Annihilation of a Pair Particle-Antiparticle

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Abstract: Annihilation of particles and antiparticles attracts considerable interest to a broad audience but its basics are difficult to understand. In addition this process is also relatively hardly accessed and monitored experimentally. But there exist analogous phenomena in condensed matter systems where the role of particles (anti-particles) is played by topological defects (anti-defects). Making use of this analogy we demonstrate the annihilation process in nematic liquid crystals, where this event is easier to visualise and comprehend.

Key Words: defects, nematic liquid crystals, annihilation, numerical simulation

1 Introduction

Preparing learning material for high school students is a demanding task. The material should be informative, clear and exciting. With this respect the computer based learning material is particularly adequate. It is often desirable to present high school students of science broad perspective of the topic rather than strict mathematical and physical model that is hidden behind the phenomenon. With this focus we have developed a numerical simulation of a possible annihilation scenario of a pair particle-antiparticle into the vacuum state. The annihilation is shown on the case of an analogous phenomenon in nematic liquid crystals (LC) where it can be clearly visualised and relatively easily understood.

The plan of the paper is as follows. In Section 2 (Liquid crystals: Laboratory of physics) the adequacy of liquid crystals as a testing ground of physics is explained. Basic properties of the nematic LC phase and nematic defects are described. The model used in our simulations is briefly described in Section 3 (Theory). A possible annihilation scenario of a pair nematic defect-antidefect, playing the role of a particle and antiparticle, is given in Section 4 (Results) and is also accessible on the Internet [1]. In the last section the results are summarised.

2 Liquid crystals: Laboratory of physics

Liquid crystalline [2,3] phases are often referred as a 4th state of matter. The materials that can potentially form liquid crystalline phases are commonly called liquid crystals. LC phases represent an intermediate state between ordinary liquids and crystals. They flow like an ordinary liquid. In addition they posses some long range ordering in the orientational or translational order or both of them.

It is well known that various applications based on liquid crystalline phases are inevitable in every days life. But it is perhaps less known that LCs also represent a convenient testing ground of fundamental physics [4,5,6]. The main advantages of liquid crystalline phases and structures over the other systems are the following. (i) LCs are typical representatives of "soft matter" systems. They earn this name because a relatively small amount of locally supplied energy is needed for a response on a macroscopic scale. (ii) Their response is on experimentally accessible length and time scales. (iii) LC phases are transparent for light and have electro-optic anisotropic properties. Therefore they can be studied with visible light or can be used to manipulate it. (iv) The samples with different LC structures are relatively easy prepared because they can be readily shaped with confining surfaces or external fields due to their liquid and "soft" characteristics. The chemistry of LCs is relatively well developed so that desirable behaviour can also be tailored by chemists. (v) A large variety of different LC phases and structure within them display a rich gallery of physical phenomena. With this respect phenomena exhibiting universal laws are of particular interest.

The molecules that can potentially form liquid crystalline phases are in most cases rod like. The nematic phase represents the simplest LC phase [2]. In addition to a liquid-like behaviour (it flows) it also exhibits orientational long-range ordering: the molecules tend to be oriented locally parallel. Consequently in a bulk sample (i.e. the influence of confining boundaries is negligible) the molecules are in thermodynamic equilibrium aligned on average parallel along a single symmetry breaking direction. In confined samples other nematic structures can emerge. In Figs.1-5 we show some different nematic structures realised within a long cylindrical capillary. The local average orientation of molecules is traditionally given by the unit vector field

$\vec{n}(\vec{r})$, called the *nematic director field*. Note that in the nematic phase the molecules display the so called "head to tail" invariance. A rotation of an angle π about the axis perpendicular to $\vec{n}(\vec{r})$ (i.e. the transformation $\vec{n}(\vec{r}) - > -\vec{n}(\vec{r})$) does not influence the physics of the problem.

