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Dual-frequency MPS enables direct MNP size re-construction: Verification with micromagnetic simulation data

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Abstract

Magnetic Particle Spectroscopy (MPS) allows for direct characterization of magneto-physical properties of magnetic nanoparticles (MNP), which are widely researched as imaging tracers, biosensing units and therapeutic heating agents. All these applications rely primarily on the core size-dependent magnetic particle relaxation dynamics. Therefore, knowledge about core size of any MNP sample is crucial. Dual-frequency MPS increases the characterization potential by considering frequency mixing terms of the received signal of MNP, from which their sizes can be approximated. In this work, preliminary feasibility and interpretation of a proposed size recon-struction method is tested against precisely simulated input data from stochastically coupled Néel-Brownian relaxation modeling using Monte Carlo implementation.

I. Introduction

The core size (and thus magnetic moment) distribution of magnetic nanoparticles (MNP) is among the fundamental constituents for their effective utilization in biomedical applications in MPI, Magnetic Fluid Hyperthermia (MFH) and MPS-based biosensing. Measuring it quickly and precisely in a non-destructive manner directly from native MNP sample establishes a vital step towards large(r) scale application of MNP. Last year we proposed a method [1] for magnetic moment reconstruction under assumption of equilibrium solution and using a dual-frequency read-out scheme, allowing direct probing of the magnetization response's curvature. In this work we apply this reconstruction scheme to controlled MNP samples from dynamic magnetization simulations using a Monte Carlo implementation of Landau-Lifshitz-Gilbert (LLG)-Langevin coupled model and evaluate its performance upon these results.

II. Methods and materials

We performed Monte-Carlo-based dynamic magnetic simulations to model the response of monodisperse magnetite MNPs ($M_s = 476$ kAm^{-1}, $K_u = 11$ kJ·m^{-3}, $T = 298$ K) under dual-frequency magnetic excitation, $H(t) = H_1 \sin(2\pi f_1 t) + H_2 \sin(2\pi f_2 t)$, with $f_1 = 40$ kHz, $f_2 = 10$ Hz, $H_1 = 0.5$ mT, and $H_2 = 0.5 \div 26$ mT, chosen to fulfill statistical interpretability criteria per [1]. We assume uniaxial excitation field, $\mathbf{H} = (0, 0, H(t))$ and uniaxial anisotropy [2]. We simulate four MNP systems of different core sizes, $d_C = \{12, 18, 24, 30\}$ nm, each with

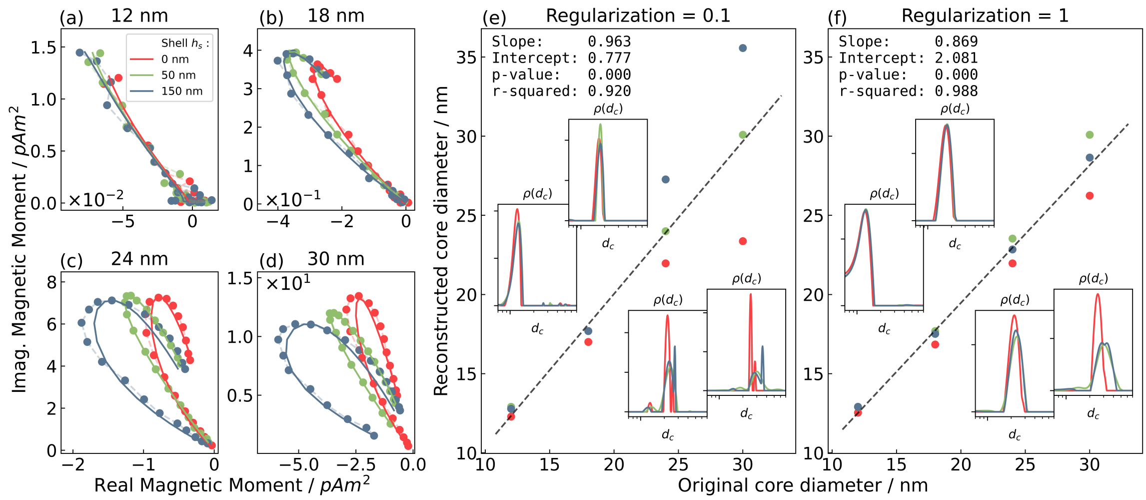

Figure 1: (a-d) Simulation results for mixing frequency term $A_{f_1+2f_2}$, core diameters (12, 18, 24, 30) nm, shell thicknesses (+0, +50, +150) nm. Dots: simulation points, solid lines: reconstructed signal. (e-f) Linear regression analysis between original and reconstructed core diameters. Regularization (e): 0.1 ,(f) :1. Insets show the reconstructed probability density functions $\rho(d_c)$ per sample.

