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Critical Line near the Zero-Density Critical Point of the Kosterlitz–Thouless Transition

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Using low-fugacity expansions, we study the exact behavior of the Kosterlitz–Thouless critical line near the zero-density critical point. We show that the critical temperature deviates from its zero-density value by a term proportional to the square root of the density.

KEY WORDS: Kosterlitz–Thouless transition; Coulomb gas; fugacity expansions; critical line.

The two-dimensional Coulomb gas is a charge-symmetric two-component plasma with charges e and $-e$ which interact through the logarithmic potential $-\ln(r/L)$, where r is the distance between the particles and L is an arbitrary length that determines the zero of the potential. This system is of great interest, since it is the archetype of a universality class of 2D transitions induced by a condensation of topological excitations (such as defects in quasicrystals or vortices in ^{4}He films). Indeed, because of the long range of the confining logarithmic interaction, opposite charges form neutral pairs at sufficiently low temperatures and low densities, and the system undergoes the well-known Kosterlitz–Thouless (KT) transition.[1] (see ref. 2 for a rigorous proof). On the other hand, the Coulomb gas is interesting in itself; in particular, when the density becomes large enough, the KT transition, which is of infinite order, is expected to bifurcate into a first-order transition between a conductive liquid and an insulating gas. This transition has been studied by numerical simulations[3] and approximate theories.[4,5] Of course, when the dimensionless coupling

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constant $\Gamma = e^2/(k_B T)$ is larger than 2, a short-range repulsive potential must be introduced in order to prevent the collapse of opposite charges. In the following, we consider a system of charged hard disks with diameter σ and we fix $L = \sigma$.

The point of this short communication is to emphasize that, in the phase diagram in temperature versus density, the tangent to the critical line $T_c(\rho)$ is vertical at the zero-density critical point $k_B T_c(\rho = 0) = 1/4$ [$T_c(\rho)$ is the critical temperature when the total density of particles is equal to ρ]. This property does not appear in the usual approaches of either the iterated mean-field model introduced by Kosterlitz and Thouless or the renormalization group applied to the sine-Gordon field theory, which is equivalent to the Coulomb gas.[6] In all these approaches, the KT critical line is given in terms of the parameters T and z, where z is the dimensionless fugacity of both species of charges. It reads

$$\Gamma_c \equiv \frac{e^2}{k_B T_c} = 4 + 8\pi z + o(z) \tag{1}$$

On the other hand, our microscopic approach based on first principles and developed in ref. 7 allows us to relate the dimensionless fugacity to the density of particles. Our result for $T_c(\rho)$ has been observed in recent approximate theories.[2] However, there are still critical lines in the figures found in the literature that ignore this property. We mention that, in fact, simulations are more adapted to the finite-density regime than to the zero-density limit of the original KT transition.

In our microscopic approach, we start from the low-fugacity expansions of the equilibrium quantities. The Mayer z-graphs are convergent when Γ is greater than 4.[8] This allows us to study the behavior of the quantities of interest in the dielectric phase when both z and $(\Gamma - 4)$ are small parameters. In particular, the large-distance behavior of the internal particle correlations $\rho^T_{++} = \rho^T_{--}$ and $\rho^T_{+-} = \rho^T_{-+}$ is controlled by the fluctuations of dipolar potentials, and we find that ρ^T_{++} and ρ^T_{+-} decay as $1/r^4$ (for a rigorous proof see ref. 9) with the same coefficient. Subsequently, the internal charge correlation, defined as

$$C(\mathbf{r}) = e^2\{2[\rho^T_{++}(r) - \rho^T_{+-}(r)] + \rho\delta(\mathbf{r})\} \tag{2}$$

falls off faster than ρ^T_{++} and ρ^T_{+-}. We have shown that the leading term in the large-distance behavior of the internal charge correlation $C(r)$ decays

[2] M. E. Fisher, private communication, based on work with X.-J. Li and Y. Levin extending the analysis of ref. 4.

as $1/r^{\Gamma/\varepsilon}$, where ε is the dielectric constant given by the linear response formula,

$$\frac{1}{\varepsilon} = 1 + \frac{\pi}{2k_B T} \int d\mathbf{r}\, r^2 C(r) \tag{3}$$

Each term of order z^{2n} in the z-expansion of $C(r)$ contributes a term of order $z[z/(\Gamma-4)]^{2n-1}$ to $1/\varepsilon$. Thus all these contributions must be resummed near the zero-density critical point. This mechanism arises from collective effects which characterize critical points. In our analysis, the signal of the KT transition appears as the nonanalyticity of $1/\varepsilon$ as a function of the parameter $z/(\Gamma-4)$: the critical line is determined by the radius of convergence of the above series, and it reads $\Gamma/\varepsilon = 4$, as conjectured in the literature. Notice that, at the KT transition, $1/\varepsilon$ jumps from a finite value in the dielectric phase (where the screening is only partial) to the value zero in the conductive phase (where the screening is perfect).

