Atomistic spin dynamics for studying magnons

*Joseph Barker[1]
University of Leeds, UK[1]
Keywords: spin dynamics, magnons, computation

We will introduce the computational method of atomistic spin dynamics. This method models magnetic materials on an atomic level, larger than electronic structure calculations but smaller than micromagnetic methods. The atomistic spin dynamics method includes both temperature and magnon-magnon interactions so spin correlation functions can be calculated accurately even at elevated temperatures or near to phase transitions. It is therefore ideally suited for comparison to quantum beam measurements such as neutron diffraction.

We will present result from recent work on yttrium iron garnet (YIG). We will show how spin models can be parameterized either from neutron diffraction measurements [1], or from first principles calculations [2], allowing an independent verification of experimental results. Our results include calculations and measurements of magnon polarization which has long been known theoretically but never measured directly. Combining theoretical calculations and cutting-edge polarized neutron diffraction experiments we were able to confirm it's existence (see Fig. 1) [3].

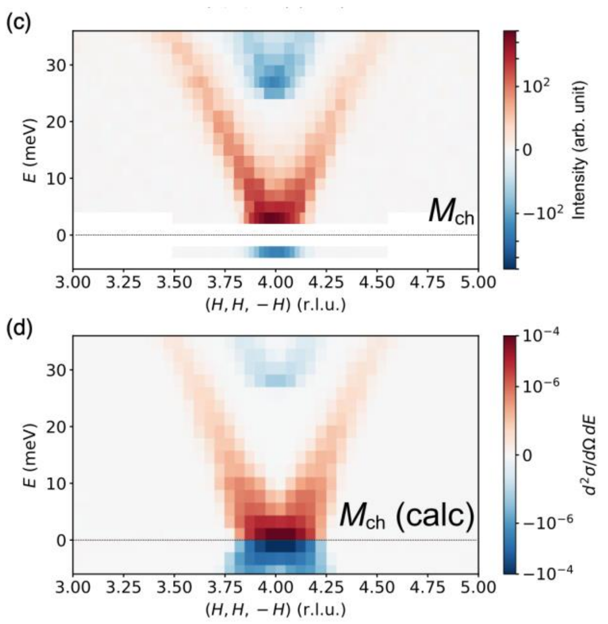

Fig. 1 *Comparison of (c) polarized neutron diffraction measurement of magnon polarization in YIG (d) atomistic spin dynamics calculation of polarized neutron scattering cross-section from polarized neutrons in YIG after instrument resolution convolution.*

[1] J. Barker & G.E.W. Bauer, *Phys. Rev. Lett.* **117**, 217201 (2016)
[2] J. Barker, D. Pashov & J. Jackson, *Electron. Struct.* **2**, 044002 (2020)
[3] Y. Nambu, J. Barker, Y. Okino et al., *Phys. Rev. Lett.* **125**, 027201 (2020)