

Kosterlitz-Thouless phase transitions in two-dimensional liquid crystals

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A renormalization-group analysis, used by previous authors to study the critical properties of the two-dimensional ferromagnetic x - y model, leads to a universal jump in the Franck constant of a two-dimensional nematic liquid crystal as the critical temperature is approached from below. The results obtained are different from those obtained for the x - y model by previous authors because vortices of half-integral strength must be taken into account. Experimental implications of these results are discussed.

Kosterlitz and Thouless¹ have demonstrated the possibility of a phase transition in certain two-dimensional systems which do not possess long-range order in the conventional sense.²⁻⁴ Above the critical temperature, topologically stable singularities (such as vortices in the ferromagnetic x - y model or planar superfluid ⁴He) appear spontaneously in unbound pairs and the response of the system to external perturbations changes accordingly. Much attention recently has been focused in particular on the critical properties of the x - y model,⁵⁻¹⁰ but there is some disagreement as to the properties of this model near the critical temperature T_c . It might be possible to decide experimentally between conflicting theories, however, since Kosterlitz and Nelson¹¹ have predicted a universal jump in the superfluid density $\rho_s(T)$ of planar ⁴He as $T \rightarrow T_c^-$, and analogous results were claimed to hold for planar magnets and liquid crystals. For the latter, a jump was predicted for the Franck coefficient $J_i(T)$, $i=1,3$ as T_c was approached from below.

In this note, it is pointed out that a two-dimensional nematic liquid crystal is *not* directly analogous to a two-dimensional x - y model in that the lowest energy "vortices," on which the critical properties near T_c crucially depend, are different from those in the x - y model. Because a nematic director $\vec{n}(\vec{r})$ has no meaningful direction [that is, $\vec{n}(\vec{r}) = -\vec{n}(\vec{r})$] the lowest-energy vortex is of strength $\frac{1}{2}$ rather than unity as in the x - y model; that is, as one makes a closed circuit about the lowest-energy vortex in a liquid crystal, the director changes by an amount π , as opposed to an amount 2π for the corresponding strength one vortex in the x - y model (see Fig. 1). That this brings about an important difference can be shown by a simple argument: using the method in Refs. 1 and 6, a rough approximation to the free energy of an isolated vortex is

$$F = E - TS = 2(\pi J/8 - k_B T) \ln(R/a_0), \quad (1)$$

where R is the size of the system and a_0 is the core radius of the vortex, and therefore the critical temperature, to first approximation, is $T_c = \pi J/8k_B$, which is one-fourth the value expected if one uses strength-one vortices. This value is renormalized in the full theory presented in Ref. 1, but the critical temperature is, nevertheless,

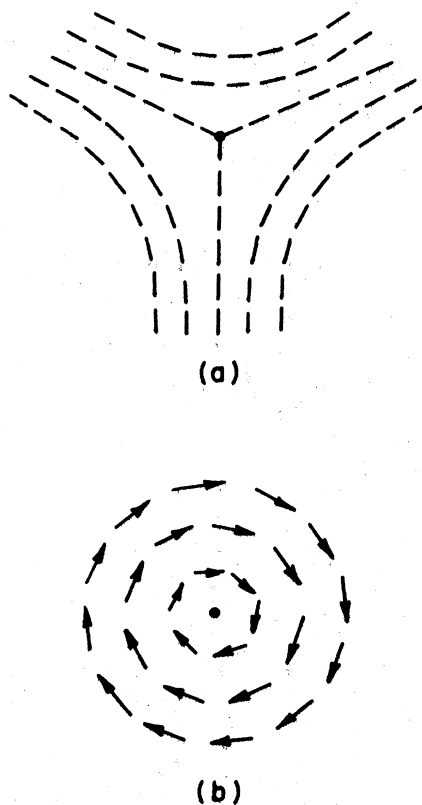


FIG. 1. (a) $m = -\frac{1}{2}$ vortex in a nematic liquid crystal; the line segments represent the director $\vec{n}(\vec{r})$. (b) $m = -1$ vortex in the x - y model; the arrows represent spin directions.

lowered from the value obtained when strength-one vortices are used. This leads us to expect that other predictions of the critical properties for nematics will be changed, and it will now be shown how these considerations affect the universal value of $J(T)/T$.

