

# Heavy fermion state in the $f^2$ periodic Anderson model

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The crystal-field levels of the  $\text{Pr}^{3+}(4f^2)$  ion in  $\text{PrOs}_4\text{Sb}_{12}$  are believed to be the ground state  $\Gamma_1$  singlet and the first excited state  $\Gamma_4^{(2)}$  triplet with the excited energy  $\sim 10\text{K}$ . To elucidate the effect of the crystal-field levels on the heavy fermion behaviour, we study the two-orbital periodic Anderson model at half-filling where the average  $f$ -electron number per site is 2, using the dynamical mean-field theory combined with the exact diagonalization method[1]. We assume a semielliptic DOS for the bare conduction band with the half-bandwidth  $W = 1$  and we set the  $c$ - $f$  hybridization  $V_{\text{cf}} = 0.1$ .

The renormalization factor  $Z$  and the local moment  $\langle \vec{S}^2 \rangle$  are obtained as functions of the on-site Coulomb interaction  $U$ , the on-site exchange coupling  $J$  and the crystal-field splitting  $\Delta$ . In the case of  $V_{\text{cf}} = 0$ , the ionic ground state is singlet ( $\langle \vec{S}^2 \rangle = 0$ ) for  $\Delta > \Delta_c = 3J$ , while it is triplet ( $\langle \vec{S}^2 \rangle = 1$ ) for  $\Delta < \Delta_c$ . In the strong correlation regime  $U \gtrsim W$ , the heavy fermion state with  $m^*/m = Z^{-1} \gg 1$  and  $\langle \vec{S}^2 \rangle \sim 1$  is realized for  $\Delta < \Delta_c$ , while it is not realized for  $\Delta > \Delta_c$ . When the ground state singlet and the excited state triplet form a quasi-quartet ( $\Delta \approx \Delta_c$ ), the system shows a moderate enhancement of the effective mass  $m^*/m \sim 10 - 50$  and a large enhancement of the orbital fluctuation.

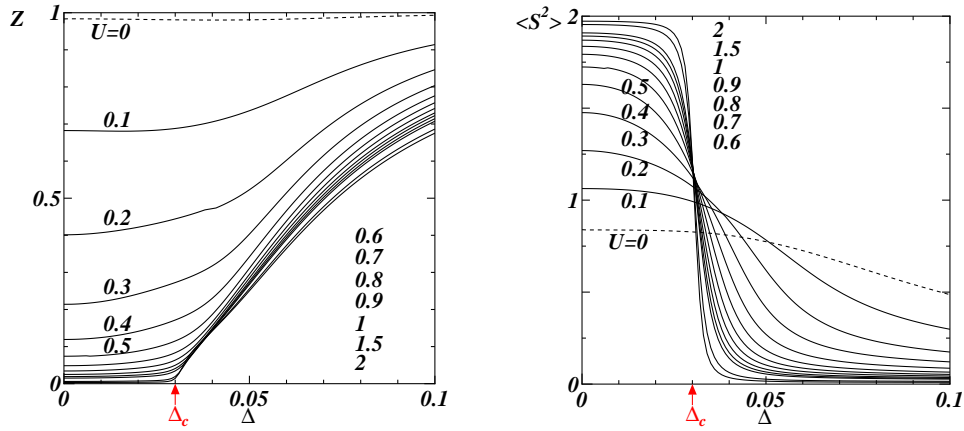


Figure 1:  $Z$  and  $\langle \vec{S}^2 \rangle$  as functions of  $\Delta$  for several  $U$  at  $J = 0.01$ .

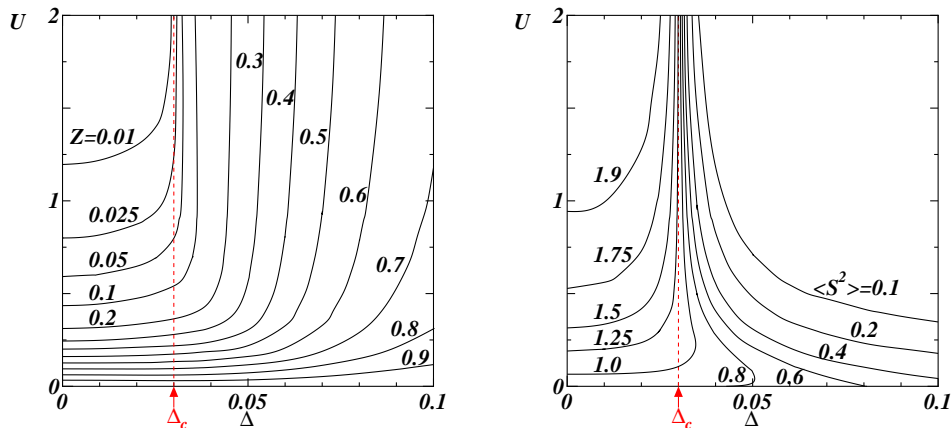


Figure 2: Contour maps for  $Z$  and  $\langle \vec{S}^2 \rangle$  on  $\Delta - U$  plane at  $J = 0.01$ .

[1] Y. Ōno, M. Potthoff and R. Bulla, Phys. Rev. **B 67** (2003) 035119.