The regions where the nematic director field is not uniquely defined are referred as nematic *defects* [2,7]. They are origin of strong localised elastic distortions resulting in relatively large free energy density costs. In nematics we meet either point (Fig.6) or line (Fig.7) defects in which the singular region is limited either to a "point" or a "line" (from the mesoscopic point of view) in space. Defects are characterised by a *topological charge* M defined with the director field surrounding the defect [2,7]. Point defects are characterised by an integer M (i.e. M=1,2,3…). For line defects also half integer values are allowed (M=1/2, 3/2..). The total topological charge M_{total} of defects within a volume is conserved for a fixed boundary condition (analogous to laws of conservation of electric and other physical charges). This conservation law regulates decay and merger of defects, their creation, annihilation and mutual transformation

In general, defects in a nematic phase behave to some extent similar to conventional electrically charged particles or lines of charge $q=Mq_o$, where q_o is the unit charge. The defects of different charge sign attract each other and repel for the same sign of M. If point/line defects are separated for a distance much larger than the typical molecular size they can be described as localised "points" or "lines" interacting via nematic director field. In general the attracting defects of opposite charge (e.g. M=M_1=1 and M=M_2=-1) approach each other, collide and then gradually decay into the defectless state in which M_{total}= M_1+M_2=0. The released energy due to the disappearance of defects is transformed into heat. This phenomenon is to some extent analogous to the annihilation of a pair particle-antiparticle transforming into the vacuum state where the released energy transforms into electromagnetic waves.

3 Theory

3.1 Model interaction

In our simulation a pair of rod like LC molecules located at $\vec{r}_1$ and $\vec{r}_2$ of a hexagonal lattice and pointing along unit vectors $\vec{e}_1$ and $\vec{e}_2$ respectively, interact via a simple pairwise interaction [3]

$$f = -\frac{J}{r^6}\left(\vec{e}_1.\vec{e}_1\right)^2 \qquad (1)$$

Here the positive constant J measures the strength of the coupling tending to enforce parallel orientation of interacting molecules and $r = \left|\vec{r}_2 - \vec{r}_1\right|$. The nematic director field at the i-th lattice site is defined as $\vec{n}(\vec{r}_i) = \left\langle \vec{e}_i \right\rangle$, where <…> stands for the average over fast molecular motions (with respect to the sampling time used in an experimental observation). The interaction energy W_{int} of the whole sample is given as a sum over all pair interactions. In calculations we limit only to the first neighbours. In addition we limit to relatively low temperatures, where W_{int} and the free energy of the system are almost equal.

In our study the LC phase is confined to a cylindrical cavity of radius $R=N_r a_0$ and length $L=N_z a_0$. Here a_0 is a hexagonal lattice unit size and $2N_r$ and N_z integers that are in our simulations typically varied in the range from 40 to 80. The cylinder axis is set along the z-direction of the Cartesian coordinate system (x,y,z). The lateral cylinder wall strongly enforces molecules to point along the surface normal. In the z direction we impose periodic boundary conditions simulating an infinite cylindrical cavity.

The local orientation of molecules is parameterised as

$$\vec{e} = \vec{e}_x \sin\theta \cos\phi + \vec{e}_y \sin\theta \sin\phi + \vec{e}_z \cos\theta, \qquad (2)$$

where θ and ϕ are the variational parameters given at a discrete time and points of the lattice. The unit vectors $(\vec{e}_x, \vec{e}_y, \vec{e}_z)$ point along the axes of the coordinate system.

The molecular orientations are updated in a time interval Δt via [8]

$$\theta(x, y, z, t + \Delta t) = \theta(x, y, z, t) - \Delta t\, A\frac{\partial W_{int}}{\partial \theta} + \theta_r,$$

$$\phi(x, y, z, t + \Delta t) = \phi(x, y, z, t) - \Delta t\, A\frac{\partial W_{int}}{\partial \phi} + \phi_r. \qquad (3)$$

The constant A depends on temperature and viscous properties of the liquid crystal system. The temperature T is introduced in the model via random variables θ_r and ϕ_r. The corresponding probabilities are described by Gaussian distributions centred at zero angles and the distribution width proportional to $\sqrt{T}$. The molecules are also allowed to fluctuate about lattice sites in order to get rid of lattice induced preferred orientations [8].

3.2 Geometry and topology of the problem

We study annihilation of a pair of nematic point defects of charge M=1 (monopole) and M=-1 (antimonopole) in a cylindrical cavity characterised by $2N_r$=40 and N_z=72.

The equilibrium nematic director configurations of our system is the so called [9] *escaped radial* (ER) structure, shown in Fig.5. In this defectless structure on approaching radially the cylinder axis $\vec{n}(\vec{r})$ gradually reorients ("escapes") from the radial orientation at $\rho=N_r a_0$ towards $+\vec{e}_z$ (or $-\vec{e}_z$) at $\rho=0$, where ρ measures the distance from the cylinder symmetry axis. By this "escape" along the axis the structure avoids energetically costly line defect at $\rho=0$. Note that the structure with the line defects can be stable for small enough radia [8].

