An alternative field theory for the Kosterlitz-Thouless transition

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Abstract. We extend a Gaussian model for the internal electrical potential of a two-dimensional Coulomb gas by a non-Gaussian measure term, which singles out the physically relevant configurations of the potential. The resulting Hamiltonian, expressed as a functional of the internal potential, has a surprising large-scale limit: The additional term simply counts the number of maxima and minima of the potential. The model allows for a transparent derivation of the divergence of the correlation length upon lowering the temperature down to the Kosterlitz-Thouless transition point.

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1. Introduction

The two-dimensional Coulomb gas has found an abundant number of applications, ranging from the melting of two-dimensional crystals \[1,2\] , vortices in superfluid films \[3\] and thin superconductors \[4\] and arrays of Josephson contacts \[5\] to topological defects of thin liquid-crystal films \[6\]. Common to these systems is the existence of two types of topological, point-like defects (positive and negative ‘charges’), which interact according to the two-dimensional Coulomb law, i.e. the potential energy grows logarithmically with distance. At low temperatures positive and negative defects are bound together and form neutral dipoles, which start to unbind at a certain critical temperature – the Kosterlitz-Thouless transition point \[7,8\]. In fact, an energy of the order of \[\Delta E \sim \log A\] (\(A\) is the system size) is needed to break up two bound charges.

On the other hand, the unbinding process implies a gain of entropy, which is also of the order of \(\log A\). Above the critical temperature entropy wins and a plasma-like gas of free charges is formed. The high-temperature phase is characterized by the existence of a screening length: The Coulomb interaction is shielded beyond the so called Debye-Hückel length due to the formation of a cloud of opposite charges around a (test-) charge. This phase is well described by a Gaussian model for the continuous charge density \(\rho\) (Debye-Hückel model) with the Hamiltonian

\[
\mathcal{H}/T = \frac{K_A}{2} \int d^2 x \int d^2 x' \rho(x) G(x-x') \rho(x') + \int d^2 x \frac{\rho^2}{2z},
\]

where \(G_r \sim -(2\pi)^{-1} \log(r/\ell) + \text{const}\) (\(\ell\) is a microscopic lengthscale) is the Green function of the two-dimensional Laplacian \((-\nabla^2 G(r) = \delta(r))\), \(K_A\) is the charge-charge coupling strength and the mass \(z\) measures the distance to the transition temperature.
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The screening length (Debye-Hückel length $\ell_{DH}$) is given by $\ell_{DH} = (K_A z)^{-1/2}$.

The Gaussian functional (1.1) applies to temperatures well above the transition temperature - it does not predict the essential singularity of the correlation length $\xi \sim \exp(b/\sqrt{T - T_c})$ closer to the transition point.

The aim of this paper is to propose a novel model Hamiltonian for the high temperature phase of the two-dimensional Coulomb gas, describing the fluctuations of the internal electrical potential. Contrary to the sine–Gordon theory, which has an unphysical auxiliary variable as its fundamental field, our model is based on a physical quantity (the potential) and, therefore, leads to a more intuitive understanding of the Kosterlitz–Thouless transition.

The resulting continuum model displays the correct divergence of the correlation length in the vicinity of the critical point, as will be demonstrated within a variational calculation and, in addition, within renormalized perturbation theory.

2. The model

We start with the (Gaussian) Debye-Hückel model (1.1) and introduce the internal electrical potential $\phi$ via $-\nabla^2 \phi = \rho$. The partition function for the model reads

$$Z = \int D[\phi] W[\phi] \exp \left( -\frac{K_A}{2} \int d^2 x (\nabla \phi)^2 - \frac{\mu}{2} \int d^2 x (\nabla^2 \phi)^2 \right)$$

with the (trivial) measure $W[\phi] \equiv 1$. Can we do better and find an appropriate measure $W[\phi]$ for the internal potential, which singles out the relevant configurations and, therefore, go beyond the Gaussian case? Here is a suitable candidate:

$$W[\phi] = \exp \left( -\frac{u}{4} \int d^2 x (\nabla^2 \phi)^2 \delta_\lambda(\nabla \phi) \right) \equiv \exp (-\mathcal{H}_1/T)$$

with the Gaussian (‘delta function’) $\delta_\lambda(E) = (2\pi\lambda)^{-1} \exp(-E^2/(2\lambda))$.

