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Defects in liquid crystals and cosmology

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Defects are a universal feature in systems of broken symmetry. They occur for example equally well in liquid crystals and cosmological field theories. The basic facts of defect theories in both systems are reviewed. It is reported how cosmologists have used liquid crystals to check theories on the defect evolution of the early universe and how in this way they have contributed considerably to the insight into defect creation and dynamics in liquid crystals.

1. Defects in liquid crystals

Nematic liquid crystals are named after their defect lines: the dark threads $(v\tilde{\eta}\mu\alpha\tau\alpha)$ visible in the polarizing microscope. Textures and defects are striking properties of liquid crystalline systems, used to identify them. Focalconics, for example, point to the existence of layers with constant separations and thus mark smectic or cholesteric liquid crystals.

Defects are a consequence of the universal concept of 'broken symmetry' [1,2], which is amply realized in liquid crystals. It says that there is a unique high symmetry phase, which in the case of nematic liquid crystals is the isotropic phase, invariant under the unbroken symmetry group SO(3) of all rigid rotations. The symmetry is reduced in a phase transition, here into the uniform nematic phase, which is uniaxially symmetric and of broken symmetry group $D_{\infty} < SO(3)$. But the axis of symmetry is arbitrary, so there is an entire set of minima, denoted the vacuum manifold.

To describe symmetry breaking requires a non-linear theory, which in the case of nematics is the Landaude Gennes (L-G) theory [3]. There, the free energy density is expanded up to quartic terms of an order parameter, which is a symmetric and traceless 'alignment tensor' Q. The value $\hat{v} Q \ \hat{v} = \sum_{ij} v_i Q_{ij}v_j$ is a measure for how much the probability of a molecule pointing along the unit vector \hat{v} deviates from an isotropic distribution (1/4 π).

The equilibrium order parameter Q_0 taken by the nematic is the minimum of the L–G free energy density:

$$f(T,p,Q) = \frac{1}{2}a(T,p)\operatorname{tr} Q^2 - \frac{1}{3}b\operatorname{tr} Q^3 + \frac{1}{4}c(\operatorname{tr} Q^2)^2 \quad (1)$$

where the coefficient at the quadratic term depends on temperature and pressure (mostly assumed in a linear fashion), and where b, c>0. The density is invariant under rotations of the order parameter Q by elements of the unbroken symmetry group SO(3).

The type of minimum order parameter is determined by the sign of the coefficient *a*. The absolute minimum is attained at Q=0 for $24ac/b^2 \ge 1$. It is of unbroken symmetry. When *a* changes sign, at $24ac/b^2 \le 0$, the minimum is taken by uniaxial alignment tensors of the form

$$Q = \frac{3}{2^{1/2}} S\left(\hat{n} \otimes \hat{n} - \frac{1}{3}\right).$$
 (2)

Q=0 still forms an extremum, but now a maximum (denoted 'false vacuum'). The symmetry is broken, but \hat{n} (which according to equation (1) is equivalent to $-\hat{n}$), is an arbitrary unit vector. Hence the degenerate set of minima or the vacuum manifold is the sphere S^2 with identified antipodal points, which forms the projective plane P^2 . For $0 \le 24ac/b^2 \le 1$ there are two minima resulting in the coexistence of the two phases, as the transition is of first order.

If the isotropic phase is cooled or compressed into the nematic phase rapidly, nucleation occurs in domains or bubbles with different director orientations, i.e. of different 'vacua'. It might occur that three domains meet along a line such that on a loop about the line the director rotates by an integer multiple of π (see the figure). The line forms a singularity in the sense that on it the director is not defined, which means that the order parameter Q must have left the vacuum manifold. The core of the singularity is of a different phase and of higher energy than the surroundings. One might assume



Figure. Kibble mechanism for formation of a defect line in a nematic. (a) Three domains with different director orientations; the bars indicate molecule orientations. (b) The domains have merged leaving a linear singularity (extending out of the paper plane); the thin lines denote director orientations. Upon encircling the singularity, the director rotates by 180°; on the singular line the director orientation is undefined.

that the core consists of the 'false' vacuum Q=0, but a closer analysis shows that in nematics the core is a biaxial phase of variable axes length with $tr Q^2 = const$ [4]. The core diameter is of the 'biaxial coherence length' $(K/b|Q_0|)^{1/2} \sim 20$ nm, and the energy per cm of the singularity is $4\pi^3 KQ_0^2$ (~10⁻⁵ erg in MBBA), where $K \sim 10^{-6}$ dyn is an elastic constant and Q_0 is estimated ~0.6.

