Wang-Landau Monte Carlo simulation of isotropic - nematic transition under confinement

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Liquid crystals exhibit a weakly first order transition from a disordered isotropic phase at high temperatures to an ordered nematic phase at low temperatures. What happens to the nature and content of the phase and of the phase transition when the liquid crystal is confined? The importance of this question to a technologist involved in making display and switching devices with confined liquid crystals, needs no emphasis; for a scientist involved in basic studies also, this question is important since a confined system exhibits interesting phenomena: for example, upon confinement, the isotropic-nematic phase transition temperature is lowered [1]; also confinement softens the transition [2]. Monte Carlo simulation of lattice models has emerged as a useful tool for investigating these and related issues; but simulation of small confined systems is beset with problems arising due to large statistical fluctuations that tend to completely hide any Monte Carlo signal that would otherwise capture the interesting phenomena. Hence attempts were made to model the effect of confinement in terms of quenched orientational disorder in the bulk; the advantage of such a scheme is that we can them simulate reasonably large systems. Indeed liquid crystals confined to a porous matrix can be simulated by incorporating quenched disorder at randomm locations in the bulk; periodic boundaries would reduce the finite size effects in the simulation; we can also employ finite size scaling to further take care of finite size effects. Recently Venu, Sastri and

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Murthy [3] reported a phenomenological relation that expresses the strength of quenched disorder in terms of the Monte Carlo system size, the average size of a pore in the porous medium and the size of a liquid crystal molecule; a preliminary study showed the usefulness of the empirical relation; it predicted correctly the experimental results on the suppression of transition temperature, the enthalpy of the transition and softening of the transition from the first to the second. Metropolis sampling was employed in the Monte Carlo simulations. Metropolis sampling is not very efficient for simulating large systems especially if we are interested in studying first order phase transition; the low probable microstates describing the phase coexistence never appear in a statistically significant number in a finite Metropolis sample; non-Boltzmann sampling technique are required. To this end we simulated the system with entropic/multicanonical Monte Carlo techniques; in fact we employed the recent Wang-Landau algorithm [4] in the simulation. Wang-Landau algorithm has been found to be efficient for simulating systems with discrete energy like Ising and Potts models; however there are problems when we simulate systems with a continuous energy. Hence in our study we discretized the Lebwohl-Lasher (LL) [5] potential; we first checked the performance of the discrete model by simulating the bulk transition. We found that the discrete model correctly predicts the nature of the transition and the transition temperature. The discrete LL model was then used in conjunction with the Wang-Landau algorithm and a series of simulations were carried out with different system sizes and different strengths of disorder. We find that the transition temperature is lowered when the disorder strength increases; also we find definitive signatures of softening of transition upon increase of disorder.

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