First, we investigate the mathematics of this ansatz. For $\lambda \to \infty$ the measure $W[\phi]$ is Gaussian and simply renormalizes the mass $z$. For small $\lambda$, on the other hand, the function $\delta_\lambda(\nabla \phi)$ picks up zeros of $\nabla \phi$, i.e. local maxima, minima and saddle points of the potential $\phi$. We expand $\phi$ in the vicinity of an extremal point $x_0$ (where $\nabla \phi(x_0) = 0$) up to second order in $\xi = x - x_0$:

$$\phi(x_0 + \xi) \approx \phi(x_0) + (1/2)\alpha_{ij} \xi_i \xi_j \quad i, j = 1, 2$$

(summation over double indices is assumed) and find for the contribution of this extremum (for $\lambda \to 0$)

$$\mathcal{H}_1/T = \frac{u}{4} \int d^2 x (\nabla^2 \phi)^2 \delta_\lambda(\nabla \phi)$$

$$\approx \frac{u}{4} \int d^2 \xi (\alpha_{ii})^2 \frac{1}{2\pi\lambda} \exp \left( -\frac{\alpha_{ij} \xi_i \xi_j}{2\lambda} \right)$$

$$= u \left( \frac{\eta_1 + \eta_2}{2} \right)^2 / |\eta_1 \eta_2|$$

(2.3)
where $\eta_{1,2}$ are the eigenvalues of the second derivative $\partial_i \partial_j \phi = \alpha_{ij}$ right at the extremal point. Maxima/minima yield a contribution $\mathcal{H}_1/T \geq u$, since $\eta_1 \cdot \eta_2 > 0$. For a symmetric maximum/minimum $\eta_1 = \eta_2$ and consequently $\mathcal{H}_1/T = u$; on the other hand, a ‘symmetric’ saddle point yields zero, since $\eta_1 = -\eta_2$. Therefore, the nonlinear term acts as a kind of chemical potential for the number of extremal points

$$\mathcal{H}_1/T \geq u \times \#(\text{local maxima and minima of } \phi).$$

(2.4)

To summarize this point, the nontrivial measure $\mathcal{W}[\phi]$ favours potentials with only few maxima and minima, which are in fact the physically relevant ones. Consider a typical charge configuration of a Coulomb gas system right above the transition temperature. Apart from a large number of dipoles, which give rise to an effective dielectric constant, we find few free charges $q_i = \pm 1$ at positions $r_i$. The corresponding potential $\phi(r) = \sum q_i G(r - r_i)$ has (few) maxima and minima at the locations of the charges $r_i$ (if we use a short-distance regularized Green function $G$, otherwise the potential $\phi$ would diverge at the locations $r_i$) and symmetric saddle points elsewhere, since $\Delta \phi(r) = 0$ for $r \neq r_i$.

We rescale the potential $\sqrt{\mu} \phi \rightarrow \phi$ and the constant $\mu \lambda \rightarrow \lambda$, define the mass $\tau \equiv K_A/\mu$, and obtain as the final model

$$\mathcal{H}/T = \int d^2 x \left( \frac{1}{2} (\nabla^2 \phi)^2 + \frac{\tau}{2} (\nabla \phi)^2 + \frac{u}{4} (\nabla^2 \phi)^2 \delta_\lambda (\nabla \phi) \right).$$

(2.5)

The coupling constants $u, \lambda$ are dimensionless, whereas $\tau$ is a relevant coupling with dimension $\tau \sim \text{length}^{-2}$—it is a measure for the deviation from the critical point $\tau \sim T - T_c$.

