8.334 Statistical Mechanics II: Statistical Physics of Fields
Spring 2008

VII.C Renormalization Group for the Coulomb Gas

The two partition functions in eq.(VII.58) are independent and can be calculated separately. As the Gaussian partition function is analytic, any phase transitions of the XY model must originate in the Coulomb gas. As briefly discussed earlier, in the low temperature phase the charges appear only in the small density of tightly bound dipole pairs. The dipoles dissociate in the high temperature phase, forming a plasma. The two phases can be distinguished by examining the interaction between two *external* test charges at a large separation X. In the absence of any *internal* charges (for $y_0 = 0$) in the medium, the two particles interact by the *bare* Coulomb interaction $C(X)$. A finite density of internal charges for small y_0 partially screens the external charges, and reduces the interaction between the test charges to $C(X)/\varepsilon$, where ε is an effective *dielectric* constant. There is an *insulator to metal* transition at sufficiently large y_0. In the metallic (plasma) phase, the external charges are completely screened and their effective interaction decays exponentially.

To quantify the above picture, we shall compute the effective interaction between two *external* charges at $\mathbf{x}$ and $\mathbf{x}'$, perturbatively in the fugacity y_0. To lowest order, we need to include configurations with two *internal* charges (at $\mathbf{y}$ and $\mathbf{y}'$), and

$$\begin{aligned}
&e^{-\beta\mathcal{V}(\mathbf{x}-\mathbf{x}')} = e^{-4\pi^2KC(\mathbf{x}-\mathbf{x}')}\times\\
&\frac{\left[1+y_0^2\int d^2\mathbf{y}d^2\mathbf{y}'\,e^{-4\pi^2KC(\mathbf{y}-\mathbf{y}')+4\pi^2K\left[C(\mathbf{x}-\mathbf{y})-C(\mathbf{x}-\mathbf{y}')-C(\mathbf{y}'-\mathbf{x})+C(\mathbf{x}'-\mathbf{y}')\right]}+\mathcal{O}(y_0^4)\right]}{\left[1+y_0^2\int d^2\mathbf{y}d^2\mathbf{y}'\,e^{-4\pi^2KC(\mathbf{y}-\mathbf{y}')}+\mathcal{O}(y_0^4)\right]}\\
&=e^{-4\pi^2KC(\mathbf{x}-\mathbf{x}')}\left[1+y_0^2\int d^2\mathbf{y}d^2\mathbf{y}'\,e^{-4\pi^2KC(\mathbf{y}-\mathbf{y}')}\left(e^{4\pi^2KD(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')}-1\right)+\mathcal{O}(y_0^4)\right],
\end{aligned} \tag{VII.60}$$

where $D(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')$ is the interaction *between* the internal and external dipoles. The direct interaction between internal charges tends to keep the separation $\mathbf{r} = \mathbf{y}' - \mathbf{y}$ small. Using the center of mass $\mathbf{R} = (\mathbf{y}+\mathbf{y}')/2$, we can change variables to $\mathbf{y} = \mathbf{R} - \mathbf{r}/2$ and $\mathbf{y}' = \mathbf{R} + \mathbf{r}/2$, and expand the dipole–dipole interaction for small $\mathbf{r}$ as

$$\begin{aligned}
D\left(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}'\right) =&C\left(\mathbf{x}-\mathbf{R}+\frac{\mathbf{r}}{2}\right)-C\left(\mathbf{x}-\mathbf{R}-\frac{\mathbf{r}}{2}\right)-C\left(\mathbf{x}'-\mathbf{R}+\frac{\mathbf{r}}{2}\right)+C\left(\mathbf{x}'-\mathbf{R}-\frac{\mathbf{r}}{2}\right)\\
=&-\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}-\mathbf{R})+\mathbf{r}\cdot\nabla_{\mathbf{R}}C(\mathbf{x}'-\mathbf{R})+\mathcal{O}(r^3).
\end{aligned} \tag{VII.61}$$

To the same order

$$\begin{aligned}
e^{4\pi^2KD(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}')}-1=&-4\pi^2K\mathbf{r}\cdot\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\\
&+8\pi^4K^2\left[\mathbf{r}\cdot\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\right]^2+\mathcal{O}(r^3).
\end{aligned} \tag{VII.62}$$

After the change of variables $\int d^2\mathbf{y}d^2\mathbf{y}' \to \int d^2\mathbf{r}d^2\mathbf{R}$, the effective interaction becomes

$$e^{-\beta\mathcal{V}(\mathbf{x}-\mathbf{x}')} = e^{-4\pi^2KC(\mathbf{x}-\mathbf{x}')}\Bigg\{\Bigg[1 + y_0^2\int d^2\mathbf{r}d^2\mathbf{R}\,e^{-4\pi^2KC(\mathbf{r})}\times$$
$$\Big(-4\pi^2K\mathbf{r}\cdot\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)+8\pi^4K^2\left[\mathbf{r}\cdot\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\right]^2$$
$$+\mathcal{O}(r^3)\Big)+\mathcal{O}(y_0^4)\Bigg]\Bigg\}. \tag{VII.63}$$

