Phase transition in the two-dimensional frustrated x-y model: scaling equations

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Received 27 April 1981

Abstract. We establish scaling equations for the two-dimensional x-y model with weak frustration using the electrostatic analogy of Kosterlitz and Thouless. In the limit of small disorder we find a shift in the critical temperature

$$T_c(x) - T_c(0) = -(Jx/k_B)(2\pi^2 - \pi/2 \ln 2x)$$

and the exponents are unchanged from the pure values.

1. Introduction

Villain (1977) initiated the study of the two-dimensional x-y model with (quenched) frustrated disorder, as an interesting example of a system with a continuous symmetry which exhibits discrete (Ising-like) two-level systems. The Ising-like variables arise as manifestations of frustration and are characterised by half-integral vortices (textural singularities), a relationship which appears to be of a general character (Alexander and Lubensky 1979). The model is also interesting when viewed as a gauge theory with a Z_2 gauge field symmetry in addition to the U(1) matter symmetry (Fradkin et al 1978).

Villain investigated the ground state of the system and suggested that the Kosterlitz-Thouless (1973: KT) transition of the pure model may be destroyed by an arbitrarily small amount of disorder for the case of a random distribution of frustrated cells. For the case of randomly distributed negative bonds, however, Shastry (1979) gave an intuitive argument that the KT transition would be stable against weak disorder since the disorder provides an effective fugacity to control the number of vortex-like combinations of two-level systems. A similar conclusion may be reached by using the Harris criterion (Harris 1974) which is satisfied by a big margin in the x-y model since the specific heat exponent in the pure case $\alpha \to -\infty$ (Imry 1979). José (1979) reached a similar conclusion by examining the two-spin correlation function, using the techniques developed by José et al (1977) for the pure case. He also examined the case of strong disorder where the correlations decay exponentially rather than as power laws. His approach, however, does not give a result for the shift in T_c from the pure value. This shift is of considerable interest and is widely studied in Ising-like systems where some exact results are known (Au-Yang et al 1976).

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In this work we calculate the behaviour of $T_c(x)$ for small x, using a generalisation of the elegant scaling argument of Kosterlitz and Thouless, which was shown by Young (1978) to be equivalent to the more conventional renormalisation group argument of Kosterlitz (1974). Our work uses the electrostatic analogy which reduces the problem to that of a two-component (neutral) Coulomb gas in two dimensions with polarisable dipoles at randomly distributed sites. The theory uses the simplification arising from low (vortex) density and low concentration assumptions (we restrict attention to the lowest powers of x, the disorder variable), and is limited in the sense that the correlation functions are not tractable. Thus our study complements that of José (1979) and also that of Fradkin *et al* (1978), whose work shows that we may expect a reduction in the magnitude of the correlation function due to weak disorder. We hope to generalise our techniques to study the case of dilution, which is of considerable experimental interest in the context of phase transitions in granular (2d) superconductors.

The paper is organised as follows. In § 2 we outline the Coulomb gas analogy which was given by Villain (1977) and discuss the reduction of the problem to an effective vortex gas with polarisable dipoles. We set up the recursion relations in analogy with the pure case (Young 1978) and the dipoles are taken into account through a 'shape function'. In § 3 we discuss the nature of the shape function and in § 4 we obtain the $T_c(x)$ to the lowest order in x by adjusting the initial conditions such that the scaling trajectory passes through the fixed point. The stability of the pure fixed point is pointed out. In § 5 we discuss our results. Appendix 1 summarises the duality argument leading to the Coulomb gas. Appendix 2 contains a novel relationship between the $\varepsilon(R)$ as defined by KT and a wavevector-dependent ε_q which is exploited to give a reasonable shape function.

2. Recursion relations for the dipole screened Coulomb gas

2.1 The effective Coulomb Hamiltonian

The system we consider is a two-dimensional classical x-y model in which the exchange constants are random variables with allowed values +J or -J. We may conveniently write the Hamiltonian as

$$H = J \sum_{\langle ij \rangle \in L} \left[1 - \cos(\theta_i - \theta_j - \pi n_{ij}) \right]$$
 (2.1)

where L is the (square) lattice of N points, and the n_{ij} are integer valued random variables attached to the 2N bonds with a probability distribution

$$p(n) = x\delta_{n,1} + (1-x)\delta_{n,0}. \tag{2.2}$$

Clearly bonds with n = (1), 0 have (anti)ferromagnetic interactions. The disorder is assumed to be quenched, i.e. the set $\{n_{ij}\}$ is assigned initially in accordance with the distribution law (2.2) and the average over these taken after computing $\log Z$, where Z, the partition function, may be written as

$$Z = \operatorname{Tr}_{\{\theta_i\}} \prod_{\langle ij \rangle} \exp(A_{ij}). \tag{2.3}$$

Here $\Pi_{(ij)}$ represents a product over each nearest-neighbour bond (singly) and the 'action' is given by

$$\exp(A_{ii}) = \exp\{-K[1 - \cos(\theta_i - \theta_i - n_{ii}\pi)]\}$$
(2.4)

where $K = J/k_BT$. We assume a simplification of equation (2.4) which was first introduced by Villain (1975):

$$\exp(A_{ij}) \simeq \sum_{m_{ij}=0,\pm 1...} \exp\left[-\frac{K}{2}(\theta_i - \theta_j - \pi n_{ij} - 2\pi m_{ij})^2\right]. \tag{2.5}$$