three shell thicknesses of h_S={0, 50, 150} nm, thereby defining a hydrodynamic size of d_H=d_C+2·h_S. From this we used the routine, described in [1], to reconstruct the distribution $\rho(d_c)$ of core diameters. This routine assumes a maximum curvature of $M(H)$, probed by low-frequency amplitude H_2-variation in dual-frequency excitation, with its position at a particular field scan value, H_2^*, being related to a specific core diameter d_C in equilibrium. We identify two potential origins of curvature: (a) caused by varying number of aligned particles in equilibrium, which arises from the interplay of random forces, anisotropy effects, and the orientational force of the external magnetic field (aligning in-phase along the imaginary axis with the excitation field); (b) particle's dynamic $M(H)$ trajectory, which contributes out-of-phase (along real axis) and is presumably caused by damping (double cross-product) term present in both the LLG and Langevin equations. ()()In cylindrical coordinates without random forces, these equations reduce to the same nonlinear differential equation for component along external field $u_z(t)$, $\frac{d\mathbf{u}}{dt} = \alpha[\mathbf{u}\times\mathbf{H}]\times\mathbf{u} \Rightarrow \frac{du_z}{dt} = \alpha\cdot H(t)\cdot\left(1-u_z^2\right)$, where $\mathbf{u}$ is a unit vector showing the orientation of particle and the solution is,

$$u_z(t) = \tanh\left(\operatorname{arctanh}(u_z(0)) + \alpha\int_0^t H(\tau)\,d\tau\right), \quad (1)$$

where $\alpha = \mu_0 m_0/\left(2\tau_{eff} k_B T\right)$ $\left[\mathrm{mA^{-1}s^{-1}}\right]$ is the damping parameter, m_0 is magnetic moment of the particle, τ_{eff} relaxation time. Solution (1) shows that the Fourier component $A_{f_1+2f_2}$=$\mathcal{F}[u_z(t)]\left(f_1+2f_2\right)$ reaches its absolute maximum at a specific low-frequency field amplitude $H_2^{\star}\propto\alpha^{-1}$, too, similar to equilibrium solution's H_2^* but out-of-phase due to $H(t)$ integration over time.

III. Results and discussion

Figure 1 (a-d) shows simulation results for the mixing frequency signal $A_{f_1+2f_2}(H_2)$ (dots) and the reconstructed signal from fitted distributions (solid lines), demonstrating good agreement for both Tikhonov (0^{th} order) regularization parameters ($R^2 > 0.9$), which highlight the effects of regularization and the critical value beyond which artifacts emerge. In Figure 1(e,f), the accuracy of core size reconstruction is evaluated through linear regression (N=12) for two regularization settings (0.1 and 1) with reconstructed distribution $\rho(d_c)$, $d_c \in [7, 70]$ nm per simulated batch (inset). Comparison shows slight underestimation of the reconstructed core diameter (slope less than unity), and increased variance for $d_c > 20$ nm, presumably due to further deviation from equilibrium. Imaginary-axis (equilibrium) projection dominates the contribution to the hook shape, explaining the strong agreement with equilibrium-based reconstruction, as the H_2^*-feature remains hydrodynamic-size invariant despite non-monotonous amplitude variations over h_s (compare Fig. 1 (b) and (c)).

IV. Conclusion

Dual-frequency magnetic excitation enables core size reconstruction of magnetic nanoparticles (MNPs) between 12-30 nm for various hydrodynamic diameters. Preliminary feasibility is demonstrated, with future work focusing on identifying the approach limitations and physical interpretation of the hook plot.

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Author's statement

Authors state no conflict of interest.

References

[1] T. Bikulov, *Multicontrasting MPS by dual-tone nonlinearity probing.*, IJMPI, vol. 10.1, Jan. 2024.

[2] U. M. Engelmann, *Magnetic Nanoparticle Relaxation in Biomedical Application* in Magnetic Nanoparticles in Human Health and Medicine, 1st ed., C. Caizer, Ed. Hoboken, John Wiley & Sons, 2021.

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