Low-temperature behavior of the dipolar hard sphere fluid

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We describe the self-assembly in magnetic nanocolloids by using a dipolar hard sphere (DHS) model. A DHS consists of a point dipole embedded in the center of a hard sphere that generates long-range anisotropic interactions. At low temperature DHS particles self-assemble into complex structures, with primary structures composed by rings and chains; understanding the emerging structures of the system is fundamental for designing new magnetic fluids-based devices for technological and medical applications.

We base our theoretical approach on classical Density Functional Theory, an approach that is able to capture the density and temperature dependence of the ring-chain equilibrium.[1] In order to estimate the ability of the theory to predict (i) the cluster size distribution of rings and chains at different values of the temperature and (ii) the individual cluster partition functions, we perform grand-canonical Monte Carlo simulations. We introduce specialized Monte Carlo biased moves, which favor the breaking and reforming of bonds. The knowledge of the cluster partitions functions, together with our analytical approach, allows us to calculate the free energy of systems at low-to-intermediate densities, where the clusters can be considered as weakly interacting.[2]

We confirm that for low concentrations and low temperatures, the majority of magnetic nanoparticles is aggregated in rings; for higher concentrations, low temperature clusters merge together into more complex branched structures, characterized by junctions between chains and rings. Our results will allow us to describe the next hierarchical level of self-assembly in magnetic nanocolloids: the aggregation of basic branched clusters into complex networks.

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[1] S.S. Kantorovich, A.O. Ivanov, L. Rovigatti, J.M. Tavares and F. Sciortino,*Phys. Chem. Chem. Phys.* **17**, 16601 (2015)

[2] M. Ronti, A.O. Ivanov, L. Rovigatti, F. Sciortino and S.S. Kantorovich, in preparation