New phase diagram for the two-dimensional Coulomb gas

Petter Minnhagen and Mats Wallin
Department of Theoretical Physics, Umeå University, S-901 87 Umeå, Sweden
(Received 23 March 1987)

The phase diagram for the two-dimensional Coulomb-gas model is deduced from a set of renormalization equations. For small fugacities the well-known Kosterlitz-Thouless phase transition is regained. For larger fugacities a new phase-transition line is found. It is argued that the phase transition across this new line is discontinuous in contrast to the continuous Kosterlitz-Thouless transition. From a physical point of view, the new transition line reflects new aspects of the charge unbinding in the Coulomb-gas system, with possible implications for related models.

The two-dimensional Coulomb gas may be regarded as the prototype for a system undergoing a Kosterlitz-Thouless transition.[1] It consists of equal numbers of positive and negative two-dimensional Coulomb-gas charges interacting with the logarithmic Coulomb interaction in two dimensions.[2] The phase transitions taking place in the Coulomb gas may intuitively be interpreted in terms of charge unbinding: for low enough temperatures the gas consists of neutral bound pairs of Coulomb-gas charges while for higher temperatures it consists of a mixture of free charges and bound pairs.[3]

For small dipole-pair fugacities the critical properties of the charge-unbinding transition are contained in the Kosterlitz renormalization-group equations[4] and the transition characterized by these renormalization-group equations is usually referred to as the Kosterlitz-Thouless transition.[1,2] It is a continuous transition of infinite order.[3]

Most predictions and conclusions concerning the charge-unbinding transition have so far been based on the Kosterlitz renormalization-group equations.[1] For example, these renormalization-group equations lead to the famous universal-jump prediction for the superfluid density in case of ^{4}He films.[5] However, it has recently been suggested, on the basis of a new set of renormalization equations for the two-dimensional Coulomb gas, that the conclusions based on the Kosterlitz renormalization-group equations may break down for larger dipole-pair fugacities.[6] As a consequence charge-unbinding transitions with nonuniversal jumps may, in principle, be possible[6] and it has been suggested that some frustrated *XY* models might be possible candidates for such charge-unbinding transitions.[6,7]

In this Brief Report we present the new and unexpected phase diagram contained in the renormalization equations constructed by Minnhagen.[6] A more detailed account will be given in a separate paper.[8]

The two-dimensional Coulomb-gas model is defined through the grand partition function Z (modulo precise cutoff prescriptions)[2]

$$Z=\sum_{N=0}^{\infty}\prod_i\int\frac{d^2r_i}{a^2}\frac{z^N}{(\frac{1}{2}N!)^2}\times\exp\left[\frac{1}{2T}\sum_{i\neq j}s_is_j\ln(r_{ij}/a)\right], \quad (1)$$

where N is the number of particles in a neutral configuration (only neutral configurations contribute to the partition function[2]), i and j numerate the particles, r_{ij} is the distance between particles i and j, a is the linear dimension of a particle, $s_i=\pm 1$ is the charge of a particle, z is the fugacity, and T is the temperature. The object is to determine the phase diagram for the Coulomb gas with T and z as variables.

The basis for the renormalization equations,[6] to be used in the present paper in order to construct the phase diagram, is the *exact* relation[8]

$$\langle\Delta n(r)\Delta n(0)\rangle=\frac{2z_{\mathrm{eff}}^2}{a^4}\{\exp[-U_{\mathrm{eff}}^{++}(r)/T]-\exp[U_{\mathrm{eff}}^{+-}(r)/T]\}, \quad (2)$$

where $\langle\Delta n(r)\Delta n(0)\rangle$ is the charge-density correlation for the Coulomb gas $[\Delta n(r)=\sum_i s_i\delta(\mathbf{r}-\mathbf{r}_i)]$, z_{eff} is an effective fugacity, and $U_{\mathrm{eff}}^{++}(r)=U_{\mathrm{eff}}^{--}(r)$ $[U_{\mathrm{eff}}^{+-}(r)]$ is the effective interaction between two Coulomb-gas charges of equal (opposite) sign. To lowest order in charge the effective particle interactions reduce to $U_{\mathrm{eff}}^{++}(r)=U_{\mathrm{eff}}^{+-}(r)=V_L(r)$, where $V_L(r)$ is the linearly screened potential and to this order Eq. (2) reduces to

