Annihilation of point defects on a line

Robert Holyst[1] and Patrick Oswald[2]
[1]*Institute of Physical Chemistry of the Polish Academy of Sciences, Department III, 01224 Warsaw, Poland and College of Science, Kasprzaka 44/52, 01224 Warsaw, Poland*
[2]*Laboratoire de Physique, École Normale Superieure de Lyon, 46 Allée d'Italie, F-69364 Lyon Cedex 07, France*
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We discuss the evolution of the distribution function of distances between point defects of opposite signs distributed on a line of finite length interacting via a potential attractive at short distances and repulsive at large distances. The standard deviation of the distribution grows quickly at short times, attains maximum, and decreases logarithmicaly at longer times. The distance between the defects increases monotonically and at equilibrium is about two times larger than the distance at which the repulsive force attains maximum. The distance dependent viscosity does not change qualitatively these conclusions, but only increases the time scale of evolution by one order of magnitude.

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I. INTRODUCTION

Disclination lines are ubiquitous in nematic liquid crystals. They spontaneously form in cylindrical capillary tubes treated in homeotropic anchoring (molecules perpendicular to the surface) [1]. If the tube diameter is small enough [2,3] (usually less than 0.1 μm) a planar disclination line of rank $+1$ forms along the tube axis. ''Planar'' means that that the director lies in a plane perpendicular to the line, forming a pure radial configuration with a singular core. For larger diameters, and providing that the bend elastic constant K_3 is not too large, the director escapes along the tube axis, forming a continuous configuration without singularity. Such a configuration allows the formation of an array of point defects: hyperbolic (H) and radial (R) [4,5]. This is due to the fact that the director field, while translationally invariant along the disclination line, can escape in two opposite directions (0 or π), leading to two energetically equivalent configurations. Thus, breaking the symmetry along the line involves the formation of point defects. These opposite defects annihilate when brought together. One of the questions, which is still a matter of controversy is the interaction potential between them, especially at large distances.

There are three conflicting model calculations [6–8] that give completely different interaction potentials between the defects despite the fact that they describe exactly the same physical situation. Vilfan, Vilfan, and Zumer [6] calculated a free energy for the linear, periodic array of RH defects as a function of their separation. Although they have not explicitly calculated the potential between the defects their result suggested that this potential should be linear and attractive between RH defects at short distances and repulsive at large distances. The characteristic distance of attraction is roughly equal to $0.1D$, where D is the diameter of the capillary. Peroli and Virga [7] got for the same system a potential that at short distances leads to an attractive force that varies logarithmically with the distances between RH defects. This force vanishes at some critical distance, which is approximately equal to $1.1D$. Finally, Semenov [8] obtained for the same system a potential always attractive between the RH defects, which at short distances agrees with the one found by Vilfan, Vilfan, and Zumer [6]. The most probable source of discrepencies in these calculations is hidden in the boundary conditions. In Ref. [6] the most natural boundary conditions have been used, namely, the bulk free energy has been supplemented with the surface free energy such that homeotropic alignment at the surface is preferred. However, for sufficiently large bulk elastic energy the director at the surface could deviate from perpendicular alignment. In the Semenov calculations [8] the director has been fixed at the surface perpendicularly to it. Peroli and Virga [7] set the director perpendicular to the cylindrical surface in a large part of the volume of the cylinder. It is interesting to note that all these models find their partial support in the molecular dynamics simulations or in the experiments. The observation of the annihilation of two point defects [9] in the bulk shows that the potential at short distances is attractive and linear as a function of the distance between R and H defects. In a capillary the potential between the defects should be the same at short distances (much smaller than the diameter) as in the bulk. This observation supports theoretical calculations done in Refs. [6] and [8]. In the molecular dynamics study of Bradac, Kralj, and Zumer [10], it was observed that the distances between the defects did not change when it was larger than D. This observation supports the calculations of Peroli and Virga. Finally, the NMR (nuclear magnetic resonance) experiments of Crawford *et al.* [5] showed that it is possible to form stable arrays of point defects along the cylinders, where the defect density does not depend on the history of the sample. This observation supports Refs. [6] or [7]. The main problem of NMR experiments is that point defects are indirectly detected so that the time evolution of their spatial distribution is out of reach.