3. Variational approach

We calculate an upper bound of the free energy $\mathcal{F}$ of our model (2.5) with the help of

$$\mathcal{F} = -\log \int D[\phi] \exp(-\mathcal{H}/T) \leq \mathcal{F}_v + \langle \mathcal{H} - \mathcal{H}_v \rangle_v,$$

(3.1)

and the ansatz

$$\mathcal{H}_v/T = \frac{A}{2} \int d^2 x \left( (\nabla^2 \phi)^2 + \omega (\nabla \phi)^2 \right)$$

(3.2)

where $A$ and $\omega$ are variational parameters, $\mathcal{F}_v$ is the free energy with respect to $\mathcal{H}_v$ and $\langle \ldots \rangle_v$ denotes the corresponding average. In fact, the optimal Gaussian fit has the form given above—a more general ansatz is not necessary and would reduce to an expression such as (3.2). To evaluate $\langle (\nabla^2 \phi(r))^2 \delta_\lambda (\nabla \phi(r)) \rangle_v$, we note that $\nabla \phi(r)$ and $\nabla^2 \phi(r)$ are uncorrelated Gaussian variables and, therefore (we drop the argument $r$ from now on),

$$\langle (\nabla^2 \phi)^2 \delta_\lambda (\nabla \phi) \rangle_v = \frac{1}{\pi} \frac{\exp(-E^2/\langle (\nabla \phi)^2 \rangle_v - E^2/(2\lambda))}{\langle (\nabla^2 \phi)^2 \rangle_v + 2\pi \lambda}$$

$$\langle (\nabla^2 \phi)^2 \rangle_v.$$ 

(3.3)

The expectation value $\langle (\nabla \phi)^2 \rangle_v$ diverges for $\omega \rightarrow 0$ and, therefore, the width $\lambda$ of the Gaussian $\delta_\lambda$ becomes irrelevant, justifying the introduction of a sharp delta-function

$\dagger$ The number of saddles is equal to the number of maxima and minima for a flat geometry.
(\lambda \to 0)$ in the model (2.3). Up to the constant $\langle \mathcal{H}_w \rangle$, we obtain the upper bound of the free energy per area $f$

$$8\pi f \leq \int_0^\Lambda^2 ds \log(A(s + \omega)) + \int_0^\Lambda^2 ds \frac{s^2}{As(s + \omega)} + \tau \int_0^\Lambda^2 ds \frac{s}{As(s + \omega)}$$

$$+ 2u \int_0^\Lambda^2 ds \frac{s^2}{As(s + \omega)} \left( \int_0^\Lambda^2 ds \frac{s}{As(s + \omega)} \right)^{-1} \quad (3.4)$$

where the first term represents $F_v$, the second and third term are the expectation value of the Gaussian part of (2.5) and the last term represents $\langle H_1 \rangle_v$. $\Lambda$ is the upper cutoff momentum and $s = p^2, \pi ds = \pi p dp = d^2 p$ using polar coordinates. Next, we set $\Lambda = 1$ (equivalently we can introduce dimensionless couplings), eliminate $A$ (variation of the bound $f$ with respect to $A$ yields $A = 1 + (\tau - \omega) \log(1 + 1/\omega)$) and arrive at

$$8\pi f \leq \log(1 + (\tau - \omega) \log(1 + 1/\omega)) + \log(1 + \omega) + \omega \log(1 + 1/\omega)$$

$$+ 2u \left( \frac{1}{\log(1 + 1/\omega)} - \omega \right). \quad (3.5)$$

It can be tested afterwards that $\omega$ and $(\tau - \omega) \log(1 + 1/\omega)$ become small enough in the critical region to approximate $\log(1 + (\ldots)) \approx (\ldots)$ in the first two terms of (3.5). The expression is especially simple for $u = 1/2$

$$8\pi f \leq \tau \log(1 + 1/\omega) + \frac{1}{\log(1 + 1/\omega)} \quad (3.6)$$

