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Duality maps for a lattice model of the smectic-A–nematic transition

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Exact duality transformations are used to study a three-dimensional lattice version of the de Gennes model of the smectic-A–nematic transition. It is shown that the partition function of this lattice model maps exactly onto that of a system of interacting dislocation loops. Analogies with other models are used to predict the behavior of this lattice model at several special points in the parameter space.

The smectic-A–to–nematic (SmA-N) transition in liquid crystals is one of the most intriguing problems in critical phenomena. Most of the theoretical studies of this transition have been based on the de Gennes phenomenological model.[1] The free energy of this model is very similar to the Ginzburg-Landau free energy for superconductors, although certain important differences remain. These differences include the absence of true long-range smectic order in three dimensions, the lack of gauge invariance of the de Gennes free energy and the inherently anisotropic nature of the smectic phase. Several years ago, Halperin, Lubensky, and Ma[2] used a fluctuation-corrected mean-field theory and a renormalization-group analysis near four dimensions to argue that both the superconducting transition and the SmA-N transition should be weakly first order in character. A recent study,[3] however, has presented strong evidence that the phase transition in type-II superconductors in three dimensions is a continuous one with XY exponents, but with the temperature axis reversed. Experimentally the SmA-N transition often appears to be continuous. However, the observed critical behavior[4] differs considerably from what is expected for an inverted X-Y transition.

In a parallel line of development, it has been suggested[5–8] that the SmA-N transition in three dimensions is driven by an unbinding of dislocation loops.[9] Nelson and Toner[7] have argued that this mechanism leads to anisotropic scaling with the correlation length exponents $\nu_{\parallel}$ and $\nu_{\perp}$ for fluctuations parallel and perpendicular to the direction of smectic order having the ratio 2:1. However, this conclusion has recently been questioned by Toner[8] who has presented strong evidence that the dislocation loop model also exhibits an inverted X-Y transition in three dimensions.

With a view towards shedding some light on this confused situation, I have constructed a lattice version of the de Gennes model in three dimensions, and used exact duality transformation to study its properties. I find that the partition function of the lattice de Gennes model (LDM) maps exactly onto that of a dislocation loop model which is very similar to the model studied in Refs. 6–8. I also find that the LDM is dual to a second loop model which is somewhat simpler in form than the dislocation loop model. For certain special values of the parameters involved, these loop models map onto other lattice models which have been studied previously. Using known results about the properties of these lattice models, I am then able to make definite predictions about the behavior of the LDM at these special points in the parameter space.

The lattice model studied in this paper is a straightforward generalization of the de Gennes model. It is defined by the partition function

$$Z=\int_{-\pi}^{\pi}\frac{d[\theta_i]}{2\pi}\int_{-\infty}^{\infty}d[A_{ix}]\int_{-\infty}^{\infty}d[A_{iy}]\sum_{[n_{i\mu}]=-\infty}^{\infty}\exp\left\{-\frac{1}{2}\sum_i\left[C_1(\Delta_z\theta_i-2\pi n_{iz})^2+C_2\sum_{\mu=x,y}(\Delta_\mu\theta_i-2\pi n_{i\mu}-A_{i\mu})^2 +K_1\left(\sum_{\mu=x,y}\Delta'_\mu A_{i\mu}\right)^2+K_2(\Delta_x A_{iy}-\Delta_y A_{ix})^2 +K_3\sum_{\mu=x,y}(\Delta_z A_{i\mu})^2\right]\right\} . \quad (1)$$

Here θ_i is an angular (phase) variable at site i of a three-dimensional simple cubic lattice with lattice constant equal to unity. The integer-valued variables $[n_{i\mu},\ \mu=x,y,z]$ and the real variables $[A_{i\mu},\ \mu=x,y]$ are defined on the directed links between adjacent sites. Δ_μ and Δ'_μ represent lattice derivatives:

$$\Delta_\mu f_i\equiv f_{i+\hat\mu}-f_i,\quad \Delta'_\mu f_i\equiv f_i-f_{i-\hat\mu}\ , \quad (2)$$

where $\hat{\mu}$ is a unit vector in the μth direction. This model is of the Villain type where the exponential of a cosine has been replaced by a periodic Gaussian function. The integer-valued variables $[n_{i\mu}]$ are the usual ones appearing in the Villain form. The phase variable θ describes the smectic order. In the continuum de Gennes model, the smectic order parameter has both an amplitude and a phase. The justification for considering only the phase in the lattice version comes from the well-known equivalence of fixed-length spin models defined on a lattice to continuum Landau-Ginzburg–type models which allow magnitude fluctuations. The real variables A_x, A_y represent fluctuations in the director field, with $A_z = 0$. C_1 and C_2 are the "bare" stiffness constants for fluctuations parallel and perpendicular to the direction of smectic order, and K_1, K_2, K_3 are the bare Frank constants. The temperature has been adsorbed in the definition of the coupling constants, and I have chosen the scale of length such that the wave number associated with the smectic order is equal to unity.

