# Emergence of two quantum critical points in $Yb_2Pd_2Sn$ under pressure: the modified Doniach phase diagram

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Abstract: In intermetallic compounds with Ytterbium ions, the fluctuations between magnetic Yb 4f 13 and nonmagnetic 4f 14 electronic configuration (EC) with different ionic volumes, provide an additional degree of freedom for the pressuredriven competition among the electronic ground states. This can lead to novel features in the phase diagram, as observed in $Yb_2Pd_2Sn$, the first compound exhibiting the two consecutive, pressure-driven quantum critical points (QCP). The novel phase diagram is explained applying Doniach approach to the Anderson model with the crystal field (CF) split f states. Such a model is characterized by the position of the f level Ef , the conduction band density of states, the hybridization strength Γ, and the coupling constant g = Γ/π |Ef |. For the CF states, the f-f correlation is infinite, i.e., the total f occupancy is always less than one. Since the ionic radius of Yb is very small, we assume that pressure does not affect, initially, the hybridization with ligands, so that Γ does not change. The main effect of pressure is, then, to make the nonmagnetic 4f 14 EC energetically unfavorable, due to it's large volume. This increases it's separation from the small-volume magnetic 4f 13 EC, which makes Ef more negative and favors the magnetic ground state. For higher pressures Ef saturates, but as the lattice constant is now reduced, the hybridization Γ increases. In this pressure range, the magnetic moment of f ions is quenched and the non-magnetic ground state is restored. The theoretical phase diagram is constructed by comparing the mean-field free energies of the local moment (LM) and aniferromagnetic (AFM) phases. The Kondo temperature TK(g) of the CF split 4f-octet of Yb ions is calculated by the NCA approximation which replaces the lattice model with the single impurity Anderson model. This Kondo scale agrees very well with the scaling result of Hanzawa, and we use it to estimate the energy gain due to the singlet formation. The RKKY temperature TRKKY (g) is estimated from the 2nd-order expansion for interaction energy of two magnetic impurities. The mean-field phase diagram obtained in such a way captures the essential features of the experimental data. A more sophisticated approach should obtain both solutions, the non-magnetic and the magnetic one, directly from the free energy of the periodic Anderson model. The experimental data regarding this work can be found in the papers:
E. Bauer et al., The magnetic instability of Yb2Pd2 (In; Sn) in a non-Fermi liquid environment, J. Phys.: Condens. Matter 17, S999-1009 (2005). T. Muramatsu et al., Pressure induced magnetic ordering in Yb2Pd2 Sn with two quantum critical points, arXiv:0704.3307v2 [cond-mat.str-el] (2007).