yielding the minimum $\log(1 + 1/\omega) = 1/\sqrt{\tau}$ or

$$\omega \approx \exp \left( -\frac{1}{\sqrt{\tau}} \right) \quad (3.7)$$

where we have used $1 + \omega^{-1} \approx \omega^{-1}$ for $\tau \to 0$. $\xi = \omega^{-1/2}$ is the correlation length of the best Gaussian fit, hence an estimate for the correlation length as a function of $\tau$

$$\xi \sim \exp \left( \frac{1}{2 \sqrt{\tau}} \right) \quad (3.8)$$

which is the celebrated essential singularity of the correlation length in the vicinity of the Kosterlitz–Thouless transition. For general $u$ we obtain $\omega = \exp(-\sqrt{2u}/\tau)$.

4. Renormalized perturbation theory

We have also studied the model Hamiltonian (2.3) within a simple (renormalized) perturbation expansion. Using the formalism presented in [9, 10, 11], we have calculated the two-point vertex function $\Gamma_2(p)$, which is the reciprocal Fourier transform of the Green function $\langle \phi(x)\phi(y) \rangle$, to lowest order in the coupling constant $u$. Details of the derivation can be found in the appendix. The vertex function displays a highly unconventional large-scale behaviour if compared to usual critical field theory. The resulting effective couplings are in fact finite in the limit $\tau \to 0$ and fixed cutoff. Since an instability shows up as a mere artefact of the expansion, we have to introduce a (finite) shift of the mass $\tau \to \tau + u \Delta \tau$, where we treat $u \Delta \tau \int d^2 x (\nabla \phi)^2 / 2$ along with the interaction term as a perturbation. For fixed spatial dimension $d = 2$, fixed
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cutoff momentum $\Lambda = 1$, a sharp delta function $\lambda \to 0$ and up to $O(u^2)$, the two-point vertex function reads (see appendix)

$$\Gamma_2(p) = A_{\text{eff}} (p^4 + \tau_{\text{eff}} p^2)$$

(4.1)

with the effective couplings

$$\tau_{\text{eff}} = \tau + u \Delta \tau - \frac{2u}{(\log(1 + 1/\tau))^2}$$

(4.2)

$$A_{\text{eff}} = 1 + \frac{2u}{\log(1 + 1/\tau)}.$$  

(4.3)

As a consequence of the $\delta(\nabla \phi)$—term and in contrast to ordinary field theories, the log—terms show up in the denominator and, consequently, the effective couplings remain finite in the critical limit $\tau \to 0$. However, at a particular $\tau$, provided $\Delta \tau = 0$, the effective mass becomes negative, signalling the breakdown of the naive perturbation theory. Even worse, the correction to the mass, divided by $\tau$ itself, tends to infinity in the limit $\tau \to 0$. To absorb this divergence, we renormalize the mass by setting

$$\Delta \tau = \frac{2}{(\log(1 + 1/\tau))^2}.$$  

(4.4)

Now, the effective mass reads $\tau_{\text{eff}} = \tau$ and the deviation from the critical point is $\tau_0 = \tau + u \Delta \tau \approx u \Delta \tau$ for small $\tau$. We arrive at

$$\tau_0 = \frac{2u}{(\log(1 + 1/\tau_{\text{eff}}))^2}$$

(4.5)

or $\tau_{\text{eff}} \sim \exp \left( -\frac{\sqrt{2u}}{\tau_0} \right)$ in agreement with the variational calculation.

5. Conclusions

We have proposed an alternative model for the high-temperature phase of the two-dimensional Coulomb gas. It describes the fluctuations of the internal electrical potential with the help of a measure term, which favours potentials corresponding to configurations of only few charges. The range of validity of this model apparently extends down to the critical point—the model yields the correct singular behaviour of the correlation length while approaching the Kosterlitz–Thouless point from above, as shown within a simple (renormalized) perturbation expansion. In addition, a Gaussian variational approximation scheme turned out to be successful, in contrast to the sine–Gordon theory [12], where an analogous Gaussian variational ansatz fails and yields a wrong singularity for the correlation length [13].