Following the angular integrations in $d^2\mathbf{r}$, the term linear in $\mathbf{r}$ vanishes, while the angular average of $(\mathbf{r}\cdot\nabla_{\mathbf{R}}C)^2$ is $r^2|\nabla_{\mathbf{R}}C|^2/2$. Hence eq.(VII.63) simplifies to

$$e^{-\beta\mathcal{V}(\mathbf{x}-\mathbf{x}')} = e^{-4\pi^2KC(\mathbf{x}-\mathbf{x}')}\times$$
$$\left[1 + y_0^2\int(2\pi r dr)e^{-4\pi^2KC(r)}8\pi^4K^2\,\frac{r^2}{2}\int d^2\mathbf{R}\big(\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\big)^2+\mathcal{O}(r^4)\right]. \tag{VII.64}$$

The remaining integral can be evaluated by parts,

$$\begin{aligned}
&\int d^2\mathbf{R}\,\left[\nabla_{\mathbf{R}}\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\right]^2\\
=&-\int d^2\mathbf{R}\,\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\left(\nabla^2C(\mathbf{x}-\mathbf{R})-\nabla^2C(\mathbf{x}'-\mathbf{R})\right)\\
=&-\int d^2\mathbf{R}\,\left(C(\mathbf{x}-\mathbf{R})-C(\mathbf{x}'-\mathbf{R})\right)\left(\delta^2(\mathbf{x}-\mathbf{R})-\delta^2(\mathbf{x}'-\mathbf{R})\right)\\
&=2C(\mathbf{x}-\mathbf{x}')-2C(0).
\end{aligned} \tag{VII.65}$$

The short distance divergence can again be absorbed into a proper cutoff with $C(x)\to\ln(x/a)/2\pi$, and

$$e^{-\beta\mathcal{V}(\mathbf{x}-\mathbf{x}')} = e^{-4\pi^2KC(\mathbf{x}-\mathbf{x}')}\left[1+16\pi^5K^2y_0^2C(\mathbf{x}-\mathbf{x}')\int drr^3e^{-2\pi K\ln(r/a)}+\mathcal{O}(y_0^4)\right]. \tag{VII.66}$$

The second order term can be exponentiated to give an effective interaction $\beta\mathcal{V}(\mathbf{x}-\mathbf{x}')\equiv 4\pi^2K_{\text{eff}}C(\mathbf{x}-\mathbf{x}')$, with

$$K_{\text{eff}} = K - 4\pi^3K^2y_0^2a^{2\pi K}\int_a^\infty drr^{3-2\pi K}+\mathcal{O}(y_0^4). \tag{VII.67}$$

We have thus evaluated the dielectric constant of the medium, $\varepsilon = K/K_{\text{eff}}$, perturbatively to order of y_0^2. However, the perturbative correction is small only as long as the integral in r converges at large r. The breakdown of the perturbation theory for

$K < K_c = 2/\pi$, occurs precisely at the point where the free energy of an isolated vortex changes sign. This breakdown of perturbation theory is reminiscent of that encountered in the Landau–Ginzburg model for $d < 4$. Using the experience gained from that problem, we shall reorganize the perturbation series into a renormalization group for the parameters K and y_0.

To construct an RG for the Coulomb gas, note that the partition function for the system in eq.(VII.59), involves two parameters (K, y_0), and has an implicit cutoff a, related to the minimum separation between vortices. As discussed earlier, the distinction between regions inside and outside the core of a vortex are arbitrary. Increasing the core size to ba modifies not only the core energy, hence y_0, but also the interaction parameter K. The latter is a consequence of the change in the dielectric properties of the medium due to dipoles of separations between a and ba. The change in fugacity is obtained from eq.(VII.46) by changing a to ba as

$$\tilde{y_0}(ba) = b^{2-\pi K} y_0(a) \quad . \tag{VII.68}$$

The modified Coulomb interaction due to dipoles of all size is given in eq.(VII.67). (The perturbative calculation at order of y_0^2 incorporates only dipoles.) From dipoles in the size range, a to ba, we obtain a contribution

$$\tilde{K} = K\left[1 - (2\pi^2 K)\int_a^{ba} (2\pi r dr)\left(y_0^2 e^{-4\pi^2 K C(r)}\right) r^2\right], \tag{VII.69}$$

where the terms are grouped so as to make the similarity to standard computations of the dielectric constant apparent. (The probability of creating a dipole is multiplied by its polarizability; the role of $\beta = (k_B T)^{-1}$ is played by $2\pi^2 K$.)

