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Studies of the classical X-Y model

Moshe Schwartz
Department of Physics and Astronomy, Tel Aviv University, Ramat Aviv, Israel
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The high-temperature expansion is used, to all orders, to obtain an equivalent description of the X-Y model in terms of a quantized vector field interacting with itself and with a system of quantized charges. This description is used to all orders to obtain some exact and some approximate results. The exact results are (a) an alternative description in terms of integer Ising spins interacting via a nearest-neighbor interaction; (b) upper bounds on the correlation length and transition temperature in two and three dimenisions. It is also shown that at low temperatures the system can be viewed as a system composed of a few kinds of charges (the number depends on the dimensionality), where the interaction between charges of a given kind is electrostatic, while the interaction between charges of different kinds is zero.

I. INTRODUCTION

Two-dimensional systems possessing a continuous symmetry pose a very interesting problem. On one hand, it is rigorously known that such a system cannot exhibit spontaneous symmetry breaking,[1-3] while there are indications that some systems undergo a transition of some kind.[4-9] The classical X-Y model is special, because according to current beliefs models possessing higher than O(2) symmetries do not have a phase transition.[10] The relation of the X-Y model to the sine-Gordon field-theoretical model adds to the importance of understanding its behavior.[11]

The main purpose of this paper is to present exact and approximate analog descriptions of the X-Y model that may enable better understanding of the system.

The high-temperature expansion for the classical X-Y model is obtained in Sec. II, and given a graphical representation. In Sec. III it is shown that evaluation of the X-Y partition function is equivalent exactly to the evaluation of the partition function of a system composed of a quantized field (generated by the interaction terms of the X-Y model), that interacts with itself and with a system of quantized charges (generated by the external field appearing in the x-y Hamiltonian). In Sec. IV, it is shown that in the absence of an external field the two-dimensional system may be viewed as a system of spins in the Z direction attaining only integer values and interacting via a nearest-neighbor interaction. The spin must obey a subsidiary condition such as the requirement that the total magnetization is zero. It is shown that this transformation is the analog of expressing quantities that depend on a divergence-free vector by its vector potential. An upper bound is obtained in Sec. V for the transition temperature of the two and three-dimensional X-Y models. Above this bound the spin-spin correlation function has a factor that decreases exponentially with distance. Sec. VI describes an equivalence of the model to a plasma model at low temperatures. It is shown, that the longitudinal degrees of freedom of the field mediate an interaction between the charges that is electrostatic at large distances. This result was earlier derived by Zittartz[12] using an entirely different approach. In Sec. VII we show also that the transverse degrees of freedom are equivalent to systems of charges interacting via the Coulomb potential. In two dimensions we find only one kind of charge, while in the three-dimensional case we have two kinds of charges, corresponding to the transverse degrees of freedom, that are mutually noninteracting. This result agrees with the description given by Thouless and Kosterlitz[13] in the two-dimensional case, in the absence of an external field.

The treatment given in Secs. VI and VII reveals the origin and relation between the charges discussed by Zittartz[12] and the charges discussed by Thouless and Kosterlitz.[13] The charges of the first kind are generated by the external magnetic field and their long-range Coulomb interaction arises from the longitudinal degrees of freedom of the vector field. The charges of the second kind and their electrostatic interaction form an alternative description of the system of transverse modes. The fact that enables this description is that the Hamiltonian describing the transverse modes of the field can be also expressed in terms of its curl.

In Sec. VIII we discuss a model that is more general than the X-Y model, the cos interaction between the angular variables being replaced by a general periodic function. It is shown that the structure of the high-temperature series is the same, except for the weights attached to the ele-

ments of the graphs composing the expansion. The different derivation of the high-temperature expansion may be used as an alternative to the derivation presented in Sec. II for the X-Y model. One of the reasons to consider a more general model is its possible importance in the construction of coordinate-space renormalization procedures for O(2) symmetries.

The results are discussed in Sec. IX. The approach of this article is related to the approach of Kadanoff *et al.*[14] for the X-Y case, to the treatment of the roughening transition by Chui and Weeks[15] and to the discussion by Kogut *et al.*[16] of extended dual models.

II. HIGH-TEMPERATURE EXPANSION OF THE FREE ENERGY OF THE X-Y MODEL

Consider a large but finite ν-dimensional cubic lattice, consisting of N sites. The X-Y model describes a system of unit-length classical spins restricted to rotate in the X-Y plane. The spins are coupled via a nearest-neighbor ferromagnetic interaction and subject to an external magnetic field, tending to align them in the X direction. The X-Y Hamiltonian is

$$H = -J\sum_P \cos(\varphi_{P_1} - \varphi_{P_2}) - B\sum_i \cos\varphi_i\ , \qquad (1)$$

where J and B are positive, the summation over P is over nearest-neighbor pairs, P_1 and P_2 are the members of the pair P, and φ_i is the angle variable attached to the site i.

It may be easily verified that the partition function of a system described by a Hamiltonian of the form

$$H = -J\sum_P F(\varphi_{P_1}, \varphi_{P_2}) - B\sum_i G(\varphi_i) \qquad (2)$$

may be written as

$$Z = \sum_{\text{all } n_i=0}^{\infty}\ \sum_{\text{all } n_P=0}^{\infty} \int_0^{2\pi}\cdots\int_0^{2\pi}\prod_{K=1}^{N} d\varphi_K \prod_P \frac{(\beta J)^{n_P}}{n_P!}$$
$$\times [F(\varphi_{P_1}, \varphi_{P2})]^{n_P}\prod_i \frac{(\beta J)^{n_i}}{n_i!}[G(\varphi_i)]^{n_i}\,. \qquad (3)$$

In the case of the X-Y Hamiltonian it will prove useful to give the integral a graphical representation. This may be done by denoting the term $e^{-i(\varphi_{P_1}-\varphi_{P_2})}$ appearing in the integrand by an arrow from the lattice point P_1 to the lattice point P_2, a term $e^{i\varphi_i}$ will be denoted by a $\oplus$ at the site i and $e^{-i\varphi_i}$ will be denoted by a $\ominus$. The $\oplus$ and $\ominus$ will be called positive and negative charges, respectively. To each configuration of arrows and charges corresponds a term in the expansion of the integrand.

