

Liquid crystals and the Coulomb gas

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Abstract We propose that the Liquid Crystal nematic phase can be described by a lagrangian that also describes a Coulomb gas. Using this lagrangian, we show that the Coulomb charges appears as defects in the nematic state. Using this approach, we calculate the nematic isotropic phase transition temperature value and argue that it is a Kosterlitz-Thouless phase transition.

1. Formulation of Problem

Liquid crystals (L.C) have a variety of phases that have been studied mainly with the use of the Landau approximation (or mean field approximation)^{1,2,3}. The results describe efficiently the observed phenomenology, although one still lacks a realistic visualization of the L.C. microscopic structure. The expansion constants are adjusted to give the observed results. This is the essence of the mean field approximation. If we wish a real microscopic description, this approximation must be abandoned.

This is by no means an easy task. There are so many systems with the nematic isotropic phase transition that, if we make a detailed study of a specific microscopic system, we can miss the transition's generality. In this way, if we want be in a general case, it is difficult to abandon the mean field approximation.

In a sense, this work intends to present an intermediate approach. We make a microscopic description of the L.C, making an idealization of the nematic phase structure, and study the dynamics and interaction of some L.C. defects⁴. Using these defects, we make a detailed study of the nematic isotropic phase transition mechanism, and claim that these defects have an important role in this transition mechanism. Finally, our nematic isotropic phase transition approach will explain why specific details of the nematic rods interaction are not important when they are close to the critical point. That is; why, in spite of the variety of nematic

Liquid crystals and the Coulomb gas

molecule structures, do the nematic isotropic phase transitions appear to be independent of the molecule details?

A- The Nematic Phase

We begin by defining what will be here understood by the L.C. nematic phase. The L.C. elements are assumed to be one-dimensional hard rods, with length l , randomly distributed in the sample, in a way that we can say that, in the mean, at low temperatures, they are aligned in a local \vec{n} direction, as showed in figure 1. We impose also, that independently of its structure, the hard rods are: a-) Indistinguishable by 180° rotations around any axis perpendicular to their center of mass; b-) The system is locally invariant by translations along a local axis \vec{e}_z .

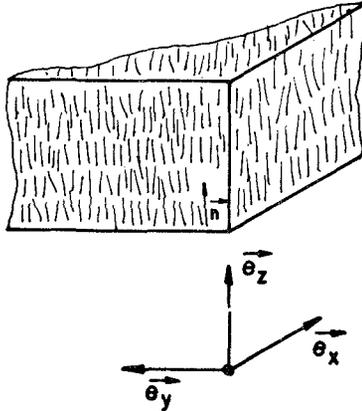


Fig. 1 - Nematic phase representation of a Liquid Cristal aligned in the direction \vec{n}

B- The Hamiltonian

To build up the hamiltonian that describes our system, we request that it should have two terms. The first one describes the interaction between the nearest hard rods. The second, the action on a rod, of a mean field produced by the others and/or the action of a external field.

To write down the first term, we look at figure 2 and suppose that, at the point $\vec{r} = (x, y, z)$, there is a rod inclined at an angle $\theta = \theta(x, y)$ in relation to an arbitrary global direction \vec{n} (not necessarily the direction of the director which will be discussed below). We made use of the translational invariance of the system with relation to \vec{e}_z , supposing that θ depends on both x and y . We will use the azimuthal invariance of the halmiltonian making it dependent only on θ ; no dependence on the spherical ϕ angle is assumed. We postulate that neighbour rods interaction, at low temperatures, minimizes their center of mass distances

and the difference between their θ angles. Thus, the rods at the positions \vec{r} and $\vec{r} + \vec{s}$ will contribute to this term as

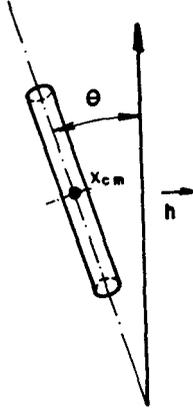


Fig. 2 - A hard rod inclined by an angle θ in relation to the arbitrary direction \vec{n} .

$$T_1 = \frac{1}{2} K_\theta \{ (\theta(x + s_x, y + s_y) - \theta(x, y)) \}^2 + \frac{1}{2} K_{X_{cm}} \{ (\vec{X}_{cm}(\vec{r} + \vec{s}) - \vec{X}_{cm}(\vec{r})) \}^2 \quad (1)$$

and, when, $s \rightarrow 0$, we rewrite it as

$$T_1 = \frac{1}{2} K_\theta \left\{ \left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right\} + \frac{1}{2} K_{X_{cm}} \left\{ \left(\frac{\partial X_{cm}}{\partial x} \right)^2 + \left(\frac{\partial X_{cm}}{\partial y} + \left(\frac{\partial \theta}{\partial z} \right)^2 \right) \right\} \quad (2)$$

Now we go to the second term, describing the interaction of the rod with the mean field produced by the others or with an external field. If we knew exactly the internal structure of a rod we could write down this term. But we make no hypothesis about the rod's internal structure. So, we only use the general hypotheses a-) and b-) made above.

This term must depend on the difference between the rods θ angle and the direction of the director, which is determined by the mean direction of the other rods (let us say that the director points in θ_o direction). We write it as

$$V = V(\theta - \theta_o) = V(\varphi) \quad \text{where} \quad \varphi = \theta - \theta_o \quad (3)$$

From the hypothesis a-) we know that $V(\varphi)$ is periodic, with period π , that is

$$V(\varphi + \pi) = V(\varphi) \quad (4)$$

Liquid crystals and the Coulomb gas

At very low temperatures, the system must be aligned with the director direction; then at $\varphi = 0 - 0 = 0$ we have a minimum in $V(\varphi)$, or

$$\left. \frac{dV(\varphi)}{d\varphi} \right|_{\varphi=0} = 0 \quad \left. \frac{d^2V(\varphi)}{d\varphi^2} \right|_{\varphi=0} > 0 \quad (5)$$

There is also the possibility of center of mass dependence in this term. Therefore, we shall say that this term must have the general form

$$T_2 = V(\varphi) + U(\vec{x}_{cm}) \quad (6)$$

From this, we conclude that the hamiltonian becomes

$$\begin{aligned} H = & \frac{1}{2} K_{X_{cm}} \left\{ \left(\frac{\partial X_{cm}}{\partial x} \right)^2 + \left(\frac{\partial X_{cm}}{\partial y} \right)^2 + \left(\frac{\partial X_{cm}}{\partial z} \right)^2 \right\} + U(\vec{x}_{cm}) + \\ & + \frac{1}{2} K_{\theta} \left\{ \left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right\} + V(\theta - \theta_0), \end{aligned} \quad (7)$$

which can be rewritten as

$$H = H_{cm} + H_{\theta}, \quad (8)$$

where the expressions for H_{cm} and H_{θ} are evident from equation 7.

