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Numerical Implementation of a General Spinwave Model to Simulate Spinwave Excitations Found in Inelastic Neutron Scattering Data
D. CASAVANT, I. BRODSKY, G. J. MACDOUGALL, Dept. of Physics, Univ. of Illinois at Urbana-Champaign — Many important details regarding magnetism in a material can be inferred from the magnetic excitation spectrum, and in this context, general calculations of the classical spinwave spectrum are often necessary. Beyond the simplest of lattices, however, it is difficult to numerically determine the full spinwave spectrum, due primarily to the non-linearity of the problem. In this talk, I will present MATLAB code, developed over the last few years at the University of Illinois, that calculates the dispersions of spinwave excitations out of an arbitrarily defined ordered spin system. The calculation assumes a standard Heisenberg exchange Hamiltonian with the incorporation of a single-ion anisotropy term which can be varied site-by-site and can also simulate the application of an applied field. An overview of the calculation method and the structure of the code will be given, with emphasis on its general applicability. Extensions to the code enable the simulation of both single-crystal and powder-averaged neutron scattering intensity patterns. As a specific example, I will present the calculated neutron scattering spectrum for powders of CoV_2O_4 , where good agreement between the simulated and experimental data suggests a self-consistent picture of the low-temperature magnetism.

David Casavant
Dept. of Physics, Univ. of Illinois at Urbana-Champaign

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