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Origin of magnetic anisotropy in *f*-electron systems with inversion symmetry

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Many heavy fermion systems show phase transition into anisotropic magnetic states. For systems without inversion symmetry, it is expected that the magnetic anisotropy is induced by the Dzyaloshinski-Moriya interaction. On the other hand, for systems with the inversion symmetry, the origin of the magnetic anisotropy has not been clarified yet. Furthermore, it is considered that in the magnetic ordered state, higher order multipole moments breaking time reversal symmetry are also induced as well as the magnetic moment. With respect to this point, it is infered that quasi-degeneracy of f-electron is responsible for the multipole moments. Thus, in order to clarify the magnetic anisotropy of f-electron systems with inversion symmetry, we develop a microscopic theory based on a quasi-degenerate microscopic model.

Based on j=5/2 multiplet as local bases of f-electron, we construct a theory of magnetic anisotropy, where j is total angular momentum. Then, any state of f-electron is described by both of pseudo-spin σ and orbital exhibiting the crystalline electric field (CEF) state γ . At first, we describe multipole moments by second-quantized operators irreducible for both orbital and pseudo-spin spaces, instead of irreducible tensors. These second-quantized operators are classified according to irreducible representations of corresponding point group. Next, according to established procedures, generalized RKKY interactions are extracted from a quasi-degenerate periodic Anderson model. Then, mean-field equations are given for every ordered states, that are specified by the irreducible representation Γ and the ordered wave vector \mathbf{Q} .

Now, to clarify magnetic anisotropy in the ordered state, we examine the mean-field equation on the symmetry property. In systems with D_{4h} point group, there are two irreducible representations accompanying magnetic moment, where the magnetic moment parallel (perpendicular) to z-axis should be observed in the ordered state belonging to A_2^- (E⁻) irreducible representation. From careful consideration of the inversion symmetry, it is concluded that RKKY interaction between pseudo-spins of same kind of CEF state induces no magnetic anisotropy in the system. Thus, it is understood that the orbital degrees of freedom is essential for explaining not only multipole ordering but also magnetic anisotropy in the system with inversion symmetry. Furthermore, considering features of the tetragonal system, we reach a conclusion for origin of magnetic anisotropy in *f*-electron systems with inversion symmetry. When the ground state of *f*-electron level scheme belongs to Γ_7 irreducible representation, the magnetic anisotropy in the ordered state is induced only by RKKY interaction between components of magnetic moment that are pseudo-spin with symmetric and off-diagonal properties in Γ_7 orbital space. On the other hand, when the ground state is classified to Γ_6 , magnetic anisotropy is expected to be much weaker than that of the previous case.