow for a pair singlet, we introduce a fictitious $4f$ orbital index $\gamma = 1, 2$ with identical energy ϵ_f, which is negative. We allow for f^0, f^1 and f^2 configurations of which the f^2 energy is the lowest. The hybridization V and band width D are identical for both orbitals γ. We adopt the NCA for this model to derive dynamics and thermodynamics on equal footing. Some results are shown in the figure.

It is seen that at temperatures higher than $I = 30$K and comparable to the f^1 Kondo temperature $T_K \sim 70$K, the CEF splitting does not affect the Kondo peak in the density of states. At low temperatures, there depelops a pseudo-gap of about $2I$ around the Fermi level. The entropy increases toward $\log 4$ with smaller characteristic energy with smaller I. We are currently deriving the dynamical susceptibility and try to adopt a more realistic model.

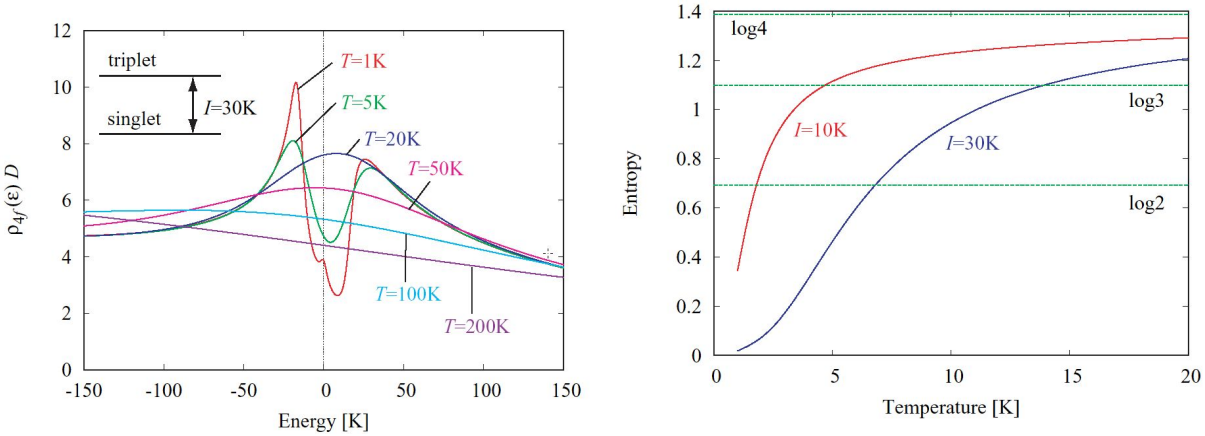

Figure 1: Density of states of 4f electrons (left), and the entropy (right) computed in the NCA. The parameters are: $\epsilon_f = -1200$K, $V^2\rho_c = 120$K, $D = 10^4$K.