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Kosterlitz-Thouless Transition in the Two-Dimensional Plane Rotator and Coulomb Gas

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(Received 4 August 1980)

We describe a rigorous argument establishing the Berezinski-Kosterlitz-Thouless transition in a class of two-dimensional models including the plane rotator and the Coulomb gas. The main idea is to rewrite correlations in the Coulomb gas as superpositions of correlations in gases of *neutral molecules* of variable size and small effective activity.

PACS numbers: 64.60.Cn

In recent years a number of authors have given fairly convincing arguments for the existence of a phase transition and a line of critical points in a class of two-dimensional (2D) models, including the rotator model, the related Villain model, and the lattice Coulomb gas. (See Refs. 1 and 2 and references given therein.) All models are known to have a high- T (T =temperature) phase with exponentially decaying correlations. The presumed transition is one from the high- T to a low- T phase characterized by a power-law falloff of correlations and scaling, so that all temperatures T below some positive T_c are critical points. Since the rotator model, and the Villain model, have a continuous, global $U(1)$ symmetry, this transition is not accompanied by symmetry breaking, and there is no spontaneous magnetization—a well-known consequence of Mermin's theorem.³

Perhaps the best arguments for the existence of the transition described above are based on analyzing the low- T behavior of the 2D Coulomb gas. Consider a positive and a negative charge separated by some distance l . They can be viewed as forming a neutral dipole whose Boltz-

mann factor is $\propto \exp[-(\beta/2\pi)\ln(l+1)]$, where β is the inverse temperature. Moreover, when the gas is very dilute, dipoles are the dominant configurations, and the exponential of the mean entropy of a dipole of length l is $\propto l^3$. Thus, the probability for such a dipole to be present is $\propto l^3 \exp[-(\beta/2\pi)\ln(l+1)]$ which is summable in l when $\beta > 8\pi$. Therefore, the 2D Coulomb gas at large β is expected to behave like a dipole gas. It is known that correlations in a dipole gas have a power-law falloff.^{4,5} In this paper we sketch a proof of existence of the transition described above—henceforth called the Kosterlitz-Thouless (KT) transition—for the simplest model, namely a dilute 2D Coulomb gas, which is inspired by the above heuristic argument. Details of our proof, as well as extensions to other 2D models and higher-dimensional, Abelian lattice gauge theories, will appear elsewhere.⁶

We now describe some of our main results concerning 2D models: For sufficiently low temperatures, (i) the spin-spin correlation in the plane rotator and the Villain model has a power-law falloff and (ii) the Coulomb gas does not screen;

and at high temperatures, (iii) the expectation of $[\varphi(0) - \varphi(x)]^2$ in the discrete Gaussian model, dual to the Villain model, diverges like $\ln|x|$, as $|x| \rightarrow \infty$ ("roughening transition").

Our methods extend to other 2D models, such as the solid-on-solid model and the z_n models, for n large enough (existence of an intermediate, massless phase). We can also prove transitions for the 1D Ising model with ferromagnetic, $1/r^2$ interactions and the 3D or 4D Abelian lattice gauge theories.

Next, we outline our proof of existence of a low-temperature, dipole phase without screening in the 2D Coulomb gas, in contrast to the high-temperature plasma phase which is known to exhibit Debye screening.⁷ The Coulomb potential on the simple square lattice Z^2 is given by $V(i-j) = (-\Delta)^{-1}(i,j) \approx -(1/2\pi) \ln|i-j|$, for large $|i-j|$, where Δ is the finite-difference Laplacian. Each site $j \in Z^2$ is assigned a charge variable, $q(j)$, with values $0, \pm 1$. The function $\vec{q} = \{q(j)\}$ describes a configuration of charges in the Coulomb gas. Its electrostatic energy (self-energies included) is given by

$$E(\vec{q}) = \frac{1}{2} \sum_{i,j} q(i)q(j)V(i-j) \equiv -\frac{1}{2} \langle q, \Delta^{-1}q \rangle. \quad (1)$$

The total charge, $\sum q(j)$, is required to vanish. The grand partition function of the Coulomb gas is given by

$$Z_{\text{Coul}}(\beta, z) = \sum_{\{q(j)=0, \pm 1\}} \prod_i \left(\frac{1}{2}z\right)^{|q(i)|} e^{-\beta E(\vec{q})}, \quad (2)$$

where β is the inverse temperature and z the bare activity of a particle with charge ± 1 .

