Inclusion of Dipolar Interactions in the Mathematical Modelling of Magnetic Hyperthermia through the Landau-Lifshitz-Gilbert Equation

PJ Cregg, Kieran Murphy & Mangolika Bhattacharya

Waterford Institute of Technology, Ireland

Introduction

Magnetic Hyperthermia Treatment (MHT) continues to occupy clinicians, and experimental & theoretical magneticians alike. The many modelling approaches for non-interacting magnetic nanoparticles(MNPs) were outlined by Carrey *et al.* [1] at ICCSAMC 2014 in Dresden. Several authors have outlined the important role interparticle interactions are likely to play in MHT for closely spaced particles [1–6]. Modelling of MHT for non-interacting MNPs through the Landau-Lifshitz-Gilbert (LLG) equation was undertaken by Châtel *et al.* [7].

Our aim is to incorporate the dipole-dipole interactions in the LLG analysis. The effects of interactions on the frequency response of the heating mechanism are presented for two identical MNPs.

Relaxation mechanisms: Debye and Néel

- **Debye** relaxation: Brownian rotation of particle.
- **Néel** relaxation: Internal motion of magnetic moment - gyromagnetic.

For a fixed particle - Debye blocked, Néel mechanism only - this can be described by LLG equation.

The Landau-Lifshitz-Gilbert (LLG) Equation

The LLG equation describes the average damped precessional motion of the magnetic moment, $\boldsymbol{\mu}$ (expressed as the normalised volume magnetisation, $\mathbf{M}$, where $\boldsymbol{\mu} = V M_s \mathbf{M}$) of an MNP in a magnetic field $\mathbf{H}$ [7,8].

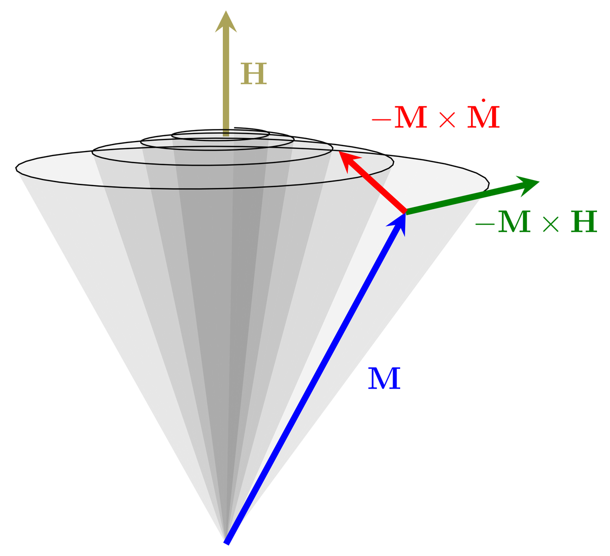
$$\dot{\mathbf{M}} = \left(\frac{\mu_0\gamma}{1+\alpha^2}\right)\mathbf{M}\times\mathbf{H} + \alpha\left(\frac{\mu_0\gamma}{1+\alpha^2}\right)(\mathbf{M}\times\mathbf{H})\times\mathbf{M}, \qquad (1)$$

where

- α is the dimensionless damping parameter, defined by

$$\alpha = \eta\gamma M_s$$

- η is the Gilbert dissipation constant,
- γ is the effective gyromagnetic ratio,
- μ_0 is permeability in vacuum,
- M_s is (volume) saturation magnetisation, and
- V is the volume of the MNP.



Inclusion of Interactions

The dipole-dipole interaction between MNPs can be included through the addition of the interaction field, (experienced by MNP 1 due to MNP 2), which for spherical MNPs of radius R, reduces to

$$\mathbf{H}_{\text{int}_1} = M_s\left(\frac{R}{|\mathbf{r}|}\right)^3\left[\left(\mathbf{M}_2\cdot\frac{\mathbf{r}}{|\mathbf{r}|}\right)\frac{\mathbf{r}}{|\mathbf{r}|} - \frac{1}{3}\mathbf{M}_2\right] \qquad (2)$$

where $\mathbf{r}$ is the vector between the MNP centres.

Calculation of Work done

We calculated the heating energy (per unit volume, per cycle), E, through the work done, i.e., damping force × distance

$$E = \mu_0\alpha M_s^2\int_0^{2\pi/\omega}\dot{\mathbf{M}}\cdot d\mathbf{M} = \mu_0\alpha M_s^2\int_0^{2\pi/\omega}|\dot{\mathbf{M}}|^2\,dt \qquad (3)$$

This can be shown to be analytically equivalent to that of Châtel *et al.* [7] where ω is the angular frequency of $\mathbf{H}$,

