

Chapter 2

d -Dimensional Coulomb Gas

2.1 Introduction

As was discussed in the previous chapter, renormalization group serves as a very powerful tool in the study of strong interactions and fluctuations, which occur near continuous phase transitions. This powerful method presents a conceptual framework which allows for capturing complex natural phenomena in terms of a few mesoscopic variables. In this chapter we will consider an equilibrium system of charges, however, the concept can also be applied in the context of dynamic critical phenomena, which will be the subject of later chapters.

The d -dimensional Coulomb gas is a statistical mechanical problem where particles of equal or opposite charge interact through the Coulomb potential. The model has been extensively studied in the past and forms one of the classical problems in field theory [1].

To this end, most of the theoretical investigations have been centered around the particular case of two dimensions. In this regime the model undergoes the celebrated Kosterlitz-Thouless phase transition [2]. The integer-charged particles interact via a logarithmic potential. Alternatively, the charges can be viewed as vortices which carry integer vorticity. At low temperature these vortices are bound in pairs and carry zero vorticity and thus form an insulating state. At higher temperatures the binding of vortices decreases until at some critical temperature, T_c , the vortices are completely unbound, thereby forming a conducting state.

The special property of the Kosterlitz-Thouless phase transition is the behavior of the correlation functions. In the metallic state one observes screening because the charges are unbound. As a result, the correlation function decays exponentially fast. In the insulating phase the correlation function decays algebraically, meaning that charge fluctuations are correlated over infinite distances, hence the correlation length is divergent throughout the insulating phase. By contrast, in the Ising model and other second-order phase transitions, the correlation function, above and below some critical temperature, T_c , decays exponentially fast and only at the critical temperature

the correlation functions decays algebraically. For that reason the insulating phase is referred to as a phase of quasi-long-range order.

The two-dimensional Coulomb gas falls into the same universality class as other statistical mechanical models such as the XY-model and the two-dimensional sine-Gordon model [1, 3]. Such mappings provide a relationship between seemingly different physical systems and provide an efficient tool for analyzing two dimensional problems in statistical mechanics [4, 5].

A part from the connection of the Coulomb gas to other physical systems, the d -dimensional Coulomb gas can be used as a model of a classical one-component plasma [5, 6]. Such plasmas are found in astrophysical systems such as white dwarfs, for example. In this thesis we will be primarily concerned with the plasma characteristics of the Coulomb gas rather than its connections to other physical models. Although the system does not undergo a phase transition for spatial dimensions $d > 2$, a renormalization group analysis can be utilized to study the role of the intrinsic length scales of the system in the behavior physical quantities such as the Debye length. Such calculations can be important in numerical simulations of plasma [7]. In the next section we will give an overview of renormalization group (RG) techniques used so far in the study of the Coulomb gas, before we present the Coulomb gas model formally and analyze it using a somewhat simpler RG method.

2.1.1 Renormalization Group Methodologies

If we go back to the particular case of $d = 2$, it must be stressed that while the argument in favor of Kosterlitz-Thouless phase transition can be relatively easily demonstrated by means of a perturbative RG analysis, the extrapolation of the behavior of the correlation function to the whole phase-space has proved to be a difficult task [1]. So, here we acknowledge some of the rigorous results which have been established for the $d = 2$ Coulomb gas [8]. Consider the metal-insulator phase space diagram:

Consider the red region in the Fig. 2.1, which represents the region of phase space sufficiently far from the critical line. It has been shown by [9] that the correlation function does indeed follow a power law decay for any z . For the opposite region, shaded blue, which is also sufficiently far from the critical line a somewhat similar result, but slightly weaker, consists of a proof that the correlation function decays exponentially for $|z| > 0$, subject to a specific boundary condition [10]. A number of other results which are concerned with rigorous proofs on the behavior of the correlation functions in different regions of the phase-space can be found here [8, 9, 11]. In this thesis we will not be concerned with these matters any further. Our analysis will be limited strictly to the vicinity of critical points.