The terms that contribute to the integral correspond to configurations obeying the two following rules: (a) the number of arrows leaving a site minus the number of arrows entering it equals the net charge at the site. (The net charge is the number of positive charges minus the number of negative charges); and (b) the total charge on the lattice is zero. The partition function is

$$Z = (2\pi)^N \sum_C \prod_P \frac{1}{n_{P_1}(C)!\,n_{P_2}(C)!}\left(\frac{\beta J}{2}\right)^{n_P(C)}$$
$$\times \prod_i \frac{1}{n_{i+}(C)!\,n_{i-}(C)!}\left(\frac{\beta B}{2}\right)^{n_i(C)} \qquad (4)$$

(see Fig. 1). The summation is over all contributing configurations C of arrows and charges, $n_{P_1}(C)$ is the number of arrows connecting the pair P in a given direction, $n_{P_2}(C)$ the number of arrows connecting the same pair in the opposite direction and

$$n_P(C) = n_{P_1}(C) + n_{P_2}(C). \qquad (5)$$

The numbers of positive and negative charges at the site i are n_{i+} and n_{i-}, respectively, and

$$n_i = n_{i+} + n_{i-}. \qquad (6)$$

It is convenient to restrict the summation to a subset $\{C'\}$ of the configuration set $\{C\}$, defined as the subset for which either n_{P_1} or n_{P_2} and either n_{i+} or n_{i-} are all zero. This may be achieved by noting that each configuration in $\{C\}$ can be obtained from a configuration in $\{C'\}$ by adding pairs of arrows connecting the same pairs of sites in opposite directions and adding pairs of opposite charges to the sites. One obtains

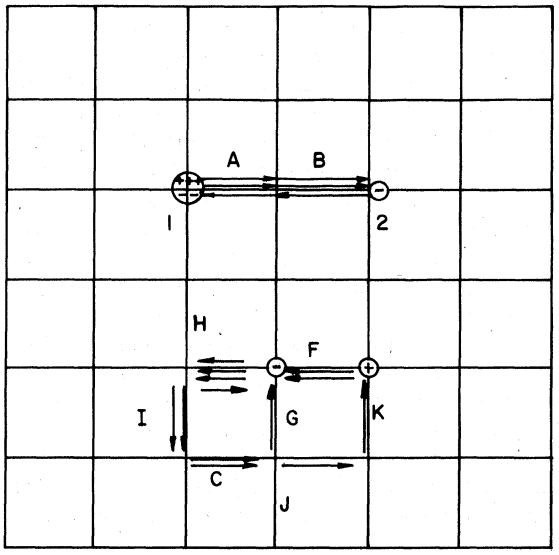

FIG. 1. A typical C configuration.

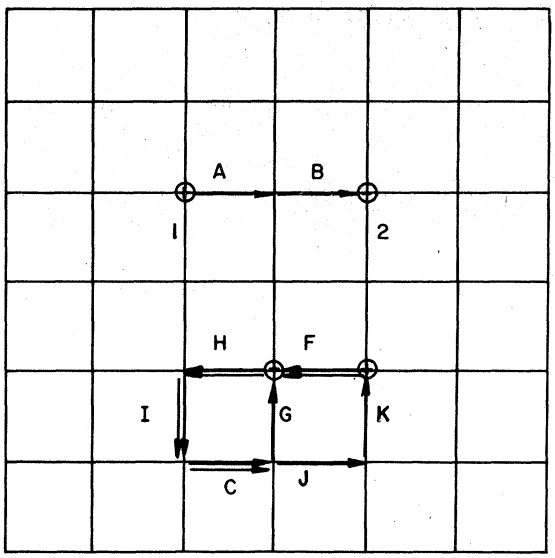

FIG. 2. A typical C' configuration.

$$Z=(2\pi)^N[\Phi(\beta J)]^{N'}[\Phi(\beta B)]^N\sum_{C'}\prod_l[Q(l,\beta J)]^{n_l(C')}\times\prod_n[Q(n,\beta B)]^{K_n(C')},$$

(see Fig. 2), where N' is the number of nearest-neighbor pairs, $n_l(C)$ is the number of pairs connected by l arrows (by definition of C' all the arrows connecting a given pair are in the same direction), $K_n(C)$ is the number of sites occupied by n charges. The functions are

$$\Phi(x)=\sum_{n\ \text{even}=0}^{\infty}\frac{1}{[(n/2)!]^2}\left(\frac{x}{2}\right)^n=J_0(ix), \tag{8}$$

and

$$Q(l,x)=\sum_{n=l,l+2}^{\infty}\frac{1}{[(n+l)/2]![(n-l)/2)]!}\frac{(x/2)^n}{\Phi(x)}=\frac{J_l(ix)}{J_0(ix)}, \tag{9}$$

where J_l denotes the Bessel function of order l. Note that

$$Q(l,x)\leq 1,\ \text{for all } l \text{ and } x\geq 0. \tag{10}$$

III. EQUIVALENCE TO A VECTOR-FIELD HAMILTONIAN THE REDUCED PARTITION FUNCTION

The reduced partition function

$$Z_R=\sum_{C'}\prod_l[Q(l,\beta J)]^{n_l(C')}\prod_n[Q(n,\beta B)]^{K_n(C')} \tag{11}$$

may be viewed as a partition function of the allowed configurations. The distribution of arrows may be thought of as a distribution of a ν-dimensional vector field, having integer components. The reduced-partition function may be expressed in terms of the integer field components E_i^m at the site i

$$Z_R=\sum_{\{E_i^m\}}\prod_i\prod_{k=1}^{\nu}Q(|E_i^k|,\beta J)Q\left(\left|\sum_{l=1}^{\nu}E_i^l-E_{i-\hat{L}}^l\right|,\beta B\right), \tag{12}$$

where E_i^x, for example, is the number of arrows starting at the site i and pointing along the edge in the x direction and where $\hat{L}$ is a unit vector in the l direction. We see that the charge density is in fact the discrete divergence of the field.

