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User-friendly software for modeling collective spin wave excitations

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SpinWaveGenie is a Python/C++ software library that simplifies the modeling of collective spin wave excitations, allowing scientists to analyze neutron scattering data with sophisticated models fast and efficiently. Furthermore, one can calculate the scattering function $S(Q, E)$ to directly compare and fit calculations to experimental measurements. Its generality has been both enhanced and verified through successful modeling of a wide array of magnetic materials. By adding features such as the Python bindings, we have moved SpinWaveGenie from an early prototype to a free open source software package accessible to the scientific community. Usability has been improved by simplifying the edit, build and debug cycle. Furthermore, SpinWaveGenie can be leveraged in larger workflows using the large ecosystem of open-source scientific software written in Python or with a Python API. For example, the Atomic Simulation Environment has been used to help build the spin structures, LMfit has been used to fit exchange parameters, and Paraview has been used to visualize results. Several examples of its use to model the spin wave spectrum of powder and single crystal MnO and compare it to measurements from HYSPEC will be discussed.

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