Henceforth we schematically indicate the ER-like structure by <<<. The structures with escapes along $+\vec{e}_z$ (>>>) and $-\vec{e}_z$ (<<<) are equivalent. Therefore on cooling the liquid crystal from the high temperature isotropic (i.e. ordinary liquid) to the nematic phase domains of ER-like structures with alternative preference along $+\vec{e}_z$ and $-\vec{e}_z$ are expected to form due to the symmetry breaking (schematically: <<<><<<>>>). The domain collision sites give rise to nematic monopoles (collision sites >>><<<) and antimonopoles (collision sites <<<>>>). The corresponding structure is called the *escaped radial structure with point defects* (ERPD) [10]. This structure is metastable with respect to the ER. The ERPD->ER transition can be realised continuously via annihilation of neighbouring monopole-antimonopole pairs. Note that in most experimental (also numerical simulations [8]) situations the defects of the ERPD structure are frozen if the distance between neighbouring defects is larger than 2R [10]. For such distances the attractive force between defects is negligible small and is overshadowed by thermal fluctuations or deviations from the topological and geometrical conditions described in our model.

4 Results

In our simulation we initially placed a monopole and antimonopole on the cylinder axis (Fig.1). This was achieved by enforcing 3 alternative ER-like domains (i.e. >>><<<>>>), using the analytic ansatz [9]. The initial separation of defects is $D=34a_0$ and $R=20a_0$. Therefore the ratio $D/(2R)=0.85$ is small enough so that the interaction between defects is strong enough to drive the system into the defectless ER structure (i.e. the vacuum state) in a computationally accessible time (in approximately 10000 sweeps).

The most important stages of annihilation are shown in Figs.2-5. A more detail simulation is available on the Internet [1]. In Fig.1 the initial configuration is shown in which we enforce a "point" like monopole and antimonopole (right and left side of the picture, respectively). After some 1000 sweeps (Fig.2) the "point"

like defects broaden in to the "ring" like defects [11,12] corresponding to the equilibrium defect core structure. The corresponding elapsed time is $t=1000$ t_0. Here t_0 stands for the time unit in the simulation (1 sweep) which depends on the elastic and viscous properties of the nematic LC and cylinder radius [8]. Note that to most experimental observations this "ring" like defect appears as a point because the "ring" radius ξ length is few molecular sizes (typically $\xi \approx 10$ to 50 nm). In our simulation the equilibrium "ring" radius is $\xi_{eq} \approx 7a_0$. Due to relatively small radius the "rings" after the creation tend to orient with their axes perpendicular to the cylinder axis (Fig.3). The two "rings" gradually attract each other and their axis slowly (on the time scale of 1000 sweeps) rotates due to fluctuations and inertial effects. In the regime where $D > \xi_{eq}$ the "ring" radia are constant within the experimental error and defects can be distinguished. We refer to this stage as the *pre-collision* regime. When $D \approx \xi_{eq}$ (approximately 5500 sweeps, Fig.3) the core structure of defects become influenced by each other. We refer to the stage, in which the defects core structures gradually merge and then decay into the defectless structure, as the *post-collision* regime. In this regime at first the "ring" radia apparently increase. Then the "rings" touch and merge into a single "ring" (Fig.4). In this event the "central" ER like structure, that was necessary for the topological stability of defects is lost. The defects now merge to the extent that they are indistinguishable and gradually decay into the defectless ER structure (Fig.5) (after 8000 sweeps).
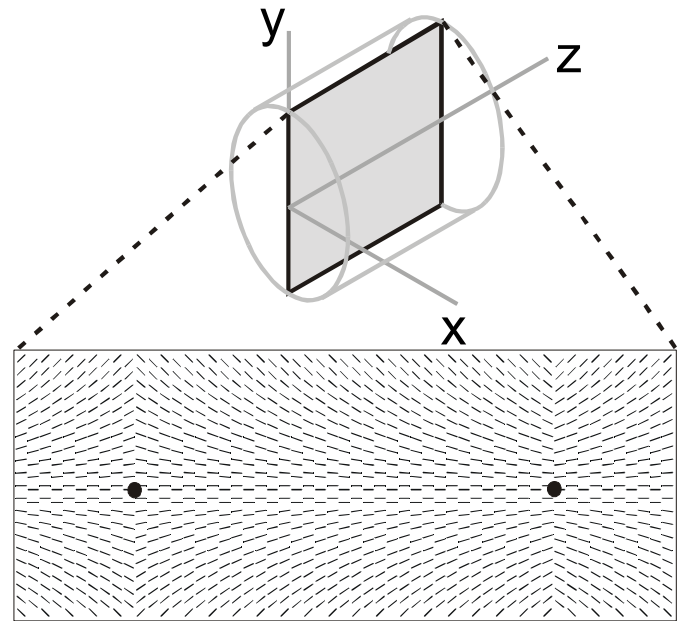

