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Luttinger-Tisza method applied to frustrated magnetic systems

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A frustrated magnetic system is one in which a spin ‘wants’ to align with some of its neighbors, but ‘wants’ to anti-align with others, and a long range ordered state that completely satisfies all interactions is not possible. This can lead to many interesting spin structures, including helical phases with incommensurate ordering wavevectors. In order to determine the magnetic structure of a given frustrated Hamiltonian, we developed a program that uses the Luttinger-Tisza method to predict the ground state spin configuration. This is used to compare to neutron scattering data on materials thought to embody the frustrated spin models. The program has been tested for the $J_1 - J_2 - J_3$ Heisenberg model on a honeycomb lattice, for which the exact results are known. The method was then applied to a $J_1 - J_2$ Heisenberg model for the three dimensional lattice appropriate to the highly frustrated material Fe_3PO_7 . The result for the relevant parameter regime for Fe_3PO_7 ($\frac{J_2}{J_1} = 1.9$) is a quasi-degenerate ring of \vec{k} -vectors, in excellent agreement with observations from neutron scattering. Our result for Fe_3PO_7 gives insight as to why this material does not form a fully long range ordered state, but instead forms nanosized domains of partial helical order.

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