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Variation of superconducting transition temperatures due to different crystalline electric field orbital-states

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$CeMIn_5$ (M=Co, Rh, and Ir) have attracted much attention due to relatively high superconducting transition temperature T_c among heavy-fermion materials. $CeMIn_5$ have the same crystal structure and f-electron number per Ce is also the same. In addition, from the de Haas-van Alphen experiments and band-structure calculations, the topology of the main Fermi surfaces are similar to each other among these materials [1]. However, T_c varies significantly among them: At ambient pressure, $T_c = 2.3$ K for $CeCoIn_5$ and $T_c = 0.4$ K for $CeIrIn_5$. $CeRhIn_5$ is an antiferromagnet at ambient pressure with a Néel temperature $T_N = 3.8$ K, while it becomes superconducting with $T_c \simeq 2$ K under pressure $p \gtrsim 1.6$ GPa. It is an important issue to find the controlling parameter of the superconductivity other than the f-electron number and the Fermi surface topology.

A possible controlling parameter is considered to be related to crystalline electric field (CEF) effect, but the CEF level splittings deduced from inelastic neutron scattering experiments are almost the same for these materials [2]. Note, however, that a CEF potential can affect not only the level splitting but also the wave-functions. Indeed, the wave-functions of the CEF states are different among $CeMIn_5$ [2], even though the splitting is almost the same. To study the role of the CEF orbital-states in these materials, we apply fluctuation exchange approximation to an f-electron model based on a j-j coupling scheme with orbital degeneracy on a square lattice [3]. In this study, we consider electrons with total angular momentum $j = 5/2$. These $j = 5/2$ states split into one Γ_6 and two Γ_7 doublets under a tetragonal CEF. By choosing appropriate CEF potentials, we can actually control the wave-functions of Γ_7 states without changing the level splitting. Although the Fermi surface does not change so much as long as the level splitting is fixed, the ground state changes depending on the Γ_7 wave-functions among paramagnetic, antiferromagnetic, and d-wave superconducting states. Thus, in addition to the Fermi-surface topology and the f-electron number, we claim that the orbital state under a CEF is an important ingredient to control the appearance of superconductivity in such systems.

Finally, we also analyze the CEF orbital-states in $CeMIn_5$ with due care, by considering experimental results of the inelastic neutron scattering [1] and the thermal expansion [4]. By using the CEF orbital-states deduced from this analysis, we show that the variations of T_c and T_N in $CeMIn_5$ are well explained within our theory.

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