

Microscopic approach to many-body effects in Pr skutterudites

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Skutterudites filled by Pr for the rare-earth sites show characteristic behaviors depending on combination of ligands. We are particularly interested in identifying the key elements which give rise to diversity among $\text{PrFe}_4\text{P}_{12}$, $\text{PrRu}_4\text{P}_{12}$ and $\text{PrOs}_4\text{Sb}_{12}$. Explicit results of theoretical calculation along this line are given by J. Otsuki (PS37) and A. Kiss (8b1). In the present contribution, we shall discuss microscopic approach toward understanding the following fundamental issues which remain unsolved.

CEF level scheme

The overall CEF splittings in $\text{PrRu}_4\text{P}_{12}$ and $\text{PrOs}_4\text{Sb}_{12}$ are clearly known by recent neutron scatterings as presented by Iwasa (8a2). We have proposed that coexistence of Coulomb interaction and hybridization is responsible for the different behaviors among Pr skutterudites [1]. If we assume that transition metal ligands are nearly divalent or trivalent, the overall CEF splitting is of the order of 10 meV. On the other hand, polycrystalline $\text{PrFe}_4\text{P}_{12}$ does not show clear CEF levels in neutron scattering. In single crystalline samples measured by Iwasa et al, however, we can recognize faint inelastic peaks around 1.5 meV even above the quadrupole ordering temperature $T_Q = 6.5\text{K}$. If we interpret this feature as CEF excitations, the overall CEF splitting seems to be of the order of 4 meV, which is less than half of Ru and Os counterparts. The small overall splitting is necessary to have the high-field ordered phase distinct from the low-field phase [2]. The small CEF splitting should enhance the Kondo effect drastically.

Origin of non-Fermi liquid behavior in $\text{PrFe}_4\text{P}_{12}$

The most strange behavior in $\text{PrFe}_4\text{P}_{12}$ is the non-Fermi liquid behavior in magnetic field H along [111]. Around this direction, the resistivity takes a sharp maximum [3]. For $H \parallel [111]$, the NMR relaxation shows a non-Korringa-like temperature dependence, as discussed by Kikuchi (PS15). These properties are likely to come from the level crossing of CEF levels occurring only for the high-symmetry direction of H . In this connection, a new ordered phase in high magnetic field found by Tayama [2] is important. The resistivity maximum is naturally explained in terms of inter CEF level scattering as discussed by Kiss (8b1). It remains to understand why the non-Fermi liquid appears under this CEF scheme.

NMR in skutterudites

It has been shown by Tokunaga (6b4) for $\text{UFe}_4\text{P}_{12}$ that anisotropy in the ^{31}P Knight shift is roughly consistent with the dipole interaction between the Pr electron moment and ^{31}P nuclear moment. The Knight shift in $\text{PrFe}_4\text{P}_{12}$ as measured by Kikuchi (PS15) in the ordered phase reflects the growth of the quadrupole order parameter. We argue that the induced antiferro octupole moment of the type $5z^3 - 3zr^2$ is responsible for the unique splitting pattern of the NMR spectra.

References

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- [3] E. Kuromachi et al: Acta Physica Polonica **B34** (2003) 1129.