If we want to know the system thermodynamics, we have to calculate its partition function,

$$Z = \int D[X_{cm}] D[\theta] \cdot \exp \left(- \frac{1}{K_B T} \int \{ H_{cm} + H_{\theta} \} dx dy dz \right), \quad (9)$$

which is separable in two terms

$$\begin{aligned} Z = & \int D[X_{cm}] \exp \left(- \frac{1}{K_B T} \int \{ H_{cm} \} dx dy dz \right) \\ & \int D[\theta] \exp \left(- \frac{1}{K_B T} \int \{ H_{\theta} \} dx dy dz \right) \\ = & Z_{cm} \cdot Z_{\theta} \end{aligned} \quad (10)$$

This separation has some consequences in the study of many issues of the L.C. For example, the H_{cm} term may be the agent for the nematic crystalline phase transition, while the term H_{θ} give us the nematic isotropic phase transition. Obviously, the formalization and demonstration of it will require a detailed study of these two terms. In this report we will concentrate on the H_{θ} term.

C- Nematic Lotropic Phase Transition

We give, now, a qualitative argument that shows how the H_θ term can give the nematic isotropic phase transition. We show, below, a demonstration of this statement.

Take the Z_θ partition function, given by eq.(10)

$$Z_\theta = \int D[\theta] \exp \left(-\frac{1}{K_B T} \int \left\{ \frac{1}{2} K_\theta \left\{ \left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right\} + V(\theta - \theta_o) \right\} dx dy dz \right) \quad (11)$$

The \underline{z} integration that appears in the exponent can be easily . Therefore, the system dynamics is essentially bidimensional, a fact widely known and that seems to be a fundamental ingredient that characterizes the L.C. properties, as we will see.

Let us call the term in the exponent of eq.(11), thermal hamiltonian; we have

$$H(\theta, T) = \frac{1}{K_B T} L \int \left\{ \frac{1}{2} K_\theta \left\{ \left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right\} + V(\theta - \theta_o) \right\} dx dy \quad (12)$$

where \underline{L} is the system's length along the \vec{e}_z direction

Changing the variable to $\phi = \left(\frac{K_\theta}{K_B T} \right)^{\frac{1}{2}} \theta$, eq.(12) becomes

$$H(\phi, T) = L \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right\} + \frac{1}{k_B T} \cdot V \left(\left(\frac{k_B T}{K_\theta} \right)^{1/2} (\phi - \phi_o) \right) \right\} dx dy \quad (13)$$

We emphasize that, in this hamiltonian, the temperature dependence becomes restricted to the "potential" term. We study now what happens when we couple this fact to the properties given by eqs. (4) and (5). In eq. (13) we can define the "thermal potential".

$$\mathcal{U}(\phi) = \frac{1}{K_B T} \cdot V \left(\left(\frac{K_B T}{K_\theta} \right)^{1/2} (\phi - \phi_o) \right) \quad (14)$$

and because $V(\theta)$ has period $p = r$, $\mathcal{U}(\phi)$ has period $P = \left(\frac{K_\theta}{K_B T} \right)^{\frac{1}{2}} \pi$; therefore, the ϕ periodicity of $\mathcal{U}(\phi)$ has temperature dependence. With these elements we make a heuristic analysis of the high and low temperatures limits and see the indication of a nematic isotropic phase transition.

If we assume that the $V(\theta)$ function has upper and lower bounds, we see that, if $T \rightarrow 0$, the potential amplitude, that is, the term $\frac{1}{K_B T}$ of eq. (13), becomes arbitrarily large, which suppresses the fluctuations around the minima

Liquid crystals and the Coulomb gas

of the potential. So when $T \rightarrow 0$ the most stable configuration is $\theta = \theta_o$, which **suppresses** the term $\frac{1}{2}\{(\frac{\partial\phi}{\partial x})^2 + (\frac{\partial\phi}{\partial y})^2\}$. Therefore, the potential given by (14) is the only relevant term in the hamiltonian: we are in the nematic phase (**viz**, the Maier-Saupe approximation⁵).

In the other temperature limit, when $T \rightarrow \infty$, we see that the potential amplitude goes to zero. At the same time, the potential minima get arbitrarily close because the period, $P = (\frac{K_\theta}{K_B T})^{\frac{1}{2}}\pi$, goes to zero. So the **rod's** direction **fluctuates freely** around these minima. The dynamics of the system is dominated by the term $\frac{1}{2}\{(\frac{\partial\phi}{\partial x})^2 + (\frac{\partial\phi}{\partial y})^2\}$. There is no order in the system, the θ_o **director's** direction is suppressed from the hamiltonian. We have the isotropic phase. In this way, we see that the nematic isotropic phase transition has no **dependence** on the detailed form of $V(\theta)$; we only request its periodicity.

2. Nematic Defects

We proposed the hamiltonian, (7), to describe L.C. nematic phase. We **will show**, in this section, how this hamiltonian can be treated to describe L.C. nematic defects. In this way, we will analyze the ϕ configurations that are extrema of H. We will see that there are solutions that agree with some observed L.C. defects.

A- The Defects

We rewrite eq.(12) as

$$H = \frac{LK_\theta}{K_B T} \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial\theta}{\partial x} \right)^2 + \left(\frac{\partial\theta}{\partial y} \right)^2 \right\} + \alpha V(\theta - \theta_o) \right\} dx dy, \quad (15)$$

where $\alpha = \frac{1}{K_\theta}$

In a L.C. sample the director direction depends on the conditions that we impose on the system. We will show here how we can calculate the director direction from these conditions.

When we sum, in the partition function, **over all** configurations that the system admits, the most probable ones, at low temperatures, will be those which are energy extrema, and therefore are solutions of the equation

$$\nabla^2\theta + \alpha V'(\theta - \theta_o) = 0, \quad (16)$$

which is the equation that determines the L.C. most probable configurations.

