Where are the Hedgehogs in Nematics?

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Abstract

In experiments which take a liquid crystal rapidly from the isotropic to the nematic phase, a dense tangle of defects is formed. In nematics, there are in principle both line and point defects ("hedgehogs"), but no point defects are observed until the defect network has coarsened appreciably. In this letter the expected density of point defects is shown to be extremely low, approximately $10^{-8}$ per initially correlated domain, as result of the topology (specifically, the homology) of the order parameter space.

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An outstanding puzzle in the formation of defects after rapid quenches is the absence of point disclinations ("hedgehogs" or "monopoles") in nematic liquid crystals. One might naively expect of order one defect per initially correlated domain. However, experiments with rapid pressure quenches [1] do not find any monopoles at all to begin with, although the expected dense network of line disclinations ("strings") is present, and rapidly reaches a scaling regime in which the string length density decreases as $t^{-1}$. This can be understood to be a result of the $t^{1/2}$ growth law of the network scale length $L(t)$. If there is on average about 1 segment of string of length $L$ per volume $L^3$, the scaling of the length density $L^{-2}$ is explained. The monopoles do not make their appearance until relatively late in the scaling regime, forming from collapsing loops of string.

In this letter a solution to this puzzle is presented. The answer lies in the topology of the order parameter space, which is the projective plane $\mathbb{RP}^2$. In order for there to be a monopole inside some sphere in the liquid crystal, the order parameter field has to cover its entire space twice. It turns out that this is very hard to arrange out of the random initial conditions produced by a rapid quench. There is an underlying mathematical formulation of the solution, in terms of the homology of the order parameter space, which is outlined briefly at the end of this work.

The order parameter of a liquid crystal is a traceless symmetric rank 2 tensor $Q_{ij}(x)$. The normalized eigenvector with the largest eigenvalue is known as the director field $n_i(x)$, for it defines the average local orientation of the liquid crystal molecules. In a nematic the other two eigenvalues are equal, and we may write [2]

$$Q_{ij} = A(n_in_j - \frac{1}{3}\delta_{ij}).$$

(1)

The free energy of the liquid crystal is

$$F[Q] = \int d^3x (L_1\partial_hQ_{ij}\partial_hQ_{ij} + L_2\partial_iQ_{ij}\partial_kQ_{ik} + L_3\partial_hQ_{ij}\partial_jQ_{ik} + V(Q))$$

(2)

where $V(Q)$ is the bulk free energy. Near the phase transition we are justified in expanding to quartic order, and

$$V(Q) = \frac{1}{2}\alpha\text{tr}(Q^2) + \frac{1}{3}\beta\text{tr}(Q^3) + \frac{1}{4}\gamma\text{tr}(Q^2)^2 + \cdots.$$ (3)

The condition that the system be in the nematic phase, i.e. that $A \neq 0$ minimize the free energy, is just $\alpha\gamma/\beta^2 \leq 1/9$. In this phase the symmetry group of the bulk free energy density, which is the group of spatial rotations $\text{SO}(3)$, is reduced to the cylinder group $D_\infty$, or $O(2)$. The manifold $M$ of possible equilibrium states is defined by the condition $\delta F/\delta Q = 0$, subject to the constraints of tracelessness and symmetry. This is isomorphic
to the coset space SO(3)/O(2), or the real projective plane $RP^2$, which can be thought of as a 2-sphere with antipodal points identified.