This approximation reproduces the small-angle expansion of the cosine function in equation (2.4) and restores the 2π periodicity, thereby leading to vortices in addition to the harmonic spin waves. A partial trace over the continuous degrees of freedom can be performed (Villain 1977, José 1979) and after a duality transformation the partition function factors out into a (non-singular) spin wave part and a Coulomb part. For completion the argument is summarised in Appendix 1 and we obtain the Coulomb part (Villain 1977)

$$Z_{c} = \operatorname{Tr}_{\{m_{i}=0,\pm 1,\pm 2,...\}} \exp(-\beta H_{c}) \, \delta_{0,\Sigma_{i}m_{i}}$$
 (2.6)

where

$$H_{c} = -q^{2} \sum_{i,j \in L} \ln(|\mathbf{r}_{i} - \mathbf{r}_{j}|/a_{0}) \,\mu_{i}\mu_{j} + \mu_{0} \sum \mu_{i}^{2}$$
(2.7)

$$\mu_i = m_i + \nu_i/2, \qquad q^2 = \pi J, \qquad \mu_0 = q^2(\gamma + \frac{3}{2}\ln 2).$$
 (2.8)

In equations (2.7) and (2.8) a_0 is the lattice constant, γ is Euler's constant, the sum ij runs over the dual lattice (again a square lattice) and the m_i are integers attached to each (dual) lattice point. The variables v_i are fixed by the distribution of the J in the original lattice (or equivalently the n_{ij}) and can be written as $v_i = n_{\text{East}} + n_{\text{North}} - n_{\text{West}} - n_{\text{South}}$, where n_{East} etc are the bond variables in the appropriate direction in a plaquette surrounding the dual lattice point i. Thus ± 2 , ± 1 , 0 are the allowed values of the quantum numbers v_i . The lattice point is frustrated in the sense of Toulouse (1977) if $v_i = \pm 1$ and non-frustrated if $v_i = \pm 2$ or 0. We may recognise equations (2.6)–(2.8) as the problem of a Coulomb gas in two dimensions with a short-distance cut-off a_0 . The charges μ_i (in units of $q = (\pi J)^2$) are half-odd integer or integer, depending on whether the site i is frustrated or otherwise. The assembly is neutral and a chemical potential μ_0 tends to suppress the creation of free vortices. The problem reduces to precisely the Coulomb gas considered by KT if the ν are set equal to zero.

In the disordered problem our analysis follows that of Villain (1977) closely. Firstly we note that it is sufficient to confine ourselves to states having the smallest possible values of charge since these represent the best compromise between energy and entropy (Kosterlitz and Thouless 1974). Thus we may set $\mu_i = \pm 1$, or 0 for $i \in R$, where R is the set of unfrustrated lattice points and F is the frustrated set $(R \cup F = L)$. (Thus the sites having trivial disorder corresponding to two antiferromagnetic bonds and hence $\nu_i = \pm 2$ have been 'gauged away' by setting $m_i = \mp 1$ on these sites.) On the frustrated set F we have $\nu_i = \pm 1$ and hence $\mu_i = m_i \pm \frac{1}{2}$. On these we restrict ourselves to $m_i = \mp 1$, so that $\mu_i = \pm \frac{1}{2}$. Furthermore, it is easy to verify that $\Sigma \nu_i = 0$ by construction, and hence $\Sigma \nu_i = 0$ and $\Sigma m_i = 0$ together imply $\Sigma \mu_i = 0$. Thus we may regard μ_i as the fundamental set of variables with values ± 1 or 0 on R and $\pm \frac{1}{2}$ on F. This procedure was introduced by Villain (1977) and has the advantage of removing trivial disorder at the very outset.

The ground state of the model corresponds to setting $\mu_i = 0$ on all unfrustrated sites (R). The μ_i on the frustrated set (F) may be $\pm \frac{1}{2}$ and hence the ground state energy is higher than in the pure case. It can be seen that the ground state has a macroscopic degeneracy which is especially clear in the weak disorder limit $x \le 1$. In this case the distribution of the frustrated plaquettes is very simple: we have

$$N_{\rm f} = 4xN + O(x^2)$$

where $N_{\rm f}$ is the number of frustrated cells. These occur in pairs (since flipping the sign of one bond in the x-y model frustrates the two squares which share the bond) and we may further regard the distribution of the pairs as random to O(x). A given pair will clearly be neutral in the ground state in order to prevent a build-up of charge locally. Thus the ground state consists of $N_{\rm f}/2$ 'dipoles', each having the possible orientations $(\pm \frac{1}{2}, \mp \frac{1}{2})$ and neglecting the dipole-dipole interaction, the ground state degeneracy is $2^{N_{\rm f}/2}$. Considerations of dipole-dipole interactions would change the picture and presumably lead to a 'dipolar spin glass' (Vannimenus 1980, private communication) but we shall not pursue this further.

At elevated temperatures one would create (thermal) vortices in neutral pairs on the non-frustrated sites, as in the pure case. However, in the disordered case we may also create a 'mertex' configuration by considering a dipole and flipping one of the two charges, giving rise to a net charge of ± 1 . We may visualise the mertex configurations as vortices which are constrained to lie on the lattice F', where each point in F' is the mid-point of a dipolar pair in the F lattice. (Clearly the number of lattice points in $F' = N_{f'} 2 = 2xN + O(x^2)$.) Charge neutrality requires compensating this configuration by creating another vortex (or mertex) with charge ∓ 1 . In the subsequent work we will be interested in taking the continuum limit, and in this limit the distinction between a mertex and a vortex is artificial. We now show that mertex-like configurations may be absorbed into vortex-like excitations provided the fugacity is redefined suitably. The argument is exact in the continuum limit and is most directly seen in the trivial case of two excitations. We consider the Hamiltonian (2.7) in the subspace of two excitations (we have subtracted the ground state energy shift). The (canonical) partition function is

$$Z^{(2)} = \left[\sum_{i,j \in F'} + \exp(-2\beta\mu_0) \sum_{\substack{i,j \in R}} + \exp(-\beta\mu_0) \sum_{\substack{i \in F' \\ j \in R}} + \exp(-\beta\mu_0) \sum_{\substack{i \in R \\ j \in F'}} \right] \times \exp 2q^2\beta \ln(|\mathbf{r}_i - \mathbf{r}_j|/a_0).$$
(2.9)

