

## Surface Roughening and the Sine-Gordon Model

*The Coulomb gas model representing vortices in the XY model describes the Kosterlitz-Thouless transition where vortices unbind. A very similar phase transition (same universality class) arises in the problem of “surface roughening” described by the so-called Sine-Gordon (SG) model. We show how the two models can be related by a “duality” transformation. This is convenient, since the SG model can be studied using the same momentum shell RG procedure of Wilson which we are already familiar with.*

### Mapping the Coulomb gas to the Sine-Gordon model



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We have already seen that the energy of a system of vortices takes the same form as that of a system of charges interacting through a two-dimensional Coulomb potential  $V_c(\mathbf{x}) = \frac{1}{2\pi} \ln |\mathbf{x}|$

$$S_{vort}[n_i] = \sum_i \beta E_o n^2(\mathbf{x}_i) - \frac{4\pi^2}{g} \sum_{i < j} n(\mathbf{x}_i) V_c(\mathbf{x}_i - \mathbf{x}_j) n(\mathbf{x}_j).$$

Here, we can restrict our attention to charge  $n = \pm 1$  vortices, since those dominate near the vortex-unbinding KT transition. Here it proves convenient to use the grand canonical ensemble, where the number of vortices is not conserved, and each site in the lattice can have  $n(\mathbf{x}_i) = 0, \pm 1$  vortices sitting on it [to be rigorous, vortices “live” on a dual lattice, whose lattice sites are located at the centers of “plaquettes” of the original lattice]. The corresponding (grand) partition function can be written as

$$Z_{vort} = \sum_{\{n(\mathbf{x}_i)=0\pm 1\}} \exp\{-\beta E_{vort}[n(\mathbf{x}_i)]\}.$$

We now perform a Hubbard-Stratonovich transformation to decouple the interaction term by introducing a “potential” field  $\varphi(\mathbf{x}_i)$

$$-\frac{1}{2} \frac{4\pi^2}{g} \sum_{i \neq j} n(\mathbf{x}_i) V_c(\mathbf{x}_i - \mathbf{x}_j) n(\mathbf{x}_j) \longrightarrow i \sum_i n(\mathbf{x}_i) \varphi(\mathbf{x}_i) - \frac{1}{2} \frac{g}{4\pi^2} \sum_{i \neq j} \varphi(\mathbf{x}_i) V_c^{-1}(\mathbf{x}_i - \mathbf{x}_j) \varphi(\mathbf{x}_j).$$

The partition function takes the form

$$Z_{vort} = \int D\varphi(\mathbf{x}) \exp \left\{ -\frac{1}{2} \frac{g}{4\pi^2} \sum_{i \neq j} \varphi(\mathbf{x}_i) V_c^{-1}(\mathbf{x}_i - \mathbf{x}_j) \varphi(\mathbf{x}_j) \right\} \\ \times \prod_{\mathbf{x}_i} \left\{ \sum_{n(\mathbf{x}_i)=0\pm 1} \exp \{ i n(\mathbf{x}_i) \varphi(\mathbf{x}_i) - \beta E_o n^2(\mathbf{x}_i) \} \right\}.$$

Finally, we sum over the vortex occupation numbers  $n(\mathbf{x}_i) = 0 \pm 1$

$$\sum_{n(\mathbf{x}_i)=0\pm 1} \exp \{ i n(\mathbf{x}_i) \varphi(\mathbf{x}_i) - \beta E_o n^2(\mathbf{x}_i) \} \approx 1 + 2y \cos(\varphi(\mathbf{x}_i)),$$

where the “fugacity”  $y_o = \exp\{-\beta E_o\}$ . The last step is valid for  $y_o \ll 1$ , which, as we shall see, is the relevant regime near the KT transition.

Using the fact that in Fourier space  $V_c(k) = 1/k^2$ , in the continuum limit we can write

$$V_c^{-1}(\mathbf{x} - \mathbf{x}') \longrightarrow -\delta(\mathbf{x} - \mathbf{x}') \nabla^2,$$

and we find the partition function of the Sine-Gordon (SG) model

$$Z_{vort} = \int D\varphi(\mathbf{x}) \exp \left\{ -\frac{1}{2\tilde{g}} \int d\mathbf{x} (\nabla\varphi(\mathbf{x}))^2 + \lambda \int d\mathbf{x} \cos \varphi(\mathbf{x}) \right\},$$

where  $\tilde{g} = 4\pi^2/g$ , and  $\lambda = 2y_o/a^2$  ( $a$  is the lattice spacing). Note that the high temperature phase of the SG model ( $g^* \ll 1$ ) corresponds to the low temperature phase of the Coulomb

gas (CG) model. This is an example of duality. One can say that the SG model is dual to the CG model.

