Nonuniversal Jumps and the Kosterlitz-Thouless Transition

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A new set of renormalization equations for the two-dimensional Coulomb gas is derived. Within this new description, the prediction of a universal jump or the prediction that the exponent η is $\frac{1}{4}$ at the critical line breaks down below a certain temperature. Consequently it should be possible to have a Kosterlitz-Thouless transition without a universal jump. A realization is suggested.

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A new set of renormalization equations for the Kosterlitz-Thouless transition[1,2] of a two-dimensional (2D) Coulomb gas is presented. In the present paper I give the main line of arguments, results, and some consequences. A full account with detailed derivations will be given elsewhere.[3]

The Kosterlitz-Thouless transition is of recent interest in many contexts.[4] Some obvious implications of the present work are to XY models and to superfluid- and superconducting films. One striking manifestation of the Kosterlitz-Thouless transition for these cases is the universal jump[5] of the helicity modulus[6] or equivalently of the superfluid density.[5,7] A consequence of my new equations is that it is possible to have a Kosterlitz-Thouless transition *without* a universal jump. I suggest that this may be the case for some of the frustrated XY models.

The model under consideration is the 2D Coulomb gas[8]; it consists of particles with charge $s=\pm 1$ interacting through a Coulomb interaction. In two dimensions this interaction is logarithmic. The model is defined through the grand partition function (modulo precise cutoff prescriptions)

$$Z=\sum_{N=0}^{\infty}\prod_{i}\int\frac{d^2r}{a^2}i\exp\left[\frac{1}{2T}\sum_{ij}s_is_j\ln\left(\frac{r_{ij}}{a}\right)\right](\tfrac{1}{2}N)!,\tag{1}$$

where N is the number of particles in a neutral configuration, i and j numerate the particles, r_{ij} is the distance between particles i and j, a is the linear dimension of a particle, z is the particle fugacity, and T is the temperature. We address the problem of describing the Kosterlitz-Thouless transition with T and z as variables.

The thermodynamic averages for the Coloumb-gas model may be mathematically transformed into a Euclidean sine-Gordon field-theory formulation.[9] An average in the sine-Gordon formulation has the following appearance:

$$\langle O[\phi]\rangle\equiv\frac{\int d\phi\exp[-\int d^2r\,\mathscr{H}_{\rm sG}(\bar r)]O[\phi]}{\int d\phi\exp[-\int d^2r\,\mathscr{H}_{\rm sG}(\bar r)]},\tag{2a}$$

with the sine-Gordon Hamiltonian density given by

$$\mathscr{H}_{\rm sG}(\bar r)=\frac{(\bar\nabla\phi)^2}{2}-\frac{2z}{a^2}\cos\left[\left(\frac{2\pi}{T}\right)^{1/2}\phi(\bar r)\right],\tag{2b}$$

and $\phi(r)$ is a real field.

The basis for the present treatment is very straightforward in the sine-Gordon formulation. It is simply the first term in a systematic cumulant expansion, namely,

$$\mathrm{Re}\langle\exp\{i(2\pi/T)^{1/2}[\phi(\bar r)-\phi(0)]\}\rangle=\exp\{-(\pi/T)\langle[\phi(\bar r)-\phi(0)]^2\rangle\}.\tag{3}$$

Note that this is a natural approximation without any obvious limitation. It also turns out to have an appealing physical interpretation.

In order to get to the physics of Eq. (3) we translate it back to the Coulomb-gas language. It then reads[3]

$$\langle n(r)n(0)\rangle=-\frac{2z^2}{a^4}\exp\left[\frac{1}{T}[V(0)-V(r)]\right].\tag{4}$$

Here $n(r)$ is the charge density, the brackets stand for thermodynamic averages in the grand canonical ensemble, and $V(r)$ is the linearly screened potential. The transformation from Eq. (3) to Eq. (4) is valid as long as the screening length in the Coulomb gas is infinite, i.e., in the low-temperature phase.[3] The linearly screened potential is related to the charge-density correlations. This relation may be expressed in terms of Fourier transforms and a dielectric function as

$$V(\bar k)=2\pi/k^2\epsilon(k),\tag{5a}$$

$$\frac{1}{\epsilon(k)}=1-(2\pi/Tk^2)\langle n(\bar k)n(-\bar k)\rangle.\tag{5b}$$

The dielectric constant $\epsilon_0\equiv\lim_{k\to 0}\epsilon(k)$ will play an important role. Note that Eqs. (4) and (5) are self-consistent equations for the charge correlations. This is the key of the present approach.