We may define now an equivalent field Hamiltonian be defining

$$\epsilon_J(l)=-\ln Q(l,\beta J), \tag{13}$$

and

$$\epsilon_B(l)=-\ln Q(l,\beta B). \tag{14}$$

It may be easily verified that

$$Z\,Z_R=\mathrm{Tr}e^{-H^*}, \tag{15}$$

where

$$H^*=\sum_i\sum_{k=1}^{\nu}\epsilon_J(|E_i^k|)+\sum_i\epsilon_B\left(\left|\sum_{k=1}^{\nu}E_i^k-E_{i-\hat{k}}^k\right|\right). \tag{16}$$

The requirement that the total charge is zero can be written as a condition on the E field, that is the discrete analog of $\int_s\vec{E}\cdot d\vec{s}=0$, where S denotes the boundary of the system. (17)

IV. THE CASE OF ZERO EXTERNAL FIELD

An interesting mapping of the $X-Y$ model is obtained, when the external magnetic field B is zero. The only configurations, that have to be considered are those for which the number of arrows entering a site equals the number of arrows leaving it. Let us consider first the two-dimensional case. In two dimensions the field E is completely determined by a field D defined on the lattice squares in such a way that the difference of the D on two adjacent squares is the number of arrows on the common edge. For the sign convention see Fig. 3. Clearly each distribution of the E field corresponds to many distributions of the D field. To have a one to one correspondence, we have to fix one of the degrees of freedom of D. The most convenient choice is

$$\sum_l D_l=0, \tag{18}$$

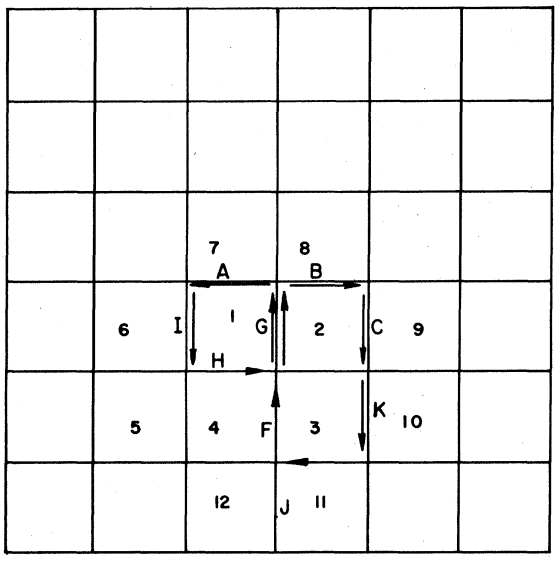

FIG. 3. The numbers denote squares while the capitals denote edges, E is positive on a vertical (horizontal) edge if it points to the right (up). The value of E on a horizontal (vertical) edge is the difference between D above the edge and D below the edge (D to the left of the edge minus D to its right).

where the summation is over all lattice squares. The equivalent Hamiltonian, H^* becomes, in terms of the D field,

$$H^* = \sum_{(l,m)} \epsilon_J(|D_l - D_m|), \tag{19}$$

where the summation is over nearest-neighbor pairs of squares. We see that H^* describes a system of Ising spins attaining all integer values and interacting via a two-body nearest-neighbor interaction. The spins must obey the subsidiary condition (18) that means that we have to consider only configurations of zero-total magnetization. It is interesting to obtain also the spin-spin correlation function in terms of the D field.

Let $g(i,j)$ be the spin-spin correlation function,

$$g(i,j) = \langle \vec{S}_i \cdot \vec{S}_j \rangle = \langle e^{i(\varphi_i - \varphi_j)} \rangle$$

$$= \frac{\int_0^{2\pi} \int \prod d\varphi_K \, e^{i(\varphi_i - \varphi_j)} e^{-\beta H}}{\int_0^{2\pi} \int \prod d\varphi_K \, e^{-\beta H}} . \tag{20}$$

The numerator in Eq. (20) may be expanded in a similar way to the expansion of the partition function. The graphs are the same except that the net number of arrows leaving the site i and entering j is one instead of zero (Fig. 4).

Since for most purposes we will be interested in the behavior of $g(i,j)$ at large separations, we may simplify matters by taking i and j to be colinear. It may be easily seen that the spin-spin correlation function may be written in terms of the D field as

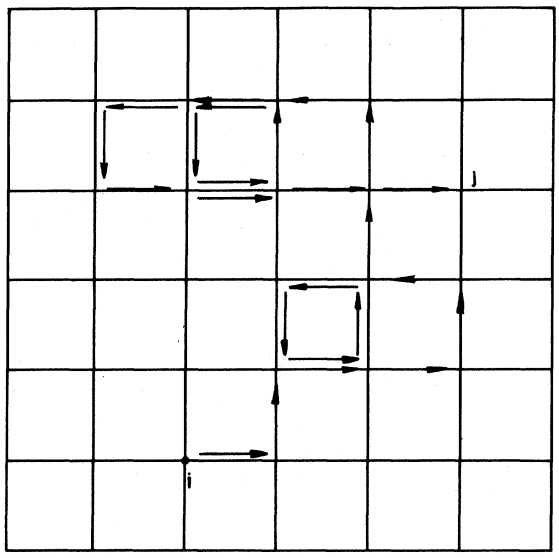

FIG. 4. A typical graph contributing to the numerator in Eq. (20).

$$g(i,j) = \left\langle \exp\left(\sum_R \epsilon_J(|D_R - D_L|) - \epsilon_J(|D_R - D_L - \mathrm{sgn}(D_R - D_L)|) \right) \right\rangle_{H^*}, \tag{21}$$

where the average is taken with respect to H^* [Eq. (16) $B=0$], and the summation is over near-

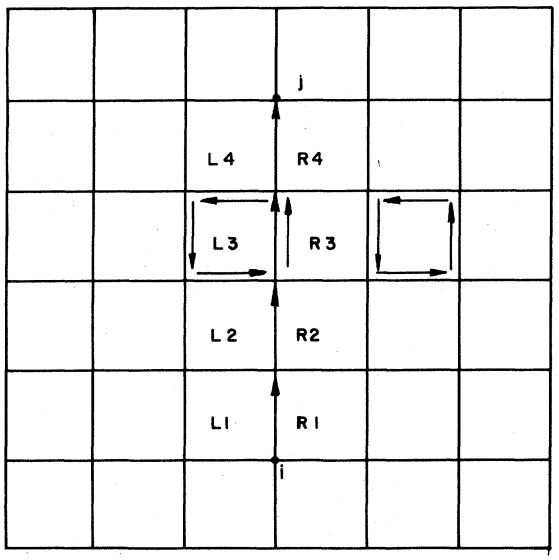

FIG. 5. The right and left squares adjacent to the line joining i and j.

est-neighbor pairs of squares (R, L), the member R of the pair is located to the right of the straight line connecting i and j and L is located to its left (Fig. 5).

