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Dynamics of paramagnetic squares in uniform magnetic fields

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The magnetic forces between paramagnetic squares cannot be calculated using a classic dipolar model because the magnetic field distribution is not uniform within square particles. Here, we present the calculation of magnetic forces and torques on paramagnetic squares in a uniform 2-D magnetic field using a Laplace's equation solver. With these calculations, we simulate the variations in equilibrium configurations as a function of number of interacting squares. For example, a single square orients with its diagonal directed to the external field while a system of multiple squares will assemble into chain-like structures with their edges directed to the external field. Unlike chains of spherical magnetic particles, that easily stagger themselves to aggregate, chains consisting of magnetic squares are unable to aggregate due to interchain repulsion.

1. Introduction

The manipulation of superparamagnetic colloidal particles using magnetic field has been employed in a variety of applications, such as altering fluid rheology [1,2], directed motion [3,4], force probing [5,6] as well as model systems for investigating physical phenomena like phase behavior [7,8]. In these applications, the colloidal particles are typically spherical in shape and their mutual interaction forces are classically calculated by dipole-based models [9]. The basis of dipole-based models is that in the presence of a uniform magnetic field, a spherical paramagnetic particle acquires uniform magnetization and thus generates a dipolar magnetic field around the particle [10]. Predictably, dipole-based models cannot be used to calculate the magnetic forces between non-spherical magnetized bodies. Alternatively, these forces can be calculated more accurately using a Maxwell stress tensor combined with solving Laplace's equation for magnetostatics [11], which is referred to as the Laplace's equation solver (LES) method. This method is inherently capable of calculating the magnetic force on any enclosed magnetized body, thus it is not restricted by shape.

With new interesting synthesis methods, colloidal squares are easily realized. Square particles show interesting packing behavior and have been reported as a model system for molecular liquid crystals [12–14]. Most recently, an analytical study on ferromagnetic squares situated periodically on a cubic lattice site has been reported [15]. However, there are few reports that describe the ability to tune the interaction potential between square colloids or describe their assembly dynamics. Here, we perform calculations of the magnetic force and torque on arbitrarily placed paramagnetic squares in a uniform magnetic field using the LES method. The squares or rectangles used in this work have a short edge length D = 2 μm, a volumetric magnetic susceptibility $\chi = 1$, and an external magnetic field strength with a magnitude of B_0=10 G in the positive x-axis direction. These calculations reveal how particles with four-fold symmetry aggregate in a uniform magnetic field.

2. Numerical methods

In the perspective of scalar magnetic potential, the Maxwell equations for magnetostatics can be simplified to Laplace's equations for different media [11]:

$$\nabla^2\phi_i = 0$$
$$\nabla^2\phi_{DM} = 0 \tag{1}$$

where ϕ_i is the scalar magnetic potential for particle n, and ϕ_{DM} is the magnetic potential for the dispersion media. The boundary conditions at the surfaces of the squares are

$$\phi_i = \phi_{DM}$$
$$\mu_p\frac{\partial\phi_i}{\partial r_i} = \mu_0\frac{\partial\phi_{DM}}{\partial r_i} \tag{2}$$

where $\mu_p = \mu_0(1+\chi)$ is the particle permeability. The boundary condition at $r_i \to \infty$ is

$$\phi_{DM} = -\mathbf{H}_0\cdot\mathbf{r}_i \tag{3}$$

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Due to the complex boundary conditions, the profile of permeability is smoothed using indicator functions [11]. The indicator function $\lambda_i(\mathbf{r})$ for the ith particle is

$$\lambda_i(\mathbf{r}) = \frac{1}{2}\left[\min\left(\tanh\left(\frac{1-|r'_{ix}|}{\xi}\right),\ \tanh\left(\frac{1-|r'_{iy}|}{\xi}\right)\right)+1\right] \tag{4}$$

Here ξ is the thickness of the interface between the particle and the surrounding medium, r'_{ix} and r'_{iy} are the x and y components of $r'_i = M\cdot(r - r_{c,i})$ where $r_{c,i}$ is the central position of the ith particle, and M is the orientation matrix defined as $M = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ where θ is the orientation angle between the edge of the square and the external magnetic field. An overall indicator function for the entire system is given by summing up the indicator functions over all particles.

$$\lambda(\mathbf{r}) = \sum_{i=1}^{n} \lambda_i(\mathbf{r}) \tag{5}$$

The discontinuous physical property in the equation is in the permeability μ, therefore the overall indicator function is used to smooth the profile of it.

$$\frac{1}{\mu(\mathbf{r})} = \frac{1}{\mu_p(\mathbf{r})}\lambda(\mathbf{r}) + \frac{1}{\mu_0(\mathbf{r})}(1-\lambda(\mathbf{r})) \tag{6}$$

By using the smoothed profile, the boundary conditions at the interfaces will be automatically satisfied. A two-grid method is used to numerically solve smoothed Eq. (1) [11].