In order to extract the physics and make contact with earlier work and renormalization-group (RG) equations we introduce a logarithmic length scale $l\equiv\ln(r/a)$ and a length-dependent dielectric function[1]

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$\tilde{\epsilon}(l)$ where (from now on we set $a=1$)

$$\frac{1}{\tilde{\epsilon}(l)} \equiv 1+\frac{\pi^2}{T}\int_0^l d\,l'\{r'^4\langle n(r')n(0)\rangle\}. \quad (6)$$

One notes that $\tilde{\epsilon}(\infty)=\epsilon_0$. After some algebra Eqs. (4) and (5) may be expressed in differential form[3]:

$$\frac{d}{dl}\left\{\frac{1}{T\tilde{\epsilon}(l)}\right\}=-\frac{2z^2(l)\pi^2}{T^2}, \quad (7a)$$

$$\frac{d}{dl}z(l) = \frac{z(l)}{2}\left\{4-\int_0^\infty dx\, e^{-x}x\frac{1}{T\tilde{\epsilon}(l+\frac{1}{2}x)}\right\}, \quad (7b)$$

with the boundary conditions $\tilde{\epsilon}(0)=1$ and $z(0)=z$; $z(l)$ may be thought of as a "renormalized" fugacity. Integrating the equations from $l=0$ to ∞ gives ϵ_0. From this one gets the position of the critical line in the (T,z) plane and the critical properties of ϵ_0 as the critical line is approached. Equations (7) bear a strong resemblance to Kosterlitz renormalization-group equations.[10] However, there is a structural difference: Equations (7) contain an integrodifferential equation whereas the renormalization-group equations are differential equations. This structural difference turns out to carry new implications for the renormalization-group flow diagram.

We now come to the physical interpretation of the difference between Kosterlitz RG equations[10] and Eqs. (7). Imagine that a test dipole pair is introduced into the Coulomb gas. Equations (7) then correspond to the following force, F, acting between the test-pair particles[3]:

$$F=F_1+F_2+F_3, \quad (8a)$$

$$F_1(r_0)=1/r_0\tilde{\epsilon}(r_0), \quad (8b)$$

$$F_2(r_0)=(r_0\pi^2/T)\int_{r_0}^\infty dr'\langle n(r')n(0)\rangle, \quad (8c)$$

$$F_3(r_0) =(2\pi^2/T)r_0\int_{r_0}^\infty dr'r'\ln(r'/r_0)\langle n(r')n(0)\rangle, \quad (8d)$$

where r_0 is the distance between the test particles. F_1 may be interpreted as the force due to the electric field between the test particles screened by Coulomb-gas dipole pairs with separation less than r_0.[1,11] F_2 may be interpreted as arising from the dipole field from the test pair screened by Coulomb-gas dipole pairs with separation larger than r_0 while F_3 arises from the orientational energy of the test pair in the electric field due to Coulomb-gas dipoles with separation larger than r_0.[3]

If the contributions from the Coulomb-gas dipoles with separation larger than the test-pair separation is ignored, i.e., if F is set equal to F_1, then Eqs. (7) reduce to Kosterlitz RG equations.[8,11] Thus from this viewpoint Eqs. (7) contain more of the physics than do Kosterlitz RG equations. They may be viewed as the length-dependent screening reasoning[1,11] carried one step further.

I have deduced the properties of Eqs. (7) by numerical integration.[3] Figure 1 shows the position of the critical line in the (T,z) plane (solid line). For comparison, I have also plotted the result from Kosterlitz RG equations[10] (dashed line) and the next order renormalization-group correction[12] to this (dotted line). In this comparison Eqs. (7) come out as a respectable approximation; they correct the lowest-order RG equations in the right direction with respect to the next order RG equations. In this comparison it must be kept in mind that the second-order RG equations are by construction only valid close to $T=\frac{1}{4}$ and $z=0$,[12] the Kosterlitz equations are valid close to $z=0$, whereas the limitations of Eqs. (7) are less obvious.