After a rapid quench, the order parameter is uncorrelated beyond a certain distance $\xi_0$, which is determined by the relative magnitudes of the quench time and the relaxation time of the system. The isotropic-nematic transition is weakly first order, which means that the correlation length grows by a large factor as the phase transition is approached [2], although the transition itself appears to proceed by bubble nucleation and growth [3]. The substance of the present argument should not depend on the order of the transition: it is only the existence of uncorrelated domains that is important. Defects form at the interstices of domains where the order parameter is in some sense maximally misaligned, in what is known in cosmology as the Kibble mechanism [4]. One can estimate the density of defects by applying the so-called “geodesic rule” [5, 6, 7]. This assumes that if we pick two points $x_1$ and $x_2$ in adjacent domains with order parameters $Q_1$ and $Q_2$, the most likely interpolation $Q_{12}(x)$ on a line between the points is the shortest path in $M$, for this locally minimizes the bulk free energy. Since $M$ comes equipped with a metric by virtue of its embedding in the Euclidean field space, this path is by definition a geodesic. Now consider three adjacent domains, and pick three points $\{x_1, x_2, x_3\}$. The geodesic rule can be applied separately to each pair of domains, and then to all three: the interpolation $Q_{123}(x)$ to the interior of the triangle $\{x_1, x_2, x_3\}$ is a geodesic surface in $M$. There may be an obstruction to the procedure: if the loop $\{Q_{12}, Q_{23}, Q_{31}\}$ is in the non-trivial homotopy class of $\pi_1(M)$, a line defect must pass through the triangle $\{x_1, x_2, x_3\}$, at the junction of the three correlated domains. A similar argument involving four domains is applied to the formation of point defects [4], which are obstructions to the construction of an interpolating geodesic 3-simplex $Q_{1234}$. We shall see, however, that four uncorrelated domains are not enough for a point disclination in a nematic liquid crystal.

Calculating the probability of finding a defect associated with non-trivial $\pi_n(M)$ at the interstices of $n + 1$ domains is a problem in geometric probability on the manifold of equilibrium states $M$. This problem has been solved only for $M \simeq S^n$ [8], and for 1-dimensional defects in $RP^2$ [5] and $S^3/\mathbb{Z}_2$ [4]. The solution is rather neat for the spheres. Consider first $n = 1$, where the order parameter is a 2 component field $\phi_a$ with $\sum_a \phi_a^2$ constant. The problem consists essentially of placing 3 points $\phi^1, \phi^2, \phi^3$ at random on the circle of constant $\sum_a \phi_a^2$, and asking the probability for $\phi^3$ to lie between $-\phi^1$ and $-\phi^2$ (taking the shortest route). In that case, and in only that case, will the geodesic rule supply a loop which wraps around $M$. Now, $\pm \phi^1$ and $\pm \phi^2$ divide the circle into 4. Given that $\phi^1$ and $\phi^2$ are isotropically distributed, one can convince oneself that the average length of the line segment between $-\phi^1$ and $-\phi^2$ is $1/4$. This is then the probability of finding a line defect at the junction of three adjacent domains, and the number of defects...
per unit area is therefore $1/4\xi_0^2$. This generalizes for arbitrary $n$ to $1/2^{n+1}$. For strings in $RP^2$ the calculation is more involved, but it emerges that the probability is $1/\pi$.

The problem with trying to extend these calculations to point defects in $RP^2$ is that four neighbouring uncorrelated domains can never generate such a defect. To construct a hedgehog configuration of the order parameter we must cover $M$ twice, because the director field has an $x \rightarrow -x$ symmetry. One cannot unambiguously do this with four domains, for the geodesic rule produces a mapping from the tetrahedron $\{x_1, x_2, x_3, x_4\}$ which is either trivial or contains a string passing through two of the faces. The point is that in order to cover $M$ twice, each face of the tetrahedron must cover on average half of it, which means that there will always be faces trying to cover more than half. This cannot happen with the geodesic rule. Thus we need more domains, which inevitably lowers the probability of finding a defect.

