Phase diagram of a single magnetic filament in bulk, an approach via numerical simulations and theory.

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Magnetic filaments constitute a novel type of unconventional magnetic materials. Basically, magnetic filaments can be conceived like supramolecular polymers at the scale of tenths of nanometers that may exhibit permanent magnetic properties at room temperatures in contrast with chemical 1D polymers which are magnetic only at $T < 100K$[1].

Despite the idea of magnetic filaments is not new at all, since the Cretaceous nature has been using systems very similar to the magnetic filaments inside magnetostatic bacterias to help them to orientate[2], the humankind has only very recently begun to caress its potential for novel applications[3,4]. Among the many new plausible applications there is the chance of using them as an improved substitute for current ferrofluids or magnetorheological fluids. In turn, these new magnetic systems pose an interesting case of research for Soft Matter community due to the non-isotropic character of the magnetic interaction combined with the physics of traditional polymers.

The current state of the art in which still very little is known about the physical behavior of such novel magnetic systems is the perfect scenario for the use of numerical simulations which can contribute in a decisive way to unravel and understand how such filaments may behave under different experimental conditions. Furthermore, numerical simulations can help in assessing the usefulness or not of the magnetic filaments for certain kinds of technologies.

After the study of the properties of a single magnetic filament close to an adsorptive wall[5], in this contribution we will present our recent advances in the characterization of magnetic filaments in bulk. In particular we will focus in the phase diagram of such magnetic filaments as a function of the temperature, the value of the magnetic moment of the beads that constitute the magnetic filament, the length of the chain, and the intensity of the interaction (attractive or repulsive) among those beads of the magnetic filaments. Furthermore, the dependence of the phase diagram with the value of an applied external magnetic field will be also studied in detail.

As we will show, our results predict a very complex phase diagram which includes many types of structural transitions ranging from globular and pseudo-helicoidal states till the case of rings and rods. In addition to our numerical simulations we will present a simple theoretical statistical-mechanics model which will be compared stringently with our simulations in order to validate it. The new theoretical model will help us to explain the physics behind the phase transitions we have observed, and it will contribute to pave the way in the study of solutions containing magnetic filaments as solutes.

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