

Computer simulation study of liquid crystal ordering near a colloid particle

Guido Germano¹, Denis Andrienko², Michael P. Allen²

¹ Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld, Germany

² H. H. Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, England

1 Nematic emulsions

Macroparticles introduced into liquid crystals considerably influence their electro-optical properties. One of the reasons is the formation of new supramolecular structures, i.e. threadlike structures consisting of colloid particles. The physical mechanism is long-range interaction of the macrodroplets. A macrodroplet distorts the director distribution and thus provides an effective long-range interaction with another similar droplet.

2 Defects make the description difficult

The complexity of such emulsions is caused by the presence of defects. Due to the topological mismatch between the local director on the particle surface and the uniform director at large distances, a drop with homeotropic boundary conditions will create a hedgehog director configuration in its immediate vicinity.

Two defect structures can result in the case of strong anchoring [1, 2]:

1. A quadrupolar structure with a ring defect (Fig. 1).
2. A dipolar structure with a satellite defect (Fig. 2).

There are no defects in the case of weak anchoring (Fig. 3).

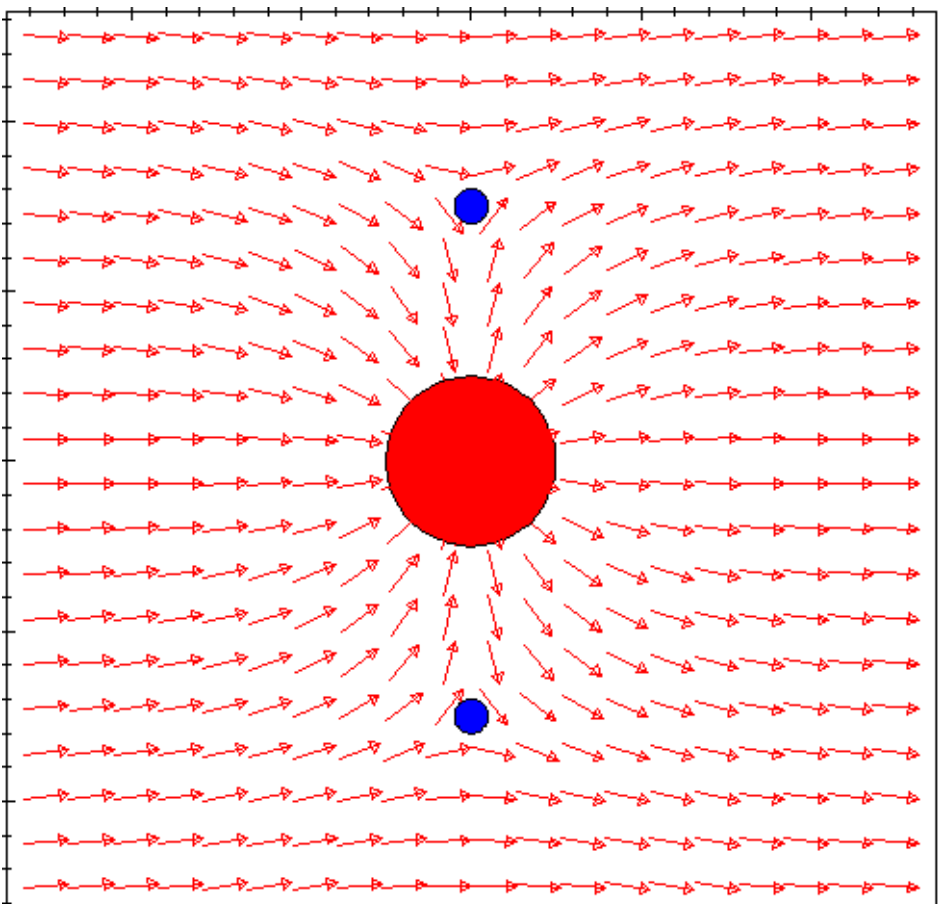


Figure 1: Particle with homeotropic boundary conditions and disclination ring.

