Multiscale Approach to Coupled Brownian and Néel Dynamics for Collections of Magnetic Nanoparticles: Application to Magnetic Particle Spectroscopy for Biological Sensing

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Magnetic Particle Spectroscopy (MPS) is a potentially powerful, highly sensitive, and inexpensive platform for pathogen detection, cell labelling and tracking, biological and biomedical assays, and blood analysis. [1] In addition to the biological applications, it can also detect environmental pollutants in liquids and foods.

MPS depends on the change in the rotational motion of magnetic nanoparticles when a pathogen or or particle of interest is attached to a functionalized magnetic nanoparticle. Creating and underdstanding the long-time behavior of these rotating particles is vital to interpretation and evaluating the presence of the pathogens.

Long time (seconds) simulations of magnetic nanoparticles in oscillating magnetic fields (kHZ) are computationally difficult due to having coupled dynamics with two different time scales. The Néel motion of moments within particles occurs with a timescale of nanoseconds. This is 3-6 orders of magnitude smaller than that for Brownian rotation. To capture the coupled Néel motion, usually calculated with LLG dynamics, and Brownian motion, one often uses time steps of 10 fs. This is computationally intractable, especially when one examines thousands of nanoparticles, a number appropriate for experiments.

We have developed a method of simulating the results from smaller time scale dynamics using a telegraph scheme which is based on rate equations. This considers interwell transitions via rate equations. This scheme allows for larger time steps while still accurately simulating Néel dynamics. Because of this we can explore longer time scales which are not computationally feasible when using LLG. We show this method works well for temperatures below 350 K and arbitrary orientations of the anisotropy axis, by matching relaxation times calculated from LLG. With this approach one can investigate relaxation times in various cases, dynamics in oscillating fields at lower frequencies, hysteresis curves, and mixed Brownian and Néel motion.