In the continuum limit, we have (since the number of lattice points is (1 - 2x)N in R and 2xN in F')

$$\sum_{i \in R} \to (1 - 2x) \int \frac{\mathrm{d}^2 r_i}{a_0^2}$$

$$\sum_{i \in F} \to (2x) \int \frac{\mathrm{d}^2 r_i}{a_0^2}.$$
(2.10)

Inserting into equation (2.9) we find

$$Z^{(2)} = z_0^2(x) \int \int \frac{\mathrm{d}^2 r_i}{a_0^2} \frac{\mathrm{d}^2 r_j}{a_0^2} \exp[2q^2 \beta \ln(|\mathbf{r}_i - \mathbf{r}_j|)/a_0]$$
 (2.11)

where

$$z_0(x) = \exp(-\beta\mu_0) + 2x + O(x^2). \tag{2.12}$$

This is precisely the result obtained by taking the continuum limit for vortices with an effective fugacity given by equation (2.12). Proceeding similarly one can see that the replacement (2.12) takes care of the mertices to all orders.

To summarise, we have seen that the low lying excitations of equation (2.7) for the case of weak disorder may be viewed as vortex-antivortex pairs with an effective (x dependent) fugacity (equation (2.12)). The interaction between the vortex pairs is no longer purely Coulomb since the dipoles form a polarisable medium and partially screen the interactions. (The conscientious reader may object that the mertex configurations occur on the same sites where the dipoles are located and hence one must introduce 'exclusion' effects; however, it is readily seen that this effect is irrelevant provided we work to the lowest order in x.)

The polarisability of the dipoles leads to a bulk dielectric constant which is readily estimated as follows (Shastry 1979). We have 2xN dipoles of which a half (xN) lie along the E-W direction and the other half (xN) along the N-S direction on the average. On applying an external electric field E_0 , the induced polarisation is $(\Delta = \frac{1}{2}\beta qa_0)$

$$\langle \mathbf{P}_{\rm in} \rangle = \left(\frac{q}{2} a_0\right) x N i \left\{ \sum_{\sigma = \pm 1} \sigma \exp[\sigma \Delta (\mathbf{E}_0 \cdot i)] \right\} / \sum_{\sigma} \exp[\sigma \Delta (\mathbf{E}_0 \cdot i)]$$

$$+ \left(\frac{q}{2}a_0\right)xNj\left\{\sum_{\sigma=\pm 1}\sigma\exp[\sigma\Delta(\boldsymbol{E}_0\cdot\boldsymbol{j})]\right\} / \left\{\sum_{\sigma}\exp[\sigma\Delta(\boldsymbol{E}_0\cdot\boldsymbol{j})]\right\}$$
(2.13)

$$= \beta \left(\frac{q}{2} a_0\right)^2 x N E_0 + O(x^2). \tag{2.14}$$

Hence the dielectric constant

$$\varepsilon_{\rm D} = 1 + \pi \beta q^2 x + \mathcal{O}(x^2). \tag{2.15}$$

In the above equations, we have neglected local field corrections since these would contribute to $O(x^2)$ only. We observe that equation (2.15) results if we relax the constraint that the 2xN elementary dipoles only align in the E-W or N-S direction, and allow these to orient in all directions in the plane, provided we assign to each dipole a polarisability $\alpha = \frac{1}{8}\beta q^2 a_0^2$. This assumption is used in § 3 to simplify the problem.

2.2. Recursion relations

In this section we set up the recursion relations for the Coulomb gas with dipolar screening in the spirit of the Kosterlitz-Thouless theory. Following KT, we define a scale-dependent dielectric function $\varepsilon(r)$ which may be defined in terms of the force experienced by a test charge pair kept at a distance r in the medium

$$F_{\text{medium}} = F_{\text{vacuum}}/\varepsilon(r). \tag{2.16}$$

(Implicit in the definition is an averaging of the force over all orientations and positions in the medium with the distance r kept fixed.) Following KT we define an effective interaction energy between a test pair of charges $\pm q$ as

$$U_{\rm eff}(r) = 2\mu_{\rm eff} + 2q^2 \int_{a_0}^r \frac{\mathrm{d}r'}{r'} \frac{1}{\varepsilon(r')}$$
(2.17)

where $\mu_{\rm eff} \equiv -(k_{\rm B}T) \ln z_0(x)$. This energy is the integral over the force in equation (2.16) and acts as a Boltzmann weight for a pair. The 'iterated mean-field theory' of KT is based upon the use of $U_{\rm eff}(r)$ in place of $\ln r$ in equation (2.11) and the assumption that this replacement incorporates the major effects of $Z^{(4)}$, $Z^{(6)}$ etc. Following Kosterlitz and Thouless, we now establish a differential equation for $\varepsilon(r)$ by enlarging the length scale from r to r+dr. On changing the separation of the test pair from r to r+dr, we have additional polarisable (vortex–antivortex) pairs to screen the test pair since the vortex pairs are distributed at various length scales. Hence we may equate $d\varepsilon(r)/4\pi$ to the polarisability times the density of all the additional polarisable entities which are brought into play by the increase in the test pair separation. We therefore write

