Computer simulation of a 2D liquid crystal confined in a circular cavity

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Nematic fluids in confined geometries are a subject of much interest from both fundamental and technological points of view. In these systems there exists competition between orientational ordering, anchoring (favoured director alignment at surfaces) and elasticity. The equilibrium configuration depends sensitively on the imposed conditions. This interplay involves frustration and formation of defects. Here we consider two-dimensional (2D) nematics, which are easier to analyse and at the same time present some interesting peculiarities[1,2]. Recently vibrated quasimonolayers of macroscopic particles with anisotropic shape have been studied, using circular containers; patterns and behaviours similar to those found in thermal anisotropic fluids were observed, including nematic and smectic ordering[3]. Our recent, exploratory theoretical work on this problem considered the thermodynamics, phase behaviour and structure using a simple version of density-functional theory[4,5].

In the present work we use Monte Carlo (MC) simulation to study the ordering properties of a fluid of rectangles in a circular cavity. The rectangles have a length-to-width ratio of 40, with L the length and σ the width; this value was dictated by the recent experiments on vibrated quasimonolayers of Galanis et al.[6]. Our aim is to compare our simulation results with those obtained from the density-functional theory, on the one hand, and with those coming from the experiments on granular matter, on the other, in an effort to shed some light on the true properties of the equilibrium system, and also on the similarities between a thermal system and a granular system driven by dissipation.

In bulk conditions, our model fluid presents stable isotropic and nematic phases, with a continuous phase transition at some critical value of density. In the confined geometry, and due to the circular geometry, the fluid is subject to frustration since particles try to respect the orientation favoured at the surface (long axes of particles along the tangential direction), while at the same time elastic modes are excited due to the director distorsion. These factors imply the existence of defected regions in the fluid, where the nematic director is not defined.

In our MC experiments on small cavities ($R < 15L$), we obtain a collection of equilibrium configurations from the very dilute régime to high packing densities[7]. Particles are added one by one, and every time a particle is added we thermally equilibrate the fluid. Fig. 1 shows two structures for $R = 7.5L$: one at low density (top panels), where the fluid adopts an isotropic configuration; and another at high density (bottom panels), where the fluid is in a nematic state, but two line structures (domain walls) are created at opposite sides with respect to the cavity centre. The walls fluctuate in position quite rapidly. In this configuration director distortion is minimised, while at the same time surface energy is optimised. For such small cavity radii we do not observe the expected structure with tangential symmetry and a point defect at the centre[5]. Changes in the structure of the fluid for larger cavities and connection with density-functional theory are discussed.

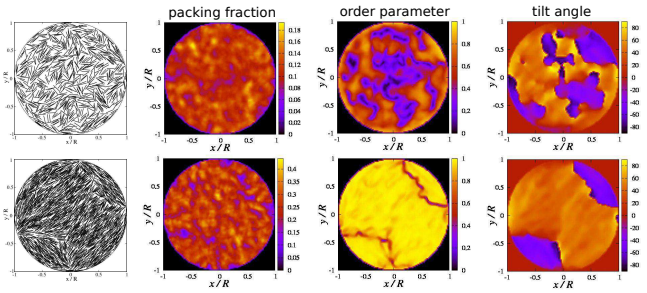

FIG. 1. Panels from left to right: particle configurations and packing fraction, uniaxial order parameter and director tilt angle local fields. Top panels correspond to a number of particles $N = 800$, while the bottom panels pertain to the case $N = 1970$. In all cases the cavity radius is $R = 7.5L$.

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