As the reader may have already observed the transformation from the E field to the D field presented above for the two-dimensional case, is just the two-dimensional example of expressing a divergence free-vector field by its "vector" potential. (In the two-dimensional case the D field may be thought of as the Z component of a vector that is perpendicular to the lattice plain.)

V. UPPER BOUND ON THE TRANSITION TEMPERATURE

The high-temperature expansion obtained in Sec. II can be used to obtain an upper bound on the transition temperature in a similar way to that discussed in Ref. 17 when considering the Ising model.

The x-y Hamiltonian in the absence of an external magnetic field can be written in the form

$$H_{x-y} = -J \sum_{P} (S^x_{P_1} S^x_{P_2} + S^y_{P_1} S^y_{P_2}) , \tag{22}$$

where the spin components, S^x_i and S^y_i must obey

$$(S^x_i)^2 + (S^y_i)^2 = 1 . \tag{23}$$

We consider now a very similar system for which the spin components can attain any value between $-\infty$ and ∞, but for which the important configurations are those where $(S^x_i)^2 + (S^y_i)^2$ is in the vicinity of 1. Such a system is described by the Hamiltonian

$$H_\lambda = -J \sum_{P} (S^x_{P_1} S^x_{P_2} + S^y_{P_1} S^y_{P_2}) + \lambda \sum_i (S^2_i - 1)^2 , \tag{24}$$

where

$$S^2_i = (S^x_i)^2 + (S^y_i)^2 . \tag{25}$$

When λ is increased the range of important configurations narrows around the configurations obeying Eq. (23). It is clear that

$$\lim_{\lambda \to \infty} \langle F(\{S^x_i, S^y_i\}) \rangle_{H_\lambda} = \langle F(\{S^x_i, S^y_i\}) \rangle_{H_{x-y}} , \tag{26}$$

where F does not depend explicitly on λ and $\langle\ \rangle_H$ denotes thermal average with respect to H. (Remember the lattice is finite. For an infinite system we must take first λ to infinity and only then take the volume limit.) We may apply now the equipartition theorem to obtain

$$-J \sum_{n(i)} \langle S^x_{n(i)} S^x_j \rangle_{H_\lambda} + 4\lambda (\langle S^2_i S^x_i S^x_j \rangle_{H_\lambda} - \langle S^x_i S^x_j \rangle_{H_\lambda}) = 0 \tag{27}$$

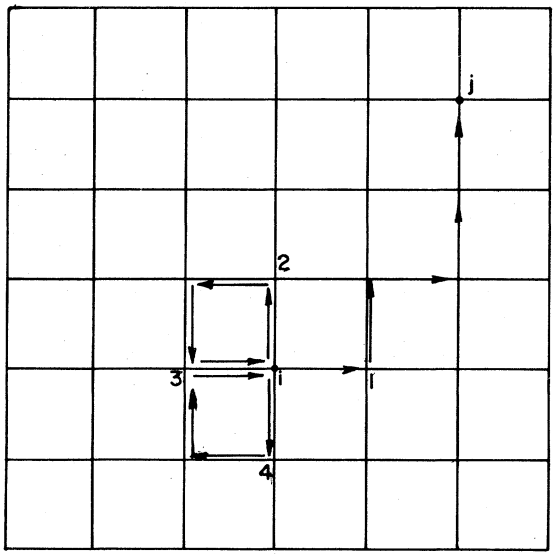

FIG. 6. In the given graph $l_1 = 1$, $l_2 = 1$, $l_3 = 2$, $l_4 = 1$.

for $i \neq j$, where the $n(i)$'s are the nearest neighbors of i. The $x-y$ results are obtained by taking λ to infinity. The procedure is similar to the corresponding procedure for the Ising model outlined in Ref. 17. The details are discussed in Appendix A. For each configuration contributing to the numerator in Eq. (18) one may define a quantity

$$M_{ij}(C') = \sum_{n(i)} \frac{\frac{\partial}{\partial(\beta J)} Q(l^{c'}_{ni}, \beta J)}{Q(l^{c'}_{ni}, \beta J)} , \tag{28}$$

where $l^{c'}_{n_i}$ is the number of arrows connecting the site i and the site $n(i)$ (Fig. 6).

We define now M_{ij} to be the average of $M_{ij}(C')$ over all configurations C' contributing to the numerator of Eq. (18).

Some algebra is required to obtain

$$-\sum_{n(i)} \langle \vec{S}_{n(i)} \cdot \vec{S}_j \rangle_{H_{X-Y}} + \left(\frac{1}{\beta J} + Z \frac{\Phi'(\beta J)}{\Phi(\beta J)} + M_{ij} \right) \langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 \tag{29}$$

for $i \neq j$, where Z is the coordination number of the lattice. Equation (29) can be put in a more convenient form

$$\sum_{n(i)} (\langle \vec{S}_{n(i)} \cdot \vec{S}_j \rangle - \langle \vec{S}_i \cdot \vec{S}_j \rangle) - \left[\frac{1}{\beta J} + Z \left(\frac{\Phi'(\beta J)}{\Phi(\beta J)} - 1 \right) + M_{ij} \right] \langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 . \tag{30}$$

At large distances the functions depend on the distance only and Eq. (30) becomes

$$\nabla^2 g(r) - F(r) g(r) = 0 , \tag{31}$$

where $g(r)$ is the spin-spin correlation function at large separations and

$$F(r) = \frac{1}{\beta J} + Z\left(\frac{\Phi'(\beta J)}{\Phi(\beta J)} - 1\right) + M(r) . \tag{32}$$