One way to bypass this difficulty is to work in another geometry that is easier to produce experimentally. This experiment consists of preparing a homeotropic sample between two parallel glass plates and looking at the circular meniscus that forms near the sample sides at the nematic-air interface [11]. In usual conditions, a $-1/2$ disclination line forms in the vicinity of the meniscus due to antagonistic boundary conditions on both the glass and the free interface. This line has a singular core but is not necessarily planar:

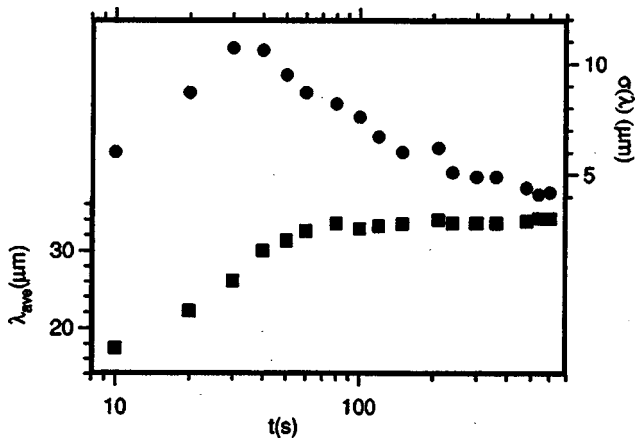

FIG. 1. The experimental results for the evolution of the distribution of point defects. The average distance between point defects (the left scale, filled squares) and the standard deviation (the right scale, filled circles) as a function of time. The average is taken here over 12 independent initial configurations (after Ref. [14]).

which means that the director may partially escape along the dislination line [12,13]. Again there are two possibilities for the director to escape, which are energetically equivalent, so that point defects of opposite signs ($\pm$) can form on the line. The main advantage of this experiment is that it is possible to prepare arrays of point defects with various initial densities. One method is to apply an external electric field to expulse the line out of the sample (it becomes virtual): then, decreasing or switching off the field leads to various distributions of defects [14]. The initial distribution is usually unstable because point defects of opposite signs attract at short distances as ''RH'' defects do in a capillary. As a consequence, the distribution evolves toward a stable configuration via the annihilation of neighboring defects at long time. In this experiment, it was possible to measure directly in the microscope both the average distance between the defects and the standard deviation of the distribution function for the distances between the defects as a function of time. The results are summarized in Fig. 1. We observe that initially the defects annihilate and both the average distance between them and the standard deviation of the distribution of the distances grow. Next, the average distance attains its equilibrium value (as it does in capillary tubes of Crawford *et al.* [5]), while the standard deviation attains a maximum. Later the standard deviation decreases logarithmically with time.

Here we would like to simulate this process (that we expect to be very similar in circular capillary tubes) and see which of the three potentials (i.e., always attractive, or attractive at short distances and zero at large distances, or attractives at short distances and repulsive at large distances) is consistent with the experimental results shown in Fig. 1.

II. INTERACTIONS AND DYNAMICS OF POINT DEFECTS

We have studied the evolution of point defects distributed on the line interacting with a force $f(x)$, where $x>0$ is a distance between neighboring defects. We have used three different models for $f(x)$ consistent with three proposals made in the literature [6–8], i.e.,

$$f(x)=-(1-x)\exp(-x), \tag{1}$$

which is attractive at short distances and repulsive at longer distances as suggested by the calculations done in Ref. [6] (model I).