Duality maps for Villain-type models have been studied by several authors.[10] Following the usual procedure, I use the Poisson sum formula to replace the integer-valued variables $n_{i\mu}$ by real variables $\phi_{i\mu}$ and new integer-valued variables $m_{i\mu}$. After performing the $\vec{\phi}$ and θ integrations, the partition function of Eq. (1) can be written as

$$Z \propto \int d[A_{ix}] \int d[A_{iy}] \sum_{[m_{i\mu}]}' \exp\left\{ -\sum_i \left[\frac{1}{2C_1} m_{iz}^2 + \frac{1}{2C_2}(m_{ix}^2 + m_{iy}^2) + i(A_{ix}m_{ix} + A_{iy}m_{iy}) + \frac{1}{2}K_1 \left(\sum_{\mu=x,y} \Delta'_\mu A_{i\mu} \right)^2 + \frac{1}{2}K_2(\Delta_x A_{iy} - \Delta_y A_{ix})^2 + \frac{1}{2}K_3 \sum_{\mu=x,y} (\Delta_z A_{i\mu})^2 \right] \right\} . \tag{3}$$

In the equation above, $\sum'$ denotes a restricted sum in which the link variables $[m_{i\mu}, \mu = x,y,z]$ have zero divergence at each lattice site,

$$\sum_{\mu=x,y,z} \Delta'_\mu m_{i\mu} = 0 \quad \text{for all } i \ . \tag{4}$$

This restriction implies that the $m_{i\mu}$'s form closed loops. This constraint can be satisfied by writing

$$m_{i\mu} = (\vec{\Delta}' \times \vec{l}_i)_\mu \ , \tag{5}$$

where $[l_{i\mu}, \mu = x,y,z]$ are new integer-valued variables on the links. I then use the Poisson sum fromula once again to replace the sum over $[l_{i\mu}]$ by integration over real variables $[\psi_{i\mu}]$, and perform the $\vec{A}$ and $\vec{\psi}$ integrations. The integrations involve using Fourier transforms which are defined in the usual way:

$$f(\vec{k}) = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} f_i \ , \qquad \vec{k} = \frac{2\pi}{L}(\hat{x}l_1 + \hat{y}l_2 + \hat{z}l_3) \ , \tag{6}$$

where $N = L^3$ is the total number of sites, $\vec{R}_i$ represents the radius vector of the ith site, and l_1, l_2, l_3 are integers. Defining

$$\alpha_\mu(\vec{k}) \equiv 1 - e^{ik_\mu}, \quad \mu = x,y,z \ , \tag{7}$$

I can write Eq. (3) as

$$Z \propto \sum_{[n_{i\mu}]}' \exp\{-H_L([n_{i\mu}])\} \ , \tag{8}$$

where

$$H_L([n_{i\mu}]) = 2\pi^2 \sum_{\vec{k}} \left\{ \frac{[K_1 + K_3|\alpha_z|^2/(|\alpha_x|^2 + |\alpha_y|^2)][|\alpha_x^* n_y(\vec{k}) - \alpha_y^* n_x(\vec{k})|^2]}{|\alpha_z|^2 + [K_1(|\alpha_x|^2 + |\alpha_y^2|) + K_3|\alpha_z|^2]\left[\frac{1}{C_1}(|\alpha_x|^2 + |\alpha_y|^2) + \frac{1}{C_2}|\alpha_z|^2\right]} + \frac{[K_2 + K_3|\alpha_z|^2/(|\alpha_x|^2 + |\alpha_y|^2)]|n_z(\vec{k})|^2}{1 + \frac{1}{C_2}[K_2(|\alpha_x|^2 + |\alpha_y|^2) + K_3|\alpha_z|^2]} \right\} . \tag{9}$$

H_L represents the Hamiltonian of an ensemble of interacting dislocation loops. The connection of this Hamiltonian with previously studied dislocation loop models[5–9] can be seen by taking the long wavelength limit of Eq. (9). If we keep only the lowest relevant powers of $\alpha_\mu(\vec{k})$, Eq. (9) becomes

$$H_L \underset{k \to 0}{\longrightarrow} 2\pi^2 \sum_{\vec{k}} \left\{ \frac{K_1|\alpha_x^* n_y(\vec{k}) - \alpha_y^* n_x(\vec{k})|^2}{|\alpha_z|^2 + \frac{K_1}{C_1}[|\alpha_x|^2 + |\alpha_y|^2]^2} + K_2|n_z(\vec{k})|^2 + K_3[|n_x(\vec{k})|^2 + |n_y(\vec{k})|^2] \right\} . \tag{10}$$