The minimal triangulation of $RP^2$ has in fact 6 vertices (see Figure 1). One can think of this as a triangulation of $S^2$ by an icosahedron, with antipodal points then identified. Thus in order to cover $RP^2$ twice we need a roughly spherical arrangement of a minimum of 12 uncorrelated adjacent domains. A great deal of calculation can now be saved by an approximation which uses a fixed triangulation of $RP^2$ directly. For example [10, 11], if we approximate $S^1$ by three equidistant points labelled 0, 1, 2, and assign a string to a spatial triangle $\{x_1, x_2, x_3\}$ when all three values of $\phi$ are different, the probability of having a string passing through the triangle is just the number of different arrangements of 0, 1, and 2 divided by the total number of possible assignments $3^3$. Thus the probability in this discrete approximation of 1-dimensional defect passing through the triangle is

$$P'_1(S^1) = 3!/3^3 = 2/9,$$

where the prime is used to denote the approximation to the true geometric probabilities $P_n(M)$. For general $n$ we have

$$P'_n(S^n) = (n + 2)!/(n + 2)^{n+2}.$$  

This approximation gets worse for large $n$. Using Stirling’s approximation, one sees that $P'_n(S^n)/P_n(S^n) \sim n^{1/2}e^{(\ln 2-1)n}$.

For line defects in $RP^2$ the calculation proceeds as follows. The first two values of the order parameter $Q^1$ and $Q^2$ can be any two different vertices of the triangulation. The last point must be one of the two which are connected to both of the first two. Thus

$$P'_1(RP^2) = 6 \cdot 5 \cdot 2/6^2 = 10/36$$

which is close to the true value $P_1(RP^2) = 1/\pi$. For point defects, we must calculate the number of different ways of assigning values of $Q$ to the 12 domains. Picking any two
adjacent domains, the first values can once again be any two vertices of the triangulation. In a third domain, adjacent to both the first two, one must correspondingly pick one of the vertices connected to both those already selected. Thus

$$P'_2(RP^2) = 60/6^{12} \simeq 2.76 \times 10^{-8}. \quad (7)$$

A quick way of calculating this number is to note that the assignment of vertices to domains is just a map from one icosahedron to another with opposite points identified. Therefore $P'_2(RP^2)$ is just the order of the icosahedral group, which is 120, divided by 2.

The configuration of domains occupies a volume of approximately $\xi_0^3$, and so the density of point defects $N_p$ is roughly

$$N_p \simeq 10^{-8} \xi_0^{-3}. \quad (8)$$

This is a very small number, as promised. If the discrete calculation is here as good an approximation as for the spheres, then it explains why the point defects of a nematic liquid crystal are not found after a rapid quench: they require a very special arrangement of the order parameter over many uncorrelated domains [12].

The icosahedral arrangement of domains can be extended into the body of the material by the addition of a further domain in the centre. One then realises that the “point” disclination is actually a small loop of size $\sim \xi_0$ encircling the central domain. The value of the order parameter here merely controls the loop’s orientation. Thus there is a sense in which there are no point disclinations at all. What we have calculated is merely the density of the smallest possible loops which can form hedgehogs.

To conclude, I outline the mathematical structure implicit in the geodesic rule. Recall that the construction starts with points $\{x_i\}$ in uncorrelated domains, and the corresponding values of the order parameter $\{Q^i\}$. One attempts to construct an approximation to the field configuration over the whole of $R^3$ by extending the points $\{x_i\}$ to a full triangulation, defining the order parameter field $Q(x)$ by the geodesic rule. This determines how to “fill in” the set of closed figures (points, lines, and triangles) in order to create others (lines, triangles and tetrahedra) of higher dimension. The result is a simplicial complex [13] in the order parameter space $M$. However, the procedure fails when some sub-complex cannot be filled in, that is, the sub-complex is not the boundary of another, higher-dimensional complex in the space $M$. The order parameter has to leave $M$ and a defect appears in the corresponding region of $R^3$. This can happen if and only if the space has a non-trivial homology group $H_n(M)$. Thus the Kibble mechanism coupled with the geodesic rule produces defects of dimension $d$ in a space of dimension $D$ only if $H_n(M)$, with $n = D - d - 1$, is non-trivial. The second homology class of $RP^2$
is zero: this is the underlying reason for the absence of point defects in nematic liquid crystals.

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Figure Captions

**Figure 1:** The minimal triangulation of $RP^2$, consisting of 6 vertices, 12 edges and 10 faces. This is essentially the top half of an icosahedron. Opposite points on the boundary are identified.