As long as

$$\lim_{r\to\infty} F(r) \equiv F(\infty) > 0 , \tag{33}$$

the behavior of $g(r)$ at large distances is determined by the equation

$$\nabla^2 g(r) - F(\infty) g(r) = 0 \tag{34}$$

that has a solution of the form

$$g(r) = g_0 \frac{e^{-r/\xi}}{r^{(\nu-1)/2}} , \quad \text{for large } r , \tag{35}$$

where

$$\xi = 1/[F(\infty)]^{1/2} . \tag{36}$$

The correlation length diverges when

$$F(\infty) = 0 . \tag{37}$$

The critical temperature T_c is the highest temperature for which Eq. (37) holds. The fact that below T_c, $F(\infty) = 0$ enables an exact evaluation of $M(\infty)$ below T_c:

$$M(\infty) = Z\left(1 - \frac{\Phi'(\beta J)}{\Phi(\beta J)}\right) - \frac{1}{\beta J} , \quad \text{for } T < T_c . \tag{38}$$

In Appendix B, it is shown that

$$\frac{\frac{\partial}{\partial x} Q(1,x)}{Q(1,x)} \leq \frac{\frac{\partial}{\partial x} Q(l,x)}{Q(l,x)} , \quad \text{for } x \geq 0 \text{ and } l \geq 1 . \tag{39}$$

If follows that

$$M(r) \geq \frac{\frac{\partial}{\partial(\beta J)} Q(1,\beta J)}{Q(1,\beta J)} , \tag{40}$$

for all r and any lattice. So

$$F(\infty) \geq \left[\frac{1}{\beta J} + Z\left(\frac{\Phi'(\beta J)}{\Phi(\beta J)} - 1\right) + \frac{\frac{\partial}{\partial(\beta J)} Q(1,\beta J)}{Q(1,\beta J)}\right] . \tag{41}$$

The critical temperature for a given lattice is bounded by

$$\frac{kT_c}{J} < \frac{1}{X^*} , \tag{42}$$

where X^* is the solution of the equation

TABLE I. Upper bounds on transition temperatures.

Lattice	Dimension	η_I	$\eta_{X-Y}^{\text{calc.}}$ (Ref.)	Upper bound on η_{X-Y} (Ref.)
hc	2	0.253		0.277
sq	2	0.284	0.675, 0.425 (13) (18)	0.353
pt	2	0.303		0.407
diamond	3	0.338		0.353
sc	3	0.376		0.407
bcc	3	0.397		0.432
fcc	3	0.408	0.402 (19)	0.456 (20)

$$\frac{1}{X} + Z\left(\frac{\Phi'(X)}{\Phi(X)} - 1\right) + \frac{\frac{d}{dX} Q(1,X)}{Q(1,X)} = 0 . \tag{43}$$

The bound we obtain depends, thus, only on the coordination number of the lattice.

The bounds for the normalized dimensionless transition temperature,

$$\eta_{X-Y} = \frac{kT_{X-Y}}{ZJ} \tag{44}$$

are presented in Table I versus

$$\eta_I = \frac{kT_I}{2ZJ} , \tag{45}$$

where T_I is the Ising transition temperature.

It is interesting to note that the transition temperatures calculated by Thouless and Kosterlitz and by Villain

$$kT_c^{TK}/J = 2.2 \text{ and } kT_c^{V}/J = 1.7 \tag{46}$$

are much higher than the upper bound found in Table I.

VI. EQUIVALENCE OF THE X-Y MODEL TO A PLASMA MODEL

In the attempt of obtaining a better understanding of the X-Y model, various authors related it to a plasma. Zittartz argued that at low temperature the excess free energy due to the introduction of the external field behaves like the free energy of a plasma. Thouless and Kosterlitz argued that in the two-dimensional case, the spin configurations, in the absence of an external magnetic field, may be described in terms of vortices, that in turn can be viewed as charges interacting via a Coulomb potential. In the following we will show how these

two descriptions follow in a most natural way from the vector field Hamiltonian, obtained in Sec. III.[21]

For $\beta J \gg 1$,

$$\epsilon_J(l) = l^2/2\beta J \ , \tag{47}$$

so that H^* can be written as

$$H^* = \sum_{i=1}^{\nu} \frac{(E_i^{\nu})^2}{2\beta J} + \sum_j \mu_j N_j \ , \tag{48}$$

where N_j is the number of sites possessing total charge j and μ_j is the corresponding "chemical potential" given by

$$\mu_j = \epsilon_\beta(|j|) . \tag{49}$$

Writing

$$\mu_j \equiv \mu_1 + \delta_j \ , \tag{50}$$

it is clear that μ_1 can be treated as a total chemical potential, while $\delta_j N_j$ can be treated as a short-range many-body interaction

$$H = \sum_i \frac{\vec{E}_i^2}{2\beta J} + \sum_j \delta_j N_j + 2\mu_1 N \ , \tag{51}$$

where N is the total positive charge. The field $\vec{E}_i$ can be written as sum of a longitudinal field and a transverse field.

$$\vec{E} = \vec{E}_L + \vec{E}_T . \tag{52}$$

Summing by parts one finds

$$H^* = \sum_i \frac{\vec{E}_{iT}^2}{2\beta J} + \frac{1}{2\beta J} \sum_{i,j} Q_i V^{\nu}(r_i - r_j) Q_j \ , \tag{53}$$

where Q_i is the charge at the site i and $V^{\nu}(r_i - r_j)$ behaves at large distances as the ν-dimensional Coulomb potential. The interaction between two charges separated by a large distance is electrostatic, so we may conclude that for $\beta J \gg 1$, H^* describes a plasma that is decoupled from the transverse degrees of freedom.

VII. TRANSVERSE MODES

It is interesting that the transverse degrees of freedom, may be also viewed as a system of charges interacting via the two-body Coulomb potential.