In the mid-1970s the richness of order parameter spaces and vacuum manifolds in liquid crystals and in the superfluid phases of ³He and ⁴He motivated the development of a 'topological theory of defects in ordered media' [5-9]. The theory first pointed out that a vacuum manifold is topologically equivalent (homeomorphic) to the set of cosets G/H, where G is the unbroken symmetry group, and H the broken one. Furthermore, the connectivity properties of the vacuum manifold determine whether there exist wall, line, point defects or textures in a phase. If the vacuum consists of disconnected parts and if vacua of adjoining domains belong to different pieces, then the domains are separated by a wall. If the vacuum is not simply connected, i.e. if there are non-contractible loops in it, there are stable line singularities. If there are non-contractible twospheres in the vacuum manifold, the system possesses stable point singularities. Finally, non-contractible threespheres within the vacuum cause stable textures.

The connectivity properties of the vacuum manifold for nematic liquid crystals, the projective plane P^2 , are such, that lines, points and textures are allowed topologically. Energetically, however, textures decay into points [10]. In the case of free boundary conditions, points will be connected by strings, which decay by 'escape to biaxiality' [11]. Thus, essentially only linear defects remain in nematics.

2. Defects in cosmology

The concept of 'broken symmetry' actually stems from high energy or particle physics [12], where it is a central guiding principle. Evidently also the notion of 'vacuum' is taken from this discipline.

It is an important objective of particle physics to describe the different forces of nature in a unified language. For this purpose, Hilbert spaces of many particle wave functions ψ are enlarged by 'inner degrees of freedom'. For example, to master the weak interaction, weak isospin is introduced, so that the wave function is a two component complex vector field $\psi \in C^2$. For the strong interaction, the colour degree of freedom is required, and $\psi \in C^3$ becomes a complex three component field. Whereas the L-G free energy density had to be invariant under rotations of the order parameter Q, the particle Lagrangian densities are invariant under unitary or special unitary operations in the extended Hilbert spaces, for example under $SU(2)_w$ or $SU(3)_c$ (w stands for 'weak', c for 'colour'). These symmetries are decoupled from spatial symmetries and form purely internal or 'dynamical' symmetries. The symmetry group of the current standard model for strong and electroweak interactions is $SU(3)_{c} \otimes SU(2)_{w} \otimes U(1)$ [13, 14]. The particle states are not invariant under this group, but transform according to certain irreducible representations. The state invariant under the group is the particlefree state of lowest energy, the literal vacuum, just as a uniform nematic is D_{∞} -invariant. With this comparison we are already implying that this vacuum is of a broken

symmetry, and that at high temperatures there is another vacuum of unbroken symmetry group, of which $SU(3)_c \otimes SU(2)_W \otimes U(1)$ is a subgroup. When this vacuum is present, all forces are of equal strength. The corresponding theory is the Grand Unification Theory (GUT), which attempts to unify the electroweak and strong interaction, starting from symmetry groups like SO(10) or SU(5) [13].

Whereas the phase transition temperatures in liquid crystals are between 240 and 400 K, in particle theories for the unbroken symmetry phase they are T = $10^{15} \text{ GeV} \sim 10^{28} \text{ K}$ and so tremendous that they were accessible only in the first instants of the big bang, namely before $t=10^{-35}$ s of the age of the universe. As the cosmos expanded it cooled down and experienced symmetry breaking phase transitions of the vacuum. There are no confirmed unbroken and broken symmetry groups, only speculations {e.g. $SO(10) \rightarrow SU(5) \times Z_2$ [15, 16]}, but it is reasonable to assume, that defects were also created, in particular as in causally unconnected regions different vacuum states had to nucleate. Just as in liquid crystals, the dimension of the defects depends on the connectivity properties of the vacuum. Out of walls, lines, points and textures essentially lines remained in the discussion (a wall separating the cosmos in two parts would have more mass than the rest of the universe, points in the form of magnetic monopoles would be too abundant).