Let us see how eq.(16) describes some observed configurations in L.C. The term $V'(\phi - \phi_o)$ gives the force, due to the L.C. molecule deviation from the director

direction, at the point (z, \mathbf{y}) . So, if the molecule is exactly in the director direction, we have $\theta(\mathbf{x}, \mathbf{y}) = \theta_o(\mathbf{x}, \mathbf{y})$ and $V'(\theta - \theta_o) = 0$. Therefore, the eq. (16) becomes

$$\nabla^2 \theta = 0. \quad (17)$$

Obviously, the solutions of (17) form a complete set for **all** the orientations of the director in a L.C. The most obvious solution is $\theta \equiv 0$, representing a pure nematic state, with the hard rods completely aligned along the same direction over the whole sample. It is observed at high external fields **or/and** low temperatura. However, this is not the **only** solution of eq. (17). Rewriting it in polar **coordinates**

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \cdot \frac{\partial \theta}{\partial r} \right) + \frac{1}{r^2} \left(\frac{\partial^2 \theta}{\partial \phi^2} \right) = 0 \quad (18)$$

and making $\theta(r, \phi) = R(r) \cdot \psi(\phi)$, we get

$$\frac{1}{\psi} \left(\frac{\partial^2 \psi}{\partial \phi^2} \right) = -k^2 \quad \text{and} \quad \frac{r}{R} \cdot \frac{\partial}{\partial r} \left(r \cdot \frac{\partial R}{\partial r} \right) = k^2 \quad (19)$$

which have, for $k = 0$, the solutions

$$\theta(r, \phi) = (A\phi + B)(C \cdot \ln r + D) \quad (20)$$

We know that the L.C. are indistinguishable by a rotations around their center of **mass**, so we can impose the condition

$$\theta(r, \phi + 2\pi) = \theta(r, \phi) + n \cdot \pi \quad , \quad n = 0, 1, 2, \dots \quad (21)$$

which **gives** us:

$$C = 0 \quad \text{and} \quad A \cdot D = \frac{n}{2} \quad (22)$$

Making $B \cdot D = \theta_o$ we arrive at

$$\theta(r, \phi) = \frac{n}{2} \phi + \phi_o \quad , \quad n = 0, \pm 1, \pm 2, \dots \quad (23)$$

that are the known L.C. defects (see ref. 4, pag 33/34). The number, $\lambda = \frac{n}{2}$, is called the charge of the defects. We will now make an energy analysis of these solutions. Their energy is given by

$$E = \int \left\{ \left(\frac{\partial \theta}{\partial r} \right)^2 + \frac{1}{r^2} \cdot \left(\frac{\partial \theta}{\partial \phi} \right)^2 \right\} r dr d\phi \quad (24)$$

For the configurations given by (23) we get $\frac{\partial \theta}{\partial r} = 0$ and $\frac{\partial \theta}{\partial \phi} = \frac{n}{2}$, therefore $E = \left(\frac{n}{2} \right)^2 \cdot 2\pi \cdot \int \frac{dr}{r}$. This integral **has** ultraviolet and infrared **divergences**. That is,

Liquid crystals and the Coulomb gas

it diverges for $r \rightarrow 0$ and $r \rightarrow \infty$. To avoid this, we insert a lower, r_{inf} , and an upper, r_{sup} , cutoff, in such a way that

$$E = \left(\frac{n}{2}\right)^2 \cdot 2\pi \cdot \ln\left(\frac{r_{sup}}{r_{inf}}\right) \quad (25)$$

In spite of the fact that we made explicit use of the inferior hard core in the equation above, it could be put directly in equation 18, if we had written

$$\nabla^2 \phi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \cdot \frac{\partial \theta}{\partial r} \right) + \frac{1}{r^2} \left(\frac{\partial^2 \theta}{\partial \phi^2} \right) \approx \frac{n}{2} \delta(r) \quad (26)$$

This is exactly the equation of a point charge electric field. But condition (21) avoids this interpretation, because it makes no electrostatic sense.

We interpret equation (25) as the necessary energy to build up, in the sample, the configuration given by (23). That is, to build this configuration we need to supply the system with this energy.

Now we make some comments about the configuration in which $k \neq 0$. With this condition the solutions of equation (19) are

$$\theta(r, \phi) = C_k r^k e^{ik\phi} \quad (k \neq 0) \quad (27)$$

And, imposing the condition (21), we arrive at

$$C_k e^{ik\phi} r^k e^{ik2\pi} = C_k e^{ik\phi} r^k + n\pi \quad (28)$$

therefore $n = 0$ and $k = p$, $p = \pm 1, \pm 2, \pm 3, \dots$

Note that in addition to the walls that we had along \vec{e}_θ , we had too, in this case, walls along \vec{e}_r . Furthermore, if $k > 1$, the distance between these walls becomes shorter as r increases, and when $r \rightarrow \infty$ we have an isotropic phase. Obviously, this is avoided by the boundary conditions imposed on the sample. In the same way, if $k < 0$, we have a singularity in the ϕ configuration as $r \rightarrow 0$, which makes no physical sense. We are, thus, left with the $k = 1$ case to study. Finally, note that due to the form of equation (24), the energy of these configurations are zero. So, we believe that they may be important when the fluctuations become large.

B- Defect Interactions

We will study here the interaction between the defects given by equation (23). We will adopt the following strategy: this equation gives us the defects at the point $(0, 0)$. Working with it, we will look for the expression of a defect at the

point $(-1,0)$. Once we find it, we have the solution for two defects, one at $(0,0)$ and another at $(-l,0)$. The sum of these two solutions is a solution too, due to the linear structure of 18. This new solution will be utilized in the study of the defect interactions.

From figure 3, we see that

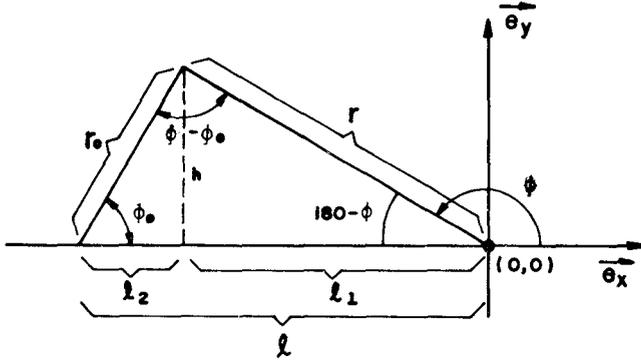


Fig. 3 - Figure used to build up a defect at the point $(-l,0)$.

$$l_1 = -r \cdot \cos(\phi), \quad l_2 = l - l_1 \quad r = r_0 \cdot \frac{\sin(\phi_0)}{\sin(\phi)}$$

and

$$\phi - \phi_0 = \arctg \frac{l_2}{h} + \arctg \frac{l_1}{h}$$

Therefore.

$$\phi_0 = \phi - \arctg \left\{ \frac{l \cdot \sin(\phi)}{r + l \cdot \cos(\phi)} \right\} \quad (29)$$

So, from eq. (23),

$$\theta(r, \phi) = \frac{p}{2} \left\{ \phi - \arctg \left\{ \frac{l \cdot \sin(\phi)}{r + l \cdot \cos(\phi)} \right\} \right\} \quad (30)$$

gives us an equation for a defect at the point $(-l,0)$.