The critical line obtained from Eqs. (7) has a nonanalytic behavior at a temperature T^* ($T^*\approx 0.1436$, see Fig. 1). This nonanalyticity is more obvious in Fig. 2 where I have plotted ϵ_c ($\equiv$ the value of ϵ_0 at the critical line) as a function of T_c ($\equiv$ the temperature on the critical line). As T^* is approached from below, ϵ_c behaves as $\epsilon_c(T_c)=1/4T^*-\mathrm{const}(T^*-T_c)^{1/2}$. Above T^* the value on the critical line is given by $\epsilon_c=1/4T_c$ which is the well-known result from RG analysis.[10,12] As the critical line is approached from the left for constant z, ϵ_0 behaves as $\epsilon_0=\epsilon_c-A_\pm(T_c)[\pm(T_c-T)]^{1/2}$ both above (+) and below (−) the temperature T^*. The coefficients $A_\pm$ are logarithmically divergent as T_c approaches T^* from above (below).

The RG trajectories are trajectories with constant

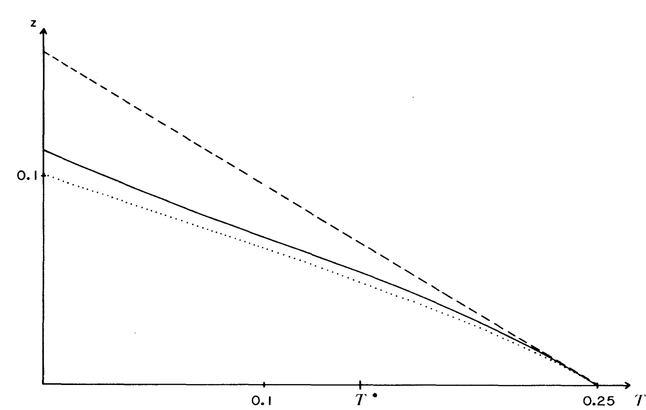

FIG. 1. Critical line in the (T,z) plane. Full line, numerical solution of Eqs. (7); dashed line, the lowest-order RG equations; dotted line, the two-lowest-order RG equations. The temperature T^* is a temperature where the solution of Eqs. (7) has a nonanalytic behavior.

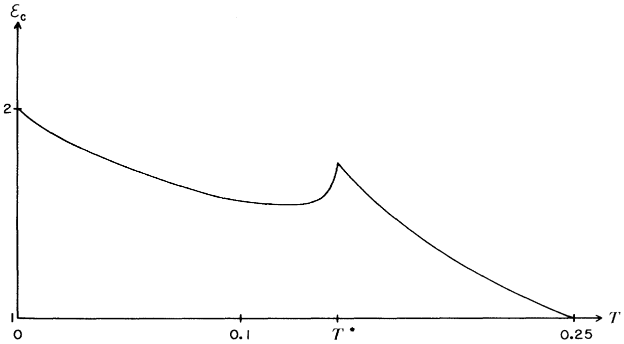

FIG. 2. The value of the dielectric constant at the critical line, ϵ_c. The nonanalytic behavior at T^* is of the form $\epsilon_c - 1/4T^* \sim (T^* - T)^{1/2}$

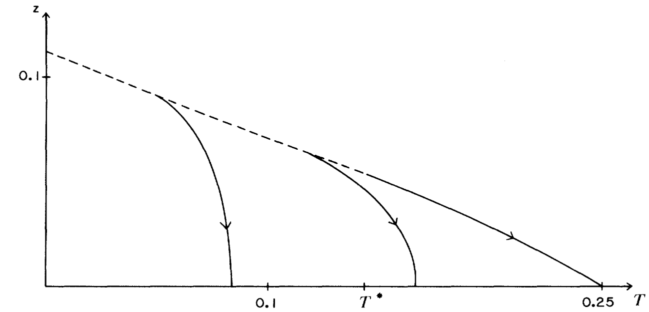

FIG. 3. Flow diagram for the RG equations corresponding to Eqs. (7). The full lines are RG trajectories corresponding, from right to left, to $1/T\epsilon_0 = 4, 6, 12$. The dashed line between $T=0$ and T^* is the locus of starting points for RG trajectories ending on the T axis.