$$\langle\Delta n(r)\Delta n(0)\rangle=\frac{2z^2}{a^4}e^{V_L(a)/T}(e^{-V_L(r)/T}-e^{V_L(r)/T}), \quad (3a)$$

where z is the fugacity associated with creating one of the particles in a neutral pair with separation a.[6,8] The linearly screened potential is related to the charge-density correlation function $\langle\Delta n(r)\Delta n(0)\rangle$ through standard linear-response theory

$$\hat{V}(k)=\frac{2\pi}{k^2}\left[1-\frac{2\pi}{Tk^2}\langle\Delta\hat{n}(\mathbf{k})\Delta\hat{n}(-\mathbf{k})\rangle\right] \quad (3b)$$

where $\hat{V}$ and $\Delta\hat{n}$ are the Fourier transforms of V and Δn, respectively. Equations (3) constitute a self-consistent set of equations.[6]

Equations (3) are exact in three independent limits: $T\rightarrow\infty$, $r\rightarrow\infty$, and $z\rightarrow 0$.[6,8] For the $z\rightarrow 0$ limit this means that Eqs. (3) reduce to the Kosterlitz renormalization-group equations for $T<\frac{1}{4}$ and for $T>\frac{1}{4}$ to the $z\rightarrow 0$ results derived earlier by sine-Gordon field-theory diagrammatics.[9] Our confidence in the results inferred from Eqs. (3) is based on the fact that they reproduce all known results in the $z \to 0$ limit and are exact in the two limits $T \to \infty$ and $r \to \infty$ irrespective of the value of z. In addition, they are based on a very natural approximation of the exact Eq. (2).

The Fourier transform of the linearly screened potential $V_L(r)$ has the leading small-k dependence $\hat{V}_L^{-1}(k) = \tilde{\epsilon}(k^2+\lambda^{-2})/2\pi$, where λ is the Debye screening length and $\tilde{\epsilon}$ is a dielectric constant, which in the intuitive charge-unbinding picture describes the polarization due to bound pairs.[2] Within the charge-unbinding picture the screening length λ may be related to the density of free particles n_F by $\lambda^{-2} = 2\pi n_F/\tilde{\epsilon}T$.[2] We will use Eqs. (3) to calculate λ as a function of T and z.

In the case $\lambda=\infty$ (which corresponds to no free charges) Eqs. (3) may be transformed into[6]

$$\frac{d}{dl}\left[\frac{l}{T(l)}\right] = -\frac{2z^2(l)\pi^2}{T^2}, \tag{4a}$$

$$\frac{d}{dl}[z(l)] = \frac{z(l)}{2}\left[4-\int_0^\infty dx\, e^{-x}x/T(l+x/2)\right], \tag{4b}$$

where $l=\ln(r/a)$, $(T(0),z(0))=(T,z)$, and $(T(\infty), z(\infty))=(\tilde{\epsilon}T,0)$. The flow diagram for Eqs. (4) is shown in Fig. 1; the arrows indicate increasing l direction. Solutions with $\lambda=\infty$ exist only in the shadowed region of the (T,z) plane.[6] The dashed border of the shadowed region is the line of starting points for the flow trajectories of Eqs. (4).[6] The dashed line ends at the special point (T^*,z^*) [$\simeq$(0.144, 0.054)] which is denoted by an asterisk in Fig. 1. For higher temperatures the boundary of the shadowed region is made up of the trajectory flowing from (T^*,z^*) into $(T,z)=(\frac{1}{4},0)$.[6] The phase transition across this later part of the boundary (solid line in Fig. 1) is the usual Kosterlitz-Thouless transition.[6]