As we have established in the first part of the thesis, there are a number of techniques to execute the RG program. One by means of field theory methods and the other by using the Wilson-Kadanoff style of RG. An extensive RG study of the Coulomb gas in two dimensions using the formalism of field theory is given by Amit [12]. In their detailed chapter the authors computed higher-order corrections in the

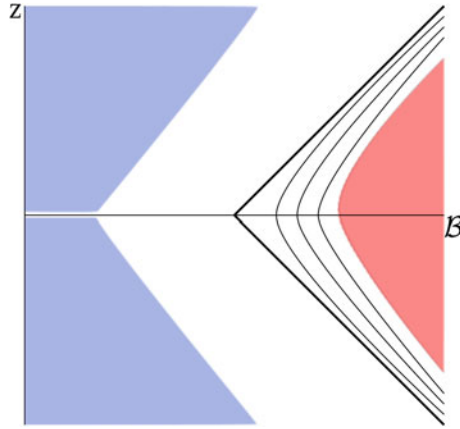


Fig. 2.1 Phase-space diagram of the $d = 2$ Coulomb gas. The two parameters of the system are z , the fugacity, and β , the inverse of the temperature. The *thick line* represents a critical line. To the *right* of the critical line, the low temperature regime, the system is in an insulating state. Vortices are bound together, with the net vorticity being zero. To the *left* of the critical line charges are unbound which forms a metallic state

flow equations, to those originally derived by Kosterlitz [2], and have shown that vortices with multiple charges are irrelevant in the RG sense. This investigations did not consider any other dimensions other than $d = 2$.

A version of real-space renormalization group RG has been given by [13]. In this chapter the RG flow has been derived for all physical dimensions. The coarse-graining of the action in the momentum space has received most of the attention in the literature. A paper exploiting the Wegner-Houghton [14] approach, for example, is [15]. A detailed calculation which exploits a standard cumulant expansion is [16].

In this thesis we present yet another RG scheme, which, to our knowledge, has not been used in the literature in the context of d -dimensional Coulomb gas. It is based on irreducible differential formulation of the Wilson-Kadanoff RG and has been successfully applied in the past to other models in statistical mechanics [17]. As suggested by the word irreducible, the object of interest is the vertex function or the Legendre transform of the free energy. The RG is formulated in terms of the integro-differential equation which describes the infinitesimal change of the vertex function under sequential mode averaging. Once compared to earlier mentioned calculations, we believe that this approach has distinct advantages in terms of conciseness and simplicity of the resultant integrals.

In the next section we will introduce the Coulomb gas model formally and derive the continuum theory in order to facilitate the Wilson-Kadanoff style of RG.

2.2 Functional Integral

2.2.1 Lattice Model

We begin by considering a d -dimensional Cartesian lattice whose spacing is a and with a total volume of V . Charges $\pm e$ can occupy the sites i_k of this lattice and there is a Coulomb interaction between these charges. For $d = 3$, the lattice Coulomb potential between sites i_j and i_k is

$$U_{ij} = \frac{1}{4\pi a |i_j - i_k|}. \quad (2.2.1)$$

There are two main reasons for putting the system on a lattice. First, the lattice avoids the singularity of the Coulomb potential at the origin, which would otherwise necessitate introducing a short-range cut-off. This issue arises when we take the continuum limit, but for the moment there are no short-range singularities. The other advantage of a lattice formulation is that we can develop a field-theoretic formulation for the partition function, which facilitates the identification with mean-field limits and perturbations therefrom.

The canonical partition function \mathcal{Z}_N for N charges $q_k = \pm e$ at positions i_k , for $k = 1, \dots, N$, is

$$\mathcal{Z}_N = \sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \frac{1}{N!} \exp \left[-\frac{\beta}{2} \sum'_{\substack{j,k \\ 1 \leq j,k \leq N}} q_j U(i_j, i_k) q_k \right], \quad (2.2.2)$$

where the factor $N!$ is to ensure correct Boltzmann counting, $\beta = 1/k_B T$, k_B is Boltzmann's constant, T is the absolute temperature, the prime on the summation indicates that the terms $j = k$ are excluded, and the factor of $1/2$ is to avoid double counting. The associated grand canonical partition function Ξ is

$$\Xi = \sum_{N=0}^{\infty} z^N a^{Nd} \mathcal{Z}_N, \quad (2.2.3)$$

where $z = e^{\beta\mu}$ is the fugacity and μ is the chemical potential.