Our derivation was rather geometrical; we just wanted to be sure that we obtain the same kind of solution as (23). Nevertheless, it must be shown that (30) is, indeed, solution of (17). This will not be done here, because it is obviously true.

We now study the interaction between two defects. Let θ_1 be a defect given by (30) and θ_2 another one given by (23), then

$$\theta(r, \phi) = \theta_1(r, \phi) + \theta_2(r, \phi) \quad (31)$$

Liquid *crystals and* the Coulomb *gas*

will be a solution of (17) too. Therefore

$$\theta(r, \phi) = \frac{n}{2}\phi + \frac{p}{2} \cdot \left(\phi - \text{arctg} \left\{ \frac{l \cdot \sin(\phi)}{r + l \cdot \cos(\phi)} \right\} \right) + \phi_0 \quad (32)$$

represents two defects with charges $\frac{n}{2}$ and $\frac{p}{2}$, a distance l appart.

From eq. (32) we can get the interaction energy of the defects. To see this we define, for simplicity,

$$E = \int e(r, \phi) r dr d\phi \quad \text{where} \quad (r, \phi) = \left(\frac{\partial \theta}{\partial r} \right)^2 + \left(\frac{\partial \theta}{\partial \phi} \right)^2 \quad (33)$$

Taking (31) we get the energy density

$$e = e_1 + e_2 + e_I \quad (34)$$

The two first terms give the defects' self-energy; its contribution has already been calculated in (25). The relevant term, showing defect interaction, is given by

$$e_I = 2 \cdot \left\{ \frac{\partial \theta_1}{\partial r} \cdot \frac{\partial \theta_2}{\partial r} + \frac{1}{r^2} \cdot \frac{\partial \theta_1}{\partial \phi} \frac{\partial \theta_2}{\partial \phi} \right\} \quad (35)$$

Using the expressions of θ_1 and θ_2 given above, we arrive at

$$E_I = -2 \cdot \frac{n}{2} \cdot \frac{p}{2} \cdot 2 \cdot \pi \cdot \ln \left(\frac{l}{r_{sup}} \right) \quad (36)$$

where r_{sup} is the upper limit defined in eq.(25)

In this equation we see that defects with the same sign are **repelled**, i.e; we have the lowest energy with the greatest separation. Obviously, when we have charges with opposite sign, the lowest energy corresponds to the shortest separation. As already noted, if it were not for the possibility of semi-integer charges, it could be said that the defects interact like **electrostatic** charges in two dimensions.

Eq. (36) can be **generalized** to the case where the two charges (or defects) are in \vec{r}_1 and \vec{r}_2 . The interaction energy is

$$E_I = -2 \cdot \frac{n}{2} \cdot \frac{p}{2} \cdot 2 \cdot \pi \cdot \ln \left(\frac{|\vec{r}_1 - \vec{r}_2|}{r_{sup}} \right) \quad (37)$$

where (26) becomes $\nabla^2 \theta \approx \frac{n}{2} \cdot \delta(\vec{r} - \vec{r}_1) + \frac{p}{2} \cdot \delta(\vec{r} - \vec{r}_2)$. Finally, the two defects' total energy is

$$E = \left(\frac{n}{2} + \frac{p}{2} \right)^2 \cdot 2 \cdot \pi \cdot \ln(r_{sup}) - \left(\left(\frac{n}{2} \right)^2 + \left(\frac{p}{2} \right)^2 \right) \cdot 2 \cdot \pi \cdot \ln(r_{inf}) - 2 \cdot \frac{n}{2} \cdot \frac{p}{2} \cdot 2 \cdot \pi \cdot \ln(|\vec{r}_1 - \vec{r}_2|) \quad (38)$$

Manuel Simões Filho

With the aid of these equations, it is **easy** to see that the interaction energy of N defects, where the i -th term has semi integer charge λ_i , is given by

$$E = \left(\sum_{i=1}^N \lambda_i \right)^2 . 2\pi . \ln(r_{sp}) - \left(\sum_{i=1}^N \lambda_i^2 \right) . 2\pi . \ln(r_{if}) - 2.2.\pi . \sum_{i>j} \lambda_i . \lambda_j . \ln(|\vec{r}_1 - \vec{r}_2|) \quad (39)$$

When $r_{sup} \rightarrow \infty$ the energy diverges. That cannot happen because, **as** we said, this is the necessary energy to construct the configuration. A way to avoid this problem is to impose

$$\sum_{i=1}^N \lambda_i = 0, \quad (40)$$

which discards infrared **divergences**. The ultraviolet ones ($r_{inf} \rightarrow 0$) are inevitable, although not real, because we always have $r_{inf} \neq 0$. That is, the system really builds up a cutoff. At **distances** shorter than r_{inf} the nematic state does not exist and the hamiltonian that we postulate makes no sense. That is, we expect that $r_{inf} \approx l$, where l is the rod's length.

Equation (39) may also have another **divergence**, that **has** not been mentioned above. **It** happens when $\vec{r}_i \rightarrow \vec{r}_j$. To avoid it, we make $\ln(|\vec{r}_i - \vec{r}_j|) \rightarrow \ln(|\vec{r}_i - \vec{r}_j + r_{if}|)$. Then

$$E = -2.\pi . \sum_{i,j} \lambda_i . \lambda_j . \ln \frac{(|\vec{r}_i - \vec{r}_j| + r_{inf})}{r_{sup}} \quad (41)$$

which is the energy of an **assembly** of defects. In the next section, when we will study the nematic isotropic phase transition, we will find again this **expression**(See, for example, equation (49)). We will suggest that these defects play an important role in this phase transition.

3 - The Nematic Isotropic Transition

We will propose an interpretation of the nematic isotropic phase transition. Through our approach we will be able to calculate exactly the **critical** temperature and also some thermodynamical variables. We will show that the **L.C** system can be thermodynamically represented by the defects discussed above.

Liquid crystals and the Coulomb gas

A- The Generalized Sine-Gordon Model

We will now show that the hamiltonian, (13), is equivalent to a sine-Gordon (S.G.) model⁶.

