# Ground state microstructures of magnetic filaments

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The synthesis of artificial magnetic filaments by mutually linking particles with magnetic properties has set the path towards the construction of supramolecular magnetic polymers at the scale of tenths of nanometers[1,2]. These novel structures, known as magnetic filaments, can hold a permanent dipolar moment at room temperature even in the absence of an external magnetic field. The potential use of magnetic filaments in technological applications, from magnetic memories to chemical and pressure nanosensors, has raised the interest in the study of their fundamental microstructure properties and to elucidate their ground state conformations.

In this work we investigate the ground state structures of stiff magnetic filaments in the bulk and in constrained 2D geometries via extensive Langevin dynamics simulations. The magnetic filament is represented by a coarse-grained bead-spring model where each bead bears a point dipole, free to rotate in 3 dimensions and located in its center. The excluded volume interaction is introduced via a soft-core repulsive potential[3].

We analyze the different topological structures that are likely to exist at low temperatures in terms of the competing dipole strength, soft-core repulsion, spring elasticity and chain stiffness interactions. In the range of parameters studied we find the majority of structures to fall in two categories: rod-like elongated chains and rings. This result reproduces the aggregates observed and predicted from density functional studies in quasi-2D ferrofluid monolayers[4,5]. Furthermore, we determine, in the limit of zero temperature and at a given dipole strength, the minimum filament length beyond which the transition from elongated towards a ring structure exists. As a difference with the ferrofluid monolayers, we find in the ring domain an optimal ring size value corresponding to configurations with a minimum energy per polymer bead. As a consequence, long filaments wish to form rings with its corresponding optimal size, leading to fascinating structures that strongly differ depending on the embedded system dimensionality (see Fig.1).

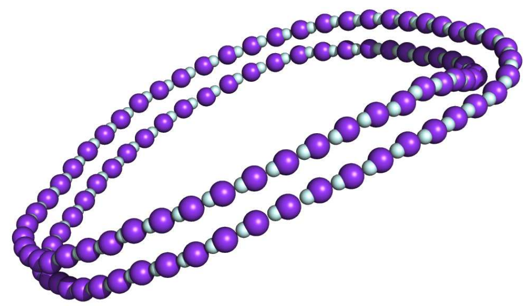

FIG. 1. Typical snapshot of an equilibrium configuration of a flexible magnetic filament in the bulk (3D)

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