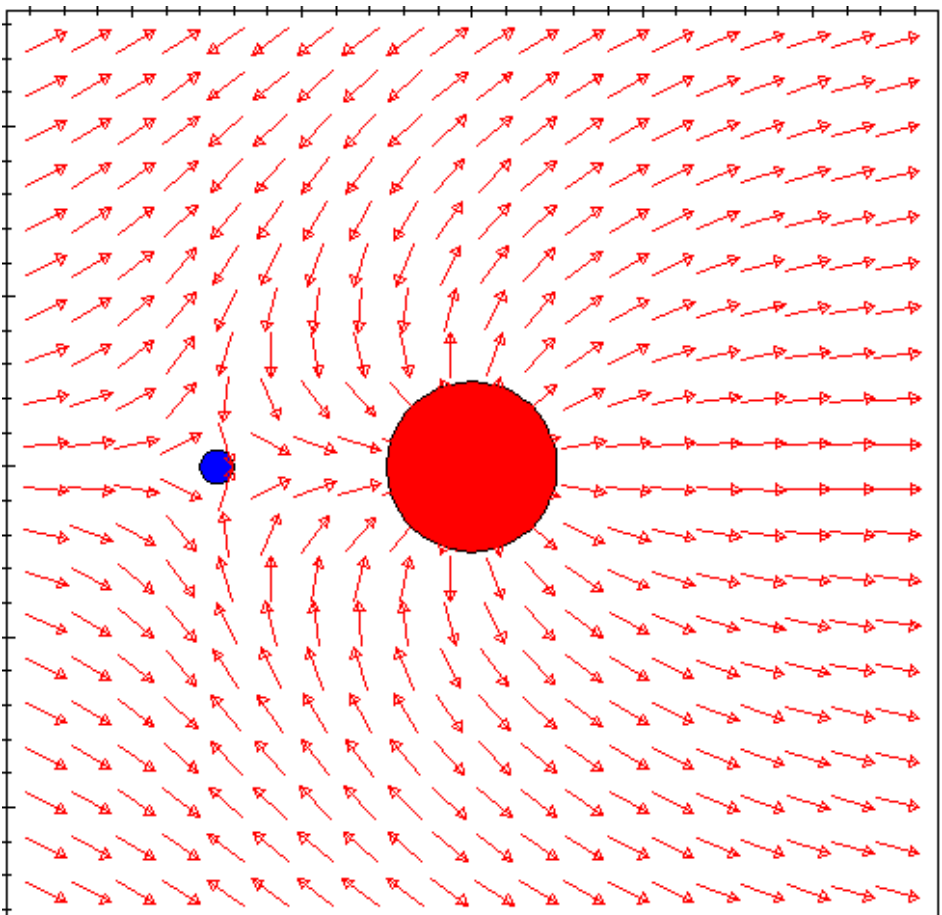


Figure 2: Particle with homeotropic boundary conditions and satellite defect.