We make use the periodicity of $U(\phi)$ to write

$$U(\phi) = \sum_{k=-\infty}^{\infty} a_k \exp(i.k.\phi) \quad (42)$$

The periodicity of the potential ($U(\phi + P) = U(\phi)$) implies that

$$k = \frac{2\pi}{P}.n, \quad n = 0, \pm 1, \pm 2, \dots \quad \text{that is } U(\phi) = \sum_n e^{i.\frac{2\pi}{P}.n.\phi} a_k \quad (43)$$

From the condition $\frac{dU(\phi)}{d\phi}|_{\phi=0} = 0$ we get $a_n = a_{-n}$ which gives

$$U(\phi) = \sum_{n>0} a_n \cos\left(\frac{2\pi}{P}.n.\phi\right) \quad (44)$$

The condition $\frac{d^2U(\phi)}{d\phi^2}|_{\phi=0} > 0$ (eq. 5) can be satisfied if we put

$$U(\phi) = - \sum_{n>0} a_n \cos\left(\frac{2\pi}{P}.n.\phi\right); \quad \sum n^2 a_n > 0 \quad (45)$$

So

$$H(\phi, T) = L \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right\} - \frac{1}{K_B T} \sum_{n>0} a_n \cos\left(\frac{2\pi}{P}.n.\phi\right) \right\} dx.dy \quad (46)$$

Therefore our model can be written as a generalization of the S.G. model. Our aim here will be to study the nematic isotropic phase transition through this generalized S.G. model.

B- The Coulomb gas

It is well known that the S.G. is equivalent to the bidimensional Coulomb gas^{7,8}. This equivalence can be extended to eq. (46). In the appendix we review how this can be done.

The L.C. thermodynamics can be obtained from the following partition function.

$$Z = \int D[\phi].e^{-Hdx.dy} \quad (47)$$

Manuel Simões Filho

where H is given by (46)

In the appendix of this work we show that this partition function can be written as

$$\begin{aligned}
 Z &= \sum_{\{n_k, p_k\}} \prod_k z(\alpha_k, \beta) \\
 z(\alpha_k, \beta) &= \left\{ \frac{(\alpha_k)^{n_k} (\alpha_k)^{p_k}}{n_k! p_k!} \right\} \\
 &\int \prod_{j=0}^{\sum_k n_k + p_k} d^2 x_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j + \epsilon|) \right) \quad (48)
 \end{aligned}$$

where $\alpha_k = \frac{L a_k}{2k_B T}$

This is the grand canonical partition function of a charged gas, whose charges, given by λ_i , are interacting through a logarithmic potential in a two dimensional world. Its total charge is zero ($\sum_i \lambda_i = 0$), in exact analogy to eq. (40); k is the absolute value of the charges (or the k-th term in the expansion (42)), and $\alpha_k = \left(\frac{L a_k}{2k_B T} \right)$ is the fugacity of this plasma, which is known as Coulomb gas.

When we compare this system's energy to the energy of the defects constructed in the previous section, we arrive at the main point of this paper. They are the same! Therefore, we claim that the defects that we obtained as solution of Laplace equation are now generated by the theory, when we take into account the inhomogeneous term and, besides that, we get the statistical mechanics of the defects. So, it is completely equivalent to describe the L.C. by the hard rod's orientations, as in equation (13), or by the statistical mechanics of the defects, as in equation (47). Besides describing the same systems, they also emphasizes different views of the same problem. Therefore, the results that we get in one formulation could be analyzed by the other formulation. That will be our strategy here.

C- The phase transition

We will now show how equation (7) can lead us to understand the nematic isotropic phase transition^{9,10}. Consider the expression

$$h \equiv \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j + \epsilon|) \quad (49)$$

Liquid crystals and the Coulomb gas

in eq. 48. It can be written as

$$h = \sum_i \lambda_i^2 \ln(|\epsilon|) + \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \quad (50)$$

One can see that

$$\sum_i \lambda_i^2 = \sum_{k>0} k^2 (p_k + n_k) \quad (51)$$

therefore

$$\begin{aligned} e^{\frac{\beta^2}{4\pi} \sum_i \lambda_i^2 \ln(\epsilon)} &= \epsilon^{\frac{\beta^2}{4\pi} \sum_{k>0} k^2 (p_k + n_k)} = \\ &= \prod_k \left\{ \epsilon^{\frac{\beta^2}{4\pi} \sum_{k>0} k^2 (p_k + n_k)} \right\} \end{aligned} \quad (52)$$

So, we can rewrite the equation (48) in a way that incorporates the self-energy that we have in equation (50). Thus,

$$z(\alpha_k, \beta) = z(\bar{\alpha}_k, \beta) \quad (53)$$

where $\bar{\alpha}_k = \alpha_k \epsilon^{\frac{\beta^2}{4\pi} k^2}$

The fact that the activity takes care of the charges' self-energy cannot surprise us, because it is given by the exponential of the chemical potential, which gives the system energy variation when we change the number of charges. Equation (53) tells that the chemical potential transforms as $\bar{\mu} \rightarrow \mu + \frac{\beta^2}{4\pi} k^2 \ln(\epsilon)$, that is, it takes care of the defect self-energy.

By transforming (48), we find the infrared behavior of the system. Making the scaling transformation $\vec{r}_i = R \cdot \vec{\bar{r}}_i$ where R gives us an arbitrary scale change in the system, we get

$$h = \sum_{i \neq j} \lambda_i \lambda_j \ln(R) + \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{\bar{r}}_i - \vec{\bar{r}}_j|) \quad (54)$$

But, from $\sum_i \lambda_i = 0$ (see the appendix or equation (40)), we have

$$\sum_{i \neq j} \lambda_i \lambda_j = - \sum_i (\lambda_i)^2 = - \sum_{k>0} k^2 (p_k + n_k) \quad (55)$$

So,

$$\begin{aligned} \exp \left(\frac{\beta^2}{4\pi} \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) &= \\ \prod_k \left\{ R^{-\frac{\beta^2}{4\pi} k^2 (p_k + n_k)} \right\} \exp \left(\sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{\bar{r}}_i - \vec{\bar{r}}_j|) \right) \end{aligned} \quad (56)$$

Therefore

$$\begin{aligned} & \int \prod_{j=0}^{\sum_k n_k + p_k} d^2 x_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) = \\ & = \prod_k \left\{ R^{(2 - \frac{\beta^2}{4\pi} k^2)(p_k + n_k)} \right\} \int \prod_{j=0}^{\sum_k n_k + p_k} d^2 \bar{x}_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) \end{aligned} \quad (57)$$

Finally we get^{11,12} :

$$z(\alpha_k, \beta) = z(\bar{\alpha}_k R^{(2 - \frac{\beta^2}{4\pi} k^2)}, \beta). \quad (58)$$

which is the basic equation to understand the nematic-isotropic phase transition.

