

Abstract Submitted
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The low-energy magnetic excitations of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxide Sr_2IrO_4 TOMONORI SHIRAKAWA, HIROSHI WATANABE, SEIJI YUNOKI, Computational Condensed Matter Physics Laboratory, RIKEN ASI — 5d transition metal oxides in a layered perovskite structure such as Sr_2IrO_4 have attracted much attention because of their unique properties caused by a strong relativistic spin-orbit coupling of 5d transition element. Recent experiments on Sr_2IrO_4 have revealed that the low-energy magnetic excitations can be described by an “isospin”-1/2 Heisenberg model with an effective exchange interaction as large as $\sim 60\text{-}100$ meV. Motivated by these experiments, we study theoretically the ground state magnetic structure and the low-energy magnetic excitations for Sr_2IrO_4 using a three-band Hubbard model with the spin-orbit coupling. Our results demonstrate that the low-energy magnetic excitations are well described by an effective antiferromagnetic Heisenberg model composed of a local Kramers doublet. The estimated value of the effective exchange interaction is as large as 79 meV, which is in good quantitative agreement with the experiments.

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