Consider the transverse Hamiltonian

$$H_T = \sum_i \frac{\vec{E}_{iT}^2}{2\beta J} . \tag{54}$$

In terms of the Fourier transform

$$[\vec{E}(\vec{q})]_T = \frac{1}{\sqrt{N}} \sum_i \vec{E}_{iT} e^{i\vec{q}\cdot\vec{R}_i} , \tag{55}$$

the Hamiltonian is

$$H_T^* = \frac{1}{2\beta J} \sum_{q\neq 0} [\vec{E}(\vec{q})]_T \cdot [\vec{E}(-\vec{q})]_T . \tag{56}$$

We do not include the $\vec{q} = 0$ term because

$$[\vec{E}(0)]_T = 0 . \tag{57}$$

We rewrite

$$H_T^* = \frac{1}{2\beta J} \sum_{q\neq 0} q^2 \frac{[\vec{E}(\vec{q})]_T \cdot [\vec{E}(-\vec{q})]_T}{q^2} . \tag{58}$$

Noting the identity

$$\sum_i q_i^2 \sum_j [E^j(\vec{q})]_T [E^j(-q)]_T = \sum_i q_i E^i(\vec{q}) \sum_j q_j E^j(-\vec{q}) + \frac{1}{2} \sum_{i,j} \{q_i [E^j(\vec{q})]_T - q_j [E^i(\vec{q})]_T\} \times \{q_i [E^j(-\vec{q})]_T - q_j [E^i(-\vec{q})]_T\} , \tag{59}$$

and using the fact that for small q

$$\sum_i q_i [E^i(\vec{q})]_T = 0 . \tag{60}$$

We obtain a Hamiltonian whose long-distance (small-q) behavior is identical to the behavior of H_T^*:

$$\bar{H}_T = \frac{1}{2\beta J} \sum_{q\neq 0} \sum_{i,j} \frac{\{q_i [E^j(\vec{q})]_T - q_j [E^i(\vec{q})]_T\}\{q_i [E^j(-\vec{q})]_T - q_j [E^i(-\vec{q})]_T\}}{q^2} . \tag{61}$$

Denoting

$$A_{ij}(\vec{q}) = i\{q_i [E^j(\vec{q})]_T - q_j [E^i(\vec{q})]_T\} \tag{62}$$

(in fact the subscript T can be omitted because the same expression vanishes for the longitudinal field), we may express the Hamiltonian as

$$\bar{H}_T = \frac{1}{2\beta J} \sum_{q\neq 0} \mathrm{Tr} \frac{A(\vec{q}) A^*(-\vec{q})}{q^2} . \tag{63}$$

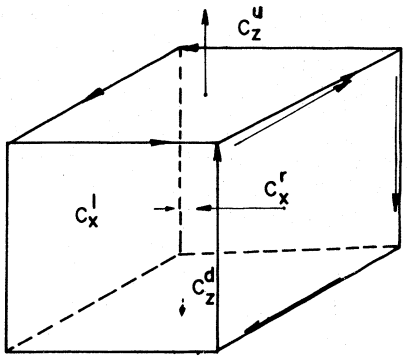

FIG. 7. The x component C_x defined at the center of the cube is the arithmetic average of C_x^l and C_x^r defined on the left and right faces of the cube. C_x^r is obtained by taking the path summation of $\vec{E}$ along the edges of the right face.

Fourier transforming we obtain

$$\overline{H}_T = \frac{1}{2\beta J} \sum_{i,j} \mathrm{Tr} A_i A_j V^{\nu}(r_i - r_j), \tag{64}$$

where A_i is the matrix Fourier transform of the matrix $A(\vec{q})$. In two and three dimensions we may write

$$\overline{H}_T = \frac{1}{2\beta J} \sum_{i,j} V^{\nu}(r_i - r_j) \vec{C}_i \cdot \vec{C}_j, \tag{65}$$

where $\vec{C}_i$ is the discrete analog of curl $\vec{E}$ (Fig. 7). (In two dimension the curl is perpendicular to the lattice plain.)

The components of the vectors $\vec{C}$ are integers or half integers since the components of $\vec{E}$ are integers. In the two dimensional case we may write

$$\overline{H}_T^{(2)} = \frac{1}{2\beta J} \sum_{i,j} V^2(r_i - r_j) Q_i Q_j, \tag{66}$$

where Q_i is the charge located at the site i and this charge must be a multiple of an elementary charge.

In the three-dimensional case we may write

$$H_T^{(3)} = \frac{1}{2\beta J} \sum V^3(r_i - r_j) \times (Q_i^{(1)} Q_j^{(1)} + Q_i^{(2)} Q_j^{(2)} + Q_i^{(3)} Q_j^{(3)}), \tag{67}$$

where instead of the single charge appearing in the two-dimensional case, we have three different charges that seem to be independent and mutually noninteracting. We have to remember, however, that the $Q_i^{(j)}$'s, being the three components of the discrete curl, are not independent. In fact they are subject to a condition

$$\mathrm{div}' \ \mathrm{curl}' \vec{E} = 0, \tag{68}$$

where div′ and curl′ denote the discrete analogues of the div and the curl, respectively.

In terms of the charges Eq. (68) can be written as (Fig. 7)

$$Q_i = Q_i^{(1)} + Q_i^{(2)} + Q_i^{(3)} = 0 \tag{69}$$

at the center of each lattice cube i.

Using the last relation we see that $H_T^{(3)}$ can be expressed in terms of two independent charges:

$$H_T^{(3)} = \frac{1}{2\beta J} \sum_{i,j} V^3(r_i - r_j)(2 Q_i^{(1)} Q_j^{(1)} + 2 Q_i^{(2)} Q_j^{(2)} + Q_i^{(1)} Q_j^{(2)} + Q_i^{(2)} Q_j^{(1)}). \tag{70}$$

We can decouple the charges obtaining two mutually noninteracting charges by introducing the two charges

$$Q_i^{(+)} = Q_i^{(1)} + Q_i^{(2)} \tag{71}$$

and

$$Q_i^{(-)} = Q_i^{(1)} - Q_i^{(2)},$$

we obtain

$$H_T^{(3)} = \frac{1}{2\beta J} \sum_{i,j} V^3(r_i - r_j) (\tfrac{3}{2} Q_i^{(+)} Q_j^{(+)} + \tfrac{1}{2} Q_i^{(-)} Q_j^{(-)}). \tag{72}$$

The same pattern will be obtained in any higher number of dimensions.