Several questions could not be addressed, for example how to extract the singular behaviour of the free energy or the universal critical superfluid density. In our opinion, the model deserves future investigations—thanks to its fascinating and unconventional properties.

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Appendix A. Calculation of the two-point vertex function

For fixed spatial dimension \( d = 2 \), \( \lambda \to 0 \) and up to \( O(u^2) \), the two-point correlation function reads

\[
\langle \phi(x)\phi(y) \rangle = \langle \phi(x)\phi(y) \rangle_0 + \frac{u}{4} \int d^2z \left( \langle \phi(x)\phi(y) \rangle_0 \left( 2 \Delta \tau \left( \nabla \phi(z) \right)^2 + \left( \nabla^2 \phi(z) \right)^2 \delta \left( \nabla \phi(z) \right) \right) \right)_0
\]

\[
- \left( \langle \phi(x)\phi(y) \rangle \left( 2 \Delta \tau \left( \nabla \phi(z) \right)^2 + \left( \nabla^2 \phi(z) \right)^2 \delta \left( \nabla \phi(z) \right) \right) \right)_0 + O(u^2)
\]

where \( \langle \ldots \rangle_0 \) denotes the (Gaussian) average with respect to the quadratic part

\[ H_0 = \frac{1}{2} \int d^2x \left( \nabla^2 \phi \right)^2 + \tau \left( \nabla \phi \right)^2 \]

As explained in the main text, we have introduced a mass shift \( \tau \to \tau + u \Delta \tau \) and treat \( u \Delta \tau \int d^2x \left( \nabla \phi \right)^2 / 2 \) as a counterterm (additional perturbation). The bare Green function reads

\[
G_0(p) = \int d^2x \langle \phi(x)\phi(0) \rangle_0 \exp(-ip \cdot x) = \frac{1}{p^2(p^2 + \tau)} \tag{A.2}
\]

The counterterm adds

\[
G_c(p) = -u \Delta \tau G_0(p)^2 p^2 = -u \Delta \tau \frac{1}{p^2(p^2 + \tau)^2} \tag{A.3}
\]

More involved are the contributions from the measure. We define the Gaussian variables \( \phi_1 \equiv \phi(x), \phi_2 \equiv \phi(y), \rho \equiv \nabla^2 \phi(z), E \equiv \nabla \phi(z) \), the five-component vector \( M \equiv (\phi_1, \phi_2, \rho, E) \), and write down the distribution of \( M \) with the help of a Gaussian transformation \[ \int \frac{1}{(2\pi)^5} d\phi_1 d\phi_2 d\rho dE d\phi_1 d\phi_2 d\rho d\phi_1 d\phi_2 d\rho dE \]

\[
= \exp \left( -\frac{1}{2} \left( \phi_1^2 + \phi_2^2 \right) + \rho^2 \left( \nabla^2 \phi \right)^2 + \nabla \phi \cdot \delta \left( \nabla \phi \right) \right)
\]

\[
+ 2\tilde{\phi}_1 \tilde{\phi}_2 \langle \phi(x)\phi(y) \rangle + 2\tilde{\rho} \tilde{\phi}_1 \langle \phi(x) \nabla^2 \phi(z) \rangle + 2\tilde{\rho} \tilde{\phi}_2 \langle \phi(y) \nabla^2 \phi(z) \rangle
\]

\[
+ 2\tilde{E} \tilde{\rho} \cdot \langle \phi(x) \nabla \phi(z) \rangle + 2\tilde{E} \tilde{\phi}_2 \cdot \langle \phi(y) \nabla \phi(z) \rangle
\]

\[
+ i \left( \phi_1 \phi_2 + \phi_2 \phi_1 + \rho \rho + E \cdot E \right) \left( \phi_1 \phi_2 \rho^2 \delta(E) \right) \tag{A.5}
\]