$T\epsilon_0$. The RG flow diagram corresponding to Eqs. (7) is shown in Fig. 3. The critical trajectory $T\epsilon_0 = \frac{1}{4}$ starts at T^* and ends on the T axis at $T = \frac{1}{4}$. The critical line for temperatures lower than T^* is the loci of starting points for the RG trajectories (dashed line in Fig. 3). Three such trajectories are shown in Fig. 3.

Above the critical line ϵ_0 is infinite. At the critical line ϵ_0 jumps from ϵ_c to infinity. The famous universal jump[5] is the jump of the quantity $1/T_c\epsilon_0$ from 4 to 0 at the critical line. The size of the jump, $1/T_c\epsilon_c$, is plotted in Fig. 4. Between $T_c = \frac{1}{4}$ and $T_c = T^*$ it has the universal value 4.[5,7] This universal value corresponds to a jump of the helicity modulus γ of $2T_c/\pi$ for XY models[6] and to a jump of $(2/\pi)k_B(m^2/\hbar^2)T_c$ for 2D superfluids[5] where, e.g., m is the mass of a He^4 atom (in the case of He^4 films) or of a Cooper pair (in the case of superconducting films). Below T^*, on the other hand, $1/T_c\epsilon_c$ has a nonuniversal value and the jump becomes *nonuniversal.* The question whether a particular system has a universal or nonuniversal jump at its Kosterlitz-Thouless transition consequently hinges on precisely what Coulomb-gas temperature the transition corresponds to.

The critical index η for the spin-spin correlations in the XY models is related to the charge-density correlations of the Coulomb gas in such a way that $\eta = T\epsilon_0$.[10,13] It follows from the present work that if a particular XY model has its Kosterlitz-Thouless transition at a Coulomb-gas T_c larger than T^* then $\eta = \frac{1}{4}$ at the critical temperature, whereas if the transition corresponds to a Coulomb-gas T_c smaller than T^* then η has a nonuniversal value less than $\frac{1}{4}$ at the critical temperature.

Into which of these two distinct classes of Kosterlitz-Thouless transitions do various current models fall? Here is a tentative answer for some models: Monte Carlo simulations for the usual 2D XY model are in good agreement with the universal-jump prediction for the helicity modulus.[14,15] The extracted ϵ_c is around 1.3,[14] corresponding to a Coulomb-gas T_c larger than T^*. The superfluid helium films are closely related to the XY model.[6,14] The experimental results are in good agreement with the universal-jump prediction[15] and the extrapolated ϵ_c is around 1.3.[14] Experiments on superconducting films show evidence of a universal jump[16] and the extracted ϵ_c is around 1.65[17] which is consistent with a Coulomb-gas T_c larger than T^*. On the other hand, Monte Carlo simulations for some of the frustrated XY models show evidence of a Coulomb-gas T_c smaller than T^* and a nonuniversal jump.[18,19] This is particularly striking for the half-frustrated XY model on a honeycomb lattice[19]; the transition is expected to be of Kosterlitz-Thouless type[19] but the jump of the helicity modulus appears to be around $0.3J$, whereas the universal-jump prediction gives $0.075J$ (J is the coupling constant of the XY model). I suggest that this is an example of a nonuniversal jump and of an XY model with the Coulomb-gas T_c smaller than T^*.

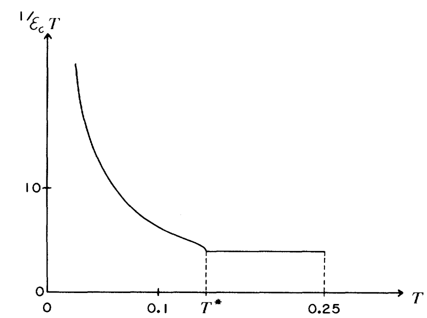

FIG. 4. Size of the jump at the Kosterlitz-Thouless transition. Between $T = \frac{1}{4}$ and T^* the jump of $1/\epsilon_0$ at the critical line has the universal value 4. Below T^* the size of the jump is nonuniversal and larger than 4.

In conclusion, I have presented a new set of renormalization-group equations for the 2D Coulomb gas. This leads to a qualitatively different renormalization-group flow diagram. A qualitatively new feature is that a nonuniversal jump at the Kosterlitz-Thouless transition becomes possible. I suggest that the transition for the half-frustrated *XY* model on a honeycomb lattice is of this new nonuniversal type.

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