From eq.(57), we see that a change of scale gives us a renormalized activity given by

$$\bar{\alpha}_k = \alpha_k R^{(2 - \frac{\beta^2}{4\pi} k^2)} \quad (59)$$

That is, as $\vec{r}_i \rightarrow R \cdot \vec{r}_i$

$$a_k \rightarrow a_k R^{(2 - \frac{\beta^2}{4\pi} k^2)} \quad (60)$$

Making the identification $R^2 \rightarrow V$ (volume), we get

$$a_k \rightarrow a_k V^{(1 - \frac{K_B T}{2L\pi K_\theta} k^2)} \quad (61)$$

We are now in position to understand the heuristic arguments presented in section I of this paper. Remember that the a_k 's, which appear in equation (44), are the expansion coefficient of the potential in cosines. But, from equation (61), we see that at low temperatures each a_k goes as some positive power of the volume. So, at these temperatures we have a big a_k , and the system is aligned with the director, due to the predominance of the potential term in the hamiltonian. As the temperature increases, the volume dependence of a_k diminishes, but it is positive for $T < \frac{2L\pi k_\theta}{K_B k^2}$. We have a completely different situation when $T > \frac{2L\pi k_\theta}{K_B k^2}$, because we can say that a_k goes to zero as $V \rightarrow \infty$.

Therefore¹³, the change of scale gives a dependence of the a_k coefficients on the temperature. At temperatures greater than $T_k = \frac{2L\pi K_\theta}{K_B k^2}$ the a_k expansion coefficient goes to zero.

From this, we see that for every coefficient there is a temperature at which it goes to zero. And the greater the k index, the lower is the corresponding temperature. So, we can conclude that, as we rise the temperature, the largest k

Liquid crystals and the Coulomb gas

coefficients become negligible, which explains the generality of nematic isotropic phase transition. At higher temperatures, only the lowest k terms survive, which shows that, at these temperatures, the details of rod's potential interaction, which is given by the highest order k terms, are not important. That is, the potential $\mathcal{U}(\phi)$, which is restricted to describe a particular rod interaction at low temperatures, becomes nearly identical when we are close to the nematic isotropic phase transition.

Obviously, the critical temperature is given by the point in which the first ($k = 1$) coefficient goes to zero

$$T_c = 2\pi L \frac{K_\theta}{K_B} \quad (62)$$

Note that this temperature depends only on K_θ .

Near the critical temperature only the first term (a_1) survives. Therefore, around this point the partition function is given by

$$Z = \sum_{n_1, p_1} \left\{ \frac{(\bar{\alpha}_1)^{n_1}}{n_1!} \frac{(\bar{\alpha}_1)^{p_1}}{p_1!} \right\} \int \prod_{j=0}^{n_1+p_1} d^2 \bar{x}_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) \quad (63)$$

but, due to the neutrality, we have $p_1 = n_1$. So, making $p_1 = n_1 = n$ and $\bar{\alpha}_k = a$ we have

$$\begin{aligned} Z &= \sum_n \frac{(\alpha)^{2n}}{(n!)^2} \int \prod_{j=0}^{n_1+p_1} d^2 \bar{x}_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i \neq j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) = \\ &= \int D|\phi| \exp \left(- \left\{ \frac{1}{2}(\partial\phi)^2 - \frac{L}{K_B T} a_1 \cos \left(\frac{2\pi}{P} \phi \right) \right\} d^2 x. \right) \end{aligned} \quad (64)$$

With equation (48) we were able to predict the temperature of the nematic isotropic phase transition, as well as the mechanism of suppression of the potential that makes the rods aligned. Now we discuss other properties related to the phase transition. As we know, as the system changes scale, we can calculate its pressure, because

$$P = K_B T \frac{\partial}{\partial V} \ln Z \quad (65)$$

So, using (61) and (64) we get

$$PV = K_B T \langle n \rangle \left(1 - \frac{K_B T}{2\pi L K_\theta} \right) \quad (66)$$

where $\langle n \rangle = \langle n_1 + p_1 \rangle$

Manuel Stmões Filho

Therefore, at the critical temperature, the system pressure goes to zero. It is easy to understand this result as due to the end of the nematic phase. At this temperature we have no more the aligned structure of hard rods near the system walls. The force of this organized structure goes to zero. The same equation applied to the second of the equations (64) gives.

$$PV = \langle La_1 \cos(2\theta) \rangle \left(1 - \frac{K_B T}{2\pi L K_\theta} \right) \quad (67)$$

The interpretation of this equation is same as (66), but now we can conclude that

$$\langle n \rangle = \frac{1}{k_B T} \langle La_1 \cos(2\theta) \rangle \quad (68)$$

Making the change of scale in (68), we see that

$$\langle n \rangle \rightarrow 0 \quad \text{when} \quad T \rightarrow T_c \quad (69)$$

because $\langle n \rangle$ is proportional to a_1

Conclusion

We have proposed a model that describes the nematic phase of a Liquid Crystal. We have shown that the hamiltonian proposed is equivalent to a Coulomb gas, in which the charges describe exactly the interaction of the defects of the nematic phase. So, the partition function of the Liquid Crystal can be written at least in two ways, one stressing the nematic alignment, and the other the interaction between the nematic defects. We have also shown that our model allows a nematic isotropic transition and argued that it is a kind of Kosterlitz-Thouless transition.

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Appendix

We will show in this appendix, that the generalized Sine-Gordon model is equivalent to a Coulomb gas.