VIII. RELATED MODELS

The $X-Y$ model is a special case of a set of models defined by the Hamiltonian

$$H = -J \sum_P F(\varphi_{p_1} - \varphi_{p_2}) - B \sum_i G(\varphi_i), \tag{73}$$

where F and G are periodic with period of 2π. Consideration of such models might prove important, for example, in the construction of coordinate space renormalization procedures for models possessing 0(2) symmetry.

We write the partition function as

$$Z = \int_0^{2\pi} \int \prod_K d\varphi_K \sum_{m_p} \psi_{m_p}(\beta J) e^{i m_p (\varphi_{p_1} - \varphi_{p_2})} \times \prod_i \sum_{n_i} \chi_{n_i}(\beta B) e^{i n_i \varphi_i}, \tag{74}$$

where

$$\psi_m(\beta J) = \frac{1}{2\pi} \int_0^{2\pi} e^{\beta J F(\varphi)} e^{-i m \varphi} d\varphi, \tag{75}$$

and

$$\chi_n(\beta B) = \frac{1}{2\pi} \int_0^{2\pi} e^{\beta J G(\varphi)} e^{-i n \varphi} d\varphi. \tag{76}$$

A graphical representation of the partition function

may be obtained by representing the term $e^{-i|m|(\varphi_{\vec{p}_1}-\varphi_{\vec{p}_2})}$ appearing in the integrand by $|m|$ arrows from the lattice point $\vec{p}_1$ to the lattice point $\vec{p}_2$ and representing the term $e^{i|n|\varphi_i}$ by $|n|$ positive charges at the site i. Integration over the φ's leads to

$$Z=(2\pi)^N[\psi(\beta J)]^{N'}[\chi(\beta B)]^N\sum_{c'}\prod_l[R(l,\beta J)]^{n_l(c')}\times\prod_n[S(n,\beta B)]^{K_n(c')}, \tag{77}$$

where

$$R(l,x)=\frac{\psi_1(x)}{\psi_0(x)}, \tag{78}$$

and

$$S(n,x)=\frac{\chi_n(x)}{\chi_0(x)}, \tag{79}$$

and all the other notations are those appearing in Eq. (7).

We conclude, that the high-temperature expansion corresponding to the general model (73) differs from the high-temperature expansion of the X-Y partition function only in the weights attached to the different elements of the configurations.

IX. DISCUSSION

Evaluation of the high-temperature expansion of the X-Y partition function was shown to be equivalent to the evaluation of the partition function corresponding to a system of quantized field and quantized charges on the lattice. The field arises from the interaction terms in the X-Y model while the charges arise from the external magnetic field. The low-temperature properties of the system are studied by considering separately the longitudinal and transverse modes of the field. It is shown that the longitudinal modes of the field give rise to an interaction between charges that is electrostatic at large distances. It is also shown that the transverse degrees of freedom, when expressed in terms of the curl of the field, may also be described as systems of electrostatically interacting charges. In the two-dimensional case, the transverse degrees of freedom, are equivalent at low temperature and small q's to a system of charges interacting pairwise via the two-dimensional electrostatic interaction. In three dimensions we have a system composed of two mutually noninteracting subsystems, or we may say that the transverse degrees of freedom correspond to a system made of two kinds of charges, that do not interact with one another. These results support the results obtained by Thouless and Kosterlitz that for the two-dimensional case showed the system to be equivalent to a system of interacting charges in the absence of an external magnetic field. These charges correspond to the transverse degrees of freedom in our description. They also support the results of Zittartz that showed equivalence of the two dimensional X-Y model to a system of interacting charges, that arise from the magnetic field. These charges arise from the magnetic field and the electrostatic interaction between any two of them is mediated through the longitudinal degrees of freedom of the field.

Another application of the high-temperature expansion is an upper bound on the transition temperature. This bound is much lower than the calculated transition temperatures obtained by Thouless and Kosterlitz,[13] by Kosterlitz,[22] and by Villain[18] for the square lattice.

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APPENDIX A: PROOF OF EQ. (29)

Proof of Eq. (29)

$$\langle S_i^2S_i^xS_j^x\rangle_{H_\lambda}-\langle S_i^xS_j^x\rangle=N_{ij}^x(\lambda)/D(\lambda), \tag{A1}$$

where

$$N_{ij}^x(\lambda)=\int_{-\infty}^{\infty}\int\prod_k dS_k^x\,dS_k^y\,e^{-\beta\lambda(S_k^2-1)^2}\exp(\beta J\sum_{(l,m)}S_l^xS_m^x+S_l^yS_m^y)\,S_i^xS_j^x(S_i^2-1)\Big/\int_{-\infty}^{\infty}\int\prod_k dS_k^x\,dS_k^y\,e^{-\beta\lambda(S_k^2-1)^2}, \tag{A2}$$

and

$$D(\lambda)=\int_{-\infty}^{\infty}\int\cdots\prod_k dS_k^x\,S_k^y\,e^{-\beta\lambda(S_k^2-1)^2}\exp(\beta J\sum_{(m,l)}S_l^xS_m^x+S_l^yS_m^y)\Big/\int_{-\infty}^{\infty}\cdots\int\prod_k dS_k^x\,dS_k^y\,e^{-\beta\lambda(S_k^2-1)^2}. \tag{A3}$$

We transform to polar coordinates

$$S_i^x = S_i \cos\varphi_i \tag{A4}$$

and

$$S_i^y = S_i \sin\varphi_i , \tag{A5}$$

and perform the configurational integration by integrating over the φ's and then integrating over the S's that are positive. Since

$$\lim_{\lambda\to\infty} N_{ij}^x(\lambda) = 0 , \tag{A6}$$

only the correction to order $1/\lambda$ of $N_{ij}^x(\lambda)$ is to be considered when calculating N_{ij}/D to order $1/\lambda$:

$$N_{ij}^x(\lambda) = \int_0^\infty \cdots \int \prod_k dS_k S_k e^{-\beta\lambda(S_k^2-1)^2} (S_i^3 S_j - S_i S_j) \int_0^{2\pi} \cdots \int \prod_k d\varphi_k \times \cos\varphi_i \cos\varphi_j \exp\Big[\beta J \sum_{l,m} S_l S_m \cos(\varphi_l - \varphi_m)\Big] \Big/ \int_0^\infty \int \prod_k dS_k S_k e^{-\beta\lambda(S_k^2-1)^2} . \tag{A7}$$

