(28b4)

Influence of CEF structures to f^2-based heavy-fermion states

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It is widely believed that degeneracy of f orbitals and plural occupation of them are a key feature in understanding a fundamental nature of heavy-fermion states observed in Pr-based Skutterudite and U-based compounds. In the case of f^1-based heavy-fermion systems, a formation of a coherent quasiparticle band with decreasing temperature and its nature in connection with the concept of the Fermi liquid are well understood so far. On the contrary, it is still obscure how the structures of crystalline electric field (CEF) affect a character of heavy fermion states for the f^2-based systems. It is a non-trivial task to connect essentially many-body local wave function of the CEF with quasiparticles in a single-particle picture. Moreover, a simple perturbation theory from a non-interacting system may not work since it does not take into account the structure of the CEF properly.

Motivated by these situation, we discuss the influence of the CEF structures to the heavy-fermion state using the slave-boson mean-field technique. Using"j-j coupling" scheme under the point group, the CEF in f^2 configuration can be expressed with the linear combination of the direct product of the f^1 states. In the case of hexagonal symmetry for instance, we have

$$|\Gamma_5^{(1)}\pm\rangle = \pm\left[a|0\pm\pm\rangle + b\left\{\sqrt{\frac{5}{14}}|\pm 0\pm\rangle + \sqrt{\frac{9}{14}}|\mp\pm 0\rangle\right\}\right], \quad |\Gamma_4\rangle = -\frac{1}{\sqrt{2}}\Big[|++0\rangle + |--0\rangle\Big],$$

where $|\alpha\beta\gamma\rangle$ represents $|\Gamma_7\alpha\rangle\otimes|\Gamma_8\beta\rangle\otimes|\Gamma_9\gamma\rangle$. In the case of Γ_5 CEF ground state, all bands (Γ_{7-9}) are heavily renormalized, while in the case of Γ_4 ground state, Γ_9 becomes irrelevant in forming heavy quasiparticle bands (see Fig. 1). The ratio of f-electron occupations in each bands is determined by the probability of each f^1 state in the f^2 CEF ground state. In the latter, the quasiparticle susceptibility does not show any enhancement since Γ_4 state has no magnetic moment, $\langle\Gamma_4|M_z|\Gamma_4\rangle = 0$. We will discuss the result of Γ_1 ground state as well.

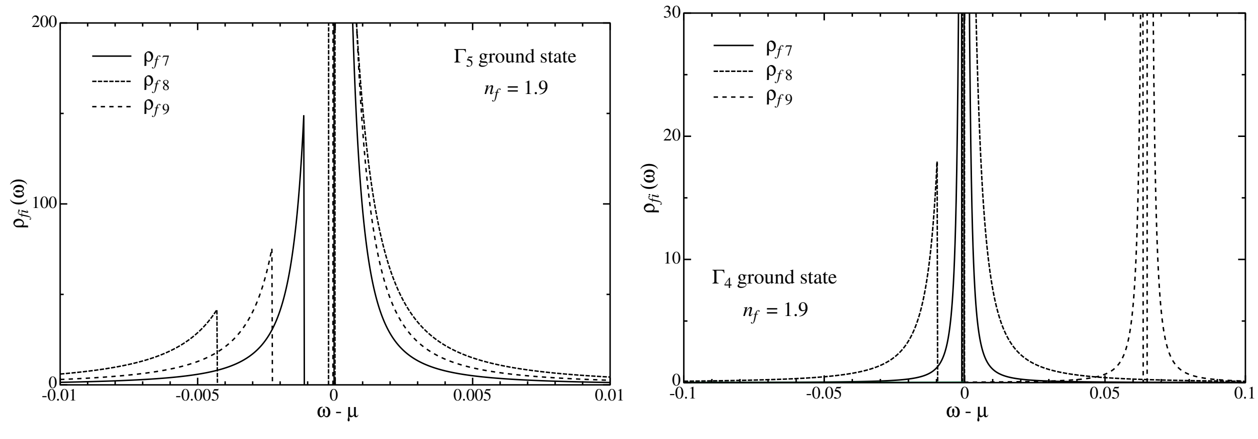

Figure 1: The quasiparticle density of states for Γ_5 and Γ_4 CEF ground states.