

Date: 13 December 2023

Selinger, J. “Nematic order parameter,” 2020, Lecture, Kent State University. (accessible at <https://youtu.be/YniRGp6CuB8?si=WZpZ0tamdgohafRa>)

In chemical physics, a mesophase (or *mesomorphic* phase) is an intermediate, anisotropic phase between solid and liquid. Gelatin is a macroscopic example, as are microscopic biological features like phospholipid bilayers, rod-like bacterial growth patterns, and other “mesogens.” Symmetric molecules that lose positional order but retain orientational order as entropy increases can be considered nematic¹. I found Professor Selinger’s discussion too lacking in topology considering Professor Beller’s focus on disclinations during my introductory meeting, so I sought out a lecture that built up the Q tensor with more geometry than (linear) algebra.

Ball, J. (2010). “The Q-tensor theory of liquid crystals.” Lecture slides, Oxford Centre for Nonlinear PDE, presented at Summer School, Benin.

Consider a nematic liquid crystal filling a container $\Omega \subset \mathbb{R}^3$, where Ω is connected with Lipschitz boundary (*i.e.*, sufficiently regular; locally a graph of a Lipschitz continuous function) $\partial\Omega$. Given a ball at position x_0 and very small radius δ , we can draw a line through the origin parallel to a dipole p , which is an element of $\mathbb{R}P^2$. The pair $\{p, -p\}$ can be interpreted as antipodal unit vectors or as a matrix (or tensor) $p \otimes p$, where $[p \otimes p]_{ij} = p_i p_j$. Notice that this method allows us to drop consideration of the antipodal unit vectors and thus have a collective direction. The distribution of orientation of molecules in $B(x_0, \delta)$ can be described as a probability measure on $\mathbb{R}P^2$. In other words, a probability measure μ on the unit sphere (or ball) S^2 so long as the measure is symmetric about its domain² ($\mu(E) = \mu(-E)$ for $E \subset S^2$).

Now, we are given a continuously distributed measure $d\mu(p) = \rho(p)dp$, where dp is the element of surface area on S^2 and $\rho \geq 0$, $\int_{S^2} \rho(p) dp = 1$ and $\rho(p) = \rho(-p)$. The first probability moment is zero. The second moment,

$$M = \int_{S^2} p \otimes p d\mu(p), \quad (1)$$

is a symmetric nonnegative 3×3 matrix satisfying $\text{trace}(M) = 1$. Let $e \in S^2$. Then,

¹ Roughly speaking, that is. The S increase concept is applicable in cases of a system largely tending to equilibrate. Our group’s study of “active matter,” from what Professor Beller mentioned, largely discards these thermodynamic principles in favor of the topological understanding of dynamical systems, particularly fluid-mechanical ones.

² Interesting Math StackExchange discussion from 10 years ago on symmetric probability measures: <https://math.stackexchange.com/questions/545566/symmetric-probability-measure>

$$\begin{aligned} e \cdot Me &= \int_{S^2} (e \cdot p)^2 d\mu(p) \\ &= \langle \cos^2 \theta \rangle, \end{aligned}$$

Where θ is the angle between p and e . If the orientation of molecules is equally distributed, the distribution is isotropic, and $\mu = \mu_0$, where

$$d\mu_0(p) = \frac{1}{4\pi} dS. \quad (2)$$

This relationship gives us the corresponding second moment tensor,

$$M_0 = \frac{1}{4\pi} \int_{S^2} p \otimes p dS = \frac{1}{3} \mathbf{1}, \quad (3)$$

where $\mathbf{1}$ is, to my knowledge, the unit tensor. Since $\int_{S^2} p_1 p_2 dS = 0$, $\int_{S^2} p_1^2 dS = \dots = \int_{S^2} p_N^2 dS$, and $\text{Tr}(M_0) = 1$. We can now introduce the **de Gennes Q-tensor** $M - M_0$ as the deviation of M from its isotropic form. It is written as

$$\mathbf{Q} = \int_{S^2} \left(p \otimes p - \frac{1}{3} \mathbf{1} \right) d\mu(p), \quad (4)$$

is symmetric ($\mathbf{Q} = \mathbf{Q}^\top$), $\text{Tr}(\mathbf{Q}) = 0$, and $\mathbf{Q} \geq -\frac{1}{3} \mathbf{1}$.

To wrap up for today, I will fast-forward to defects in constrained theory (slide 40).

Given $\mathbf{Q} = s(n \otimes n - \frac{1}{3} \mathbf{1})$ (from the constrained theory) and hedgehog function $n(x) = \frac{x}{|x|}$, we get $\nabla n(x) = \frac{1}{|x|} (\mathbf{1} - n \otimes n)$, $|\nabla n(x)|^2 = \frac{2}{|x|^2}$, and $\int_0^1 r^{2-p} dr < \infty$ (finite energy). A **disclination** occurs when $n(x) = (\frac{x_1}{r}, \frac{x_2}{r}, 0)$ and, consequentially $r = \sqrt{x_1^2 + x_2^2}$, so $|\nabla n(x)|^2 = \frac{1}{r^2}$ (more generally, disclinations command Coulomb law attractive and repulsive forces on a field). These regions are points where $\mathbf{Q} \notin W^{1,2}$.

Getting into topology I still need to learn, we get that for a variety of boundary conditions, under suitable inequalities on the L_i (material constants) such that the elastic energy

$$\psi_E(\mathbf{Q}, \nabla \mathbf{Q}) = \sum_{i=1}^N L_i I_i \quad (5)$$

has axial order, we can understand \mathbf{Q} as a minimizer of a function on the elastic energy field where we hold the weak form of a basic equilibrium equation with symmetrized elastic energy:

$$Z\mathbf{Q} = \mathbf{Q}Z, \text{ where } Z_{ij} = \frac{\partial \psi_E}{\partial \mathbf{Q}_{ij}} - \frac{\partial}{\partial x_k} \frac{\partial \psi_E}{\partial D_{ijk}} \quad (6)$$

where, for each point $x \in \Omega$, we have a corresponding measure μ_x and (potentially nematic) order parameter tensor $\mathbf{Q}(x)$, we suppose that the material is described by a free-energy density with an associated unit third-order tensor D .