

Computer Simulations of Liquid Crystals

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1. Introduction.

Liquid crystals (LC) form a state of matter intermediate between solids and liquids [1] as indicated by their contradictory name. The main characteristic of liquid crystals at molecular level is that they possess orientational order, together with a translational mobility similar to that of liquids in nematics phases and reduced in other, smectic, types. The theoretical investigation of LC can be tackled, as for any other complex fluids, by means of approximate theories or performing numerical experiments on models. Monte Carlo simulation, one of the foremost simulation techniques [2], commonly used in studying phase transitions and critical phenomena plays an important role also in the investigation of liquid crystals for which two approaches, discussed in the following, are used. The first one deals with lattice models [3,4,5] where the molecules, or tightly ordered cluster of molecules, represented by three dimensional unit vectors ("spins") are considered to have a fixed position at the lattice sites. The spins retain full rotational freedom, subject to a certain intermolecular potential, so that

this restriction does not affect the long range orientational behaviour. The second approach, which is becoming more popular in the last few years, is to use more realistic off-lattice potentials [6], with translational degrees of freedom. Only the development of more powerful computers and of suitable parallel software allows performing *computer experiments* of this type with reasonable size (roughly a thousand particles). Parallel computing is also essential in studying lattice systems with a larger number of molecules or when it is required to investigate their behaviour under many different conditions [7]. Here we wish to describe these two approaches with some recent applications and results. Moreover the implementation of the simulations on some different computers is also briefly discussed.

2. Lattice models.

2.1 Lebwohl-Lasher potential and its generalizations.

The prototype hamiltonian for liquid crystal lattice model, introduced by Lebwohl and Lasher (LL) [3] is the discretized version of the Maier-Saupe potential [8]. Although liquid crystals are in some respect the very antithesis of lattice systems no essential feature is lost by making this approximation as far as orientational ordering is concerned. The particles, assumed to have uniaxial symmetry and represented by three dimensional spins located at the sites of a cubic lattice, interact through a pair potential of the form:

$$U_{ij} = -\epsilon_{ij} P_2(\cos \beta_{ij}) \quad (78)$$

where ϵ_{ij} is a positive constant, ϵ , for nearest neighbours spins i and j and zero otherwise, P_2 is the second Legendre polynomial and β_{ij} is the angle between the molecules. This model, although very simple, gives a good representation of the orientational properties of a real nematic, showing a weak first order nematic-isotropic phase transition (at a scaled temperature $T_{NI}^* \equiv kT_{NI}/\epsilon = 1.1232$) [5] and a reasonable dependence of the orientational order parameter $\langle P_2 \rangle$ against temperature. This behaviour can be obtained also using small lattices (a few thousands of spins) in comparison with real systems (10^{23} molecules) [4]. Possibly the model works so well because a "spin" represents a closely packed group of molecules, rather than a single particle, and these local domains maintain their local structure at various temperatures and even across the nematic/isotropic phase transition [9]. As a special case these domains could comprise just one molecule but it seems more realistic to assume that they typically include a few tens

of particles [10]. Increasing the lattice size up to 10^4 ($N \langle 10^5$ particles [5] it is possible to increase the accuracy in the determination of the critical temperature of the model up to $\approx 0.1\%$ and also to reproduce pretransitional effects that diverge, like it is found for real nematics, just below T_{NI}^* .

Apart from the lattice size another very important aspect is the choice of boundary conditions, i.e. of what environment to surround the sample with. A common choice is to use periodic boundary conditions with exact replicas of the system filling the space as needed by the range of the pair interaction. Although quite satisfactory when far from a phase transition, using periodic boundary conditions (PBC) leads to large smearing and broadening of the heat capacity and order parameter vs. temperature curves. This complicates the location of the transition and demands the use of very large samples.

Another possibility is to use the Cluster Monte Carlo simulation (CMC), introduced in Ref. [11] where the space around the sample is filled with an additional layer of spins ("ghost") which have, on average, the same ordering as that inside the lattice. The orientations of such "ghosts" are sampled from a distribution obtained, using the order parameters of the system, by means of the maximum entropy principle. The CMC method gives results, for a certain system size, comparable with those obtained employing PBC on a lattice up to 2^d times larger in d dimensional systems [11]. The CMC boundaries are particularly useful when potentials with additional parameters have to be studied and a large set of independent simulation have to be performed to obtain a phase diagram [7].

2.2 Confined systems.

Apart from basic research, the use of a large number of particles allows computer simulations of certain technologically relevant systems, such as Polymer Dispersed Liquid Crystals (PDLC) [10] and Twisted Nematic LC displays [12].

PDLC consist of a polymer matrix containing cavities filled with a liquid crystal material [13]. The boundary conditions, as well as the anchoring strength of the liquid crystal molecules to the surface, are then determined by the type of polymeric material and liquid crystal chosen. PDLC also exhibits different properties according to the size of the cavities formed in the polymer, which are in the micron or even sub-micron range. MC simulations on spherical PDLC droplets [10], have been performed by carving the sample out of the cubic lattice,