Let

$$Z = \int D[\phi]. e^{-H dx. dy} \quad (A.1)$$

We have, thus, a term like

$$\exp \left(\left\{ \frac{1}{K_B T} \sum_{n>0} a_n \cos \left(\frac{2\pi}{P} . n . \varphi \right) \right\} dx. dy \right) \quad (A.2)$$

Liquid crystals and the Coulomb gas

Eq. (A.2) is of the form $e^{\sum_i z_i}$, and can be rewritten as

$$e^{\sum_i z_i} = \sum_{n>0} \frac{1}{n!} (\sum_i x_i)^n \quad (\text{A.3})$$

But $(\sum_i x_i)^n$ can be rewritten, using the multinomial expansion, as

$$\left(\sum_i x_i\right)^n = \sum_{\{n_k\}} \frac{n!}{(\prod_k n_k!)} \prod_k (x_k)^{n_k} \quad (\text{A.4})$$

where $\sum_k n_k = n$, and the notation $\sum_{\{n_k\}}$ means a sum over all the possible values in the set $\{n_k\}$. From (A.2), (A.3) and (A.4) we arrive at

$$\begin{aligned} & \exp\left(\left\{\frac{1}{K_B T} \int \sum_n a_n \cos\left(\frac{2\pi}{P} \cdot n \cdot \varphi\right)\right\} dx \cdot dy\right) = \\ & = \sum_n \frac{1}{n!} \sum_{\{n_k\}} \frac{n!}{(\prod_k n_k!)} \prod_k \left\{\left(\frac{1}{K_B T} \int a_n \cos\left(\frac{2\pi}{P} \cdot n \cdot \varphi\right) dx \cdot dy\right)^{n_k}\right\} \end{aligned} \quad (\text{A.5})$$

But

$$\begin{aligned} & \left(\frac{1}{K_B T} \int a_n \cos\left(\frac{2\pi}{P} \cdot n \cdot \varphi\right) dx \cdot dy\right)^{n_k} = \\ & = \left(\frac{1}{K_B T}\right)^{n_k} \int \left\{\prod_{l=0}^{n_k} d^2 x_l\right\} \cdot \left\{\prod_{l=0}^{n_k} a_k \cos\left(\frac{2\pi}{P} k \varphi(x_l)\right)\right\} \end{aligned} \quad (\text{A.6})$$

Noting that

$$\begin{aligned} & \prod_{l=0}^{n_k} a_k \cos\left(\frac{2\pi}{P} k \varphi(x_l)\right) = \\ & = \left(\frac{a_k}{2}\right)^{n_k} \cdot \left(e^{i\beta\varphi(x_1)} + e^{-i\beta\varphi(x_1)}\right) \dots \left(e^{i\beta\varphi(x_{n_k})} + e^{-i\beta\varphi(x_{n_k})}\right) = \\ & = \left(\frac{a_k}{2}\right)^{n_k} \sum_{l=0}^{n_k} \binom{n_k}{l} e^{i\beta k \int \rho_{n_k, l}(x) \varphi(x) d^2 z} \end{aligned} \quad (\text{A.7})$$

where $\rho_{n_k, l}(x) = \sum_{i=0}^l \delta(x - x_i) - \sum_{j=l+1}^{n_k} n_k \delta(x - x_j)$ e $\beta = \frac{2\pi}{P}$
We arrive at

$$\begin{aligned} & \left(\frac{1}{K_B T} \int a_n \cos\left(\frac{2\pi}{P} \cdot n \cdot \varphi\right) dx \cdot dy\right)^{n_k} = \\ & = \left(\frac{1}{K_B T}\right)^{n_k} \int \left\{\prod_{l=0}^{n_k} n_k d^2 x_l\right\} \cdot \sum_{l=0}^{n_k} \binom{n_k}{l} e^{i\beta k \int \rho_{n_k, l}(x) \varphi(x) d^2 z} \end{aligned} \quad (\text{A.8})$$

Substituting (A.8) in (A.5) we get

$$\begin{aligned} \exp \left(\left\{ \frac{1}{K_B T} \int \sum_n a_n \cos \left(\frac{2\pi}{P} \cdot n \cdot \varphi \right) \right\} dx \cdot dy \right) = \\ = \sum_{n>0} \sum_{\{n_k\}} \prod_k \left\{ \left(\frac{L a_k}{2 K_B T} \right)^{n_k} \sum_l^{n_k} \frac{1}{l!(n_k - l)!} \int \prod_{i=0}^{n_k} e^{i\beta k \int \rho_{n_k, l}(x) \varphi(x) d^2 x} \right\} \end{aligned} \quad (\text{A.9})$$

For every value of n_k we have, through eq. A.9, that l is the number of **positive poles** and $n_k - l$ is the number of negatives ones. In equation (A.9) the set $\{n_k\}$ is unconstrained, because in this equation the explicit n dependence disappeared: So we can rewrite it as

$$\begin{aligned} \exp \left(\left\{ \frac{1}{K_B T} \int \sum_{n>0} a_n \cos \left(\frac{2\pi}{P} \cdot n \cdot \varphi \right) \right\} dx \cdot dy \right) = \\ = \sum_{\{n_k, p_k\}} \prod_k \left\{ \frac{\left(\frac{L a_k}{2 K_B T} \right)^{n_k} \left(\frac{L a_k}{2 K_B T} \right)^{p_k}}{n_k! p_k!} \right\} \times \\ \times \int \prod_{i=0}^{\sum_k n_k + p_k} d^2 x_i \exp \left(i\beta \sum_k k \int \rho_{n_k, l}(x) \varphi(x) d^2 x \right) \end{aligned} \quad (\text{A.10})$$

Substituting this in the equation A.1 we arrive at

$$\begin{aligned} Z = \sum_{\{n_k, p_k\}} \prod_k \left\{ \frac{\left(\frac{L a_k}{2 K_B T} \right)^{n_k} \left(\frac{L a_k}{2 K_B T} \right)^{p_k}}{n_k! n_k!} \right\} \times \\ \times \int \prod_{j=0}^{\sum_k n_k + p_k} d^2 x_j D|\phi| \exp \left(- \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right\} \right. \right. \\ \left. \left. - i\beta \sum_k k \rho_{n_k, l}(x) \phi(x) \right\} d^2 x \right) \end{aligned} \quad (\text{A.11})$$

We take, in this equation, the integral

$$z(\beta) = \int D|\phi| \exp \left(- \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right\} - i\beta \rho x \phi(x) \right\} d^2 x \right) \quad (\text{A.12})$$

where we have used $\rho(x) = \sum_k k \rho_{n_k, l}(x)$. As is well known, equation A.12 can be rewritten as

$$z(\beta) = z(0) \cdot \exp \left(- \int \left\{ \frac{1}{2} \left\{ \left(\frac{\partial \phi_0}{\partial x} \right)^2 + \left(\frac{\partial \phi_0}{\partial y} \right)^2 \right\} - i\beta \rho(x) \phi_0(x) \right\} d^2 x \right) \quad (\text{A.13})$$

