Brownian Dynamics of Interacting Anisotropic Magnetic Nanoparticles

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Introduction:

Anisotropic magnetic nanoparticles (AMNPs) have irregular physical properties that differentiate them from uniform, spherical particles. Currently, anisotropic magnetic particles can be fabricated in a variety of ways, which are classified by shape anisotropy, surface anisotropy, branchiness, and internal configuration. Additionally, the magnetic dipole in these particles is oriented in a specific direction. As a result, the response of the magnetic dipole to an externally applied magnetic field can affect the orientation of the particle.

Because AMNPs combine both shape anisotropy and magnetic polarization, their positional and orientational particle-particle interactions can be directly controlled by externally applied magnetic fields. The "tunability" of AMNP interactions gives them considerable potential for a variety of uses. Generally, they are used as tunable building blocks for materials with unconventional properties. For example, AMNPs are subject to research on the development of materials with magnetically controllable optical properties, such as windows with automatic lighting control. AMNPs show potential for use in numerous other fields as well, including in microfluidics (*e.g.*, sensing artificial skin), chemical catalysis (*e.g.*, catalyzing redox reactions), biomedicine (*e.g.*, targeted drug delivery), electronics (*e.g.*, telecommunication), and nanorobotics (*e.g.*, constructing nano-robots).[1]

In this project, we will focus on binary systems of colloidal AMNPs with shape anisotropy. These pairs of particles are of particular interest in the development of materials with reconfigurable properties. When using singular AMNPs to fabricate tunable materials, the particles tend to get stuck in packed configurations where nearby particles restrict the rotation and translation of each individual particle. As a result, the tunability of the material suffers as the AMNPs respond less to the magnetic field. On the other hand, using binary AMNP systems, each pair of particles responds independently to the magnetic field, sustaining the tunability of the material. Binary AMNPs show promise in the fabrication of tunable materials, but the particle-particle interactions of magnetically controlled binary AMNPs are not fully understood. The dynamic behavior and interaction relaxation of binary AMNP systems under time-varying magnetic fields need further examination in order to verify the feasibility of building tunable materials with these particles.

Project Description:

This research hopes to directly study the dynamic configuration of AMNPs pairs under the influence of a time-varying magnetic field. In particular, we will investigate and predict the dynamic response of the binary magnetic particles to changes in the magnetic susceptibility of the particle, the aspect ratio of the particle, the aspect ratio between the two particles, and the frequency of the time-varying magnetic field. By changing these variables, we expect to learn how to control the precise characteristics and behavior of different binary AMNP systems. With this information, we plan to settle the fundamentals for developing an algorithm capable of controlling the relative alignment of AMNP assembly with a magnetic field.

Methodology:

In this work, we will calculate the force and torque of an interacting pair of magnetic particles and use these expressions to simulate the three-dimensional behavior of the pair of AMNPs over time. We plan to introduce the previous expressions in a Brownian dynamics simulation to model the relative position and orientation of the particles as the magnetic field changes. Brownian dynamics simulation is a useful technique commonly used to simulate diffusional processes in complex fluids. At its core, this technique involves integrating a stochastic differential equation forward in time to plot the trajectories of the solute particles.[2] We will use computational tools such as MATLAB, Wolfram Mathematica, and Fortran to perform these calculations and simulations. Additionally, we will use mathematical principles such as order parameters and mean-passage-time to help describe the motion of the particles.

Outcomes:

When the simulations are completed and fully analyzed, I will write a final report summarizing the project results. I plan to publish this report in Perpetua and present the project results at the Fall 2021 Research Horizons Day. In collaboration with Dr. Torres-Díaz, the extended version of the final report will be published in a peer-reviewed Journal.

Timetable:

The project will be completed during the 10 weeks between May 10 and July 16.

Contingency Plans:

In the case that UAH limits in-person interaction between faculty and students during the summer term, this project can be carried out remotely. Dr. Torres-Díaz and I will meet every other day through Zoom. We will set up a lab-computer that I have access to at UAH on which I can run simulations. Due to the digital nature of this project, is will not be difficult to transition to remote work if necessary. Moreover, I remotely worked with Dr. Torres-Díaz in an unofficial capacity last summer, researching Janus superellipsoid nanoparticles, and thus we have experience working on projects together online.

Citations:

[1] D. Lisjak and A. Mertelj. Anisotropic magnetic nanoparticles: A review of their properties, syntheses and potential applications. *Progress in Materials Science*, 95, 286-328. 2018.
[2] P.S. Doyle and P.T. Underhill. Brownian Dynamics Simulations of Polymers and Soft Matter. In: Handbook of Materials Modeling, edited by S. Yip, *Springer Dordrecht*. 2005.