These singular lines are denoted cosmic strings [16–18] and possess amazing properties. They are either infinitely long or form loops of 1 million light years across. The diameter of the defect core, 10^{-30} cm, is close to the Planck length. The core consists of the 'false vacuum' and its energy is 10^{17} tons cm⁻¹. The loops oscillate, dispersing their energy by gravitational radiation. Smaller loops, of diameter 100 light years, might have nucleated galaxies. The larger ones might be responsible for the large scale structure of the universe, for anisotropies in the cosmic background microwave spectrum and for the matter–antimatter asymmetry.

Due to the importance of defects for cosmic evolution, the 'topological theory of defects' was developed in the mid-1970s also by cosmologists [19], independent of the condensed matter physicists and mutually unnoticed. When two successive symmetry breaking phase transitions occur, bounded defects can arise; for instance line singularities terminating at a point defect, or wall singularities terminating on a line. The topological description of these defects, denoted 'semidefects' in condensed matter physics [9, 20] and 'hybrid defects' in particle physics [13, 21], was also developed in parallel by methods of algebraic topology. Hybrid defects most recently were discussed as cosmic structure forming entities [22].

To predict a defect-induced large scale structure of the universe, for cosmologists the dynamical evolution of defect networks is of the same importance as structural static properties of defects. The scenario of defect formation by coalescence of regions with different vacuum values, indicated in the previous section, was developed and evaluated statistically by Kibble [19]. Kibble estimated the defect density at formation under the assumption that there is a characteristic scale ξ beyond which the order parameter is uncorrelated. Thus initial conditions on the density of the line defect network were gained. Subsequently the defects coalesce and annihilate, straighten, recombine and emit loops that collapse, so that the network is coarsening and the density is decreasing. This process is described by a scaling theory, which goes back to Binder and Stauffer [23]. It states that at all times the defect networks look similar, differing only by the scale ξ , which informs us about the mean separation. This scale expands with a power law of time: $\xi \sim t^{\alpha}$. Relativistic strings retreat with the velocity of light, hence $\alpha = 1$, but in dispersive systems like liquid crystals α was predicted as $\frac{1}{2}$. (For a thorough review on the determination of exponents both in conserved and unconserved systems consult the articles by Bray [24], Mazenko [25] and Goldenfeld [26] in reference [27].)

But apart from computer simulations, cosmologists do not have a chance to confirm their theories in experiment. They therefore turned to condensed matter systems.

3. Cosmology in the laboratory

In 1985 Zurek [28] proposed that a check on Kibble's theory be made for liquid ⁴He. The vacuum is a circle [the set U(1) of phase factors in the complex plane], the potential is of the Mexican hat form, and the phase transition is second order as in most cosmological models. However, the line singularities in the form of vortices can be observed only indirectly, by attenuation of second sound, and the experiment has been performed only recently [29].

A system still closer to the conditions of particle theories would be a superconductor. The singularities are magnetic flux lines, the symmetry is a local gauge theory, connected with the magnetic field as gauge field. But observability is difficult.

Therefore nematic liquid crystals were used by the group of Yurke. Chuang *et al.* [10] performed a rapid transition from the isotropic to the nematic phase of 5CB through a pressure quench. The evolution of the defect network was documented by a high speed video camera. The defect dynamics indeed followed exactly the scaling law with $\alpha = 0.5$. The authors also observed string recombination and decay of a texture into a

monopole–antimonopole pair. In another experiment, also with 5CB [30], the average number of line singularities per bubble was counted as 0.6, yielding agreement with the prediction of the Kibble mechanism.

Thus the cosmologists have been given an impetus to study the dynamical evolution of liquid crystal phase transitions via defect formation and defect coarsening. Conclusive confirmation of the existence of cosmic strings, however, is not yet given. Currently many studies concentrate on the interpretation of the infrared measurement of the microwave background anisotropy by the COBE-satellite (Cosmic Background Explorer) [31].

To merge the knowledge on defects of cosmologists and condensed matter physicists, a six-month-long workshop was organized at the Isaac Newton Institute for Mathematical Sciences at Cambridge, UK, in the second half of 1994. Within this period an Advanced Study Institute took place, whose proceedings provide an excellent overview of current theories on formation and interactions of topological defects [27].

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