Where Are the Hedgehogs in Quenched Nematics?

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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 a 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] report a substantial deficit to begin with, although the expected dense network of type $\frac{1}{2}$ 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 $\xi(t)$. If there is on average about one segment of string of length L per volume ξ^3, the scaling of the length density ξ^{-2} follows. The monopoles do not make their appearance until 1–2 s after the quench, and then disappear again faster than the naive scaling law of $n_M \sim \xi^{-3}$ would predict. Chuang *et al.* [1] observed that monopoles were formed either by a collapsing type $\frac{1}{2}$ loop or at a three-way junction between two type $\frac{1}{2}$ and one (nontopological) type 1 disclinations. They were able to explain the general shape of $n_M(t)$ by proposing that the departure from naive scaling was due to the repulsive forces between self-intersecting strings.

However, it seems that monopoles were *only* formed by string interactions and that there were essentially none generated in the quench. This is the puzzle, and in this Letter a solution is presented. The answer lies in the topology of the order-parameter space, which is the projective plane 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 $Q_{ij}(\boldsymbol{x})$. The normalized eigenvector with the largest eigenvalue is known as the director field $n_i(\boldsymbol{x})$, 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]

$$Q_{ij} = A(n_i n_j - \tfrac{1}{3}\delta_{ij}). \tag{1}$$

The free energy of the liquid crystal is, in the absence of boundaries,

$$F[Q] = \int d^3x [L_1 \partial_k Q_{ij} \partial_k Q_{ij} + L_2 \partial_j Q_{ij} \partial_k Q_{ik} + L_3 \partial_k Q_{ij} \partial_j Q_{ik} + V(Q)], \tag{2}$$

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

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

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 SO(3), is reduced to the cylinder group D_∞, 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 ξ_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]. In the cosmological Kibble mechanism [4], one assumes that the order parameter in each nucleating bubble is constant, but uncorrelated with its neighbor, and defects then form at the interstices of domains where the order parameter is in some sense maximally misaligned.

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There is a complication here, for there is generally some preferred orientation of the director field at the boundary between the isotropic and nematic phases. For K15 (also known as 5CB), the nematic used by Chuang *et al.*, it is energetically favored for the director to be at an angle of 63.5° to the surface [5]. Thus every sufficiently large bubble contains a hedgehog (and a pair of boojums), provided the anchoring energy WR^2 outweighs the volume energy KR, where K is a combination of elastic constants [6]. When two such bubbles collide, a loop of string with topological charge -1 can be produced around the intersection site, which keeps the total charge in the merged bubbles unity.

Thus the substance of the present argument as applied to nematics requires that the bubbles are not of sufficient size for them to automatically contain hedgehogs. This critical size R_c can be estimated from the experimental values of W and K, which are $(4.8 \pm 1.2) \times 10^{-4}$ erg cm^{-2} rad^{-2} and $(2.1 \pm 0.3) \times 10^{-7}$ erg cm^{-1}, respectively [5]. Thus $R_c \sim K/W \sim 2 \times 10^{-4}$ cm. We can also estimate an upper bound on the initial domain size in the quenches performed by Chuang *et al.* In the light transmission studies of that group [7] they were able to pick up scaling behavior from as early as 10 ms after the quench. One can infer from the $t^{1/2}$ growth law that the network scale length was at most about 10 μm at that time, and therefore smaller right after the quench. Thus it seems very unlikely that the bubbles contained hedgehogs before merging.

One can estimate the density of defects by applying the so-called "geodesic rule" [8–10]. This assumes that if we pick two points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ in adjacent domains with order parameters Q^1 and Q^2, the most likely interpolation $Q^{12}(\boldsymbol{x})$ 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 $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$. The geodesic rule can be applied separately to each pair of domains, and then to all three: The interpolation $Q^{123}(\boldsymbol{x})$ to the interior of the triangle $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$ 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 nontrivial homotopy class of $\pi_1(M)$, a line defect must pass through the triangle $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$, 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 nontrivial $\pi_n(M)$ 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 $M \simeq S^n$ [11], and for one-dimensional defects in RP^2 [8] and S^3/Z_2 [12]. The solution is rather neat for the spheres. Consider first $n = 1$, where the order parameter is a two component field ϕ_a with $\sum_a \phi_a^2$ constant. The problem consists essentially of placing three points ϕ^1, ϕ^2, ϕ^3 at random on the circle of constant $\sum_a \phi_a^2$, and asking the probability for ϕ^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 ϕ^1 and ϕ^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 neighboring 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 $\boldsymbol{x} \rightarrow -\boldsymbol{x}$ symmetry. One cannot unambiguously do this with four domains, for the geodesic rule produces a mapping from the tetrahedron $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4\}$ 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.