$$d\varepsilon(r) = 4\pi \, dn(r) \, \frac{1}{2} (qr)^2 \, \beta + (4\pi) \, dn_D(r) \, \alpha \tag{2.18}$$

where dn(r) is the density of vortex-antivortex pairs with a separation lying between r and r + dr; the factor $\frac{1}{2}\beta(qr)^2$ is the polarisability of the pairs and the last term is the correction term due to the dipoles, with α the polarisability of each dipole and $dn_D(r)$ the density of dipoles contained within r and r + dr. The first term in equation (2.18) is expressed back in terms of $\varepsilon(r)$ using

$$dn(r) = (2\pi r \, dr/a_0^4) \exp[-\beta U_{\text{eff}}(r)] \tag{2.19}$$

which follows from equation (2.11) on using $U_{\rm eff}$ in place of $\ln r$. In the second term, we define

$$dn_D(r) = (2x/a_0^2) \frac{dg(r)}{dr} dr$$
(2.20)

where g(r) is a dipolar 'shape function' which will be elaborated upon in the following. Using $\alpha = \frac{1}{8}\beta q^2 a_0^2$ we get

$$d\varepsilon(r) = q^2 \beta 4\pi^2 r^3 (dr/a_0^4) \exp(-\beta U_{\text{eff}}(r)) + (\pi \beta q^2 x) (dg(r)/dr) dr.$$
 (2.21)

We next go over to a logarithmic length scale and define

$$l = \ln(r/a_0), \qquad K = \beta J, \qquad K(l) = K/\varepsilon(l).$$
 (2.22)

It is expedient to define a scale dependent fugacity (Young 1978)

$$y(l) = z_0(x) \exp\left(2l - \pi \int_0^l K(l') \, dl'\right)$$
 (2.23)

in terms of which equation (2.21) becomes

$$\frac{dK(l)}{dl} = 4\pi^{3}y^{2}(l) + \pi^{2}x(d\psi/dl)$$
 (2.24)

with

$$\psi(l) = g(r)|_{r=a_0e^{l}}. (2.25)$$

Differentiating (2.23) with respect to l, we get

$$dy(l)/dl = [2 - \pi K(l)] y(l).$$
 (2.26)

Thus we have replaced the integro-differential equation (2.21) by a pair of coupled differential equations which are precisely those of Kosterlitz (1974) in the absence of the term involving $\psi(l)$ in equation (2.24).

The terms involving g(r) and $\psi(r)$ can be understood in terms of the dipolar system as follows. If we neglect the vortices completely (set $z_0(x) \to 0$) the calculation sketched above reduces to that of the computation of the scale-dependent ε for a system of dipoles. Thus integrating equation (2.21) we get

$$\varepsilon_{\rm D}(r) = 1 + \pi \beta q^2 x g(r) \tag{2.27}$$

where $g(0) \equiv 0$. For $r \to \infty$, $\varepsilon_D(\infty)$ must reduce to the bulk screening constant calculated in equation (2.15) and hence $g(\infty) = 1$. Thus g(r) represents the build-up of the response of the dipolar system as the test pair separation is varied and is normalised to unity at $r = \infty$. It is at first sight surprising that one should be considering a scale dependence of ε_D at all, since there is no real dispersion (such as a distribution of vortex pairs etc) for the dipoles. The reason why we are forced to consider $\varepsilon_D(r)$ is that the dipoles are separated by a mean distance

$$a_m = a_0/(2x)^{1/2} (2.28)$$

which tends to infinity as $x \to 0$. Thus for small x the test pair has to be at least $O(a_m)$ apart before the dipolar screening can be effective, resulting in g(r) = 0 for $r \le a_m$. It is this scale dependence that we substantiate and estimate in the following section.

The disorder thus modifies the Kosterlitz recursion relations in two ways: (a) the initial condition on fugacity y(0) depends on x (through equation (2.12)) and (b) the dependence on $\psi(l)$ in equation (2.24). As $l \to \infty$, $\psi'(l) \to 0$ and hence the fixed point of the equations is the same as for the pure case $(K^* = 2/\pi, y^* = 0)$. In § 4 we calculate the shift in T_c as a result of the disorder.

3. Dipolar shape function

We place the 2xN dipoles on a lattice $\{r_i\}$ with lattice parameter a_m (equation (2.28)) and place a test charge pair $\pm Q$ at $R_0 \pm R/2$. Each dipole has a polarisability $\alpha(=\frac{1}{8}\beta q^2 a_0^2)$ and to the lowest order in x, we may disregard the dipole–dipole interactions. The interaction energy of the system is known for elementary electrostatics

$$U_{\text{int}} = \frac{1}{8\pi} \int \boldsymbol{E} \cdot \boldsymbol{D} \, d^2 r = 2Q^2 \ln |\boldsymbol{R}| / a_0 - \frac{1}{2} \sum_i \langle \boldsymbol{p}_i \rangle \cdot \boldsymbol{E}_i.$$
 (3.1)

