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Theory of Crystalline Electric Field States and Kondo Effect in Pr Skutterudites

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Heavy fermion states have been observed in some Pr skutterudites such as $PrOs_4Sb_{12}$ and $PrFe_4P_{12}$. In the inelastic neutron scattering experiment of $PrFe_4P_{12}$, crystalline electric field (CEF) excited peak cannot be detected at temperature higher than the phase transition. It seems that Kondo effect is related to heavy mass in $PrFe_4P_{12}$, while the other mechanism will be relevant in $PrOs_4Sb_{12}$. CEF singlet ground state and low lying excited triplet states are proposed in such materials. We investigate the condition for the occurrence of Kondo effect.

We consider hybridization between CEF singlet-triplet system and conduction electrons with a_u symmetry [1]. We define the projection operator $P_{\rm t}$ and $P_{\rm s}$ onto triplet and singlet, respectively. Effective exchange interaction is written either in terms of $P_{\rm t,s}$ or pseudo-spin $\boldsymbol{S}$:

$$\begin{aligned} H_{\text{s-t}} &= \epsilon_{\rm t} P_{\rm t} + \epsilon_{\rm s} P_{\rm s} + \left(I_{\rm t} \boldsymbol{X}^{\rm t} + I_{\rm s} \boldsymbol{X}^{\rm s} \right) \cdot \boldsymbol{s}_c \\ &= \Delta_{\rm CEF} \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + (J_1 \boldsymbol{S}_1 + J_2 \boldsymbol{S}_2) \cdot \boldsymbol{s}_c, \end{aligned}$$

where $\boldsymbol{X}^{\rm t} = \boldsymbol{S}_1 + \boldsymbol{S}_2$ and $\boldsymbol{X}^{\rm s} = \boldsymbol{S}_1 - \boldsymbol{S}_2$ are operators act on the triplet and between singlet and triplet, respectively. $\Delta_{\rm CEF} = \epsilon_{\rm t} - \epsilon_{\rm s}$ is the CEF splitting. In the second order perturbation theory, coupling constant J_1 becomes ferromagnetic and J_2 antiferromagnetic if the triplet wave functions mainly consist of $|\Gamma_4\rangle$ in O_h. On the other hand, both exchange interactions can be negligible if the triplet is almost composed of $|\Gamma_5\rangle$ in O_h.

We derive the dynamics of quasi-quartet using the NCA. Figure 1 shows the magnetic spectral function with CEF singlet ground state and temperature dependence of magnetic relaxation rate. While only quasi-elastic peak can be seen at $T \gtrsim \Delta_{\rm CEF}$, CEF excited peak develops as temperature decreases below $\Delta_{\rm CEF}$. Correspondingly, magnetic relaxation rate varies from $T^{1/2}$-like behavior at $T \gtrsim \Delta_{\rm CEF}$ to rapid increase as temperature decreases below $\Delta_{\rm CEF}$. The decrease below about 5K is due to the inaccuracy of the NCA. In the case of $PrOs_4Sb_{12}$, there exist sharp CEF peak at whole temperatures because both J_1 and J_2 are small.

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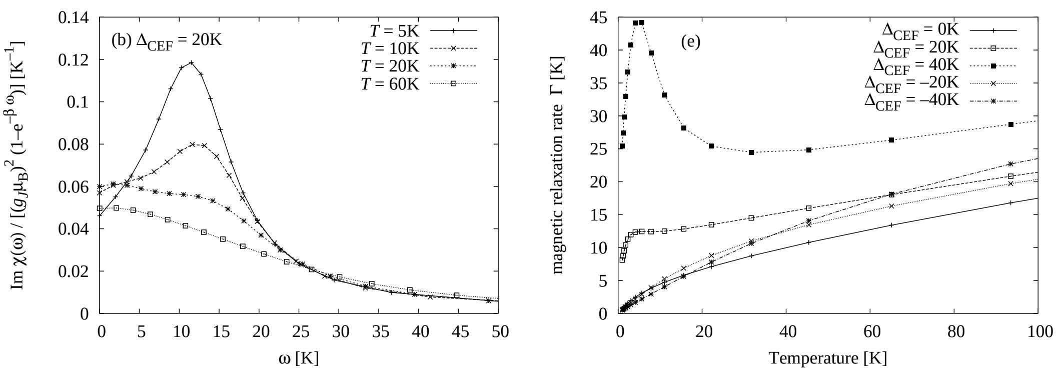

Figure 1: Magnetic spectral function (left) and magnetic relaxation rate (right) computed in the NCA. The parameters are $J_1 = 4000$K, $J_2 = 0$, and $D = 10^4$K.