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Heavy Fermion State in the f^2 Anderson Lattice with Singlet-Triplet Crystal-Field Levels

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The crystal-field levels of the $Pr^{3+}(4f^2)$ ion in the filled skutterudite $PrOs_4Sb_{12}$ are considered to be the ground state Γ_1 singlet and the first excited state $\Gamma_4^{(2)}$ triplet with a small excitation energy $\sim$ 8K. To elucidate the effect of the crystal-field levels on the heavy fermion behavior, we study the two-orbital periodic Anderson model at half-filling where the average f-electron number per site is 2 [1]. The calculations are based on the dynamical mean-field theory where the effective impurity Anderson model is solved using the exact diagonalization method. The renormalization factor Z is obtained as a function of the intraorbital Coulomb interaction U, the interorbital Coulomb interaction U' (we set $U = U'$), the exchange (Hund's rule) coupling J and the crystal-field splitting Δ. In the absence of c-f hybridization $V_{cf} = 0$, the ionic ground state is triplet for $J > \Delta$, while it is intraorbital singlet for $|J| < \Delta$ and interorbital singlet for $J < -\Delta$. In the strong correlation regime with $V_{\rm cf} \neq 0$, the heavy fermion state with $m^*/m = Z^{-1} \gtrsim 100$ is realized for $|J| > \Delta$, while it is not realized for $|J| < \Delta$. When the singlet ground state and the triplet excited state form a quasi-quartet ($J \sim \Delta$), the system shows a moderate enhancement of the effective mass $m^*/m \sim 10 - 50$, which is consistent with the experimental observation in $PrOs_4Sb_{12}$.

[1] Y. Ōno and K. Mitsumoto: *Proceedings of SCES 2005*, Physica B (in press)

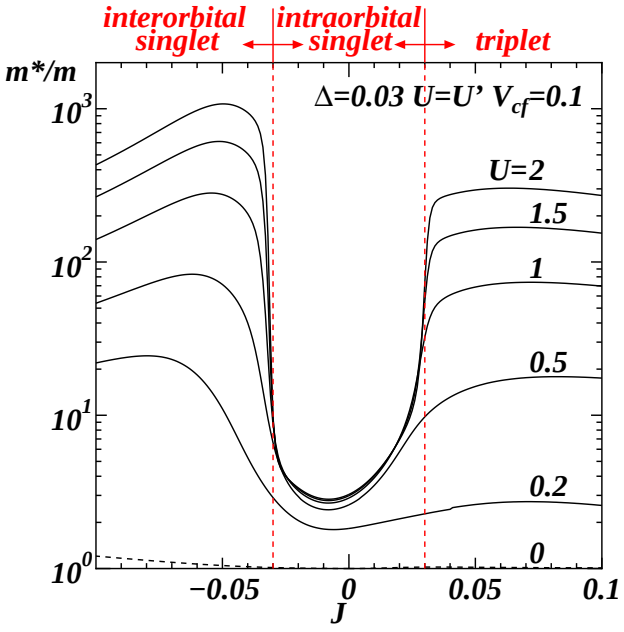

Figure 1: Mass enhancement factor.

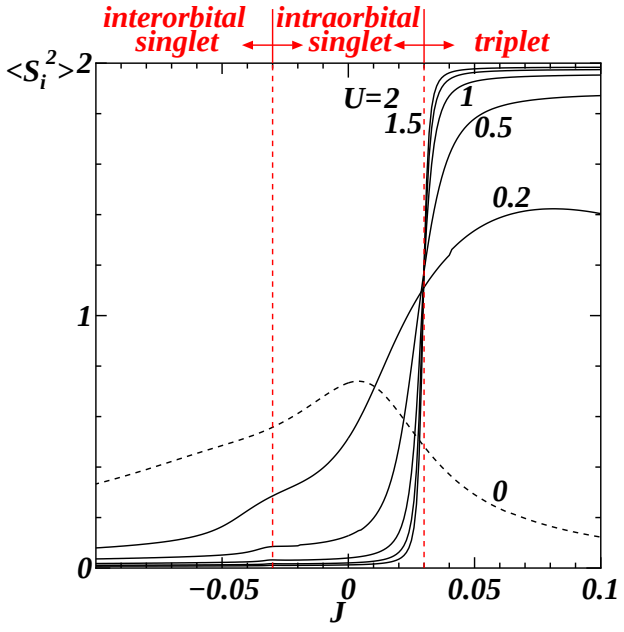

Figure 2: Local moment.