Brownian Dynamics of Interacting Anisotropic Magnetic Nanoparticles

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Motivation
Magnetized nanoparticles with shape anisotropy have potential applications in several fields, including optics (e.g., windows with controlled transparency), biomedicine (e.g., targeted drug delivery), and chemical catalysis (e.g., catalyzing redox reactions). One particularly exciting area of interest is nanorobotics. Theoretically, two attached magnetized colloidal nanoparticles can swim by deforming and reforming under the influence of a time-varying magnetic field. However, simple nanorobots face an obstacle known as the Scallop Theorem, which states that a swimmer experiencing time-periodic motion in a Newtonian fluid cannot achieve net locomotion. Thus, to controllably maneuver the nanorobot, the return path from deformation must differ from the deformation path, breaking the symmetry of the periodic motion. Using various shapes of ellipsoidal particles offers one method of breaking the symmetry. But before the goal of fabricating nanorobots from anisotropic magnetic nanoparticles can be realized, the dipole-dipole interactions of these particles must be understood. This research aims to model the Brownian motion of two close anisotropic magnetic nanoparticles under the influence of an external magnetic field.

Methodology
Brownian dynamics of a particle \( J \) is described by

\[
\left( \frac{d\mathbf{u}}{dt} \right) = -\nabla U + \mathbf{f},
\]

where the dipolar interaction force results

\[
\mathbf{F}_{\text{dd}} = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{P}_d \cdot \mathbf{d}_d}{r_d^3},
\]

and the dipolar interaction torque is

\[
\mathbf{M}_{\text{dd}} = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{P}_d \times \mathbf{d}_d}{r_d^5}.
\]

Dipole-field interaction force results

\[
\mathbf{F}_{\text{df}} = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{P}_d \cdot \mathbf{d}_f}{r_f^3},
\]

Dipole-field interaction torque results

\[
\mathbf{M}_{\text{df}} = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{P}_d \times \mathbf{d}_f}{r_f^5}.
\]

A repulsive potential is considered to avoid particle overlapping:

\[
\mathbf{U}_{\text{rep}} = 2e^{-\kappa r}.
\]

Brownian force and torque is generated using a Box-Muller transform with a normal distribution of vectors:

\[
r = \sqrt{\frac{2\ln(\alpha)}{\kappa^2}}, \quad \theta = 2\pi \cdot \cos(2\pi \cdot \alpha).
\]

Quaternion parameters are used to track particle orientation, and the transformation matrix \( \mathbf{A} \) relates the fields in laboratory and particle coordinate systems:

\[
\mathbf{A} = \begin{bmatrix}
\sqrt{\xi^2 - \eta^2 - \zeta^2 - \xi^2} & 2(\eta \xi - \chi \zeta) & 2(\eta \chi + \xi \zeta) \\
2(\xi \eta + \zeta \chi) & \xi^2 - \eta^2 + \zeta^2 - \xi^2 & 2(\xi \chi - \eta \zeta) \\
2(\xi \eta - \zeta \chi) & 2(\xi \chi + \eta \zeta) & \chi^2 - \eta^2 + \zeta^2 + \xi^2
\end{bmatrix}
\]

References

Conclusions and Future Work
We developed a reliable model to quantify the dynamics of the dipole interaction between multi-shaped ellipsoids. In the future, the dynamics of longer and larger systems will be considered. We aim to use the dipole interaction model to simulate the motions of nano-robots.

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Figure 1. Left to right, ellipsoidal particles as spheres, circular disks, rectangular disks, and elliptical disks.

Figure 2. Dipole-dipole dynamics with \( \beta_2 = 10 \). The force (top) and torque (bottom) fields are represented over the dipolar interaction energy.

Figure 3. Simulation snapshots with various particle shapes and in various conditions. All using 2000 time steps and \( \Delta t = 0.12 \). The magnetic moment of each particle points in the positive x-direction (red axis), \( t_0 \) represents the initial configuration.