The distortion free energy in a two-dimensional nematic is given by¹²

$$F_d = \frac{1}{2} J_1 [\vec{\nabla} \cdot \hat{\mathbf{n}}(\vec{\mathbf{r}})]^2 + \frac{1}{2} J_3 [\hat{\mathbf{n}}(\vec{\mathbf{r}}) \times [\vec{\nabla} \times \hat{\mathbf{n}}(\vec{\mathbf{r}})]]^2, \quad (2)$$

since twist distortions are absent. Nelson and Pelcovits¹³ have shown, using a renormalization-group analysis, that $J_1 - J_3$ is an irrelevant variable in the low-temperature regime and so we may use the one constant approximation

$$F_d = \frac{1}{2} J \sum_{\vec{\mathbf{r}}} [\vec{\nabla} n^i(\vec{\mathbf{r}})]^2. \quad (3)$$

We are thus led back to the x - y model, the only difference being that we must consider vortices with strength $m = \pm \frac{1}{2}$.

The analysis now follows that of Kosterlitz and Nelson¹¹ and will only be sketched here. Defining

$$K = J/k_B T, \quad (4)$$

we can express K in terms of a correlation function

$$K_R^{-1} = \int d^2 r \langle m(\vec{\mathbf{r}}) m(\vec{\mathbf{0}}) \rangle, \quad (5)$$

where $m(\vec{\mathbf{r}})$ is the vortex strength at $\vec{\mathbf{r}}$ and K_R is the renormalized K . To evaluate (5), the approach of Jose *et al.*⁹ is used: neglecting "spin-wave" contributions (which cancel out in the end, anyway), the partition function due to vortices may be written

$$Z_c(y_0) = \sum_{m(\vec{\mathbf{r}})} e^{A_c(m(\vec{\mathbf{r}}))}, \quad (6)$$

where

$$A_c(m(\vec{\mathbf{r}})) = \sum_{\vec{\mathbf{r}}} m^2(\vec{\mathbf{r}}) \ln y_0 + \sum_{\text{pairs}} 2\pi K m(\vec{\mathbf{r}}) G'(\vec{\mathbf{r}} - \vec{\mathbf{r}}') m(\vec{\mathbf{r}}'), \quad (7)$$

and the prime constrains the sum to configurations with total vorticity zero. Here $G'(\vec{\mathbf{r}} - \vec{\mathbf{r}}')$ is the Green's function for a square lattice given for large r by

$$G'(\vec{\mathbf{r}}) \approx \ln(r/a_0) + C, \quad (8)$$

where C is a constant and a_0 a lower cutoff. The parameter $\ln y_0$ is thermodynamically conjugate to the "enstrophy," or squared vorticity,¹¹ and is assumed to be much less than one. Using (6)–(8),

and noting that the dominant contribution arises from a single excited vortex pair of $m = \pm \frac{1}{2}$, we find, to lowest order in y ,

$$\langle m(\vec{\mathbf{r}}) m(\vec{\mathbf{0}}) \rangle \approx -\frac{1}{2} y^{1/2} (r/a_0)^{-\pi K/2}, \quad (9)$$

for large r , where $y = y_0 e^{-CK}$. In a self-consistent theory, K_R rather than K should enter into (9); it can then be shown that K_R^{-1} has the following expansion^{9,11}

$$K_R^{-1} = K^{-1} + \pi^3 y^{1/2} \int_{a_0}^{\infty} \left(\frac{dr}{a_0} \right) \left(\frac{r}{a_0} \right)^{3-\pi K/2} + O(y), \quad (10)$$

where vortex pairs of order higher than $\pm \frac{1}{2}$ are neglected. As described in Ref. 9, we may re-scale (10), integrating between a_0 and $a_0 e^l$, to obtain

$$K_R^{-1}(l) = K^{-1}(l) + \pi^3 y^{1/2}(l) \int_{a_0}^{\infty} \left(\frac{dr}{a_0} \right) \left(\frac{r}{a_0} \right)^{3-K/2} + O(y(l)), \quad (11)$$

where $K(l)$ and $y(l)$ obey the recursion relations (expressed in differential form)

$$\frac{dK^{-1}(l)}{dl} = \pi^3 y^{1/2}, \quad (12a)$$

$$\frac{dy(l)}{dl} = [8 - \pi K(l)] y(l). \quad (12b)$$

As described in Ref. 11, the critical temperature is approached from below as

$$\lim_{l \rightarrow \infty} y(l) = 0, \quad (13)$$

so that

$$\lim_{T \rightarrow T_c^-} [J(T)/k_B T] = 8/\pi. \quad (14)$$

It was suggested by deGennes¹² that a two-dimensional nematic may be prepared by floating a nematic film on the surface of a fluid, although to the author's knowledge, experimental difficulties have so far prevented the realization of such a system. If and when such a system is prepared, however, its critical properties should obey Eq. (14) of this paper rather than the results obtained in Ref. 11. The value calculated in that letter should apply to two-dimensional *smectic* liquid crystals, which more closely approximate the standard x - y model.

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