Microscopic modeling of the S=1/2 Heisenberg ferrimagnet Cu_2OSeO_3

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Cu_2OSeO_3 is a $S = 1/2$ Heisenberg ferrimagnet with a sizable magnetoelectric coupling [1]. Recent experimental studies reported magnetic-field-induced emergence of skyrmions in this insulating material [2]. Based on extensive DFT band structure calculations, we evaluate isotropic (Heisenberg) as well as anisotropic (Dzyaloshinskii-Moriya) magnetic exchange couplings.

Five relevant magnetic couplings form a complex, non-frustrated spin model, which can be described as a pyrochlore lattice of magnetic tetrahedra. A peculiar feature of this lattice is the alternation of "strong" tetrahedra (the constituent spins are strongly coupled) and "weak" tetrahedra.

Profiting from the separation of the energy scales, we develop an effective model, treating strong tetrahedra either as a classical $S = 1$ object or as a coherent quantum superposition of classical states. For the latter case, we find an excellent agreement with the quantum Monte Carlo simulations of the full model and the experimental magnetization and neutron diffraction data.

We demonstrate that the developed effective model can be further used to model the field-induced behavior, including the formation of skyrmions.

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