$$f(x)=\ln(x), \tag{2}$$

which is attractive for $x<1$ and 0 otherwise [7] (model II). Finally, we have modeled the force calculated by Semenov by

$$f(x)=-\exp(-x^2) \tag{3}$$

attractive at all distances (model III). The force given by Eq. (1) does not follow directly from Ref. [6], although it retains its salient features suggested in Ref. [6], i.e., attraction at short distances and repulsion at large distances. We shall discuss this point further in Sec. V. In model I, we have assumed the form of the repulsive part of the potential to be exponential and checked that other forms (i.e., algebraic) do not change the final conclusions. The attractive part of the force in model I is constant at short distances in accordance with the interaction of two RH defects in the infinite space. The model III is slightly inaccurate in comparison with Ref. [8] since the force in Ref. [8] decreases at large distances as $\exp(-x)$, but with a very short correlation length, i.e., $D/6.6$. If we look at Fig. 2 of Ref. [8] it can be well approximated by Eq. (3). We have assumed that the forces act between the nearest neighbors, but we have also verified that even if we assume that every defect interacts with every other defect on the line, it does not change qualitatively and also quantitatively the results. Because the interactions between the point defects are related to the three-dimensional (3D) distribution of the director field it is reasonable to assume that the interactions between the defects are strongly screened by the nearest neighbors and therefore this justifies the assumption of the nearests neighbors interactions. The dynamics of the system depends also on translational viscosity of the defects, which is directly proportional to the rotational viscosity of the director field in the bulk. The distortions of the field decrease when two opposite defects are close together and increase when the distance between them increases. Therefore, the viscosity is directly proportional to the elastic energy stored in the director field at least for short distances for which this energy is proportional to the distance between the defects [7]. Therefore, we have also studied two cases: one when the viscosity is independent of the distance and one when it linearly depends on the distance [9] between $\pm$ defects.

We assume that we have N defects of alternating sign on the line of length L. In the model we simply assume that the defects move under the influence of force f with a velocity proportional to it. When the viscosity is independent of the distance between the moving defects, we can write the following equations for the velocity v_i of the ith defect in the array:

$$v_i = -f(x_{i,i+1}) + f(x_{i-1,i}), \tag{4}$$

$$\frac{dy_i}{dt} = v_i . \tag{5}$$

Here

$$x_{i,j} = |y_i - y_j|$$

is the distance between the ith and jth defects and y_i is the location of the ith defect on a line. For the model with a viscosity depending linearly on the distance, we use the following equation instead of Eq. (4):

$$(x_{i,i+1} + x_{i-1,i}) v_i = -f(x_{i,i+1}) + f(x_{i-1,i}). \tag{6}$$

In general, all constants in the model such as viscosity, strength of the potential or its range rescale the time and the distance and therefore they do not explicitly appear in the model. It follows that all quantities are dimensionless. We took reflecting boundary conditions with zero force acting on the defect at the boundaries and verified that the results do not change if we take as the boundary force a force produced by the mirror image of the last defect. In general, the final results do not depend on the particular form of the interaction between the last (or first) defect on the line with the boundary. As typical parameters we have used $L = 1000$ and $N = 1500$ with a random initial distribution of the defects on the line. Each defect (e.g., "$-$") had an opposite defect ("$+$") at each of its sides. Two defects were annihilated when the distance between them was less than 0.1. We used a simple Euler scheme to solve the equations with a time step of 0.1 and checked the results for the time step 0.01. We averaged the results typically over 400 runs i.e., 400 initial configurations. We have verified that the final results did not depend strongly on the initial distribution; even for an almost equidistant distribution of defects with small standard deviation (1% of the average distance) we have got the same results as with the random distribution. Also, qualitatively the model given by Eq. (4) and the one given by Eq. (6) gave the same qualitative results; one only had to rescale the time scale. We have also noted that the final distribution of defects in the case of the model force given by Eq. (1) did not depend on the initial number of defects on the line providing that N was large enough, i.e., roughly much larger than $L/4$.

III. RESULTS

First of all, we have found that the models with the attractive force between opposite defects (models II and III) give always a monotonic growth of the standard deviation of the distribution of distances between the defects. In the case of the model given by Eq. (2) (model II), the average distance and the standard deviation of the distribution of distances grow at short times reaching a plateau at longer times. The final distribution reaches the average distance 3.6 with the standard deviation 2.7. The average distance between the defects is much larger than the distance at which the force is zero in this model. In the model given by Eq. (3) (model III) the force does not vanish at any fixed distance between the defects, as in model given by Eq. (2), and therefore both the average and the standard deviation grow in time. However, the growth of the standard deviation at longer times is logarithmic. Neither the dynamic with the force given by Eq. (2) nor the one given by Eq. (3) is consistent with the experimental results shown in Fig. 1.