This Hamiltonian is identical [with $\alpha_\mu(\vec{k}) \to -ik_\mu$] to the dislocation loop Hamiltonian studied in Refs. 7 and 8. I should mention here that Eq. (10) is not the correct long-wavelength limit of Eq. (9) if either K_1 or C_1 is equal to zero. However, for K_1, $C_1 \neq 0$, the dislocation loop Hamiltonian of Eq. (9) should exhibit the same critical behavior as that of Eq. (10) because they have the same form at long distances. This exact mapping between the LDM and the dislocation loop model shows conclusively that a description of the SmA-N transition within the framework of the de Gennes model is completely equivalent to a description based on the statistical mechanics of interacting dislocation loops.

Before proceeding further, I show that the LDM is dual to a second loop model which I call the dual loop model. This model is obtained by integrating out the $\vec{A}$ fields in Eq. (3). This gives

$$Z \propto \sum_{[m_{i\mu}]}' \exp\{-H_D([m_{i\mu}])\} \ , \tag{11}$$

with

$$H_D([m_{i\mu}]) = \frac{1}{2C_1}\sum_i m_{iz}^2 + \frac{1}{2C_2}\sum_i (m_{ix}^2 + m_{iy}^2) + \frac{1}{2}\sum_{\vec{k}}\left[\frac{|m_x(\vec{k})|^2 + |m_y(\vec{k})|^2}{K_2[|\alpha_x|^2+|\alpha_y|^2]+K_3|\alpha_z|^2} + |m_z(\vec{k})|^2\left(\frac{K_2}{K_3}\frac{1}{K_2(|\alpha_x|^2+|\alpha_y|^2)+K_3|\alpha_z|^2} - \frac{K_1}{K_3}\frac{1}{K_1(|\alpha_x|^2+|\alpha_y|^2)+K_3|\alpha_z|^2}\right)\right] \ . \tag{12}$$

This model is somewhat simpler in form and often easier to handle than the dislocation loop model of Eq. (9). For $K_1 = 0$, this model reduces to an anisotropic version of the generalized Villain model considered in Ref. 3, which should have an X-Y transition. Since the temperature is inverted in going from the LDM to the dual loop model, the LDM should exhibit an inverted X-Y transition for $K_1 = 0$. This is, of course, what one would expect, because for $K_1 = 0$, $K_2 = K_3$, and $C_1 = C_2$, the LDM is equivalent, via a gauge transformation, to the lattice superconductor model of Ref. 3.

The duality maps as such do not tell us very much about the nature of the phase transition in the LDM for $K_1 \neq 0$. However, for certain special values of the coupling constants, the loop models of Eq. (9) and Eq. (12) map onto other lattice models whose properties are known. This then provides us with exact information about the behavior of the LDM at these special points in the parameter space. Several such special cases will be discussed below. Before proceeding further, however, I note that all the terms involving $1/C_2$ in Eq. (9) come with higher powers of $\alpha_\mu(\vec{k})$ than terms already present. Thus, the terms involving $1/C_2$ are quite unimportant in determining the long-distance form of the interactions, and neglecting them should not affect the critical behavior. This allows me to simplify matters by puttig $1/C_2 = 0$. In the following discussion, I also put $K_2 = K_3 = K$. The conclusions are not affected if $K_2 \neq K_3$. Let us now consider the following special cases.

(i) $K = 0$, K_1, C_1 *finite*. In this limit, Eq. (9) reduces to

$$H_L = 2\pi^2 K_1 \sum_{\vec{k}} \frac{|\alpha_x^* n_y(\vec{k}) - \alpha_y^* n_x(\vec{k})|^2}{|\alpha_z|^2 + \frac{K_1}{C_1}(|\alpha_x|^2+|\alpha_y|^2)^2} \ . \tag{13}$$

Defining a new integer-valued variable l_i by

$$l_i \equiv (\vec{\Delta} \times \vec{n}_i)_z \ , \tag{14}$$

I can write Eq. (8) as

$$Z \propto \sum_{[l_i]} \exp\left[-2\pi^2 K_1 \sum_{\vec{k}} |l(\vec{k})|^2 \Big/ \left(|\alpha_z|^2 + \frac{K_1}{C_1}(|\alpha_x|^2+|\alpha_y|^2)^2\right)\right] \ . \tag{15}$$

This partition function describes an ensemble of point charges interacting via an anisotropic logarithmic potential. In fact, for $K_2 = K_3 = 0$, $1/C_2 = 0$, the LDM reduces to a model studied recently by Amit *et al.*,[11] and they have also found this mapping to a system of point charges. Grinstein[12] has shown that this system of point charges is always in the disordered (plasma) phase. Hence, the LDM is always disordered for $K_2 = K_3 = 0$.

