

Exercise sheet #12

Problem 1. What does “short range order” mean in the context of molecules in a fluid? How does that compare to the structure of a liquid?

Solution: Short range order means that there is some order in the orientation or spacing of molecules (or atoms) over a short distance (there is a correlation between the distances of nearest neighbors), but there is no order over longer distances. The order of liquid crystals is higher than that in liquids, that have no long or short range order at all. \square

Problem 2. Liquid crystals are phases of matter that are intermediate between solids and liquids. In the nematic phase, molecules have no positional order (they can flow like a liquid), but they exhibit long-range orientational order: their long axes tend to align along a common direction called the director. At first glance, this seems surprising. Pure liquids are disordered, why would molecules in a “liquid” spontaneously align? Explain qualitatively why the nematic phase can be thermodynamically stable, even though the molecules are still mobile like in a liquid. Why does raising the temperature eventually destroy the nematic order, leading to an isotropic liquid?

Solution: A nematic phase can be stable because, although aligning rod-like molecules reduces their orientational freedom, it allows them to pack more efficiently and reduces the amount of space they exclude to one another. When the molecules point in similar directions, they interfere less with each other’s motion, so each molecule gains more room to translate and move around, which increases the system’s translational entropy. The loss in orientational entropy is therefore outweighed by the gain in positional entropy, making the partially ordered nematic phase thermodynamically favorable even though it remains fluid. As the temperature is raised, however, thermal motion increases and the benefit of orientational alignment becomes insufficient to compensate for the entropic drive toward randomness, causing the system to transition to an isotropic liquid in which molecular orientations are fully randomized. \square

Problem 3. In a nematic liquid crystal, the rod-like molecules tend to point roughly in the same direction, called the director. The amount of alignment is measured by the order parameter S , which is close to 1 when molecules are well aligned and close to 0 when they are almost random.

Light polarized parallel to the director experiences a refractive index n_{\parallel} , while light polarized perpendicular to it experiences n_{\perp} . The birefringence¹ is

$$\Delta n = n_{\parallel} - n_{\perp}.$$

Explain qualitatively why a higher order parameter (stronger molecular alignment) leads to a larger birefringence.

Solution: As the order parameter S increases, the molecules in the nematic phase become more consistently aligned with each other, meaning that their long axes point in nearly the same direction. Because each molecule interacts differently with light depending on the orientation of its long axis, this increased alignment amplifies the difference between how the material responds to light polarized parallel versus perpendicular to the director. When molecules are well aligned, light polarized parallel to the director couples strongly to the long-axis polarizability of many molecules at once, giving a larger effective refractive index in that direction. Light polarized perpendicular to the director mostly interacts with the short axes of the molecules, which produce a weaker response and therefore a smaller refractive index. With weak alignment (small S), these directional differences mostly average out, so the refractive indices become nearly equal and the birefringence is small. But when the alignment becomes stronger (large S), the optical anisotropy becomes more pronounced, and the difference $n_{\parallel} - n_{\perp}$ increases accordingly. Thus, higher orientational order directly enhances the material’s birefringence because it sharpens the contrast between the optical response along and across the director. \square

¹Birefringence, also known as double refraction, is the optical property of certain materials where light is refracted in two different directions, resulting in two distinct rays.

Problem 4. In a nematic liquid crystal, the rod-like molecules tend to align along a common direction called the director. However, in many situations—such as when the material is confined, rubbed surfaces impose different orientations, or temperature changes occur—this alignment cannot be maintained everywhere. As a result, topological defects (also called disclinations) appear, where the director field becomes undefined.

Consider a thin film of nematic liquid crystal confined between two parallel plates. The plates impose different anchoring directions: the bottom plate forces the director to lie horizontally, while the top plate forces the director to lie vertically. Somewhere in the film, the director field must change from one direction to the other.

- a) Explain why defects must form in this situation.
- b) A common defect in nematics is a $\pm\frac{1}{2}$ disclination, where the director rotates by $\pm 180^\circ$ around a loop enclosing the defect core. Explain qualitatively why such half-integer defects are allowed in nematic liquid crystals, and why they occur more frequently than integer defects.
- c) Describe how the elastic energy of the liquid crystal tends to influence the size and structure of the region near a defect, and why the core of the defect often behaves more like an isotropic fluid.

Solution: a) Defects must form because the boundary conditions imposed by the plates are incompatible: the bottom plate forces the director to lie horizontally, while the top plate forces it to lie vertically. The director field cannot smoothly satisfy both orientations everywhere without some singular point or line where the orientation becomes undefined. At these points, the continuous alignment breaks down, creating a topological defect. The system cannot continuously interpolate between the two orientations everywhere without introducing such a singularity.

- b) In nematic liquid crystals, the molecules are head-tail symmetric: the long axis has no intrinsic "arrow" direction. This means that a 180° rotation of the director is equivalent to no rotation at all. As a result, half-integer disclinations ($\pm 1/2$), where the director rotates by 180° around the defect, are allowed. Integer defects, which would require a full 360° rotation of the director, carry higher elastic energy and are therefore less common. The head-tail symmetry of nematic molecules makes half-integer defects energetically favorable and topologically permissible.
- c) The elastic energy of the nematic tends to penalize rapid changes in the director orientation, so the director field around a defect spreads the distortion over a finite region to reduce energy. Near the very center, or core, the elastic energy would diverge if the molecules remained aligned, so the material often becomes locally disordered or isotropic, relieving the singularity. The size of this defect core is typically on the order of a few molecular lengths, while the director distortion extends over a much larger distance, producing the characteristic pattern of alignment around the defect.

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