The first step in our proof reexpresses the Coulomb gas in the well-known sine-Gordon representation⁸: Consider the zero-mass Gaussian measure

$$d\mu_\beta(\varphi) \equiv N^{-1} \exp\{\langle \varphi, \Delta\varphi \rangle / 2\beta\} \prod_j d\varphi(j), \quad (3)$$

where $-\langle \varphi, \Delta\varphi \rangle = \sum [\varphi(i) - \varphi(j)]^2$ with i and j nearest neighbors and N is a normalization factor chosen so that $\int d\mu_\beta(\varphi) = 1$. Since the covariance of $d\mu_\beta(\varphi)$ is proportional to the Coulomb potential, namely βV ,

$$\exp\{-\beta E(\vec{q})\} = \int \prod_j \exp[i\varphi(j)q(j)] d\mu_\beta(\varphi),$$

provided that $\sum q(j) = 0$. Inserting this identity in (2), one obtains

$$Z_{\text{Coul}}(\beta, z) = \int \prod_j [1 + z \cos \varphi(j)] d\mu_\beta(\varphi). \quad (4)$$

Next, let \mathfrak{X} denote some collection of nonoverlapping charge distributions $\{\rho_\alpha\}$, $\alpha = 1, 2, \dots$. Each ρ_α describes a neutral molecule of finitely many charged particles with charge $\rho_\alpha(j) = 0, \pm 1$, at site j . We then prove the identity

$$z_{\text{Coul}}(\beta, z) = \sum_k c_k Z_k(\beta), \quad (5)$$

where Z_k denotes the partition function for a gas of molecules $\rho_\alpha \in \mathfrak{X}_k$

$$Z_k(\beta) = \int \prod_{\rho_\alpha \in \mathfrak{X}_k} [1 + K(\rho_\alpha) \cos \varphi(\rho_\alpha)] d\mu_\beta(\varphi) \quad (6)$$

and $\varphi(\rho_\alpha) = \sum_j \varphi(j) \rho_\alpha(j)$. The coefficients c_k are positive with $\sum c_k = 1$. The index k labels the various collections of molecules \mathfrak{X}_k that are formed from free charges. In (6), $K(\rho)$ is the bare activity of the molecule ρ which depends only on z , the bare activity of a single particle in the Coulomb gas, and on the shape of ρ .

The important point in this identity is that in two dimensions all particles can be grouped together in finite, neutral molecules, hence $\sum_j \rho_\alpha(j) = 0$, for all α . This fact implies that all expectations $\langle \dots \rangle_k$ corresponding to the measures

$$Z_k^{-1} \prod_{\rho_\alpha \in \mathfrak{X}_k} [1 + K(\rho_\alpha) \cos \varphi(\rho_\alpha)] d\mu_\beta(\varphi)$$

are formally invariant under the continuous symmetry $\varphi(j) \rightarrow \varphi(j) + c$, for all j , where c is an arbitrary constant. One therefore expects that by a Mermin-type argument

$$\langle |\hat{\varphi}(p)|^2 \rangle_k \geq \text{const } p^{-2} \quad (7)$$

for all k . If the constant on the right-hand side of (7) is independent of k , we obtain

$$\langle |\hat{\varphi}(p)|^2 \rangle_{\text{Coul}} \geq \text{const } p^{-2}. \quad (8)$$

At sufficiently low temperature and $z \ll \exp(\beta\epsilon)$ we shall establish (8). It is well known that $\langle [\varphi(0) - \varphi(x)]^2 \rangle$ is the effective electrostatic potential between two opposite charges in the Coulomb gas. By Fourier transformation we see that (8) implies the effective potential diverges logarithmically, hence there is no screening.