(ii) $K_1 = K \neq 0$, $C_1 \to \infty$. In this limit, Eq. (12) becomes

$$H_D = \frac{1}{2K}\sum_{\vec{k}} \frac{|m_x(\vec{k})|^2 + |m_y(\vec{k})|^2}{|\alpha_x|^2+|\alpha_y|^2+|\alpha_z|^2} \ . \tag{16}$$

Since the Hamiltonian does not depend upon m_z, the restricted sum over $[m_{i\mu}]$ in Eq. (11) reduces to an unrestricted sum over $[m_{ix}]$ and $[m_{iy}]$. The partition function in this limit is, thus, proportional to that of two mutually independent sets of point charges with Coulomb interaction at long distances. Since a

Coulomb gas in three dimensions is always in the plasma phase, the dual loop model is always disordered in this limit. This, in turn, implies that the LDM is always ordered if $K_1 = K_2 = K_3$ and $1/C_1 = 0$.

(iii) K_1, K *finite,* $C_1 \rightarrow \infty$. Using the result obtained in (ii), it can be shown that LDM is always in the ordered phase in this limit. The argument goes as follows. If there is a phase boundary in the (K_1-K) plane separating ordered and disordered phases, then it must have a negative slope everywhere, i.e., the critical value of K_1 must decrease as K is increased, and vice versa. We already know that for $K_1 = 0$, there is a phase transition at some value K_c of K. Any line with negative slope emerging from this point must intersect the line $K_1 = K$ somewhere. But the result obtained in (ii) tells us that on the line $K_1 = K$, there is no phase transition. Thus, the only conclusion consistent with all the facts is that, for any nonzero value of K_1, the LDM is in the ordered phase if $K \neq 0$ and $C_1 \rightarrow \infty$. In other words, in the $C_1 \rightarrow \infty$ limit, the inverted X-Y transition at $K = K_c$, $K_1 = 0$ disappears as soon as K_1 is turned on.

Recently, Toner[8] has used a renormalization-group analysis of the dislocation loop model of Eq. (10) to argue that the inverted X-Y transition at $K_1 = 0$ is stable with respect to turning on a finite K_1. This conclusion appears to be in contradiction with the result obtained above.

However, there are indications that this disagreement is because of the rather special nature of the $C_1 \rightarrow \infty$ limit. There is reason to believe that the properties of the LDM for finite values of C_1 are quite different from those for $C_1 \rightarrow \infty$. For a qualitative understanding of the situation, let us consider the dual loop model. The last three terms in Eq. (12) represent the interactions among loop segments. It is easy to verify that, for any finite value of K_1, the interaction energy goes to zero if $m_x(\vec{k}) \cong 0$, $m_y(\vec{k}) \cong 0$, $m_z(k_z \neq 0) \cong 0$, and $m_z(k_z = 0)$ finite. This implies that for $C_1 \rightarrow \infty$, it cost little energy to have a large number of very long loops running predominantly in the z direction. This is what makes the dual loop model disordered (and consequently, the LDM ordered) at any finite value of K_1 in the $C_1 \rightarrow \infty$ limit. A finite value of $1/C_1$ acts as a core energy per unit length for the z components of the loops, and makes it energetically unfavorable to have very long loops running along the z axis. Thus, for $1/C_1 \neq 0$, one would expect the presence of a phase boundary in the K_1-K plane, emerging from the inverted X-Y transition point $(0, K_c)$. The analysis presented here cannot predict the nature of the phase transition across this line.

It can be seen from Eq. (12) that the interaction between z components of the loops in the dual loop model changes sign as K_1 is increased above K. One may consider this to be an indication of a change in the nature of the phase transition. However, there is reason to believe that the phase transition is not sensitive to the sign of the interaction between the z components. For $1/C_1 \neq 0$, it is easy to show that due to cancellations between the last two terms of Eq. (12), the energy associated with the z components of large loops is dominated by the $1/C_1$ term, not by the interaction. Thus, it is unlikely that any dramatic change in the critical behavior will take place as K_1 is increased beyond K.

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