Liquid crystals and the Coulomb gas

where ϕ_o is the solution of the equation

$$\partial^2 \phi_o + i\beta \rho = 0 \quad (\text{A.14})$$

Noticing that

$$\begin{aligned} & \int \left\{ \frac{1}{2} (\partial \phi_o)^2 - i\beta \rho(x) \phi_o(x) \right\} d^2 x = - \\ & - \int \left\{ \frac{1}{2} \phi_o \partial^2 \phi_o + i\beta \rho(x) \phi_o(x) \right\} d^2 x = -\frac{i\beta}{2} \int \rho(x) \phi_o d^2 x \end{aligned} \quad (\text{A.15})$$

where we made use of equation A.14. Making now

$$\phi_o = i\beta \int \Delta(x-y) \rho(y) d^2 y \quad (\text{A.16})$$

where $\Delta(x-y)$ is solution of the equation

$$\partial^2 \Delta(x-y) + \delta(x-y) = 0 \quad (\text{A.17})$$

We conclude that

$$z(\beta) = z(0) \cdot \exp \left(\frac{\beta^2}{2} \int \rho(x) \Delta(x-y) \rho(y) d^2 x d^2 y \right) \quad (\text{A.18})$$

Our aim now is to calculate $\Delta(x-y)$. Fourier transforming

$$\Delta(x) = \frac{1}{2\pi} \int g(k) e^{-i \vec{k} \cdot \vec{x}} d^2 k \quad (\text{A.19})$$

and using the trick

$$\partial^2 \Delta(x) = \lim_{\mu \rightarrow 0} (\partial^2 - \mu^2) \Delta(x) = -\delta(x) \quad (\text{A.20})$$

We have (leaving out the notation $\lim_{\mu \rightarrow 0}$)

$$g(k) = -\frac{1}{(k^2 + \mu^2)} \quad (\text{A.21})$$

In this way

$$\begin{aligned} \Delta(x) &= -\frac{1}{(2\pi^2)} \int \frac{1}{(k^2 + \mu^2)} e^{-i \vec{k} \cdot \vec{x}} d^2 k \\ &= -\frac{1}{(2\pi^2)} \int \frac{\exp(-i k r \cos(\theta))}{(k^2 + \mu^2)} k dk d\theta \end{aligned} \quad (\text{A.22})$$

Manuel Simões Filho

which

$$\Delta(x) = -\frac{1}{2\pi} K_o(\mu|r|) \quad (A.23)$$

where $K_o(\mu|r|)$ is a modified second class Bessel function of zero order. But

$$\lim_{\mu \rightarrow 0} K_o(\mu|r|) = -\lim_{\mu \rightarrow 0} \left\{ \ln \left(\frac{\mu e^\gamma}{2} |r| \right) \right\} \quad (A.24)$$

Therefore

$$\Delta(x) = \lim_{\mu \rightarrow 0} \frac{1}{2\pi} \ln \left(\frac{\mu e^\gamma}{2} |r| \right) \quad (A.25)$$

We are now ready to calculate

$$h = \int \rho(x) \Delta(x-y) \rho(y) d^2x d^2y \quad (A.26)$$

But

$$\begin{aligned} \rho(x) &= \sum_k k \rho_{n_k, l}(x) = \\ &= \sum_k k \left\{ \sum_{l=0}^{p_k} \delta(x-x_l) - \sum_{m=0}^{n_k} \delta(x-x_m) \right\} = \\ &= \sum_k k(p_k + n_k) \lambda_i \delta(x-x_i) \end{aligned} \quad (A.27)$$

where the set $\{\lambda_i\}$ is given by all the charge's possible values, with $\sum_k k(p_k + n_k)$ elements.

So'

$$\begin{aligned} h &= \int \rho(x) \Delta(x-y) \rho(y) d^2x d^2y = \\ &= \frac{1}{2\pi} \lim_{\mu \rightarrow 0} \left(\sum_i \lambda_i \right)^2 \ln \left(\frac{\mu e^\gamma}{2} \right) + \frac{1}{2\pi} \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \end{aligned} \quad (A.28)$$

Therefore we have

$$z(\beta) = z(0) \cdot \exp \left(\frac{\beta^2}{2} \left\{ \frac{1}{2\pi} \lim_{\mu \rightarrow 0} \left(\sum_i \lambda_i \right)^2 \ln \left(\frac{\mu e^\gamma}{2} \right) + \frac{1}{2\pi} \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right\} \right) \quad (A.29)$$

But

$$\exp \left(\frac{\beta^2}{2} \right) \left\{ \frac{1}{2\pi} \lim_{\mu \rightarrow 0} \left(\sum_i \lambda_i \right)^2 \ln \left(\frac{\mu e^\gamma}{2} \right) \right\} = \lim_{\mu \rightarrow 0} \left(\frac{\mu e^\gamma}{2} \right)^{\frac{(\sum_i \lambda_i)^2}{4\pi}} \quad (A.30)$$

Liquid crystals and the Coulomb gas

For the theory to make sense, we need to impose $\sum_i \lambda_i = 0$, which is the same as

$$\sum_{k>0} k(p_k - n_k) = 0 \quad (\text{A.31})$$

That is, the total charge of the system is zero!

Therefore we have

$$z(\beta) = z(0) \cdot \exp \left(\frac{\beta^2}{4\pi} \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j|) \right) \quad (\text{A.32})$$

Finally

$$Z = \sum_{\{n_k, p_k\}} \prod_k \left\{ \frac{\left(\frac{La_k}{2KB^T} \right)^{n_k}}{n_k!} \frac{\left(\frac{La_k}{2KB^T} \right)^{p_k}}{p_k!} \right\} \times \int \prod_{j=0}^{\sum_k n_k + p_k} d^2 x_j \exp \left(\frac{\beta^2}{4\pi} \sum_{i,j} \lambda_i \lambda_j \ln(|\vec{r}_i - \vec{r}_j + \epsilon|) \right) \quad (\text{A.33})$$

Where we used a ultraviolet cutoff ϵ . That is exactly where we wanted to arrive. So, the system describing the nematic state of a L.C. is equivalent to a Coulomb gas with charges $\pm k$, where, $k = 1, 2, 3, \dots$

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Manuel Simões Filho

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13. A rigorous demonstration of this phase transition can be found, by example, in the ref. **12** above. We choose this **approach** because we think that doing so we have gained in conciseness and physical insight.

Resumo

Propomos neste trabalho, que a fase nemática de um Cristal Líquido pode ser descrita por uma lagrangeana que também descreve um **gás** de Coulomb. Usando essa lagrangeana, mostramos que as cargas do **gás** de Coulomb aparecem como defeitos na fase nemática dos C.L. Calculamos **então**, usando essa abordagem, a temperatura da transição nemática isotrópica e concluímos que se trata de uma transição do tipo Kosterlitz Thouless.