The electric field may be approximated by the field due to the external charges

$$E_i = (2Q) \frac{R}{|\mathbf{r}_{i+}| |\mathbf{r}_{i-}|} n \tag{3.2}$$

where $\mathbf{r}_{i\pm} = \mathbf{r}_i - \mathbf{R}_0 \pm \mathbf{R}/2$ and \mathbf{n} is a unit vector. Equation (3.2) cannot be used as it stands in the problem at hand since the denominators may vanish and lead to spurious singularities. The underlying lattice provides a cut-off ' a_0 ' which is the distance of minimum approach, and we replace equation (3.2) by

$$E_i \to \frac{(2Q) R}{[a_0 + |r_{i+1}|] [a_0 + |r_{i-1}|]} n. \tag{3.3}$$

The induced polarisation $\langle P_i \rangle = \alpha E_i$ must also be found using equation (3.3). We must also make sure that linear response theory is valid for computing P_i , since E_i becomes very small for $r_{i\pm} = 0$ and $|\langle P_i \rangle|$ is bounded by $\frac{1}{2}qa_0$. The ratio $\alpha |E_i|_{\max}/\frac{1}{2}qa_0$ is $\sim (\pi K/2)$,

and hence for $T \simeq T_c$ we may neglect this complication. Therefore using equation (3.3) in equation (3.1) we find

$$U_{\text{int}} = 2Q^{2} [\ln |\mathbf{R}| / a_{0} - f(\mathbf{R}, \mathbf{R}_{0})]$$
(3.4)

where

$$f(\mathbf{R}, \mathbf{R}_0) = \alpha \sum_{i} \frac{R^2}{[|\mathbf{r}_{i+}| + a_0]^2 [|\mathbf{r}_{i-}| + a_0]^2}.$$
 (3.5)

We may define the average of f over the location \mathbf{R}_0 and the orientations of \mathbf{R} :

$$f(|\mathbf{R}|) = \langle f(\mathbf{R}, \mathbf{R}_0) \rangle. \tag{3.6}$$

Clearly, the average over R_0 may be restricted to a unit cell since the function is periodic in R_0 . The dipolar dielectric function may be obtained from equations (2.16), (3.4) and (3.6) as

$$\varepsilon_{\rm D} = [1 - R(\partial/\partial R) f(R)]^{-1} \simeq 1 + R(\partial/\partial R) f(R). \tag{3.7}$$

The last equality in equation (3.7) follows since we expect $f(R) \sim O(x)$. We now examine f in the extreme limits of small R and large R.

 $R \le a_m$. In this case we isolate the unit cell in equation (3.5) which contains R_0 and write

$$f(R) = f_0(R) + f_1(R) \tag{3.8}$$

where

$$f_0(R) = (\alpha R^2) \int_{\text{Ucell}} \frac{\mathrm{d}^2 R_0}{a_m^2} \{ a_0 + |\mathbf{R}_0 - \mathbf{R}/2| \}^{-2} \{ a_0 + |\mathbf{R}_0 + \mathbf{R}/2| \}^{-2}$$
 (3.9)

$$f_1(R) = \alpha R^2 \sum_{i \neq 0} \frac{1}{\left[|\mathbf{r}_{i-}| + a_0|^2 \left[|\mathbf{r}_{i+}| + a_0|^2 \right] \right]}.$$
 (3.10)

Equation (3.9) contains potentially large terms since the denominators can become small. We may estimate equation (3.9) by confining our attention to $\mathbf{R}_0 \cong \pm R/2$, and obtain the leading behaviour as

$$f_0(R) \simeq C \left[\frac{8\pi \alpha}{a_0^2} \right] \left[\frac{R}{R + a_0} \right]^2 \tag{3.11}$$

where C is O(1). For $R > a_0$, f(R) is a very slowly varying function and hence does not contribute to the dielectric function (3.7).

The terms $f_1(R)$ can be estimated by neglecting the average over R_0 and we find

$$f_1(R) \cong (2\alpha x/a_0^2) (R/a_m)^2 C'$$
 (3.12)

where C' is O(1).

 $R \gg a_m$. In this limit we may replace the summation in equation (3.5) by an integration (since the lattice constant is a_m). Thus

$$\sum_{i} \to (2x) \int d^2r_i/a_0^2$$

and

$$f(R) \simeq \left(\frac{2x\alpha}{a_0^2}\right) R^2 \int \frac{d^2r_i}{[a_0 + |\mathbf{r}_i - \mathbf{R}/2|]^2 [a_0 + |\mathbf{r}_i + \mathbf{R}/2|]^2}.$$
 (3.13)

By scaling $r_i = |R|y$ and shifting,

$$f(R) \simeq \left(\frac{2x\alpha}{a_0^2}\right) \int \frac{d^2y}{[y + a_0/|R|]^2 [|y + R/|R|] + a_0/|R|]^2}.$$
 (3.14)

The regions $y \approx 0$ and $y \approx -R/|R|$ contribute equally to the leading behaviour of equation (3.9) and we get

$$f(R)_{(R \gg a_m)} = \left(\frac{8\pi\alpha\alpha}{a_0^2}\right) \ln\frac{R}{a_0}.$$
 (3.15)

It is clear from equations (3.15) and (3.7) that asymptotically

$$\varepsilon_{D(R \geqslant a_m)} = 1 + (8\pi x \alpha/a_0^2).$$
 (3.16)

This result is of course precisely what we expected from equation (2.15) in this limit. It is clear from equations (3.7), (3.12) and (3.15) that the dipolar shape function

$$g(R) = C(R/a_m)^2 \qquad (R \le a_m)$$

$$= 1 \qquad (R \ge a_m). \qquad (3.17)$$

For $R \ge a_m$ these are always cells in which the denominators become small $(O(a_0))$ but these can be handled in a manner analogous to $f_0(R)$ in equation (3.9). Therefore within the accuracy of our estimates we conclude that the dipolar shape function can be represented reasonably by an interpolation formula

$$g(R) \simeq \frac{(R/a_m)^n}{C + (R/a_m)^n}$$
 $C \simeq O(1)$. (3.18)

We expect n=2, but we shall see in § 4 that the leading behaviour of $T_c(x)$ is independent of C and n, and hence we may content ourselves with the above crude estimate. In Appendix 2 we suggest a more appropriate form for g(R) by using a novel relationship between the dielectric function in momentum space and $\varepsilon(R)$. This, however, leads to the same behaviour as equation (3.18) for the leading behaviour of $T_c(x)$. The interpolation formula (3.18) captures the essential physics of the situation, which is that a_m , the lattice constant, sets the scale for the function, and therefore for $R \ge a_m$ a substantial number of dipoles are available for screening the test pair, whereas for $R \le a_m$ one has essentially $\varepsilon_D \simeq 1$.

