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Unconventional Charge-Density Wave, Fluctuating f Orbitals, and Metal-Insulator Transition in $\text{PrRu}_4\text{P}_{12}$

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$\text{PrRu}_4\text{P}_{12}$ undergoes a metal-insulator transition at $T_c = 63\text{K}$, below which a two-sublattice modulation of the atomic displacement is experimentally observed. One of the unconventional properties of this charge density wave (CDW) order shows up in the crystal field (CF) level scheme of Pr $4f$ electrons. It is revealed by a neutron scattering experiment that a strong and characteristic temperature dependence of the CF levels is associated with the CDW ordering [1].

In the normal phase above T_c , the level scheme is homogeneous, and a singlet ground state denoted by Γ_1 is realized for all Pr sites. As temperature is lowered below T_c , the excitation energy to a triplet Γ_4 is markedly reduced in one of the sublattices, and a level crossing with the singlet takes place at 40K. Since the singlet ground state is maintained in the other sublattice, two distinct CF ground states, singlet and triplet, are realized for different sublattices at zero temperature.

Considering these facts, a mean field (MF) theory of the CDW has been proposed by Takimoto [2]. According to the theory, the CDW of conduction electrons is triggered by an interaction with f electrons, different from that with phonons in conventional cases. The temperature dependence of the CF levels is successfully explained as a manifestation of a multipolar ordering that keeps the cubic site symmetry unbroken.

In this presentation, we shall report the result of a theoretical study of the fluctuation correction to the MF theory [3]. For simplicity, we restrict f degrees of freedom into singlet and triplet levels only, and apply a variant of the dynamical mean-field theory to the simplified model. We show that a gap formation of the quasi-particle spectrum in the CDW phase is strongly influenced by a thermal fluctuation of the f states. The key to producing such a large fluctuation is a crossing of the f -electron CF levels in one of the sublattices. It is shown that the resulting characteristic temperature dependence of resistivity is qualitatively consistent with a recent experimental observation indicating an unusual thermal activation behavior at low temperature [4].

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