We employ now the identity proven in Ref. 17:

$$\frac{\int\cdots\int \prod dS_k e^{-\beta\lambda f(S_k)} \Phi(\{S\})}{\int\cdots\int \prod dS_k e^{-\beta\lambda f(S_k)}} = \Phi(\{1\}) + \frac{1}{2\beta\lambda}\left(\frac{1}{f^{(2)}(1)} \sum_l \frac{\partial^2\Phi}{\partial S_l^2}(\{1\}) - \frac{f^{(3)}(1)}{[f^{(2)}(1)]^2} \sum_l \frac{\partial\Phi}{\partial S_l}(\{1\}) + \cdots\right), \tag{A8}$$

where $\cdots$ denote higher order in $1/\lambda$, $f(x)$ has its only minimum at $x=1$, $f^{(2)}$ and $f^{(3)}$ are second and third derivatives, respectively, neither f nor Φ de pend on λ, and $\phi(\{1\})$ denotes that all the arguments of ϕ are taken as 1.

In our case

$$N_{ij}^x(\lambda) = \frac{\int_0^\infty \int \prod_k dS e^{-\beta\lambda f(S_k)} \Phi_1(\{S\}) \int_0^\infty \int \prod_k dS_k e^{-\beta\lambda f(S_k)}}{\int_0^\infty \int \prod_k dS_k e^{-\beta\lambda f(S_k)} \int_0^\infty \int \prod_k dS_k \exp[-\beta\lambda f(S_k)\Phi_2(\{S\})]} , \tag{A9}$$

where

$$\Phi_1(\{S\}) = (S_i^3 S_j - S_i S_j) \prod_k S_k \int_0^{2\pi} \cdots \int \prod_k d\varphi_k \cos\varphi_1 \cos\varphi_j \exp\left(\beta J \sum_{l,m} S_l S_m \cos(\varphi_l - \varphi_m)\right) \tag{A10}$$

and

$$\Phi_2(\{S\}) = \prod_k S_k . \tag{A11}$$

So

$$N_{ij}^x(\lambda) = \frac{D_{X-Y}}{4\beta\lambda}\left(\langle\cos\varphi_i \cos\varphi_j\rangle_{H_{X-Y}} + \frac{\partial}{\partial S_i}\int_0^{2\pi} \cdots \int \prod_k d\varphi_k \cos\varphi_i \cos\varphi_j \, e^{-\beta H_{X-Y} - \beta(S_i-1)H_i}\Big|_{S_i=1}\right), \tag{A12}$$

where

$$H_i = -J\sum_{n_i} \cos(\varphi_i - \varphi_{n_i}) , \tag{A13}$$

$$N_{ij}(\lambda) = N_{ij}^x(\lambda) + N_{ij}^y(\lambda) = \frac{D_{X-Y}}{4\beta\lambda}\left(\langle\cos(\varphi_i - \varphi_j)\rangle_{H_{X-Y}} + \frac{\partial}{\partial S_i}\int_0^{2\pi} \int \prod_k d\varphi_k \cos(\varphi_i - \varphi_j) \, e^{-\beta H_{X-Y} - \beta(S_i-1)H_i}\Big|_{S_i=1}\right).$$

This equation leads directly to Eq. (29). (A14)

APPENDIX B: PROOF OF EQ. (39)

$$\frac{[Q(1,x)]'}{Q(1,x)} - \frac{[Q(l,x)]'}{Q(l,x)} = \frac{P_1'(x)}{P_1(x)} - \frac{P_l'(x)}{P_l(x)} , \tag{B1}$$

where

$$P_l(x) = J_l(ix). \tag{B2}$$

We prove now that

$$P_l'(x)P_m(x) - P_m'(x)P_l(x) \le 0, \tag{B3}$$

for $x>0$ and $l<m$ $(l, m\neq 0)$. Consider the differential equations obeyed by P_l and P_m:

$$\frac{d^2}{dx^2}P_l(x)+\frac{1}{x}\frac{d}{dx}P_l(x)-\left(\frac{l^2}{x^2}+1\right)P_l(x)=0\,, \quad \text{(B4)}$$

$$\frac{d^2}{dx^2}P_m(x)+\frac{1}{x}\frac{d}{dx}P_m(x)-\left(\frac{m^2}{x^2}+1\right)P_m(x)=0\,. \quad \text{(B5)}$$

By multiplying (B4) by $P_m(x)$ and (B5) by $-P_l(x)$ and summing the resulting equations one obtains

$$P_m(x)\frac{d^2}{dx^2}P_l(x)-P_l(x)\frac{d^2}{dx^2}P_m(x)+\frac{1}{x}\left(P_m(x)\frac{d}{dx}P_l(x)-P_l(x)\frac{d}{dx}P_m(x)\right)=\frac{1}{x^2}(l^2-m^2)P_l(x)P_m(x)\,. \quad \text{(B6)}$$

Defining

$$F_{lm}(x)=P_m(x)\frac{d}{dx}P_l(x)-P_l(x)\frac{d}{dx}P_m(x)\,, \quad \text{(B7)}$$

and

$$G_{lm}(x)=(1/x^2)(l^2-m^2)P_l(x)P_m(x), \quad \text{(B8)}$$

Eq. (B6) can be rewritten as

$$\frac{d}{dx}F_{lm}(x)+\frac{1}{x}F_{lm}(x)=G_{lm}(x)\,. \quad \text{(B9)}$$

Solving for $F_{lm}(x)$ in terms of $G_{lm}(x)$ one obtains

$$F_{lm}(x)=\frac{1}{x}\int_0^x x'G_{lm}(x')dx'\,, \quad \text{(B10)}$$

by using the initial condition

$$F_{lm}(0)=0, \quad \text{for } l, m\neq 0. \quad \text{(B11)}$$

For $x>0$ and $l>m$

$$G_{lm}(x)<0. \quad \text{(B12)}$$

so Eq. (B10) implies (B3).

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