Finally, we define

$$l_0 = \ln(a_m/a_0) = \ln[1/(2x)^{1/2}]$$
(3.19)

so that

$$\psi(l) = \frac{\exp[(l - l_0)n]}{C + \exp[(l - l_0)n]}.$$
(3.20)

4. Behaviour of $T_c(x)$

The recursion relations (2.24) and (2.26) have the same fixed point as the pure case (since $\psi'(l) \to 0$):

$$K^* = 2/\pi y^* = 0. (4.1)$$

Linearising about this, we define

$$K(l) = 2/\pi + 4t(l). (4.2)$$

The linearised recursion relations are

$$dt/dl = -4\pi y^2(l) - x\psi'(l) \tag{4.3}$$

$$dy/dl = -4\pi t(l) y(l). \tag{4.4}$$

Multiplying these equations by 2t and 2y respectively, and on taking the difference, we find

$$\frac{d}{dt}(t^2 - y^2) = -2xt\psi'. {(4.5)}$$

On the critical trajectory, $t(\infty) = 0 = y(\infty)$ and hence integrating (4.5) from 0 to ∞ we get

$$t^2(0) - y^2(0) = 2xL (4.6)$$

$$L = \int_0^\infty \mathrm{d}l \psi'(l) \, t(l). \tag{4.7}$$

For the pure case, x = 0 and $t^2(0) - y^2(0) = 0$ on the critical trajectory. The RHS of equation (4.6) is positive and shows that the initial conditions must be modified to reach the critical point and hence leads to the shift in T_c . In view of the explicit factor 2x in the RHS of equation (4.6) we expect that the leading behaviour can be obtained by setting $t = t^0(l)$, i.e. the solution in the pure case

$$t^{0}(l) = \frac{1}{(\tau + 4\pi l)}; \qquad \tau = \frac{1}{t^{0}(0)}. \tag{4.8}$$

We have solved equation (4.3) for a model $\psi_{\text{model}}(l) = \theta(l - l_0)$, where $l_0 = \ln(1/\sqrt{2x})$, and have verified that the above replacement is sufficient provided $x < \exp(-\beta\mu_0)$, whereas for $x \gg \exp(-\beta\mu_0)$ the results are different. For the x-y model the first inequality applies and hence we may use the approximation with confidence. Thus from equations (4.7), (4.8) and (3.15) we have on integrating by parts

$$L = (4\pi) \int_0^\infty \frac{\mathrm{d}l}{(\tau + 4\pi l)^2} \frac{\exp[(l - l_0)n]}{C + \exp[(l - l_0)n]}.$$
 (4.9)

In the limit $x \to \infty$, $l_0 \to \infty$, and hence we may extract the leading behaviour of equation (4.9) by setting the lower limit as l_0 . Calling $l = l_0(1 + \sigma)$ we get

$$L \simeq \frac{1}{(4\pi) l_0} \int_0^\infty \frac{d\sigma}{(\tau/4\pi l_0 + 1 + \sigma)^2} \frac{1}{[1 + C \exp(-\sigma l_0 n)]}.$$
 (4.10)

For large l_0 , we find

$$L = 1/4\pi l_0. (4.11)$$

Combining equations (4.2), (4.7) and (4.11) we find

$$(J\beta_{\rm C}(x) - 2/\pi) = 4(y^2(0) + x/2\pi l_0)^{1/2}.$$
(4.12)

For small x we may expand the squere root in equation (4.12) and hence

$$J\beta_{\rm C}(x) = 2/\pi + 4y(0) + x/\pi l_0 y(0). \tag{4.13}$$

Using equations (2.12) and (3.14) we finally obtain

$$k_{\rm B}T_{\rm c}(x)/J = \pi/2 - \pi^2 \exp(-\beta_{\rm c}\mu_0) - 2x\pi^2 + \pi x/2 \ln(2x).$$
 (4.14)

The first two terms are known from the work of Kosterlitz (1974). The last two terms in equation (4.14) represent the corrections due to disorder which leads to a decrease in $T_{\rm c}$ as expected. The logarithmic term is, however, unusual and not found in Ising-like systems in the lowest order.

The recursion relations have the same nature as those for the pure case, and in particular the rate at which one moves away from the fixed point is identical. The exponents are therefore unchanged by weak disorder.

5. Discussion

The main result of this work is equation (4.14), which shows a different character from the results of Ising-like systems with defects. In the latter case, the quenched and annealed disorder yield an identical linear depression of T_c to the lowest order, but higher-order terms may contain non-analytic x dependences (Harris 1974). In higher orders, the exact results of Au-Yang et al (1976) for an Ising model with a periodic distribution of defects in 2d show non-analytic terms such as $x^2 \ln x$. The frustrated x-y model is thus unusual in that non-analytic contributions such as $x/\ln x$ make their appearance in the lowest order.

If we naively assume that all the Coulomb interactions are screened by the bulk dielectric constant (2.15), the screening can be incorporated into a shift of the initial conditions in the recursion relations and a trivial calculation shows that the last term in equation (4.14) is to be replaced by $-\pi^2 x$, which is clearly more effective in reducing T_c . The logarithmic dependence on x stems from the fact that the vortex pair separation has to be greater than $a_0/(2x)^{1/2}$ before they can benefit from dipolar screening.