The evaluation of Ξ proceeds by using the Hubbard–Stratonovich transformation, which is a standard operating procedure for such Hamiltonians. Based on the identity

$$\exp\left(\frac{b^2 y^2}{2a}\right) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2 + bxy} dx, \quad (2.2.4)$$

the Hubbard-Stratonovich transformation for a symmetric $N \times N$ matrix \mathbf{A} with real eigenvalues is

$$e^{\frac{1}{2} \sum_{ij} A_{ij} s_i s_j} = \left\{ \frac{1}{|\mathbf{A}| (2\pi)^N} \right\}^{1/2} \int \dots \int e^{-\frac{1}{2} \sum_{ij} (A^{-1})_{ij} \phi_i \phi_j + \sum_i \phi_i s_i} \left(\prod_{i=1}^N d\phi_i \right), \quad (2.2.5)$$

where $|\mathbf{A}|$ is the determinant of \mathbf{A} . This identity is used to represent Ξ as

$$\begin{aligned} \mathcal{Z}_N &= \sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \frac{1}{N!} \exp \left[-\frac{\beta}{2} \sum'_{\substack{j,k \\ 1 \leq j,k \leq N}} q_j U(i_j, i_k) q_k \right] \\ &= \left\{ \frac{1}{|\mathbf{U}| (2\pi)^N} \right\}^{1/2} \sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \frac{1}{N!} \int \dots \int e^{-\frac{1}{2} \beta^{-1} \sum_{jk} \phi_{i_j} (\mathbf{U}^{-1})_{jk} \phi_{i_k} + i \sum_k \phi_{i_k} q_k} \left(\prod_{k=1}^N d\phi_{i_k} \right), \end{aligned} \quad (2.2.6)$$

in which \mathbf{U} is the matrix with entries given in Eq. (2.2.1) and the factor of i on the right-hand side is necessary for consistency of signs in Eqs. (2.2.5) and (2.2.6).

2.2.2 Continuum Limit

Consider first the determination of \mathbf{U}^{-1} . In the case of continuous variables, we have the definition [18]

$$\int \mathbf{U}^{-1}(\mathbf{x}, \mathbf{y}) \mathbf{U}(\mathbf{y}, \mathbf{z}) d\mathbf{y} = \delta(\mathbf{x} - \mathbf{z}), \quad (2.2.7)$$

in which $\delta(x)$ is the Dirac delta-function. Since, according to Eq. (2.2.1),

$$U(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi |\mathbf{x} - \mathbf{y}|}, \quad (2.2.8)$$

Equation (2.2.7) is seen to be the definition of the fundamental solution for Poisson's equation:

$$\nabla^2 U(\mathbf{x} - \mathbf{x}') = -\delta(\mathbf{x} - \mathbf{x}'). \quad (2.2.9)$$

Hence,

$$\mathbf{U}^{-1}(\mathbf{x}, \mathbf{y}) = -\delta(\mathbf{x} - \mathbf{y}) \nabla_{\mathbf{x}}^2. \quad (2.2.10)$$

Thus, in the continuum limit, the first term in the exponential on the right-hand side of Eq. (2.2.6) becomes

$$\begin{aligned} \frac{1}{2\beta} \sum_{jk} \phi_{ij} (\mathbf{U}^{-1})_{jk} \phi_{ik} &\rightarrow \frac{1}{2\beta} \int \int \phi(\mathbf{x}) \mathbf{U}^{-1}(\mathbf{x}, \mathbf{y}) \phi(\mathbf{y}) d\mathbf{x} d\mathbf{y} \\ &= -\frac{1}{2\beta} \int \phi(\mathbf{x}) \nabla^2 \phi(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (2.2.11)$$

The summation over the q_k on the right-hand side can now be carried out:

$$\begin{aligned} \sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \exp\left(i \sum_{k=1}^N \phi_{i_k} q_k\right) &= \sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \prod_{k=1}^N e^{i\phi_{i_k} q_k} = \sum_{\{i_k\}} \prod_{k=1}^N (e^{-ie\phi_{i_k}} + e^{ie\phi_{i_k}}) \\ &= \sum_{\{i_k\}} \prod_{k=1}^N [2 \cos(e\phi_{i_k})] \\ &= \left[\sum_{i_k} 2 \cos(e\phi_{i_k}) \right]^N. \end{aligned} \quad (2.2.12)$$

In the continuum limit, the summation becomes an integral and this term simplifies to

$$\sum_{\substack{\{i_k\} \\ \{q_k = \pm e\}}} \exp\left(i \sum_{k=1}^N \phi_{i_k} q_k\right) = \left\{ \frac{1}{a^d} \int 2 \cos[e\phi(\mathbf{x})] d\mathbf{x} \right\}^N. \quad (2.2.13)$$