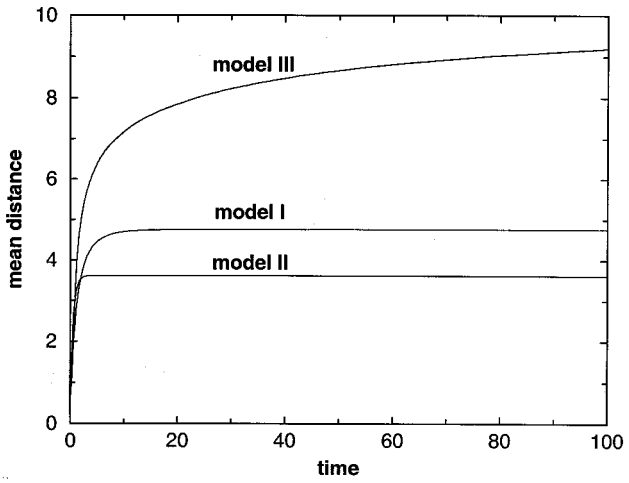

FIG. 2. The average distance between the defects as a function of time for models I, II, and III [Eqs. (1)–(3)].

The comparison of the average distance between the defects for the three models is shown in Fig. 2. The growth of the average distance between the defects reaches a constant value for model I and II, and grows, for model III, untill the last pair of opposite defects is present. In models I and II, we reach the final configuration with a comparable number of defects, while in model III defects always disappear at the end, but extremely slowly (logarithmically).

Even more different is the behavior of the standard deviation of the distribution of the distances between the defects shown in Fig. 3. The model given by Eq. (1) gives a peak in the standard deviation consistently with the experimental results while the model with purely attractive force (model III)

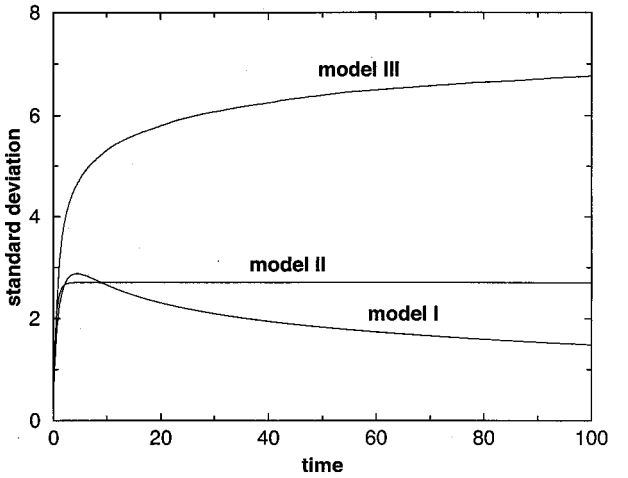

FIG. 3. The standard deviation for the distribution of distances between the defects as a function of time for models I, II, and III [Eqs. (1)–(3)].

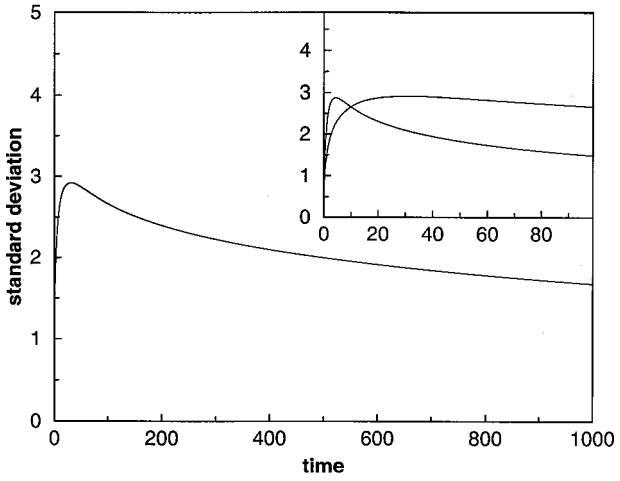

FIG. 4. The standard deviation for model I with the viscosity depending linearly on the distance between the defects [Eq. (1) and Eq. (6)]. In the inset, we show its behavior for a short time scale, i.e., the same as used in Fig. 3 together with the results of model I with constant viscosity [Eq. (1) and Eq. (4), see also Fig. 3]. Please note the change of scale between the figure and inset.

