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Systematic analysis on competition between Kondo and crystal field effect in Ce ion

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I report theoretical studies on the competition of the Kondo effect and the CEF of Ce³⁺ by using the NCA. The NCA can comparatively easily treat complicated CEF structures including the Kondo effect. Therefore, the NCA may be applied to comparisons with general experimantal results. However, systematic calculations of the magnetic specific heat have not been carried out because very careful numerical treatment is needed. Today, I deal with the magnetic specific heat, the static susceptibility, the one particle excited spectrum and the neutron inelastic scattering spectrum. In particular, I attach importance to the connection between the magnetic specific heat and the competition of the Kondo effect and the CEF. I use the one impurity N-fold degenerate Anderson model as the model Hamiltonian.

Firstly, I report theoretical calculations of the magnetic specific heat and the static susceptibility. For example, the result of specific heat is shown in Fig.1. This is equally spaced three doublets case. Two peaks appear when the splitting width becomes large. The low temperature side peak is due to the effective doublet Kondo effect and the high temperature side peak is due to the Schottky one.

Next, I apply the NCA calculation to comparisons with experimental results. Today, I target CePd₂Al₃ [1] and related compound Ce(Pd_{1-x}Cu_x)₂Al₃ [2][3]. This compound has the hexagonal symmetry CEF. Then six-fold multiplet splits into three doublets. The comparison of specific heat is shown in Fig.2. This is the x = 0.0 case. The calculated result agrees to the experimental one except for the sharp λ type peak caused by the magnetic phase transition.



Figure 1: Δ is splitting width and T_K^0 is the Figure 2: Δ_1 and Δ_2 are splitting width from Kondo temperature without the CEF. the ground multiplet. $\Delta_1 = 35K, \Delta_2 = 800K$

References

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