Carrying out the summation over N in Eq. (2.2.3) yields the continuum limit of the grand canonical partition function Ξ :

$$\begin{aligned} \Xi &= \left\{ \frac{1}{|\mathbf{U}|(2\pi)^N} \right\}^{1/2} \int \exp\left[\frac{1}{2\beta} \int \phi \nabla^2 \phi d\mathbf{x}\right] \sum_{N=0}^{\infty} \frac{z^N a^{Nd}}{N!} \left\{ \frac{1}{a^d} \int 2 \cos[e\phi(\mathbf{x})] d\mathbf{x} \right\}^N D[\phi] \\ &= \left\{ \frac{1}{|\mathbf{U}|(2\pi)^N} \right\}^{1/2} \int \exp\left[\frac{1}{2\beta} \int \phi \nabla^2 \phi d\mathbf{x}\right] \exp\left[z \int 2 \cos(e\phi) d\mathbf{x}\right] D[\phi] \\ &= \left\{ \frac{1}{|\mathbf{U}|(2\pi)^N} \right\}^{1/2} \int \exp\left\{ \int \left[\frac{1}{2\beta} \phi \nabla^2 \phi + 2z \cos(e\phi) \right] d\mathbf{x} \right\} D[\phi]. \end{aligned} \quad (2.2.14)$$

The right-hand side of this equation is the functional integral for the Debye problem. The first term represents a ‘kinetic energy’, which results from the Coulomb interaction, and the second term a ‘potential energy’, which arises from the Hubbard–Stratonovich transformation. The prefactor is not important for calculating thermodynamic averages, and will be omitted in what follows. A somewhat more concise form of this representation is obtained by introducing a new field variable $\phi = \varphi \sqrt{\beta}$, in which case we obtain

$$\Xi = \int \exp \left\{ \int \left[\frac{1}{2} \varphi \nabla^2 \varphi + 2z \cos(\alpha \varphi) \right] d\mathbf{x} \right\} D[\varphi], \quad (2.2.15)$$

with $\alpha = e/\sqrt{k_B T}$.

There are several advantages to the functional integral representation of a statistical mechanical problem over other formulations:

1. A large class of problems can be represented as functional integrals, ranging from equilibrium statistical mechanics, as the Debye problem, to non-equilibrium statistical dynamics. The Ising model serves as the canonical example for this approach, and the expression obtained in Eq. (2.2.15) has several formal similarities with the functional integral for the Ising model.
2. Mean-field limits are straightforward to identify, for example, as Gaussian field theories, corrections to which can be evaluated with various expansions. For the case at hand, the mean-field limit corresponds to the Debye–Hückel theory. This will be shown explicitly in the next section.
3. Renormalization-group calculations can be carried out using either the Wilson or field-theoretic formalism. Time-dependence, vector fields, and other degrees of freedom enter such calculations simply as summations/integrals in the evaluation of individual terms. The structure of the RG expansion is determined by the polynomial terms in the functional integral.
4. An alternative form of the functional integral in Eq. (2.2.15) is obtained by performing an integration by parts on the first term:

$$\Xi = \int \exp \left\{ - \int \left[\frac{1}{2} (\nabla \varphi)^2 - 2z \cos(\alpha \varphi) \right] d\mathbf{x} \right\} D[\varphi]. \quad (2.2.16)$$

In writing this expression, we have neglected the surface term, which is a finite constant and so does not affect our subsequent calculation.

2.3 Mean-Field Approximation

The simplest evaluation of the functional integral (2.2.15) is to expand the cosine function and retain terms only to quadratic order:

$$\cos(\alpha \varphi) = 1 - \frac{(\alpha \varphi)^2}{2} + \dots, \quad (2.3.1)$$

which yields a Gaussian field theory,

$$\begin{aligned} \Xi &= \int \exp \left\{ \frac{1}{2} \int \left[\varphi \nabla^2 \varphi + 4z - 2z(\alpha \varphi)^2 \right] d\mathbf{x} \right\} D[\varphi] \\ &= e^{2zV} \int \exp \left[\frac{1}{2} \int \left(\varphi \nabla^2 \varphi - \xi^{-2} \varphi^2 \right) d\mathbf{x} \right] D[\varphi], \end{aligned} \quad (2.3.2)$$

where V is the volume of the system and $\xi^{-2} = 2z\alpha^2$. We will again neglect the constant prefactor, since we are interested only in averages.