leads to the monotonic growth. It is interesting to note that this monotonic growth is logarithmic in time. Also, the decrease of the standard deviation is logarithmic for model I, which is also consistent with the experimental results.

We have also studied model I with the equidistant initial distribution of defects with no force at the boundary. The behavior of such array depends strongly on the initial distance between the defects. When this distance is smaller than 1 (at $x=1$ the force is exactly zero and repulsive for $x>1$) all defects disappear during the evolution. When the distance is between 1 and 2 (for $x=2$ the repulsive force is the largest) part of the defects disappears. And for $x=2$ or larger none of the defects annihilates. However, it is sufficient to introduce a small disorder in the initial configuration to find the same behavior as in the case of random distribution of defects.

We have looked at the influence of the viscosity in model I. In Fig. 4 (inset), we plot the standard deviation for model I (Eq. (1) and Eq. (4), i.e., constant viscosity) and model I with distance dependent viscosity [Eq. (1) and Eq. (6)]. As can be seen the evolution is much slower (order of magnitude) in the latter case than in the former case as shown in the figure and in the inset. But the close comparison between the figure and its inset shows that by the proper rescaling of the time scale we find the same results. It is interesting to note that this slowing down cannot be accounted for by the force $f(x)/x$ with $f(x)$ given by Eq. (1). The model with such a force gives practically the same results as model I with force f.

Finally, we have studied several potentials that had the same attractive part (linear in x) and different repulsive part (exponential or algebraic) and found that the details of the potential do not strongly influence the dynamics except for the change of the time scale (similarly as in the case of the distance dependent viscosity discussed above).

IV. CONCLUSIONS

From our results it follows that only model I characterized by the attractive force at short distances and repulsive force at large distances is consistent with the experimental results presented in Fig. 1. The evolution of point defects in this case is characterized by a peak in the standard deviation of the distribution of the distances between the defects and its logarithmic decrease at longer times. The final average distance between the defects is roughly twice as large as the distance at which the repulsive force between the defects attains its maximal value. The evolution does not depend on the initial distribution of defects. The distance dependent viscosity or different form of the repulsive potential (algebraic or exponential) does not change the results qualitatively except for the change of time scale as shown in Fig. 4. This means that from the experimental studies described in Ref. [14] one can only get the distance at which the repulsive force between the defects attains the maximum, since the qualitative and quantitative behavior of the defects is not very sensitive neither to the viscosity nor to the exact form of the potential. More information can be obtained if one predicts the time scale of the evolution from the microscopic calculations.

V. FURTHER DISCUSSION

The problem of the dynamics of the array of point defects on the line is far more complicated than described in this paper. In this last section, we shall discuss the main assumptions that have been made in the paper and the approach to the solution of the full problem.

First of all we have assumed that the system can be described by the pairwise potential. The defects on the line are a consequence of the 3D distribution of the director field **n**, and in general the nonlinear equations for the 3D distribution of the director in the capillary can give rise to the many-body potential between the defects. However, the pairwise additive potential can provide a good (but not perfect) description of the system. We have also assumed that the dissipation coefficient is either a constant or a linear function of the separation between the defects. In general, it can be a complicated nonlinear function of the distances between all the defects present on a line. Nevertheless, a simplified model for the viscosity used in this paper seems to give a reasonable description of the system. In order to see these two points more clearly let us discuss the derivation of the equations of motion for the point defects from the motion of the 3D director field.