By choosing an infinitesimal $b = e^\ell \approx 1 + \ell$, eq.(VII.69) is converted to

$$\frac{dK}{d\ell} = -4\pi^3 K^2 a^4 y_0^2 + \mathcal{O}(y_0^4) \quad . \tag{VII.70}$$

Including the fugacity, the recursion relations are

$$\begin{cases} \dfrac{dK^{-1}}{d\ell} = 4\pi^3 a^4 y_0^2 + \mathcal{O}(y_0^4) \\ \dfrac{dy_0}{d\ell} = (2-\pi K) y_0 + \mathcal{O}(y_0^3) \end{cases}, \tag{VII.71}$$

originally obtained by Kosterlitz in 1975. While $dK^{-1}/d\ell \geq 0$, the recursion relation for y_0 changes sign at $K_c^{-1} = \pi/2$. At smaller values of K^{-1} (high temperatures) y_0 is relevant, while at lower temperatures it is irrelevant. Thus the RG flows separate the parameter space into two regions. At low temperatures and small y_0, flows terminate on a *fixed line* at $y_0 = 0$ and $K_{\rm eff} \geq 2/\pi$. This is the insulating phase in which only dipoles of finite size occur. (Hence the vanishing of y_0 under coarse graining.) The strength of the effective Coulomb interaction is given by the point on the fixed line that the flows terminate on. Flows not terminating on the fixed line asymptote to larger values of K^{-1} and y_0, where perturbation theory breaks down. This is the signal of the high temperature phase with an abundance of vortices.

The critical trajectory that separates the two regions of the phase diagram flows to a fixed point at $(K_c^{-1} = \pi/2, y_0 = 0)$. To find the critical behavior at the transition, expand the recursion relations in the vicinity of this point by setting $x = K^{-1} - \pi/2$, and $y = y_0 a^2$. To lowest order, eqs.(VII.71) simplify to

$$\begin{cases} \dfrac{dx}{d\ell} =4\pi^3 y^2 + \mathcal{O}(xy^2, y^4) \\ \dfrac{dy}{d\ell} =\dfrac{4}{\pi} xy + \mathcal{O}(x^2 y, y^3) \end{cases} . \tag{VII.72}$$

The recursion relations are inherently *nonlinear* in the vicinity of the fixed point. This is quite different from the linear recursion relations that we have encountered so far, and the resulting critical behavior is non-standard. First note that eqs.(VII.72) imply

$$\frac{dx^2}{d\ell} = 8\pi^3 y^2 x = \pi^4 \frac{dy^2}{d\ell}, \quad \Rightarrow \quad \frac{d}{d\ell}\left(x^2 - \pi^4 y^2\right) = 0, \quad \Rightarrow \quad x^2 - \pi^4 y^2 = c. \tag{VII.73}$$

The RG flows thus proceed along hyperbolas characterized by different values of c. For $c > 0$, the focus of the hyperbola is along the y-axis, and the flows proceed to $(x, y) \to \infty$. The hyperbolas with $c < 0$ have foci along the x-axis, and have two branches in the half plane, $y \geq 0$: the branches for $x < 0$ flow to the fixed line, while those in the $x > 0$ quadrant flow to infinity. The critical trajectory separating flows to zero and infinite y corresponds to $c = 0$, i.e. $x_c = -\pi^2 y_c$. Therefore, a small but finite fugacity y_0 reduces the critical temperature to $K_c^{-1} = \pi/2 - \pi^2 y_0 a^2 + \mathcal{O}(y_0^2)$.

In terms of the original XY model, the low temperature phase is characterized by a line of fixed points with $K_{\rm eff} = \lim_{\ell\to\infty} K(\ell) \geq 2/\pi$. There is no correlation length at a fixed point, and indeed the correlations in this phase decay as a power law, $\langle \cos(\theta_{\mathbf{r}} - \cos\theta_{\mathbf{0}}) \rangle \sim 1/r^\eta$, with $\eta = 1/(2\pi K_{\rm eff}) \leq 1/4$. Since the parameter c is negative in the low temperature phase, and vanishes at the critical point, we can set it to $c = -b^2(T_c - T)$ close to the transition. In other words, the trajectory of initial points tracks a line $(x_0(T), y_0(T))$.