We should clarify that the results of this work do not necessarily have a direct bearing on the conjectured instability of the KT transition due to Villain. His conjecture is specifically for the case of a random distribution of frustrated cells rather than of antiferromagnetic bonds, and in that case the mean distance between half-integral charges becomes large ($\ge a_0/(x)^{1/2}$) as compared to the present work (a_0).

The fact that the exponents do not change in the limit of small x is expected from the criterion of Harris, as mentioned in the Introduction[†]. We should note, however, that a recent study (Shastry and Bruno 1981) of the effect of more general bond disorder than that studied in this work indicates that the criterion must be used with considerable care for the 2d x-y model.

[†] We should also mention that Dhar has recently analysed the same problem using a real space 'block charge' technique and obtains somewhat different results. His technique is very different in detail and it is not clear as to what approximation is responsible for the differences.

Acknowledgments

I would like to thank J Bruno, D Dhar, S Kirkpatrick and A P Young for helpful discussions, and also J José and J Villain for a useful correspondence.

Appendix 1: Duality and the Coulomb gas

We write equation (2.5) as a Fourier series

$$\exp(A_{ij}) = \sum_{m_{ij}=0,\pm 1,...} \exp[i(\theta_i - \theta_j - \pi n_{ij}) \, m_{ij}] \exp[-m_{ij}^2/2K - \ln(2\pi K)^{1/2}]. \tag{A1.1}$$

Multiplying out the expansions for the A in equation (2.3), we integrate over θ_i . Each θ_i occurs in four terms and on using

$$\int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \exp(\mathrm{i} m\theta) = \delta_{m,0}$$

we get a constraint at each site of the form $m_N + m_W = m_E + m_S$, where m_N , m_W , m_E and m_S are the Fourier expansion integers on bonds to the North, West, East and South of the site *i*. The constraint is recognised as a lattice version of potential flow and may be satisfied by going over to the dual lattice and defining at each lattice point an integer variable. We write

$$m_{\rm N} = m'_{\rm NW} - m'_{\rm NE}, \qquad m_{\rm S} = m'_{\rm SW} - m'_{\rm SE}$$
 (A1.2)

$$m_{\rm W} = -m'_{\rm NW} + m'_{\rm SW}, \qquad m_{\rm E} = -m'_{\rm NE} + m'_{\rm SE}$$
 (A1.3)

where the primed variables refer to the dual lattice. These equations clearly satisfy the constraints on the original lattice automatically. We may now express the partition function as a sum over the integers m' and after some elementary manipulations we find

$$Z = \frac{1}{(2\pi K)_i^N} \sum_{m=0,\pm 1,...} \exp\left[-\frac{1}{2} \sum_{K(ij)} (m_i - m_j)^2 - i\pi \sum_i m_i \nu_i\right]$$
(A1.4)

where we have introduced a new set of variables $\{\nu_i\}$ defined over the dual lattice in terms of the n as

$$\nu_i = n_{\rm E} + n_{\rm N} - n_{\rm W} - n_{\rm S}. \tag{A1.5}$$

Equation (A1.4) may be regarded as a Gaussian model for interfacial roughening in the absence of the ν variables (e.g. see Chui and Weeks 1976). In order to evaluate equation (A1.4) we introduce the Poisson summation formula

$$\sum_{n} g(n) = \sum_{m=-\infty} \int_{-\infty}^{+\infty} dx \exp(-2\pi i m x) g(x). \tag{A1.6}$$

at each site. This leads to

$$Z = \frac{1}{(2\pi K)^{N}} \sum_{\{m_i\}} \int_{-\infty}^{+\infty} d\varphi_i \exp\left[-\frac{1}{2} \sum_{K(ij)} (\varphi_i - \varphi_j)^2 - 2\pi i \sum_i (m_i + \nu_i/2) \varphi_i\right]. \tag{A1.7}$$

The integral over the φ is trivial since we have a gaussian form. Retaining the second cumulant of the φ we get

$$Z_V = Z/Z_{S-W} = \frac{1}{(2\pi K)^N} \sum_{(m_i)} \exp\left[-2\pi^2 K \sum_{ij} \mu_i \mu_j G(ij)\right]$$
 (A1.8)

where $\mu_i = m_i + \nu_i/2$, Z_{S-W} is the spin wave part (equation (A1.7) with $m_i = 0 = \nu_i$) and the Green function is

$$G(ij) = K^{-1} \langle \varphi_i \varphi_j \rangle = \frac{1}{2} \int \frac{\mathrm{d}k}{(2\pi)^2} \frac{\exp[ik \cdot (r_i - r_j)]}{2 - \cos k_x - \cos k_y}. \tag{A1.9}$$

The Green function diverges for all i and j due to the long-wavelength behaviour of the denominator. This may be regularised in the usual way by adding a small positive number to the denominator and defining

$$G(ij)_{\varepsilon \to 0} = G_{\varepsilon}(0) - \overline{G}(ij) \qquad G_{\varepsilon}(0) = \frac{1}{2} \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \frac{1}{\varepsilon + 2 - \cos k_x - \cos k_y}$$
(A1.10)

$$\overline{G}(ij) = \frac{1}{2} \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \frac{1 - \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j)]}{\varepsilon + 2 - \cos k_x - \cos k_y}.$$
(A1.11)

The exponential in equation (A1.8) may be written as

$$-2\pi^2K\sum_{ij}\mu_i\mu_jG_{\varepsilon}(0)+2\pi^2K\sum_{ij}\mu_i\mu_j\,\overline{G}(ij).$$