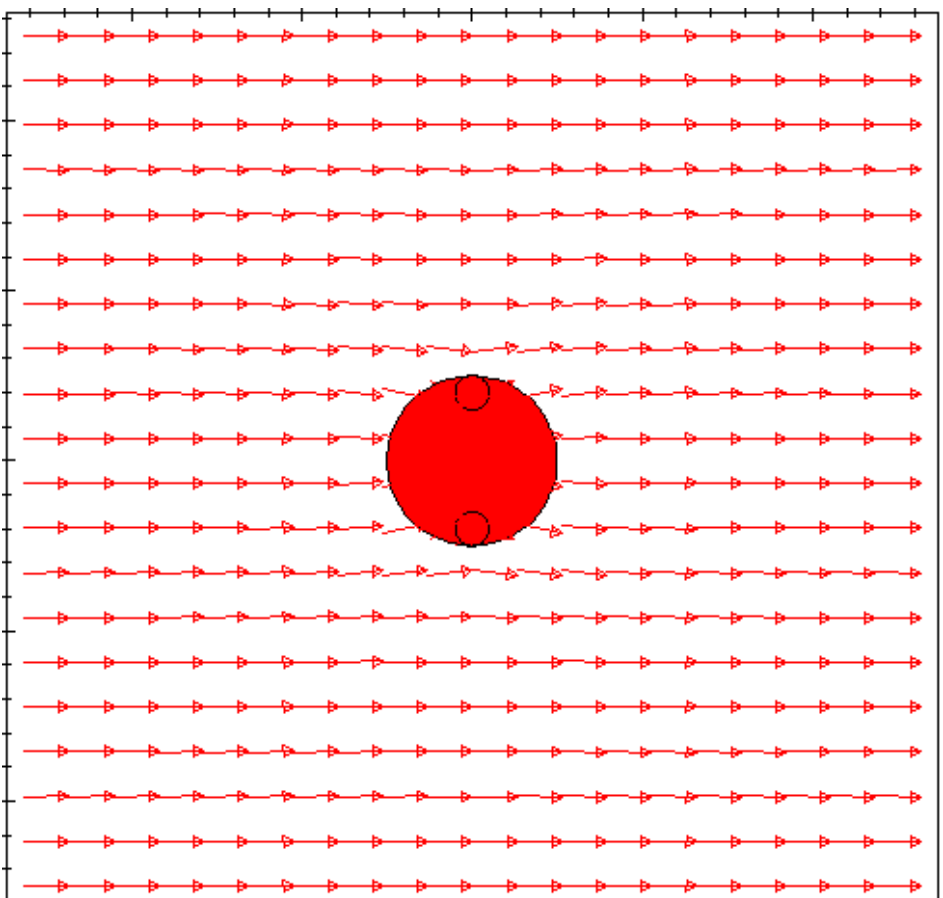


Figure 3: Particle with homeotropic boundary conditions and weak anchoring: no defect structures.

3 Disadvantages of existing theories

- The core region is treated as an isotropic inclusion with some unknown free energy [1, 3].
- The phase is treated as uniaxial (which is not true near the disclination core), and the order parameter is considered constant (which is not true either near the particle surface) [1–3].
- Dynamics is too complicated.

4 Computer simulation

Computer simulation allows to resolve the nematic orientational ordering near the particle taking into account density and order parameter variations as well as a possible biaxiality of the nematic phase close to the particle in the disclination core region.

5 Mesogen-mesogen potential

We chose the repulsive part of the soft ellipsoid potential, a variant of the Gay-Berne potential [4] with exponents $\mu = 0$, $\nu = 0$:

$$U_{ij}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) = 4\epsilon_0 [q_{ij}^{12}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) - q_{ij}^6(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j)] + \epsilon_0$$

where

$$q_{ij}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) = \frac{\sigma_0}{r_{ij} - \sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) + \sigma_0}, \quad q_{ij}^{-1} < \sqrt[6]{2}$$

$$\sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) = \sigma_0 \left\{ 1 - \frac{\chi}{2} \left[\frac{(\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{e}}_i + \hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{e}}_j)^2}{1 + \chi \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j} + \frac{\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{e}}_i - \hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{e}}_j}{1 - \chi \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j} \right] \right\}^{-1/2}$$

$$\chi = (\kappa^2 - 1)/(\kappa^2 + 1), \quad \kappa = \sigma_{end-end}/\sigma_{side-side} = 3.$$

6 Colloid-mesogen potential

The macroparticle has a radius κ and exerts a shifted Lennard-Jones repulsion on the centers of the mesogens, resulting in homeotropic anchoring of the latter on the macroparticle surface ($\sigma_c = \kappa - \sigma_0/2$):

$$U_i(\mathbf{r}_i) = 4\epsilon_0 \left[\left(\frac{\sigma_0}{r_i - \sigma_c} \right)^{12} - \left(\frac{\sigma_0}{r_i - \sigma_c} \right)^6 \right] + \epsilon_0, \quad \frac{r_i - \sigma_c}{\sigma_0} < \sqrt[6]{2}.$$

7 Computational details

The system consists of 8000 mesogens and was run on a Cray T3E with our own domain decomposition parallel molecular dynamics program for rigid bodies with axial symmetry. The colloid particle was fixed in the center of the box and the mesophase director was

constrained along the z axis.