The solutions for $\lambda\neq\infty$ may be obtained from Eqs. (3) by first transcribing them into[8]

$$\frac{V_L(r/\lambda)}{T} = \int_{r/\lambda}^\infty dx'h(x')\left\{1-\ln\left[\frac{x'\lambda}{r}\right]-\left[\frac{x'\lambda}{r}\right]^{-2}\times\left[1+\ln\left[\frac{x'\lambda}{r}\right]\right]\right\}, \tag{5a}$$

$$h(x) = -\frac{x^3}{8}\left[e^{V_L(x)/T}-e^{-V_L(x)/T}\right], \tag{5b}$$

$$T = -\left[\int_{a/\lambda}^\infty dx\, h(x)\right]^{-1}, \tag{5c}$$

$$z = \frac{Ta^2}{4\pi\lambda^2}e^{-V_L(a/\lambda)/2T}. \tag{5d}$$

Equations (5) may be solved numerically by interating Eqs. (5a) and (5b) from $r/\lambda=\infty$ to $r/\lambda=a/\lambda$ with $V_L(x)\to Ce^{-x}/\sqrt{x}$, where C is a positive constant, as the boundary condition for large $x=r/\lambda$. This is just the Debye screening condition in two dimensions. The solutions are obtained by solving for all possible values of C. The corresponding values of T and z are then obtained from Eqs. (5c) and (5d). Solutions with $\lambda\neq\infty$ exist in the region of the (T,z) plane which is shadowed in Fig. 2. Note that this region overlaps the region of solutions with $\lambda=\infty$ (the boundary for this latter region is also shown in Fig. 2). This means that in some regions of the (T,z) plane more than one λ solution exists for Eqs. (3) for a given (T,z) point, and each solution corresponds to a different boundary condition at $r\to\infty$. We conjecture that the

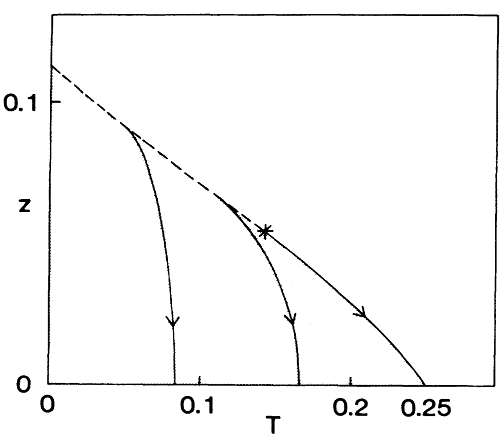

FIG. 1. Region of solutions with $\lambda=\infty$. The shadowed region is the part of the (T,z) plane where $\lambda=\infty$ solutions exist. The full drawn line with arrows are flow trajectories for Eqs. (4), the arrows indicate the direction of increasing l values. The dashed line is the line of starting points for the flow trajectories. The asterisk is the special point (T^*,z^*) where the critical trajectory starts. The phase transition across the critical trajectory is the Kosterlitz-Thouless transition. The phase transition across the dashed line is nonuniversal since every point on this line corresponds to a different flow trajectory.

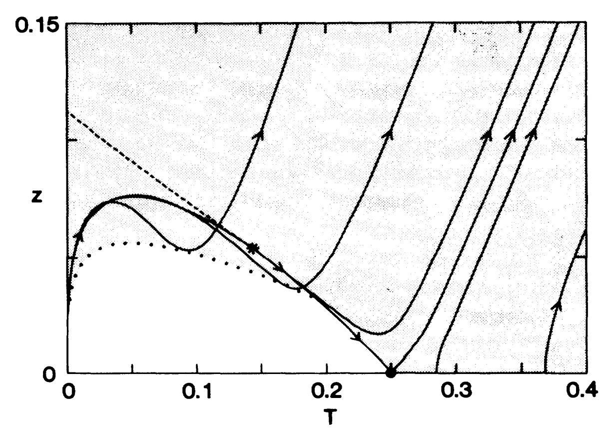

FIG. 2. Region of solutions with $\lambda\neq\infty$. The shadowed region is the part of the (T,z) plane where solutions with $\lambda\neq\infty$ exist. The full drawn lines with arrows are the flow trajectories of Eqs. (5), arrows indicate the direction of increasing a/λ. The special point (T^*,z^*) is denoted by an asterisk and lies on the critical trajectory which also passes through the point $(T,z)=(\frac{1}{4},0)$ (denoted by a dot). The dashed line constitutes part of the boundary for solutions with $\lambda=\infty$ (compare Fig. 1), whereas the dotted line is part of the boundary for solutions with $\lambda\neq\infty$. The remaining parts of these two boundaries are made up of parts of the critical trajectory going through the points $(T,z)=(T^*,z^*)$ and $(T,z)=(\frac{1}{4},0)$.

