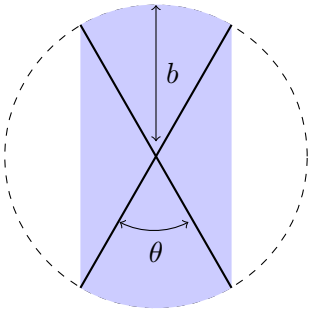
statistical physics → microcanonical ensemble ★★★

The Nematic-Isotropic Phase Transition (Model 1)

Liquid crystals are phases of matter which may flow, but tend to have some sort of ordering nonetheless. The classic way this can occur is to have a collection of rod like molecules, which may enter a nematic phase in which the rods all tend to align with each other.

In this problem, we consider a simplified model of the transition between a nematic phase, where the liquid crystal molecules all tend to align. Consider a collection of N rods of length $2b$ living on a 2 dimensional surface of area A. We assume that these rods rods typically rotate through an angle θ, and thus are associated with an excluded area $a(\theta)$ corresponding to the area in which they rotate:



The phase space volume allowed for a given rod can be approximated as

$$\text{rod's phase space volume} = \text{allowed volume in space} \times k\theta.$$

(a) Find a formula for $a(\theta)$.

(b) Find the entropy $S = \log(\text{phase space volume})$ of a configuration of N rods.

(c) Find the a relation between the rod density $n = N/A$ and the angle θ such that the entropy S is maximized: i.e., find an expression for $n(\theta)$.

(d) Using a computer program such as `Mathematica`, plot $n(\theta)$.

(e) Using your sketch, show that a phase transition occurs between a nematic (ordered) phase and an isotropic (disordered) phase. Show on the sketch the angle θ_c and the density n_c at which the phase transition occurs. Comment on the physical interpretation of why a phase transition occurs.