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Modeling the impact of finite magnetic anisotropy on systems of ferromagnetic nanoparticles

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Magnetic nanoparticles (MNPs) are an essential building block of magnetoresponsive soft matter systems and remain a subject of intense research for already more than seven decades. Even for the simple case of a single ferromagnetic monodomain nanoparticle in a liquid or viscoelastic background under thermal fluctuations, the accurate modeling of its response is challenging due to the presence of both, translational and rotational Brownian diffusion of the particle and Néel fluctuations of its magnetic moment due to finite magnetic anisotropy, whose relative importance and characteristic time scales change with the particle size and the background conditions [1]. The behavior of dispersions of MNPs becomes even more challenging when interparticle interactions, being these magnetic and/or hydrodynamic, enter into play. Thus, a large fraction of modeling efforts to date have been based on strong simplifications that neglect certain aspects of the problem, such as interparticle magnetic interactions in dilute systems or, more frequently, the interplay between finite anisotropy and hydrodynamics. The latter, however, is not valid for applications of high interest such as micro- and nanofluidic systems or magnetic hyperthermia applications.
Our goal is to put forward a computer modeling approach able to represent accurately the properties of finite dispersions of MNPs in viscous and viscoelastic environments when interparticle interactions and their finite magnetic anisotropies can not be neglected. As a first step, we implemented an extended Stoner-Wohlfarth model for uniaxial anisotropy that includes thermally activated Néel fluctuations [2] and adopts the asymptotic behavior predicted by the Fokker-Planck-Brown equation for ferromagnetic monodomain particles [1]. This model has been combined with a molecular dynamics integration scheme that calculates the Brownian diffusion of the particles and can be coupled to different hydrodynamics solvers. In this contribution we will present the first results obtained with this approach for small systems of nanoparticles under different conditions, including rotating and oscillating external fields and simple background flows.

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