Spin dynamics simulations uncover the microscopic origins of phase transitions in hematite

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Hematite (α-Fe_2O_3), the most common iron ore, is an insulating antiferromagnet, its ground state characterised by an antiparallel alignment of atomic magnetic moments and vanishing net magnetisation. Magnetic fields or increasing temperature can induce phase transitions into a weak ferromagnetic phase in which a slight canting of the magnetic sublattices leads to a small but finite macroscopic magnetisation [1, 2, 3]. In the vicinity of this phase transition, spin waves have been found to travel unusually long distances, up to the micrometer range, making this rather complex material of particular interest in modern spintronics [4]. However, much remains unknown about the details of the mechanisms driving the transition into the weak ferromagnetic state. Here, we reveal the microscopic origins of these phase transitions using atomistic spin dynamics simulations based on a semiclassical model parameterised from ab initio calculations. We find that dipole-dipole interactions play a major role in determining the equilibrium state. We compare our simulation results to spin-Hall magnetoresistance measurements and we show how the quantum nature of the thermal fluctuations leads to significant deviations from the predictions of a classical model at low temperatures. Beyond these new insights into the equilibrium properties of hematite, we hope that this model can in the future be deployed for the investigation of its dynamic properties as well, in particular the transport of spin waves.

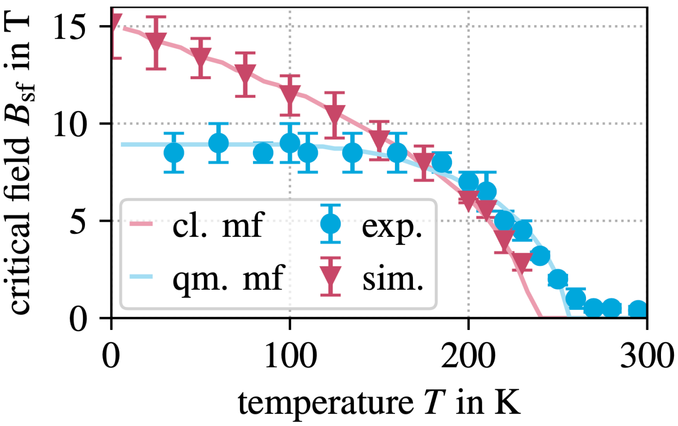

Fig. 1: *Temperature dependence of the spin flop field in hematite. Comparison of measured and simulated critical fields with rescaled mean field (mf) curves based on a classical (cl.) and a quantum (qm.) model.*

References:

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