3. Results and discussions

3.1. A single square

In two-dimensions (2-D), paramagnetic spheres can be considered as disks, which also acquire uniform magnetization when placed in a uniform magnetic field. However, paramagnetic squares do not have a uniform magnetic field distribution within the particle (Fig. 1(a) and (b)) when placed in a uniform magnetic field. Additionally the magnetic field distribution outside the square is not axisymmetric since the symmetry axis of the square does not coincide with the orientation of the external magnetic field. The highest magnetic field intensity is distributed in the vicinity of the far-left and the far-right vertices of the square, leading to a non-zero torque rotating the square towards an orientation where its long axis coincides with the direction of the external field. Fig. 1(c) shows the torque τ exerted on the square for different edge-to-field angles, θ. We set the initial angle $\theta = 0°$ for our calculations. When $-45° < \theta < 0°$, the torque is counterclockwise (Fig. 1(b)), changing θ towards $-45°$, to the orientation where $\tau = 0$. When $0° < \theta < 45°$, the torque is clockwise (Fig. 1(a)), changing θ towards $45°$ where $\tau = 0$. This indicates that at $\theta = 0°$ the configuration of the square is metastable. Though $\tau = 0$ at $\theta = 0°$, $\lim_{\theta\to 0^+}\tau = 2.6\bullet 10^{-20}$ N m and $\lim_{\theta\to 0^-}\tau = -2.6\bullet 10^{-20}$ N m, leading to a singularity at $\theta = 0°$. Therefore a paramagnetic square always

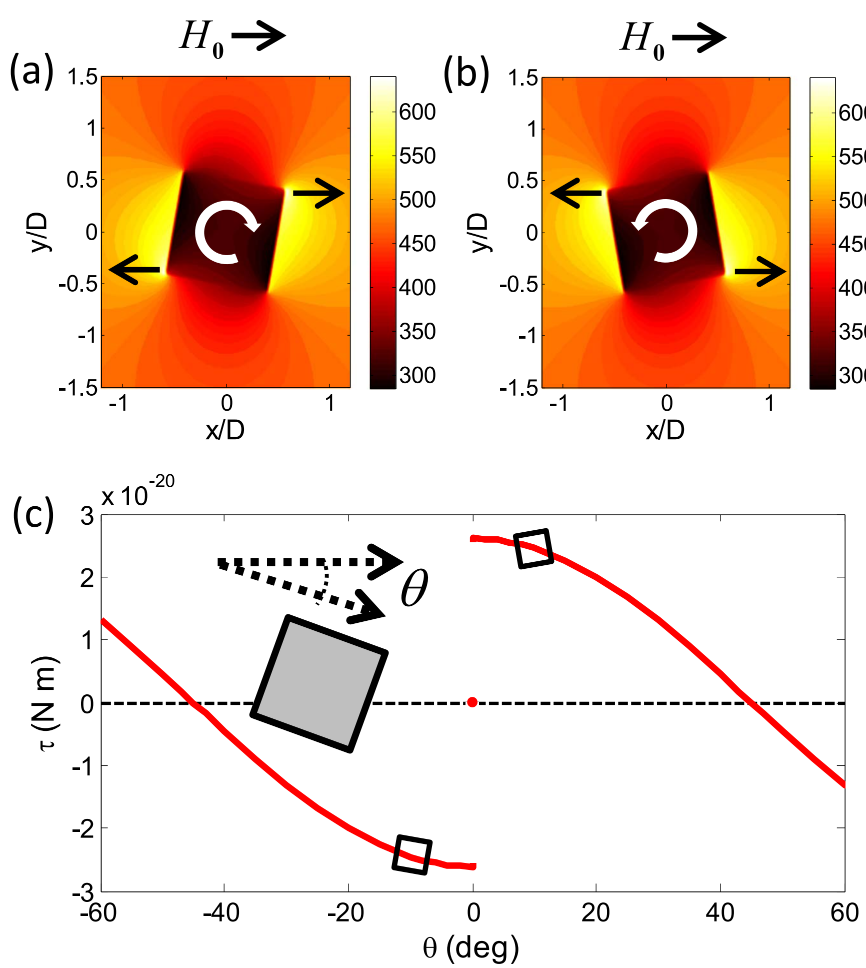

Fig. 1. A single square under a uniform magnetic field. (a) The magnetic field distribution of a square with −10° orientation. Colormaps indicate the magnetic field intensity in units of A/m. (b) The magnetic field distribution of a square with 10° orientation; (c) The torque on a square with different orientations.