Atomistic spin dynamics beyond the Landau-Lifshitz-Gilbert equation

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For nearly 100 years the Landau-Lifshitz-Gilbert (LLG) equation has been the cornerstone of modelling magnetic materials. To achieve energy efficient and high-density applications, nanoscale magnetic materials are being driven at faster speeds or with stronger stimuli. Atomistic spin dynamics (ASD)[1], based on the LLG, has been a powerful tool for prototyping and evaluating both ultrafast and nanoscale magnetic systems. However, in these systems the common assumptions that underpin this approach are being challenged. In this talk, I will introduce two recent extensions to atomistic spin dynamics that provide new directions for understanding high-frequency and ultrafast magnetic systems: longitudinal and spin-lattice dynamics.

Conventionally, the magnitude of the atomic magnetic moment is considered constant. However, for materials like FePt or Ni, where weak moments are polarised from local interactions this constraint becomes limiting. With longitudinal spin dynamics [2], the atomic spin moment is allowed to fluctuate in magnitude allowing for a more natural model of these systems. Using FePt as an example system, I will introduce a generalised spin equation where the Pt spin moment is induced by the Fe exchange interaction and show how this can successfully describe the experimentally observed two-ion anisotropy. Secondly, I will introduce spin-lattice dynamics (SLD) [3] as a technique for understanding the complex interplay between the spin and lattice sub-systems when driven by a terahertz laser excitation. Through magneto-elastic coupling the lattice motion can induce an internal field with the magnetic material that drives switching behaviour on an ultrafast timescale [4]. This technique provides a new tool for modelling how magnons and phonons interact and can provide perspectives on high-frequency and ultrafast nano-magnetic systems.

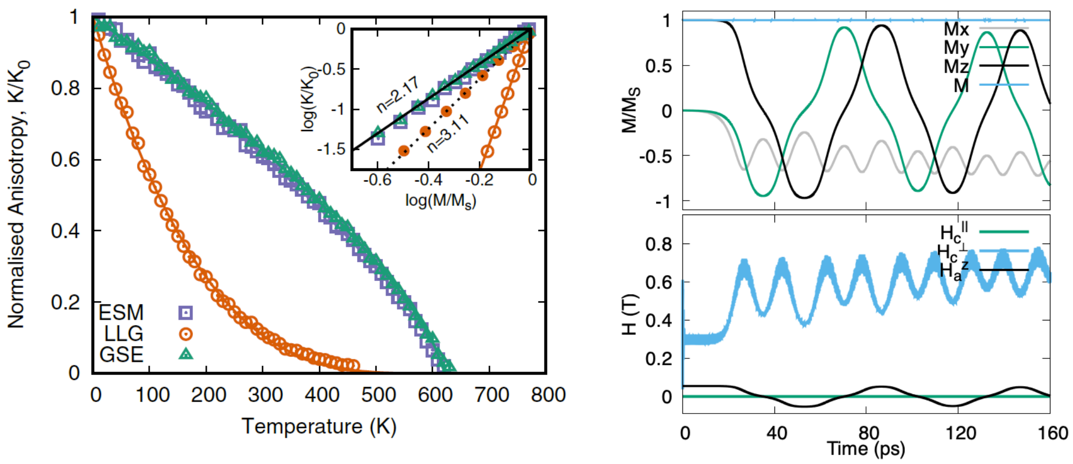

Fig. 1. (left) Comparison of the anisotropy calculated using the generalised spin equation (GSE) to conventional LLG dynamics. (right) Magnetisation switching in Spin-Lattice dynamics driven by a terahertz pulse. The lattice induces an internal coupling field (lower) that causes precessional switching of the magnetisation (top).

[1] Evans et al. *Atomistic spin model simulations of magnetic nanomaterials, J. Phys.: Condens. Matter* **26** 103202 (2014)
[2] Ellis et al. *Role of longitudinal fluctuations in L10 FePt*, Phys. Rev. B, **100** 214434 (2019)
[3] Strungaru et al. *Spin-lattice dynamics model with angular momentum transfer for canonical and microcanonical ensembles*, Phys. Rev. B **103**, 024429 (2021)
[4] Strungaru et al. Route to minimally dissipative switching in magnets via terahertz phonon pumping, Phys. Rev. B **109**, 224412 (2024)