8 Results and conclusion

Fig. 4 shows a snapshot of our system, Fig. 5 a density profile. We observed a ring defect near the colloid particle, though in the elastic theory this defect is energetically less favorable than the satellite one. This probably means that the variations of the order parameter and the density near the macroparticle play essential roles in the formation of the defect, that cannot be taken into account by theories involving just a director field. Thus computer simulations proved a useful and promising tool in the investigation of this kind of systems.

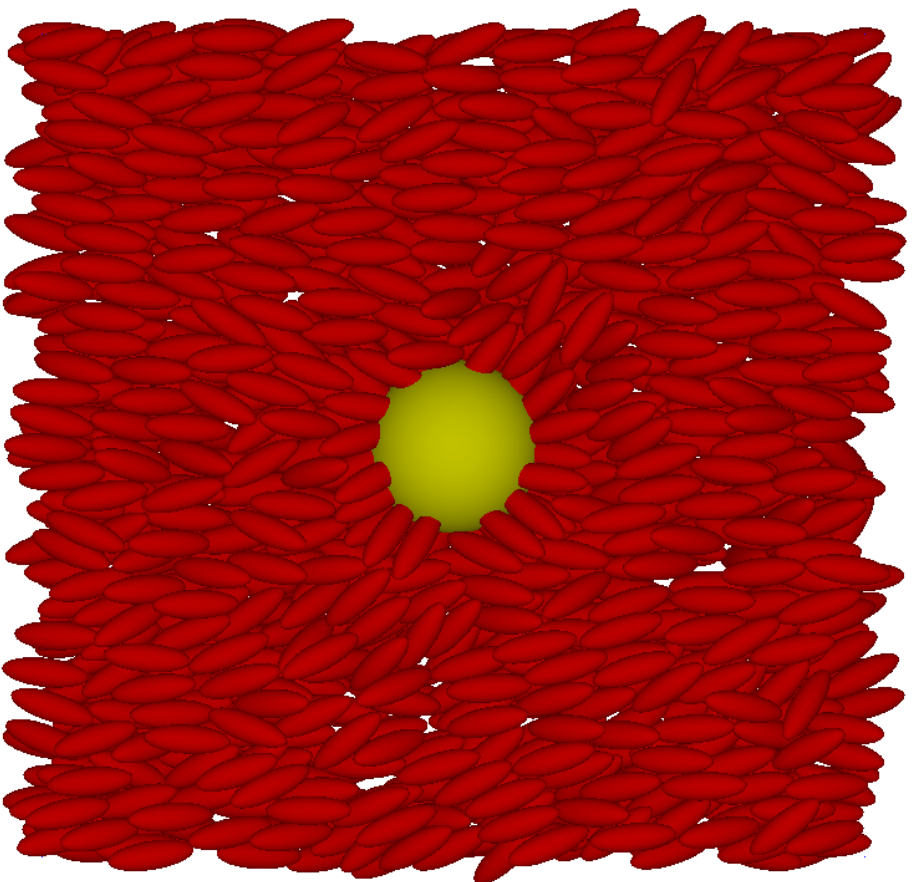


Figure 4: Slice through a configuration (zy-plane).