The solution of the equations of motion for the defects on a line should follow from the solutions of the equations of nematodynamics [9] for the director field in the capillary in the presence of point defects. The problem can be simplified, because the time scale for the reorientation of the director **n** is much shorter (few orders of magnitude) than the time scale of the translational motion of the defects on the line. Therefore, we may assume the following scenario for the process. We have N defects on a line characterized by their location $y_1 \cdots y_N$. At each instant of time the director field **n** assumes

a configuration minimizing the Franck elastic energy $\hat{F}[\mathbf{n}]$ (a functional of $\mathbf{n}$), subject to the constraint of constant location of the defects, $y_1 \cdots y_N$. After minimization we get the Franck free energy as a function of N variables $y_1 \cdots y_N$, i.e., $F(y_1 \cdots y_N)$. In Ref. [6] this function has been calculated only for a special case of constant distance between the defects $y_i - y_{i+1} = l$ for each i. Next, we have to find the equation of motion for the defects. We assume that all the elastic energy is dissipated in the process. The dissipation function D [7] is

$$D = \gamma_1 \int d\mathbf{r} \left(\frac{\partial \mathbf{n}}{\partial t} \right)^2, \tag{7}$$

where the integral is over the whole volume of the system, t is time, and γ_1 is the orientational viscosity. The director field $\mathbf{n}$ follows from the minimization of $\hat{F}[\mathbf{n}]$ and therefore is a function of $y_1 \cdots y_N$. Because of the separation of time scales, we assume that the whole dependence of $\mathbf{n}$ on time is hidden in $y_1 \cdots y_N$. Thus, we may write

$$\frac{\partial \mathbf{n}}{\partial t} = \sum_{i=1}^{N} \frac{\partial \mathbf{n}}{\partial y_i} \frac{dy_i}{dt}. \tag{8}$$

Both $F(y_1 \cdots y_N)$ and $\mathbf{n}(\mathbf{r}; y_1 \cdots y_N)$ follow from the numerical solution of the minimization of $\hat{F}[\mathbf{n}]$. Finally, we assume that during the motion of the defects the dissipation is minimized, i.e.,

$$2D_i \equiv \frac{\partial D}{\partial y_i'} = 0 \tag{9}$$

$(y_i' = dy_i/dt)$, subject to the constraint that the whole elastic energy is dissipated in the process i.e.,

$$\frac{dF(y_1 \cdots y_N)}{dt} + D = 0. \tag{10}$$

Using the Lagrange multipliers and the quadratic dependence of the dissipation on velocities, we find the following equation of motion:

$$D_i + \frac{\partial F}{\partial y_i} = 0, \tag{11}$$

where

$$D_i = \sum_{j=1}^{N} \frac{dy_j}{dt} \gamma_1 \int d\mathbf{r} \frac{\partial \mathbf{n}}{\partial y_i} \frac{\partial \mathbf{n}}{\partial y_j}. \tag{12}$$

The numerical solution of this problem is far from being trivial, but only this solution can give us a hint whether the assumptions about the constant viscosity or the pairwise additive potential are correct. For the pairwise additive potential between nearest neighbors, $V(x)$, to be a valid approximation the form of $F(y_1 \cdots y_N)$ should be as follows:

$$F(y_1 \cdots y_N) = \sum_i V(x_{i,i+1}), \tag{13}$$

where $x_{i,i+1} = |y_i - y_{i+1}|$ is the distance between the i, $i+1$ defects. For the viscosity to be a constant independent of y_i we should have

$$D_i \approx \text{const} \frac{dy_i}{dt}. \tag{14}$$

Both assumptions can be verified after the numerical solution of $F(y_1 \cdots y_N)$ and $\mathbf{n}(\mathbf{r}; y_1 \cdots y_N)$ are determined.

We conclude that despite 11 years of intensive studies of point defects on a line inside capillaries the problem of the interaction potential between them is far from being solved. The qualitative agreement of our simplified model (pairwise additive potential with attractive and repulsive part) with the results of experiment [11] provides a good (but not perfect) description of the defect motion on a line in a capillary.

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