correct boundary condition at $r \rightarrow \infty$ in such a case is the one corresponding to the largest λ. Within the charge-unbinding picture this means that the correct solution is the one corresponding to the largest fraction of bound neutral pairs. Figure 2 also shows some typical flow trajectories for Eqs. (5), i.e., trajectories connecting solutions with the same large r behavior of $V_L(r/\lambda)$. The flow direction indicated in Fig. 2 corresponds to increasing a/λ.

The phase diagram for the two-dimensional Coulomb gas may be inferred from the solutions of Eqs. (4) and (5) together with the conjecture that the correct physical solution is the one corresponding to the largest possible fraction of bound neutral pairs. The phase diagram in the (T,z) plane is shown in Fig. 3. It contains two phase-transition lines; one is the full drawn line in Fig. 3. It goes from the point (T^*,z^*) (denoted by an asterisk in Fig. 3) to the point $(T=\frac{1}{4},z=0)$ (denoted by a dot). The transition across this line is the usual Kosterlitz-Thouless transition. Within the charge-unbinding picture this transition may, in the thermodynamic limit, be associated with the breaking of an *infinitesimal fraction* of bound pairs on crossing the transition line from below. The other transition line is the dashed line in Fig. 3. This line goes from zero temperature and ends at the special point (T^0,z^0) $[\simeq(0.20,0.03)]$ denoted by an open circle in Fig. 3. Within the charge-unbinding picture the transition across this line from below is, in the thermodynamic limit, associated with the breaking of a *finite fraction* of bound pairs. It is, hence, a discontinuous transition and is consequently expected to be associated with a discontinuity in the free energy. The two transition lines join smoothly (i.e., with the same tangents) at the special point (T^*,z^*). This means that for $T<T^*$ the transition from the low-temperature $\lambda=\infty$ phase to the high-temperature $\lambda\neq\infty$ phase is discontinuous, while for $T>T^*$ it is the usual continuous Kosterlitz-Thouless transition. For T in the interval $T^*<T<T^0$ the discontinuous transition comes as an additional transition between two phases both with $\lambda\neq\infty$ where the low-temperature phase has a larger λ than the high-temperature phase. Within the charge-unbinding picture this again means that a *finite fraction* of bound pairs breaks as this transition line is crossed from below.

In summary, the approximate equations (3) lead to the prediction that the Kosterlitz-Thouless transition ceases below a certain temperature[6] and goes over into a discontinuous transition below this temperature. This prediction is corroborated by Monte Carlo simulations of the two-dimensional Coulomb gas.[10,11] The Monte Carlo confirmation suggests that Eqs. (3) are basically sound and may be trusted at least as far as one is concerned with qualitative features.[12]

