102

Coupled Brownian and Néel Relaxation in Magnetic Nanoparticles: Regimes and Losses

Author: Santiago Helbig[1]

Co-authors: Andrey Kuznetsov[2]; Deniz Mostarac[3]; Claas Abert[1]; Pedro A. Sánchez[1]; Sofia Kantorovich[1]; Dieter Süss[1]

[1] *University of Vienna*
[2] *Computational and Soft Matter Physics, University of Vienna, 1090 Vienna, Austria*
[3] *University of Edinburgh*

Colloidal magnetic nanoparticles exhibit coupled dynamics of magnetization, hydrodynamics, and thermal noise that are difficult to resolve with experiments or continuum models alone. We address this by extending the ESPResSo molecular dynamics framework [1] with magnetization dynamics governed by the Landau–Lifshitz–Gilbert (LLG) equation. We model uniformly magnetized single-domain particles with uniaxial anisotropy as macrospins using Langevin dynamics. This approach resolves Brownian and Néel relaxation in tandem and allows us to separate magnetic and friction loss channels. Losses are obtained from hysteresis loops under AC magnetic fields and are averaged over a system of 256 particles. The partition between magnetic and friction losses follows from the work done over one cycle by the field on the magnetization and the viscous rotational dissipation, respectively [2].

Validation against analytical results shows excellent agreement for equilibrium properties, thermal spectra, and dynamic susceptibility. The code also allows observation of particle clustering, polydispersity in size and anisotropy, as well as cubic and shape anisotropy, which will be briefly discussed.

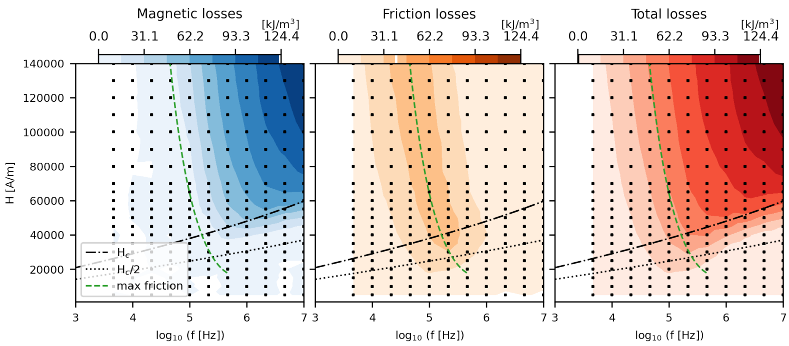

Figure 1: Three diagrams depict the energy-loss landscape for magnetic losses, friction losses, and total dissipated energy for non-interacting magnetite-like nanoparticles with $K_u = 30\,\mathrm{kJ\,m^{-3}}$ and $M_s = 400\,\mathrm{kA\,m^{-1}}$, as functions of field amplitude (up to and slightly above the anisotropy field) and frequency (4.6 kHz to 1 MHz).

Acknowledgments

This research was funded in whole or in part by the Austrian Science Fund (FWF) 10.55776/PIN4281825. We acknowledge financial support by the Vienna Doctoral School in Physics (VDSP).

References

[1] R. Weeber, J.-N. Grad, D. Beyer, P. M. Blanco, P. Kreissl, A. Reinauer, I. Tischler, P. Košovan, and C. Holm. *ESPResSo, a Versatile Open-Source Software Package for Simulating Soft Matter Systems.* In: *Comprehensive Computational Chemistry* (First Edition), edited by M. Yáñez and R. J. Boyd, pp. 578–601, Elsevier, Oxford (2024).
[2] S. Helbig, C. Abert, P. A. Sánchez, S. S. Kantorovich, and D. Suess. *Self-consistent solution of magnetic and friction energy losses of a magnetic nanoparticle.* Physical Review B, **107**, 054416 (2023).

Type:
Oral