In the present paper, we investigate the low-fugacity expansion of the particle densities,

$$\rho_+ = \rho_- = \frac{z^2}{\sigma^4} \int_{r>\sigma} d\mathbf{r} \left(\frac{\sigma}{r}\right)^{\Gamma} + O(z^4) \tag{4}$$

Now, all the Mayer graphs remain finite when $\Gamma \to 4^+$. Indeed, the KT transition is of infinite order, and the thermodynamic quantities are continuous as well as all their derivatives when Γ varies. In contrast to the case of $1/\varepsilon$, no resummations are needed. As a consequence, the total density of particles $\rho = \rho_+ + \rho_-$ behaves like

$$\rho \sim \frac{2\pi z^2}{\sigma^2} \tag{5}$$

in the regime of interest. Thus the Eq. (1) of the critical line can be rewritten as

$$\frac{k_B T_c}{e^2} = \frac{1}{4} - \frac{\pi^{1/2}}{2^{3/2}} [\rho\sigma^2]^{1/2} \tag{6}$$

where all terms of order higher than $\rho^{1/2}$ have been dropped. Consequently, the tangent to the critical line at the zero-density critical point is vertical.

In Fig. 1, we have drawn the curve extrapolated from the exact low-density form (6). This curve should represent the critical line quite

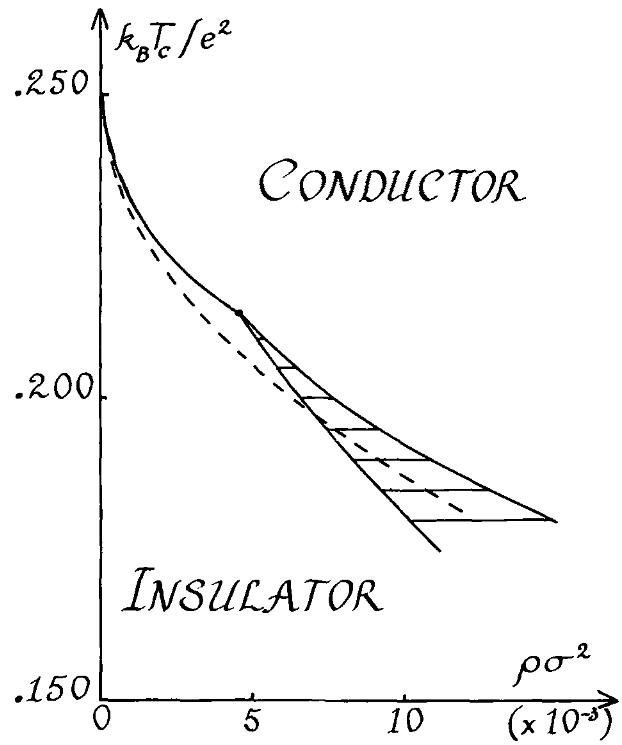

Fig. 1. Phase diagram in the plane $(\rho\sigma^2, k_B T/e^2)$. Dashed curve: the KT critical line extrapolated from the exact low-density behavior (6). Solid curve: the KT critical line and the liquid–gas coexistence curve computed by Fisher *et al.* (see footnote 2). Hatched zone: the liquid–gas coexistence region. Circle: the tricritical point $(\rho_t\sigma^2 \simeq 0.00456, k_B T_t/e^2 \simeq 0.2138)$.

accurately in the vicinity of the zero-density critical point. We also show the phase diagram recently computed by Fisher *et al.* (see footnote 2) for models which take into account finite-density effects. Notice that their tricritical point (ρ_t, T_t) is close to our extrapolated curve. The expression (6) indeed gives $T_c = 0.2077$ for $\rho_t\sigma^2 = 0.00456$, while $T_t = 0.2138$.

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