Figure 1: The geometry of the problem and the initial nematic structure shown in the (y,z) cross section. The

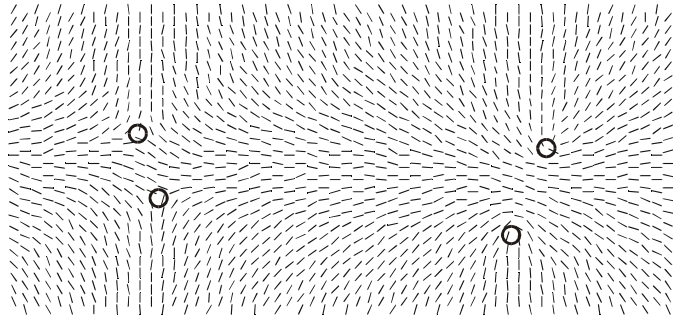point defects of strenght M=–1 (left) and M=1 (right) are denoted with full circles.

Figure 2: The nematic structure after 1000 sweeps. The "point" defects broadened into "rings" lying in the (y,z) plane. The location of the two "rings" at the left and right side of the figure in the (y,z) plane is denoted with open circles.
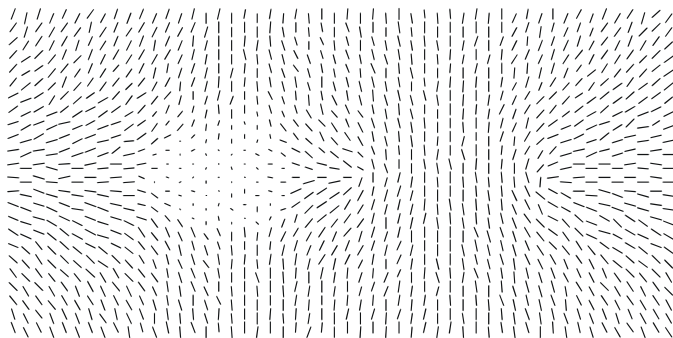

Figure 3: The nematic structure after 6000 sweeps. The "rings" are broader and rotated with respect to the structure shown in Fig.2. The left "ring" lyes in the (y,z) plane and the left in the (x,z) plane.
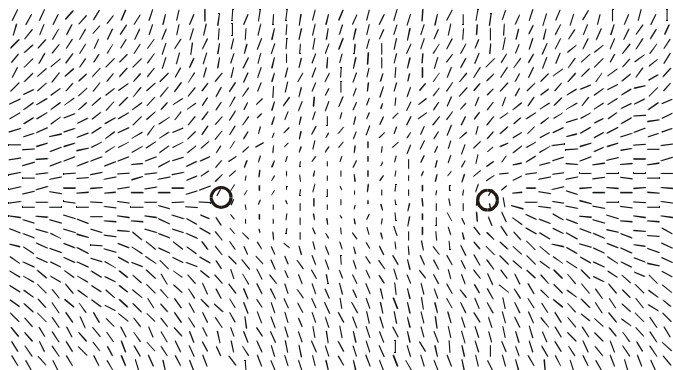
Figure 4: The nematic structure after 6500 sweeps. The two "rings" merge into a single "ring" lying predominantly in the (x,z) plane.
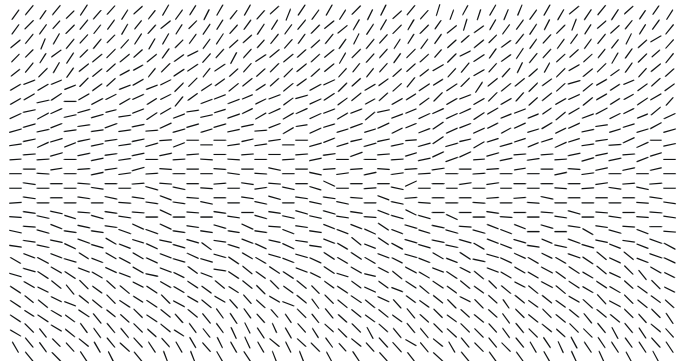

