2D liquid crystal confined in a square cavity

M. González Pinto[1], Y. Martínez-Ratón[2] and E. Velasco[1]
[1] *Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid*
[2] *Grupo Interdisciplinar de Sistemas Complejos (GISC), Departamento de Matemáticas, Universidad Carlos III de Madrid, 28911 Leganés, Madrid*

Nematic fluids in confined geometries are a subject of much interest from both fundamental and technological points of view. In these systems there is a competition between orientational ordering, anchoring (favoured director alignment at surfaces) and elasticity whose final outcome depends sensitively on imposed conditions. This interplay involves frustration and formation of defects.

3D studies of this problem, using different approaches and confinement geometries, are numerous. However, 2D fluids have not been explored in detail, and only a few simulation and theoretical works exist. Recently vibrated grains have been studied in quasimonolayers in circular cavities[1,2]. Similar behaviours to those found in thermal systems have been observed. Our recent theoretical work of this problem pointed to a rich phenomenology[3,4].

In this work we use density-functional theory, in its fundamental-measure version, to study the ordering properties of a fluid of rectangles of length L and width σ in a square cavity. The square geometry creates quite different conditions at the surfaces because of the presence of corners, and further frustration effects are expected with respect to the circular geometry.

In bulk conditions, our model fluid presents stable isotropic and nematic phases, with a continuous phase transition at a value of density which depends on the aspect ratio $\kappa = L/\sigma$. For a fixed value of κ, we study both the thermodynamics and structure of the fluid as the chemical potential is increased. Nematic ordering (capillary isotropic-nematic phase transition) is shifted in chemical potential with respect to the bulk transition and the confined nematic presents a defected structure. Changes in the structure in the nematic régime, associated with changes in the size of the square cavity, are discussed.

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