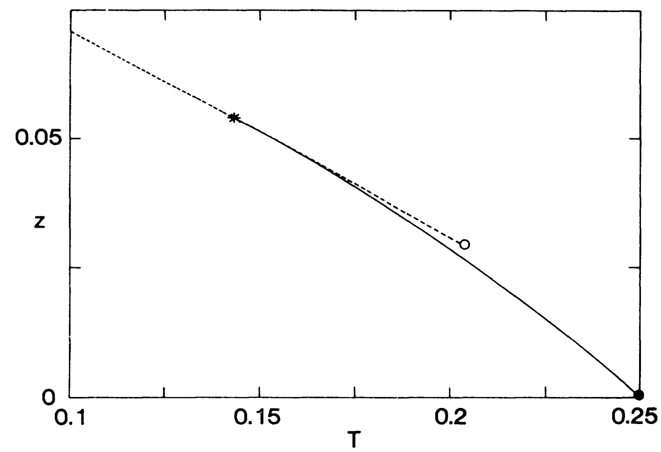

FIG. 3. Phase diagram for the two-dimensional Coulomb gas. The phase diagram in the (T,z) plane consists of two phase transition lines. The full drawn line is the Kosterlitz-Thouless phase transition line which is associated with the breaking of an infinitesimal fraction of bound pairs: it starts at the point (T^*,z^*) (denoted by an asterisk) and ends at the point $(T,z)=(\frac{1}{4},0)$ (denoted by a dot). The dashed line is the phase transition line for a discontinuous transition associated with the breaking of a finite fraction of pairs, it starts at zero temperature and ends at the special point (T^0,z^0) (denoted by an open circle). The two phase transition lines join smoothly (with the same tangents) at the point (T^*,z^*) (denoted by asterisk).

The high-temperature tail of the discontinuous transition from (T^*,z^*) to (T^0,z^0) (compare Fig. 3) leads to the new possibility of having two consecutive distinct transitions with increasing temperature; a Kosterlitz-Thouless transition followed by a discontinuous transition.

Finally, we note that if the presented phase diagram for the two-dimensional Coulomb gas is the correct one, then an interesting question is what consequences this could have for all other two-dimensional models displaying Kosterlitz-Thouless-type transitions.[1] For example, various simulations for dislocation-mediated melting in two dimensions sometimes give evidence in favor of a discontinuous transition and sometimes in favor of a continuous one, seemingly depending on the precise definition of the model.[13] This might be connected to the fact that the charge-unbinding transition in itself may be either discontinuous or continuous.

[1]For a review, see, e.g., J. M. Kosterlitz and D. J. Thouless, in *Progress in Low Temperature Physics*, edited by D. F. Brewer (North-Holland, Amsterdam, 1978), Vol. VII-B, p. 1; B. I. Halperin, in *Physics of Low-Dimensional Systems*, Proceedings of the Kyoto Summer Institute, 1979, edited by Y. Nagaoka and S. Hikami (Physical Society of Japan, Research Institute for Fundamental Physics, Kyoto, 1979), p. 53; D. R. Nelson, in *Phase Transitions and Critical Phenomena 7*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), p. 1.

[2]See, e.g., P. Minnhagen, in *Percolation, Localization, and Superconductivity*, edited by A. M. Goldman and S. A. Wolf, NATO Advanced Study Institute, Series B Physics (Plenum, New York, 1984, Vol. 109, p. 287.

[3]V. L. Berezinskii, Zh. Eksp. Teor. Fiz. **61**, 1144 (1971) [Sov. Phys. JETP **34**, 610 (1972)]; J. M. Kosterlitz and D. J. Thouless, J. Phys. C **5**, L124 (1972); **6**, 1181 (1973).
[4]J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).
[5]D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).
[6]P. Minnhagen, Phys. Rev. Lett. **54**, 2351 (1985); Phys. Rev. B **32**, 3088 (1985).
[7]P. Minnhagen, Phys. Rev. B **32**, 7548 (1985).
[8]P. Minnhagen and M. Wallin (unpublished).
[9]P. Minnhagen, A. Rosengren, and G. Grinstein, Phys. Rev. B **18**, 1356 (1978).
[10]J. M. Caillol and D. Levesque, Phys. Rev. B **33**, 499 (1986).
[11]Caillol and Levesque (Ref. 10) hypothesize that the points (T^*,z^*) and (T^0,z^0) coalesce. However, as pointed out by Caillol and Levesque this hypothesis is well beyond the resolution of their calculation. In other words, their calculation and our phase diagram are indeed consistent.
[12]P. Nozière and F. Gallet, J. Phys. (Paris) **48**, 353 (1987), have recently obtained another set of approximate equations. However, as pointed out by them, their approach is entirely different and leads to structurally very different equations compared to ours and their equations do not contain any first-order transitions.
[13]For a review see, e.g., D. R. Nelson, in *Phase Transitions and Critical Phenomena 7,* edited by C. Domb and J. l. Lebowitz (Academic, London, 1983), p. 1.