The resulting $c = x_0^2 - \pi^4 y_0^2 \propto (T_c - T)$ is a linear measure of the vicinity to the phase transition. Under renormalization, such trajectories flow to a fixed point at $y = 0$, and $x = -b\sqrt{T_c - T}$. Thus in the vicinity of transition, the effective interaction parameter

$$K_{\text{eff}} = \frac{2}{\pi} - \frac{4}{\pi^2} \lim_{\ell\to\infty} x(\ell) = \frac{2}{\pi} + \frac{4b}{\pi^2}\sqrt{T_c - T}, \tag{VII.74}$$

has a square root singularity.

The *stiffness* K_{eff}, can be measured in experiments on superfluid films. In the superfluid phase, the order parameter is the condensate wavefunction $\psi(\mathbf{x}) = \Psi e^{i\theta}$. Variations in the phase θ, lead to a superfluid kinetic energy,

$$\mathcal{H} = \int d^d\mathbf{x}\, \psi^* \left(-\frac{\hbar^2\nabla^2}{2m}\right)\psi = \frac{\hbar^2\Psi^2}{2m}\int d^d\mathbf{x}(\nabla\theta)^2, \tag{VII.75}$$

where m is the particle (helium 4) mass. The corresponding XY model has a stiffness $K = \hbar^2\rho_s/(2mk_BT)$, where $\rho_s = \Psi^2$ is the superfluid density. The density ρ_s is measured by examining the changes in the inertia of a torsional oscillator; the superfluid fraction, $\rho_s m$, experiences no friction and does not oscillate. Bishop and Reppy (1978) examined ρ_s for a variety of superfluid films (of different thickness, helium 3 concentration, etc.) wrapped around a torsional cylinder. They constructed the effective stiffness K as a function of temperature, and found that for all films it undergoes a *universal jump* of $2/\pi$ at the transition. The behavior of K for $T < T_c$ was consistent with a square root singularity.

Correlations decay exponentially in the high temperature phase. How does the correlation length ξ, diverge at T_c? The parameter $c = x^2 - \pi^4y^2 = b^2(T - T_c)$ is now positive all along the hyperbolic trajectory. The recursion relation for x,

$$\frac{dx}{d\ell} = 4\pi^3y^2 = \frac{4}{\pi}\left(x^2 + b^2(T - T_c)\right), \tag{VII.76}$$

can be integrated to give

$$\frac{dx}{x^2 + b^2(T - T_c)} = \frac{4}{\pi}d\ell, \quad \Longrightarrow \quad \frac{1}{b\sqrt{T - T_c}}\arctan\left(\frac{x}{b\sqrt{T - T_c}}\right) = \frac{4}{\pi}\ell\,. \tag{VII.77}$$

The contribution of the initial point to the left hand side of the above equation can be left out if $x_0 \propto (T - T_c) \ll 1$. The integration has to be stopped when $x(\ell) \sim y(\ell) \sim 1$, since the perturbative calculation is no longer valid beyond this point. This occurs for a value of

$$\ell^* \approx \frac{\pi}{4b\sqrt{T-T_c}}\,\frac{\pi}{2}, \tag{VII.78}$$

where we have used $\arctan(1/b\sqrt{T-T_c}) \approx \arctan(\infty) = \pi/2$. The resulting correlation length is

$$\xi \approx a e^{\ell^*} \approx a \exp\left(\frac{\pi^2}{8b\sqrt{T-T_c}}\right). \tag{VII.79}$$

Unlike any of the transitions encountered so far, the divergence of the correlation length is not through a power law. This is a consequence of the nonlinear nature of the recursion relations in the vicinity of the fixed point.

Vortices occur in bound pairs for distances smaller than ξ, while there can be an excess of vortices of one sign or the other at larger separations. The interactions between vortices at large distances can be obtained from the Debye-Hückel theory of polyelectrolytes. According to this theory the free charges screen each other leading to a screened Coulomb interaction, $\exp(-r/\xi)C(r)$. On approaching the transition from the high temperature side, the singular part of the free energy,

$$f_{\text{sing.}} \propto \xi^{-2} \propto \exp\left(-\frac{\pi^2}{4b\sqrt{T-T_c}}\right), \tag{VII.80}$$

has only an *essential singularity.* All derivatives of this function are finite at T_c. Thus the predicted heat capacity is quite smooth at the transition. Numerical results based on the RG equations (Berker and Nelson) indicate a smooth maximum in the heat capacity at a temperature higher than T_c, corresponding to the point at which the majority of dipoles unbind.

The Kosterlitz-Thouless picture of vortex unbinding has found numerous applications in two dimensional systems such as superconducting and superfluid films, thin liquid crystals, Josephson junction arrays, electrons on the surface of helium films, etc. Perhaps more importantly, the general idea of topological defects has had much impact in understanding the behavior of many systems. The theory of two dimensional melting developed in the next section is one such example.