In the limit $\varepsilon \to 0$, $G_{\varepsilon}(0) \to +\infty$ and hence we get a zero contribution to the partition function unless $\sum \mu_i = 0$. Thus the neutrality constraint is forced by the long-wavelength behaviour of G(ij). In the limit $\varepsilon \to 0$, the reduced Green function $\overline{G}(ij)$ is well behaved and has the asymptotic behaviour (Spitzer 1964)

$$\overline{G}(ij)_{r_{ij}\to\infty} = +\left(\frac{1}{2\pi}\right)\ln(|r_{ij}|/r_0) \tag{A1.12}$$

where $+\ln(r_0/a_0) = -(\gamma + \frac{3}{2}\ln 2)$, γ being Euler's constant. Using equation (A1.11), equation (A1.8) becomes

$$Z_V = \frac{1}{(2\pi K)^N} \sum_{\{m_i\}} \delta_{0, \Sigma m_i} \exp(-\beta H_c)$$
 (A1.13)

where

$$H_{c} = -\pi J \sum_{i \neq i} \ln[|r_{i} - r_{j}|/r_{0}] \,\mu_{i}\mu_{j}. \tag{A1.14}$$

Defining $q = (\pi J)^{1/2}$ and $\mu_0 = \pi J \ln(a_0/r_0)$, equation (A1.14) reduces to equation (2.6).

Appendix 2

We establish an exact relationship between a Kosterlitz-Thouless-like dielectric function $\varepsilon(R)$ and a more conventional dispersive dielectric function ε_q for a homogeneous medium. If we place a test charge pair ± 0 in a medium (at $\pm R/2$) characterised by a dielectric function ε_q , the interaction energy (3.1) may be written as

$$U_{\rm int} = (2\pi) \left\langle \frac{\rho_{-q}^{\rm ext} \rho_q^{\rm ext}}{q^2 \varepsilon_q} \right\rangle \tag{A2.1}$$

where $\rho_q^{\rm ext}$ is the external charge density (-2i) $Q \sin(q \cdot R/2)$ and the angular bracket represents a sum over all q. By taking the derivative of equation (A2.1) with respect to R and on using equation (2.16) we find the relationship

$$\frac{1}{\varepsilon(R)} = \left\langle \frac{(\boldsymbol{q} \cdot \boldsymbol{R})}{q^2 \varepsilon_q} \sin(\boldsymbol{q} \cdot \boldsymbol{R}) \right\rangle \left\langle \frac{(\boldsymbol{q} \cdot \boldsymbol{R})}{q^2} \sin(\boldsymbol{q} \cdot \boldsymbol{R}) \right\rangle^{-1}. \tag{A2.2}$$

If we assume further that ε_a is isotropic, this equation reduces to

$$\frac{1}{\varepsilon(R)} = \int_0^\infty \frac{J_1(t) \, \mathrm{d}t}{\varepsilon_{t/R}} \tag{A2.3}$$

where J_1 is the Bessel function of first order. This equation shows that $\varepsilon(R = \infty)$ is $\varepsilon_{q=0}$ and hence is the bulk value.

We can exploit the relation (A2.3) to obtain a reasonable approximation for the dipolar shape function as follows. The dipolar system has a non-dispersive (wavevector-independent) dielectric constant for most wavevectors of interest except for very high q, when the lattice makes itself felt. Hence a reasonable choice is

$$\varepsilon_a = 1 + \pi \beta q^2 x \theta (1 - |\boldsymbol{q}| a_m). \tag{A2.4}$$

Substituting equation (A2.4) into equation (A2.3), we find after an elementary calculation

$$g(R) = 1 - J_0(r/a_m) (A2.5)$$

and therefore $\psi(l) = 1 - J_0 \left(\exp(l - l_0) \right)$. For $r \le a_m$, $g(R) \sim \frac{1}{4}R^2/a_m^2$ and for $r \ge a_m$, g = 1. Thus equation (A2.5) has all the desired properties (see equation (3.17)) and we believe it is a reasonable guess.

We now show that equation (A2.5) leads to the same $\beta_c(x)$ as equation (4.13). From equations (4.7), (4.8) and (A2.5) we have

$$L = (4\pi) \int_0^{l_0} \frac{dl[1 - J_0(\exp(l - l_0))]}{(\tau + 4\pi l)^2} + (4\pi) \int_{l_0}^{\infty} \frac{dl[1 - J_0(\exp(l - l_0))]}{(\tau + 4\pi l)^2}.$$
 (A2.6)

The first integral vanishes faster than $1/l_0$ as $l_0 \rightarrow \infty$ and may be omitted. In the second integral we separate the two terms in the numerator and get

$$L_{l_0 \to \infty} \sim \frac{1}{4\pi} l_0 + \overline{L} \tag{A2.7}$$

$$\overline{L} = (-4\pi) \int_{l_0}^{\infty} \frac{J_0(\exp(l - l_0))}{(\tau + 4\pi l)^2} \, \mathrm{d}l. \tag{A2.8}$$

Clearly

$$|\overline{L}| \le \frac{(4\pi)}{(\tau + 4\pi l_0)^2} \int_{l_0}^{\infty} |J_0(\exp(l - l_0))| dl < \frac{1}{4\pi l_0^2} \int_{1}^{\infty} |J_0(z)| \frac{dz}{z}.$$

As $z \to \infty$, $|J_0(z)| \sim 1/z^{1/2}$ and hence the integral converges. Therefore the leading behaviour of L is $1/(4\pi)$ l_0 , which coincides with equation (4.11) and hence leads to equation (4.14).

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