Our proof of (7) is based on a Mermin argument³ which is applicable only if the activities $K(\rho_\alpha)$ are sufficiently small so that $\langle \dots \rangle_k$ is a positive measure. In general, however, the $K(\rho_\alpha)$ are quite large. We resolve this problem by means of a "block spin" integration: We prove the

identity

$$Z_{\text{Coul}}(\beta, z) = \sum_k c_k Z_k(\beta, z) = \sum_k c_k \int \prod_{\{\alpha | \rho_\alpha \in \mathfrak{X}_k\}} \{1 + [K(\rho_\alpha)]^{-\beta E_{10c}(\rho_\alpha)} \cos\varphi(\bar{\rho}_\alpha)\} du_\beta(\varphi), \quad (9)$$

where $E_{10c}(\rho_\alpha)$ is some portion of the electrostatic self-energy of ρ_α , and $\bar{\rho}_\alpha$ is an effective (renormalized) charge distribution not, in general, integer valued, but of total charge 0. The renormalization transformation

$$\rho_\alpha \rightarrow \bar{\rho}_\alpha, \quad K(\rho_\alpha) \rightarrow z(\beta, \rho_\alpha) \equiv K(\rho_\alpha) \exp[-\beta E_{10c}(\rho_\alpha)]$$

preserves the electrostatic interactions between distinct molecules and extracts part of the self-energy by spreading out ρ_α .⁹

The key point is now to show that, in two dimensions and for β large enough,

$$z(\beta, \rho_\alpha) \leq \exp[(-c\beta + b) \ln d(\rho_\alpha)], \quad (10)$$

$$(1 + K_a \cos a)(1 + K_b \cos b) = \frac{1}{3}(1 + 3K_a \cos a) + \frac{1}{3}(1 + 3K_b \cos b) + \frac{1}{6}[1 + 3K_a K_b \cos(a + b)] + \frac{1}{6}[1 + 3K_a K_b \cos(a - b)] \quad (11)$$

to pairs of factors in $I(\varphi; z) \equiv \prod_j [1 + z \cos\varphi(j)]$. First, all sites are grouped in nearest-neighbor pairs (i, j) , and Eq. (11) is applied to pairs of factors in $I(\varphi; z)$, with $a = \varphi(i)$, $b = \varphi(j)$, and $K_a = K_b = z$. The right-hand side of Eq. (11) is, for each pair (i, j) , substituted back into $I(\varphi; z)$, and the resulting expression is expanded in a sum of terms of the form

$$\prod_\alpha [1 + K(\rho_\alpha') \cos\varphi(\rho_\alpha')].$$

To each pair of factors indexed by charge distributions $\rho_\alpha', \rho_\gamma'$ which are not yet in desired form, in particular have nonzero total charge, identity (11) is applied again, with $a = \varphi(\rho_\alpha')$, $K_a = K(\rho_\alpha')$, $b = \varphi(\rho_\gamma')$, and $K_b = K(\rho_\gamma')$. These operations are organized inductively on a sequence of length scales 2^m , $m = 0, 1, 2, \dots$. On scale 2^m , all charge distributions which are not yet in final form (e.g., have nonzero total charge) are separated from each other by a distance $\geq 2^m$, and (11) is applied to pairs of factors corresponding to charge distributions at a distance between 2^m and 2^{m+1} from each other. Each application of (11) obviously increases bare activities by a factor of 3. Thus

$$K(\rho_\alpha) = z^{|\rho_\alpha|} 3^{N(\rho_\alpha)},$$

where

$$|\rho_\alpha| = \sum_j |\rho_\alpha(j)|,$$

and $N(\rho_\alpha)$ is the number of times identity (11)

where $d(\rho_\alpha)$ is the diameter of the molecule ρ_α . Inequality (10) is a consequence of the logarithmic growth of the 2D Coulomb potential and fails in higher dimensions. We now observe that for $\beta \gg b/c$, $z(\beta, \rho_\alpha) \ll 1$; hence large neutral molecules are suppressed and Mermin's argument can be used to prove (7).

Next we comment on the proof of the key identities (5) and (9).

