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Quantum Spin Ice for Pr Pyrochlore Magnets SHIGEKI ONODA, YOICHI TANAKA, Condensed Matter Theory Laboratory, RIKEN — We theoretically propose a new state comprising a quantum-mechanical analogue of the spin ice for pyrochlore magnets. In classical spin-ice systems like $Dy_2Ti_2O_7$, the ice rule is mainly driven by the magnetic dipolar interaction, which is proportional to the square of the total angular momentum J. Therefore, for Pr^{3+} ions having two f electrons forming the $J = 4$ localized moment, the dipolar interaction becomes an order of magnitude smaller than that for Dy ions. Then, the magnetic superexchange interaction should play a important role. In fact, the form of the exchange interaction is nontrivial because of the highly relativistic nature of f electrons with strong LS coupling and crystal-field effect. Here, we present a microscopic derivation of the effective relativistic spin-orbital Hamiltonian for the pyrochlore magnets $Pr_2TM_2O_7$ with a transition-metal element TM. Then, it is shown that the nearest-neighbor exchange interaction is significantly modified from antiferromagnetic to ferromagnetic by quantum- mechanical processes through excited states split by the crystal field. This bears a quantum-mechanical formation of the ice rule for Pr magnetic moments. Solving the Hamiltonian for a Pr_4O tetrahedral cluster, we obtain a further small energy splitting of the low-energy states, leaving doubly degenerate ground states per tetrahedron. Implications for the lattice model and possible relevance to experiments are also discussed.

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