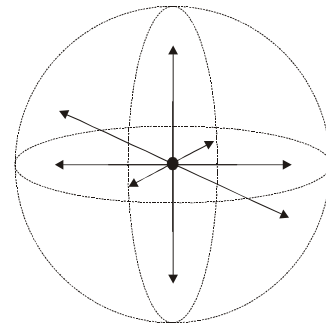Figure 5: The defectless ER structure reached after approximately 8000 sweeps.

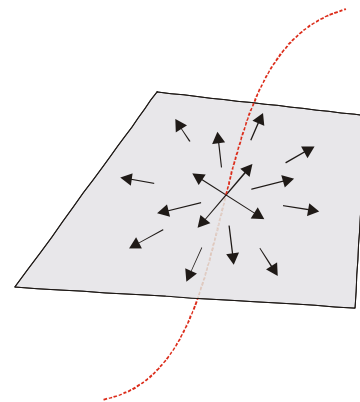Figure 6: A nematic point defect of topological charge M=1.

Figure 7: A nematic line defect of topological charge M=1.

5 Conclusions

We have developed a numerical simulation in which we study the annihilation of a pair monopole-antimonopole in nematic liquid crystals. These "point" like defects have topological charges M=1 and M=-1, respectively. The process is to some extent similar to the annihilation process between charged particle and antiparticle. In our simulation we distinguish between the pre-collision and post collision regime. In the pre-collision regime the defects are well separated. The cores of interacting defects are negligible affected by the mutual attraction and can be

clearly distinguished (i.e. they can be treated as "particles"). In the post-collision regime the core structure of defects with time progressively overlap making them indistinguishable and gradually decay into the defectless (vacuum) state. Note that in real experiments to our knowledge only the pre-collision regime can be monitored because the post-collision dynamics is to fast. In our simulation we have chosen a small enough cavity to make typical time scales of pre-collision and post-collision regime comparable.

References:

[1] http://www.pfmb.uni-mb.si/complex/intro.html

[2] R. Templer and G. Attard, The fourth state of matter, New Scientist 1767, 25 (1991).

[3] P.G. de Gennes and J. Prost, The Physics of Liquid Crystals (Oxford University Press, Oxford, 1993).

[4] M.V. Kurik and O.D. Lavrentovich, Defects in Liquid Crystals : Homotopy Theory and Experimental Studies, Sov. Phys. Usp. 31, 196 (1988) [Usp. Fiz. Nauk 154, 381 (1988)], and references therein.

[5] H. Trebin, Defects in Liquid Crystals and Cosmology, Liq.Cryst. 24, 127 (1988).

[6] D.N. Spergel and N.G. Turok, Textures and Cosmic Structure, Scientific American, March, 36 (1992).

[7] W.F. Brinkman and P.E. Cladis, Defects in Liquid Crystals, Physics Today, May, 48 (1982).

[8] Z. Bradač, S. Kralj, S. Žumer, Molecular dynamics study of nematic structures confined to a cylindrical cavity, Phys.Rev.E 58, 7447 (1998); Molecular dynamics study of isotropic-nematic quench, Phys.Rev.E (2002).

[9] C. Williams, P. Pieranski, and P.E. Cladis, Nonsingular S=1 Screw Disclination Lines in Nematics, Phys .Rev. Lett. 29, 90 (1972).

[10] G. Guidone Peroli and E.G. Virga, Role of boundary conditions in the annnihilation of nematic point defects, Phys.Rev.E 59, 3027 (1999).

[11] M. Terentjev, Phys.Rev. E 51, 1330 (1995), and references therein.

[12] S. Kralj, E.G. Virga, S. Žumer, Biaxial torus around nematic point defects, Phys.Rev.E 60, 1858 (1999); Universal fine structure of nematic hedgehogs, J.Phys.A:Math.Gen. 34, 829 (2001).