where the correlations \( \langle \nabla^2 \phi(z) \nabla \phi(z) \rangle \) vanish by symmetry. Next, we perform the trivial \( E \) integration and the \( \tilde{E} \) integration and obtain

\[
(*) = \frac{1}{(2\pi)^3} \frac{1}{\pi \left( \nabla \phi \right)^2} \int d\tilde{\phi}_1 d\tilde{\phi}_2 d\rho d\phi_1 d\phi_2 d\rho
\]

\[
\times \exp \left( -\frac{1}{2} \left( \tilde{\phi}_1^2 + \tilde{\phi}_2^2 \right) + \tilde{\rho}^2 \left( \nabla^2 \phi \right)^2 \right)
\]

\[
\times \exp \left( -\frac{1}{2} \left( \tilde{\phi}_1^2 + \tilde{\phi}_2^2 \right) \left( \phi^2 \right) + \tilde{\rho}^2 \left( \nabla^2 \phi \right)^2 \right) \]
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\[ + 2 \hat{\phi}_1 \hat{\phi}_2 \langle \phi(x) \phi(y) \rangle + 2 \hat{\rho} \hat{\phi}_1 \langle \phi(x) \nabla^2 \phi(z) \rangle + 2 \hat{\rho} \hat{\phi}_2 \langle \phi(y) \nabla^2 \phi(z) \rangle \]

\[- \frac{2}{\langle \nabla \phi \rangle^2} \left( \hat{\phi}_1 \langle \phi(x) \nabla \phi(z) \rangle + \hat{\phi}_2 \langle \phi(y) \nabla \phi(z) \rangle \right)^2 \]

\[ + i \left( \hat{\phi}_1 \phi_1 + \hat{\phi}_2 \phi_2 + \hat{\rho} \rho \right) \phi_1 \phi_2 \rho. \] (A.6)

The variables \( \phi_1, \phi_2, \rho \) are still Gaussian variables, with, however, modified correlations which can be found from (\ref{A.8}). Therefore, using Wick’s theorem

\[ \langle \phi(x) \phi(y) \rangle = \frac{\langle \nabla^2 \phi \rangle^2 \delta(\nabla \phi) \rangle}{\pi \langle \nabla \phi \rangle^2} \] (A.7)

yielding the following contribution of the measure term:

\[ G_1(p) = \frac{u}{2 \pi \langle \nabla \phi \rangle^2} \left( \frac{1}{p^2 + \tau} \right) \left( \frac{\langle \nabla^2 \phi \rangle^2}{\langle \nabla \phi \rangle^2} \right). \] (A.9)

The vertex function reads

\[ \Gamma_2(p) = (G_0 + G_c + G_1)^{-1} = p^2(p^2 + \tau) + u \Delta \tau p^2 \]

\[ + \frac{u}{2 \pi \langle \nabla \phi \rangle^2} \left( p^4 - \frac{\langle \nabla^2 \phi \rangle^2}{\langle \nabla \phi \rangle^2} p^2 \right) + O(u^2) \]

\[ \equiv A_{\text{eff}} (p^4 + \tau_{\text{eff}} p^2) \] (A.10)

with the effective coupling constants (up to order \( O(u^2) \) and cutoff momentum \( \Lambda = 1 \)

\[ A_{\text{eff}} = 1 + u / \left( \frac{1}{2 \pi} \int_{|p| < \Lambda} d^2 p \frac{1}{p^2 + \tau} \right) = 1 + \frac{2u}{\log(1 + 1/\tau)} \] (A.11)

and

\[ \tau_{\text{eff}} = \tau + u \Delta \tau - \frac{\tau u}{2 \pi \langle \nabla \phi \rangle^2} - \frac{u \langle \nabla^2 \phi \rangle^2}{2 \pi \langle \nabla \phi \rangle^2} \]

\[ = \tau + u \Delta \tau - \frac{2u}{\log(1 + 1/\tau)}. \] (A.12)

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