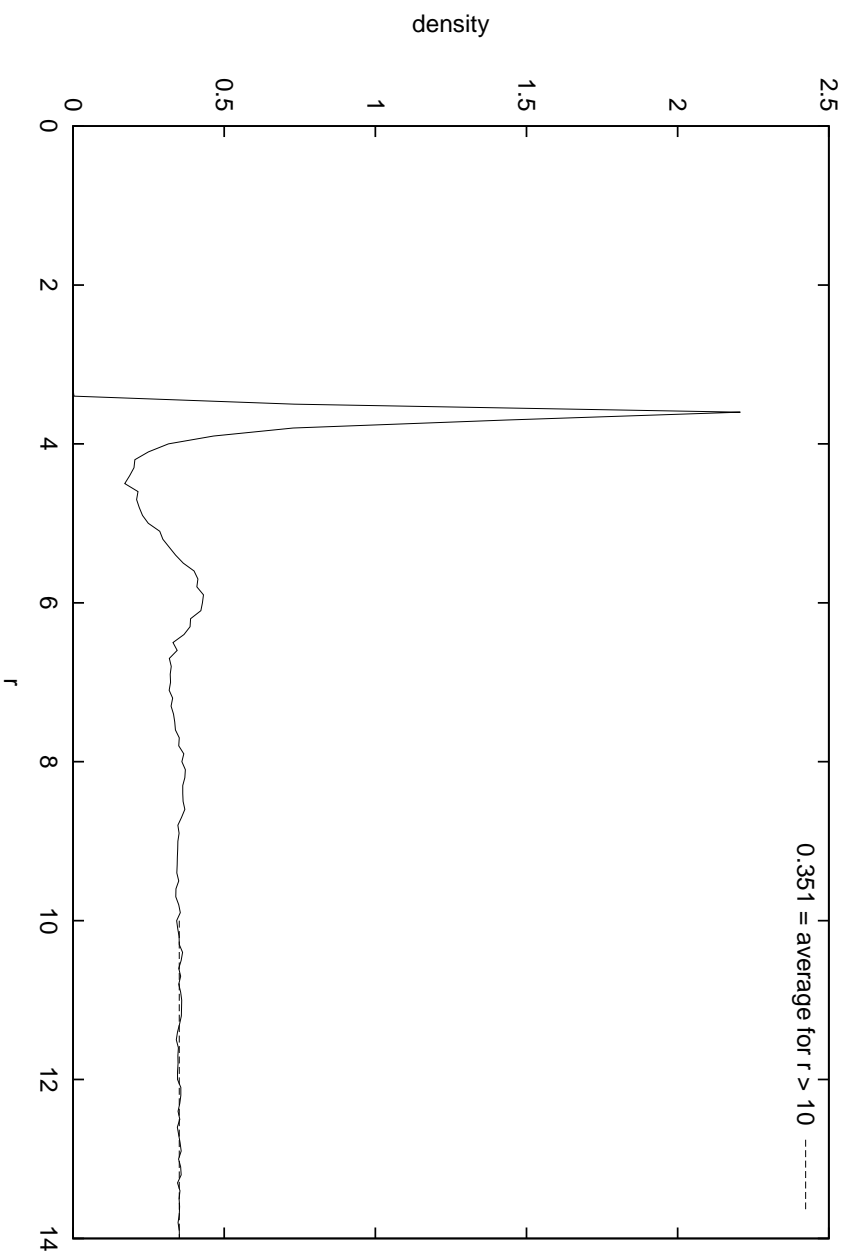


Figure 5: Density profile centered on the macroparticle; average over 100 configurations saved every 1000 steps.

9 Future work

We plan future work along the following directions:

- Different anchoring conditions.
- Study of droplet-droplet interactions.
- Inclusion of walls.
- Formation of induced supramolecular structures [5].

Acknowledgments

Financial support by EPSRC and DFG is gratefully acknowledged.

References

- [1] R. W. Ruhwandl, E. M. Terentjev, “Monte Carlo simulation of topological defects in the nematic liquid crystal matrix”, *Phys. Rev. E*, **56**, 5561 – 5565 (1997).
- [2] T. C. Lubensky, D. Pettey, N. Currier, “Topological defects and interactions in nematic emulsions”, *Phys. Rev. E* **57**, 610 – 624 (1998).

- [3] O. V. Kuksenok, R. W. Ruhwandl, S. V. Shiyanovskii, E. M. Terentjev, “Director structure around a colloid particle suspended in a nematic liquid crystal”, *Phys. Rev. E* **54** 5198 – 5203 (1996).
- [4] J. G. Gay, B. J. Berne, “Modification of the overlap potential to mimic a linear site-site potential”, *J. Chem. Phys.* **74**, 3316 – 3319 (1981).
- [5] B. I. Lev, P. M. Tomchuk, “Interaction of foreign macrodroplets in a nematic liquid crystal and induced supermolecular structures”, *Phys. Rev. E* **59**, 591 – 602 (1999).