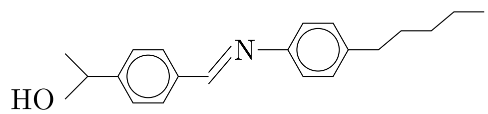
The Nematic-Isotropic Phase Transition (Model 2)

A **liquid crystal** refers to a state of matter which has properties reminiscent of both a liquid and a crystal. For example, a liquid crystal may flow like an ordinary liquid, but the molecules may tend to orient themselves along a common axis, just as would happen in a crystal. Liquid crystals can be made of both organic and inorganic compounds, and they appear in everything from electronics to (arguably) cell membranes.

The liquid crystals of interest for the purposes of this problem are called **thermotropic** liquid crystals. They exist in an ordered liquid crystal state and a disordered liquid state; by raising and lowering the temperature, we can transition between these two states. Most of these liquid crystals consist of long rod-like organic molecules such as the one below:[1]

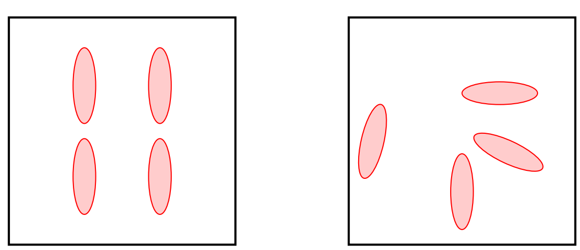


A single liquid crystal molecule such as the one above breaks most of the rotational symmetry of space. We will assume, however that the molecule does preserve a parity operation; even though it is certainly not *truly* symmetric, it is close. If a collection of them are all aligned, they macroscopically break the rotational symmetry of a fluid (and are therefore a crystal). Therefore, an appropriate order parameter for studying liquid crystals is $\hat{\mathbf{n}}(\mathbf{r})$, where $\hat{\mathbf{n}}$ is a unit vector satisfying

$$\hat{\mathbf{n}} \cdot \hat{\mathbf{n}} = 1.$$

which points in the direction of (one of the) ends of the rod.[2]

Liquid crystals can exist in two phases. In one phase, the molecules tend to all line up; this is called the **nematic phase**. (This is why they are called crystals even though they are not actually made up of an ordered lattice!) At high enough temperatures, however, this crystalline phase disassociates into an **isotropic phase** where the molecules have no preferred orientation.



(ordered) nematic phase (unordered) isotropic phase

We can use Landau theory to model this transition between isotropic and nematic phases, just as with Ising ferromagnetism. The appropriate order parameter to use is the *average* deviation from the isotropic

[1] This is MBBA, or N-(4-Methoxybenzylidene)-4-butylaniline. It is a liquid crystal commonly found in modern technologies.

[2] The Nobel Prize in Physics was awarded to Pierre-Gilles de Gennes for first using the concept of order parameters to study complex forms of matter such as polymers and liquid crystals, so this is fairly modern stuff!

case: we characterize this by a traceless tensor given by

$$Q_{ij} = \left\langle n_i n_j - \frac{1}{3}\delta_{ij} \right\rangle .$$

For example, if the liquid is isotropic, then $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3}$, as follows from the fact that $\langle x^2 + y^2 + z^2 \rangle = \langle \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} \rangle = 1$, and in this case (since off-diagonals will vanish) we get that $Q_{ij} = 0$. If the liquid is in a perfect crystal phase where $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ everywhere, then $Q_{xx} = Q_{yy} = -\frac{1}{3}$ and $Q_{zz} = \frac{2}{3}$. Using this logic, we choose to represent the order parameter in the following form

$$Q_{ij} = \begin{pmatrix} -\frac{1}{2}x & 0 & 0 \\ 0 & -\frac{1}{2}x & 0 \\ 0 & 0 & x \end{pmatrix}$$

where x is a simpler (scalar) order parameter.

(a) What is the allowed spectrum of x?

The free energy density for a nematic in the neighborhood of the nematic-isotropic transition is given by

$$\mathcal{F} = \mathcal{F}_0 + \frac{1}{2}a(T - T_0)\ \mathrm{tr}\left(Q^2\right) - \frac{1}{3}b\ \mathrm{tr}\left(Q^3\right) + \frac{1}{4}c\left(\mathrm{tr}\left(Q^2\right)\right)^2 .$$

T_0 is a temperature in the neighborhood of the transition, but as we do not know the precise nature of the transition itself it is unwise to say anything further. We can take a, b and c to all be positive constants.

(b) Express $\mathcal{F}$ as a function of x.

(c) Find the values of x for which $\mathcal{F}$ is an extremum.

(d) There exist four regimes of temperature for this Landau theory:

	isotropic phase	nematic phase
$T < T_0$	unstable	stable
$T_0 < T < T_1$	metastable	stable
$T_1 < T < T_2$	stable	metastable
$T > T_2$	stable	unstable

Draw the curve $\mathcal{F}(x)$ in each of these temperature regimes, and find expressions for T_1 and T_2.