The functional Gaussian integrals in Eq. (2.3.2) are carried out by transforming to a Fourier representation of decoupled modes. For a finite volume V , the Fourier transform $\varphi_{\mathbf{k}}$ of $\varphi(\mathbf{x})$ is

$$\varphi_{\mathbf{k}} = \int_V \varphi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} d\mathbf{x}, \quad (2.3.3)$$

where, since $\varphi(\mathbf{x})$ is real, we have that $\varphi_{-\mathbf{k}} = \varphi_{\mathbf{k}}^*$. The inverse Fourier transform is

$$\varphi(\mathbf{x}) = \frac{1}{V} \sum_{\mathbf{k}} \varphi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (2.3.4)$$

The largest wavevector in this summation is $\Lambda \equiv 2\pi/a$, where a is the lattice constant on our Cartesian lattice, and the smallest is $2\pi/L$, where $V = L^3$ is the volume of the system and which approaches zero as $L \rightarrow \infty$. These are referred to as *ultraviolet* and *infrared* cutoffs, respectively. Critical quantities should not depend on the values of these cutoffs. Since there is one wavevector per volume $(2\pi/L)^d$ in \mathbf{k} -space, summations over \mathbf{k} are converted into integrals according to

$$\sum_{\mathbf{k}} = \int d\mathbf{k} \left(\frac{L}{2\pi} \right)^d = V \int \frac{d\mathbf{k}}{(2\pi)^d}. \quad (2.3.5)$$

This transcription is exact only in the thermodynamic limit ($V \rightarrow \infty$). The transformed grand canonical partition function thereby reads

$$\Xi = \int \prod_{\mathbf{k}} d\varphi_{\mathbf{k}} \exp \left[-\frac{1}{2V} \sum_{\mathbf{k}} (k^2 + \xi^{-2}) |\varphi_{\mathbf{k}}|^2 \right]. \quad (2.3.6)$$

Consider now the evaluation of the two-point correlation function $\langle \varphi(\mathbf{q})\varphi(\mathbf{q}') \rangle$ which, in the limit $V \rightarrow \infty$, is calculated as

$$\begin{aligned} \langle \varphi(\mathbf{q})\varphi(\mathbf{q}') \rangle &= \frac{1}{\Xi} \int D\varphi(\mathbf{k}) \left[\varphi(\mathbf{q})\varphi(\mathbf{q}') \right] \exp \left[-\int_0^\Lambda \frac{d\mathbf{k}}{(2\pi)^d} (k^2 + \xi^{-2}) |\varphi(\mathbf{k})|^2 \right] \\ &= \frac{\delta(\mathbf{q} + \mathbf{q}')}{q^2 + \xi^{-2}}. \end{aligned} \quad (2.3.7)$$

Performing the Fourier transform yields the real-space correlation function

$$\langle \varphi(\mathbf{r})\varphi(\mathbf{0}) \rangle = \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{e^{-i\mathbf{q}\cdot\mathbf{r}}}{q^2 + \xi^{-2}} = \frac{e^{-r/\xi}}{4\pi r}. \quad (2.3.8)$$

The quantity

$$\xi^{-2} = 2z\alpha^2 = \frac{2ze^2}{k_B T} \quad (2.3.9)$$

is seen to correspond to a screening length. To obtain an explicit expression for this quantity, we need an expression for the fugacity z . This can be obtained from the following two standard statistical mechanical relations for the grand canonical partition function

$$\langle N \rangle = \frac{1}{\Xi} \sum_{N=0}^{\infty} N z^N a^{Nd} \mathcal{Z}_N = z \frac{\partial \ln \Xi}{\partial z}, \quad (2.3.10)$$

$$\frac{PV}{k_B T} = \ln \Xi = 2zV + \ln \left\{ \int \exp \left[\frac{1}{2} \int (\varphi \nabla^2 \varphi - \xi^{-2} \varphi^2) d\mathbf{x} \right] D[\varphi] \right\}, \quad (2.3.11)$$

where P is the pressure of the system and we have used Eq. (2.3.2) in the second equation. We now consider the high temperature limit, in which case ξ^{-2} is small. Since the second term on the right-hand side of Eq. (2.3.11) is the only term with an explicit z -dependence, this limit suppresses the contribution from this term in the derivative in Eq. (2.3.10), leaving

$$\langle N \rangle = 2zV, \quad (2.3.12)$$

or

$$2z = \frac{\langle N \rangle}{V} = n_0, \quad (2.3.13)$$

where n_0 is the average particle density. Hence, the decay length reduces to

$$\xi = \left(\frac{k_B T}{n_0 e^2} \right)^{1/2}, \quad (2.3.14)$$

which is the standard result for the Debye length [6]. The validity of this results rests on the assumption that the $\cos(\alpha\varphi)$ is a slow varying function of position, which is certainly true at high temperatures.

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