

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Bayesian Inference of Effective Classical Spin Hamiltonians from Hartree-Fock Calculation HIKARU TAKENAKA, KENJI NAGATA, Graduate School of Frontier Sciences, The University of Tokyo, TAKASHI MIZOKAWA, School of Advanced Science and Engineering, Waseda University, MASATO OKADA, Graduate School of Frontier Sciences, The University of Tokyo — A novel method is described for extracting effective classical spin Hamiltonians from mean-field type electronic structural calculations by means of Bayesian inference[1]. The method is applied to a NiS₂ triangular lattice in NiGa₂S₄ with a spin disordered ground state. Unrestricted Hartree-Fock calculations for the spin configurations of 16 Ni sites led to the estimation that not only the strongest superexchange interaction between the third nearest neighbor sites but also those between the nearest and the second nearest neighbor sites should be taken into account to extract effective classical spin Hamiltonians for NiGa₂S₄. Results obtained from the above calculations with the Boltzmann factor are also shown. It was estimated that the superexchange interaction between the nearest neighbor sites is ferromagnetic, which is consistent with magnetic experiment results. This supports the theory that the competition between the antiferromagnetic third neighbor interaction and the ferromagnetic nearest neighbor interaction may lead to the quantum spin liquid in NiGa₂S₄. [1]H. Takenaka, K. Nagata, T. Mizokawa, and M. Okada, J. Phys. Soc. Jpn. 83, 124706, (2014).

Hikaru Takenaka
Graduate School of Frontier Sciences, The University of Tokyo

Date submitted: 06 Nov 2015

Electronic form version 1.4