Identity (5) is obtained from (4) by grouping together charges in the Coulomb gas so as to form neutral molecules of finite size. This is achieved by repeatedly applying the simple identity

had to be applied to obtain a factor $[1 + K(\rho_\alpha) \times \cos\varphi(\rho_\alpha)]$. The main combinatorial estimate in this scheme is the following

$$(\ln 3)N(\rho_\alpha) \equiv S(\rho_\alpha) \leq \text{const} \sum_{m=0}^{n(\rho_\alpha)} A_m(\rho_\alpha), \quad (12)$$

where $A_m(\rho_\alpha)$ is the area of ρ_α on scale 2^m , i.e., the minimal number of $2^m \times 2^m$ squares needed to cover the support of ρ_α , $n(\rho_\alpha) = \text{const} \ln d(\rho_\alpha)$, and the constants are independent of α and the particular collection \mathfrak{X}_k to which ρ_α belongs. The quantity $S(\rho_\alpha)$ may be interpreted as the entropy of a molecule with charge distribution $\pm \rho_\alpha$. If ρ_α is a dipole of length l , $A_m(\rho) = 2$ for $m \leq \log_2 l$, and we see that $S(\rho) \propto \ln l$, in accordance with the heuristic argument made at the beginning.

The final result of the expansion is

$$I(\varphi; z) = \sum_k c_k \prod_{\{\alpha | \rho_\alpha \in \mathfrak{X}_k\}} [1 + K(\rho_\alpha) \cos\varphi(\rho_\alpha)], \quad (13)$$

with $K(\rho_\alpha) = z^{|\rho_\alpha|} \exp S(\rho_\alpha)$. After integration with the Gaussian measure $d\mu_\beta(\varphi)$, this yields (5). The details in this expansion can be arranged such that the distance between two molecules with charge distributions ρ_α, ρ_γ is at least

$$\text{const}[\min\{d(\rho_\alpha), d(\rho_\gamma)\}]^n \quad (14)$$

for some n , $\frac{3}{2} < n < 2$. This sparseness condition is needed in order to perform the renormalization transformation which we sketch next.

Our renormalization transformation (9) is based

on some elementary electrostatic identities. Consider a molecule with charge distribution ρ . Let f be a charge distribution (not necessarily integer valued) which does not overlap with ρ_α , $\alpha \geq 2$, i.e., $\sum f(j)\rho_\alpha(j) = 0$. If we set $\bar{\rho}_1 = \rho_1 + \Delta f$ then the electrostatic energy between ρ_1 and ρ_α equals the electrostatic energy between $\bar{\rho}_1$ and ρ_α for $\alpha \geq 2$ since $-\Delta V(i-j) = \delta(i,j)$. Moreover, the total charge is preserved, $\sum \rho_1(j) = \sum \bar{\rho}_1(j)$. However, we have made a change in the self-energy and to compensate for this change we set $E_{1\text{oc}}(\rho_1) = E(\rho_1) - E(\bar{\rho}_1)$.

If our gas of molecules is sufficiently sparse as in (14), we can redistribute the charge of ρ_1 over a wide region. More precisely we choose $f(j)$ to approximate $-(\Delta^{-1}\rho_1)(j)$ and so that $\sum_j f(j)\rho_\alpha(j) = 0$ for $\alpha \geq 2$. We show that f can be chosen so that $E(\bar{\rho}_1)$ is relatively small and hence $E_{1\text{oc}}(\rho_1) \approx E(\rho_1)$. A similar procedure is applied to each of the ρ_α , $\alpha \geq 2$. This renormalization together with the sine-Gordon transformation yields (9).

Finally we briefly indicate how to bound $E(\rho_1) \approx E_{1\text{oc}}(\rho_1)$ from below, so that the effective activity of the molecule ρ_1 , given by $K(\rho_1) \exp[-\beta E_{1\text{oc}}(\rho_1)]$, is small, for β sufficiently large. Recall that if $\{q(x_i)\}$ is a collection of charges $q = \pm 1$ located at points $x_i \in Z^2$, the electrostatic energy of $\{q(x_i)\}$ is larger than $\text{const} \sum_i \ln(r_i + 1)$, where r_i is $\frac{1}{2}$ the distance between x_i and the nearest charged particle. This type of inequality is applied on all distance scales 2^m , i.e., charges q_j are replaced by charged submolecules $\rho_{1,i}$ of

size 2^m . The distances $r_i(m)$, measured in units of 2^m , correspond to the distance to the nearest charged submolecule.

One of us (T.S.) wishes to thank Professor N. H. Kuiper for his hospitality at Institut des Hautes Etudes Scientifiques. We also wish to thank J. Lebowitz for several helpful suggestions. This work is supported in part by the Alfred P. Sloan Foundation and by the National Science Foundation under Grant No. NR-DMR-73-04355.

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