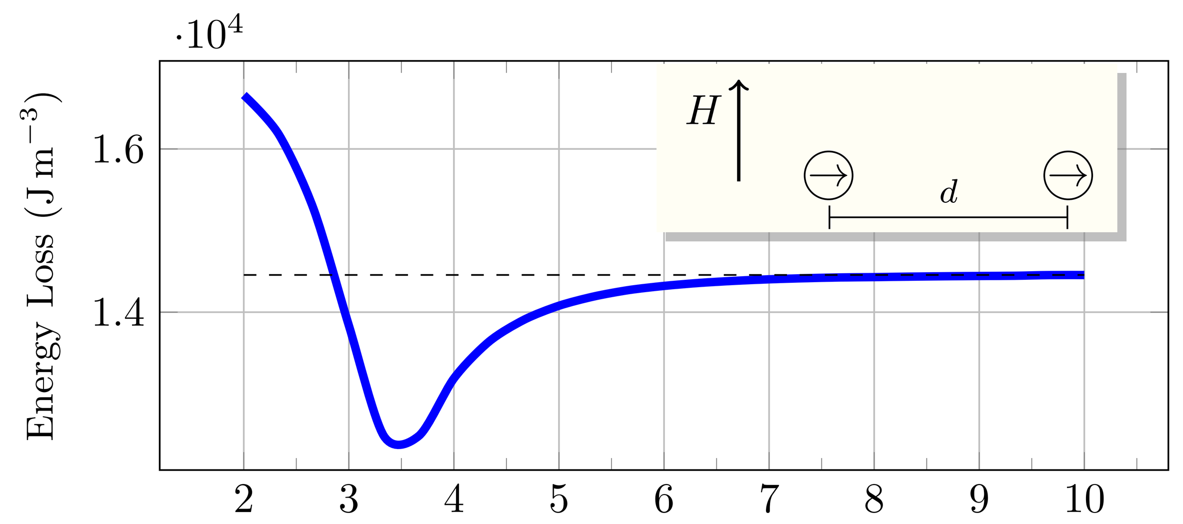
$$E = \mu_0 M_s\int_0^{2\pi/\omega}\left(\mathbf{H}\cdot\frac{d\mathbf{M}}{dt}\right)dt$$

Behaviour of two MNPs

The heating per cycle, E and the consequent Specific Absorption Rate (SAR) (taken to be the per unit volume value found from SAR $= Ef$, for frequency f) can be calculated over a range of frequencies.

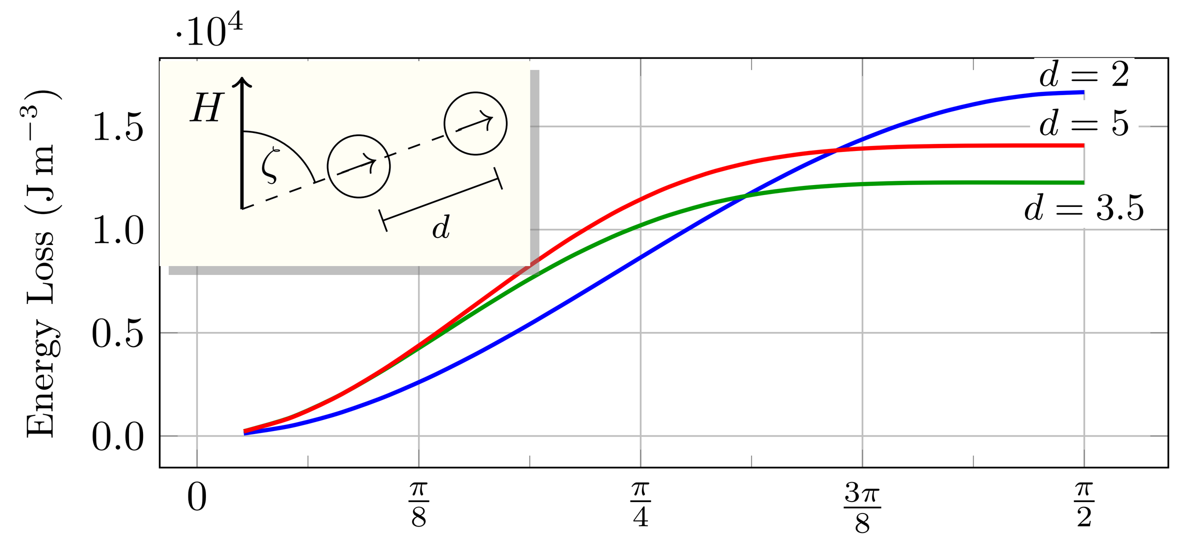
The effect of dipole-dipole interactions is investigated for different MNP orientations.

Effect of inter-particle distance



d, distance between particle centres relative to particle radius.

Effect of particle centre alignment



ζ, angle between external magnetic field and particle centres.

Conclusions

- Our results for the non-interacting case are consistent with ref. [7].
- Consistent with observations in ref. [6], the interparticle interactions are seen to hinder the heating mechanism. As expected the interaction effects fall off with $\sim|\mathbf{r}|^3$. Thus, interaction effects predominate when interparticle distance is $\leq\sqrt[3]{\frac{M_s}{H}}$.

Future Work

More complex arrangements can be considered. These include likely physical arrangements such as: • Chains • Cluster • Equi-spaced • Random

Acknowledgements

- MB acknowledges WIT PhD scholarship and is grateful to the organisers of ICSCAMC 2016 for a travel grant.
- PJC acknowledges the support of the School of Engineering & Dept. of Engineering Technology, WIT to attend ICSCAMC 2016.
- Dr Paul Southern of University College London is thanked for helpful conversations at ICSCAMC 2014, Dresden.

References

[1] J. Carrey et al. *J. Appl. Phys.*, 109(8), 2011.
[2] Luis C. Branquinho et al. *Sci. Rep.*, 3:2887, 2015.
[3] M Osaci et al. *IOP Conf. Series: Mater. Sci. Eng.*, 106:012004, 2016.
[4] D. Soto-Aquino and C. Rinaldi. *J Magn. Magn. Mater.*, 393:46 – 55, 2015.
[5] M B López et al. *Rep. Prac. Oncol. Radiother.*, 18:397–400, 2013.
[6] C. Blanco-Andujar et al. *Nanoscale*, 7(5):1768–1775, 2015.
[7] P F de Châtel et al. *J. Phys.: Condens. Matter*, 21:124202(8pp), 2009.
[8] W. T. Coffey et. al. *Adv. Chem. Phys*, pages 263–464, 1992.