To know just how many domains are needed, we need the *minimal triangulation* of RP^2, which is the triangulation with the smallest number of vertices. In order to be a proper triangulation, each edge must be connected to two different vertices, each face to three different edges, and so on. To consistently use the geodesic rule it is necessary for the director field to map the domains to a proper triangulation, for there will otherwise be ambiguities when constructing the interpolating simplices. If we have an arrangement of domains, which are connected together by edges and faces into a surface with the topology of a sphere, then that surface will contain a hedgehog only if the surface is mapped onto M twice. The minimal triangulation therefore tells us the smallest surface that can contain a hedgehog: it has twice the number of domains as the minimal triangulation has vertices. The minimal triangulation of RP^2 has, in fact, six vertices (see Fig. 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 twelve uncorrelated adjacent domains.

A great deal of calculation can now be saved by an approximation which uses a fixed triangulation of RP^2

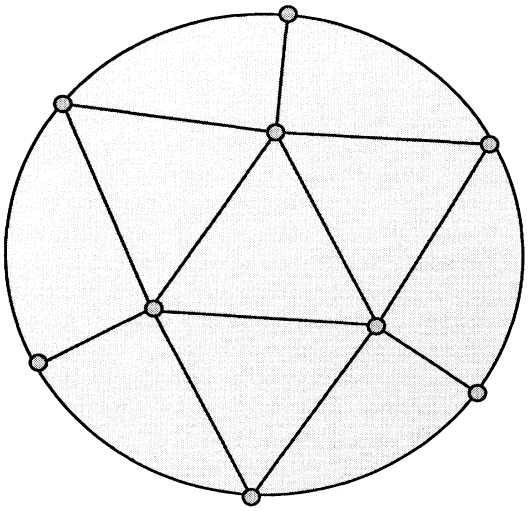

FIG. 1. The minimal triangulation of RP^2, consisting of six vertices, twelve edges, and ten faces. This is essentially the top half of an icosahedron. Opposite points on the boundary are identified.

directly. For example [13,14], if we approximate S^1 by three equidistant points labeled 0, 1, and 2, and assign a string to a spatial triangle $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$ when all three values of ϕ 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 a one-dimensional defect passing through the triangle is

$$P_1'(S^1) = 3!/3^3 = 2/9, \tag{4}$$

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

$$P_n'(S^n) = (n + 2)!/(n + 2)^{n+2}. \tag{5}$$

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

$$P_1'(RP^2) = 6 \times 5 \times 2/6^3 = 10/36, \tag{6}$$

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 twelve 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

$$P_2'(RP^2) = 60/6^{12} \simeq 2.76 \times 10^{-8}. \tag{7}$$

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 ξ_0^3, and so the density of point defects N_p is roughly

$$N_p \simeq 10^{-8} \xi_0^{-3}. \tag{8}$$

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 [15].

The icosahedral arrangement of domains can be extended into the body of the material by the addition of a further domain in the center. One then realizes 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. As the smallest loops are the most common, larger loops with unit topological charge are presumably even rarer.

The explanation in terms of the Kibble mechanism may still not be wholly satisfactory, for there is also a severe initial deficit in n_L, the number density of loops [1]. Calculations using the Kibble mechanism for Abelian strings, where $M \simeq S^1$, indicate that the fraction of string in the loops is 0.2–0.3 [13,14], whereas $n_L \xi^3$ is never greater than about 4×10^{-3}. It is possible that with $M \simeq RP^2$ the loop fraction is much lower, but preliminary measurements are not encouraging [16].

To conclude, I outline the mathematical structure implicit in the geodesic rule. Recall that the construction starts with points $\{\boldsymbol{x}_i\}$ 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 $\{\boldsymbol{x}_i\}$ to a full triangulation, defining the order-parameter field $Q(\boldsymbol{x})$ 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 [17] in the order-parameter space M. However, the procedure fails when some subcomplex cannot be filled in, that is, the subcomplex is not the boundary of another, higher-dimensional complex in 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 nontrivial 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 nontrivial. The second homology class of RP^2 is zero, which is the underlying reason for the low density of point defects.

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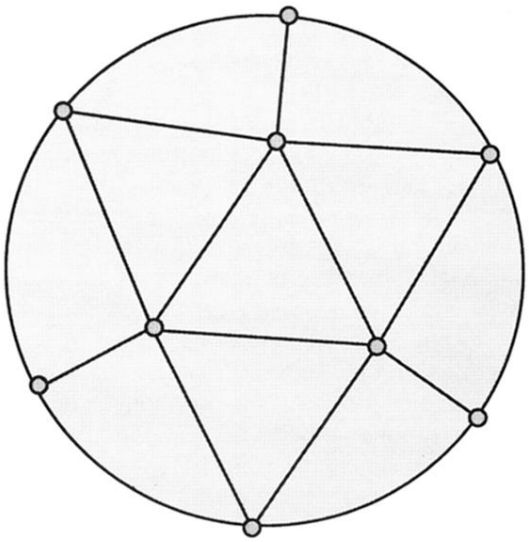

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