Before we move on to discussing the Sine-Gordon model, it is interesting to interpret the field  $\varphi(\mathbf{x}_i)$  in terms of the original Coulomb gas model. Since it is a Hubbard-Stratonovich field corresponding to the charge density, the field  $\varphi(\mathbf{x}_i)$  physically represents the electrostatic potential at site  $\mathbf{x}_i$  that is produced by all the other charges (vortices). The bare propagator for this field is  $\tilde{g}/k^2$ , i.e. it has the form of the bare Coulomb potential between the charges. The situation is completely analogous to electrostatics, where the exchange of photons “mediates” the Coulomb interaction between charges.

### Surface Roughening

The Sine-Gordon model also describes the so-called “surface roughening” problem. A good example is adsorption of hydrogen gas on a surface of silicon.

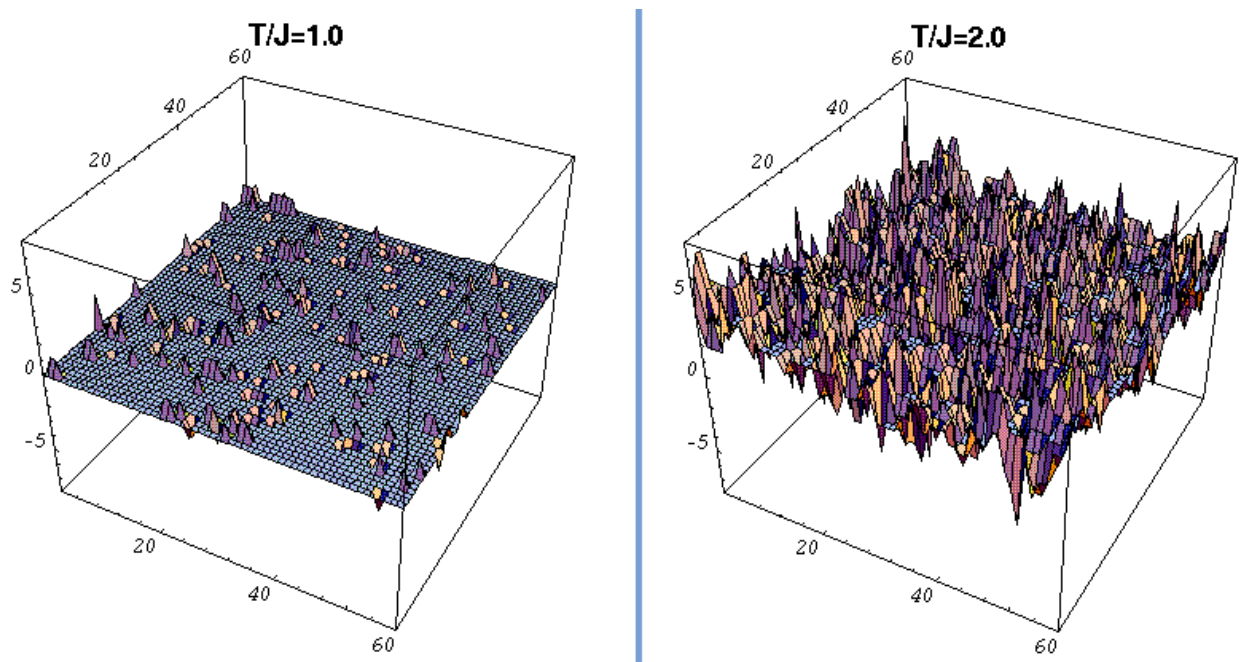


FIG. 1: Computer simulation results for the “solid-on-solid” model, which is a lattice version of the Sine-Gordon theory. As the temperature is increased, large height fluctuations of the adsorbed layers emerge, and the surface becomes “rough”.

Due to surface tension, at low temperature the adsorbed gas tends to form smooth layers

of height  $h$ . Because of the atomic structure of the gas, the preferred average coverage tends to be an integer multiple of the monatomic layer thickness  $d$ , i.e.  $h \approx nd$ . In our language,  $\varphi = 2\pi h/d$ , so that the cosine term describes the preferred coverage states, and the surface tension of the first (gradient) term is  $\sigma = \pi/2d\tilde{g}$ .

Even before we do detailed calculations, it is interesting to “guess” the result, based on the analogy with the Coulomb gas problem. In the low temperature phase of the CG (i.e. the height temperature phase of the SG model), we expect vortices to be bound and screening is absent. The Coulomb potential then reduces to its bare form, corresponding to  $y = 0$  (no vortices). In this case, we have a free elastic theory in  $d=2T$ , and the fluctuations of the surface height

$$\langle h^2(\mathbf{x}) \rangle \sim \int \frac{d\mathbf{k}}{k^2} \sim \ln(L/a),$$

i.e. huge fluctuations are found. The surface is rough. In the opposite limit of high temperatures for the CG (i.e. low  $T$  for the SG model), there are free vortices, and thus the Coulomb interaction is screened. The propagator for the  $\varphi$ -field (which corresponds to the screened Coulomb potential) is now “massive”, giving

$$\langle h^2(\mathbf{x}) \rangle \sim \int \frac{d\mathbf{k}}{k_o^2 + k^2} \sim \text{const.}$$

The surface fluctuations are now suppressed, and the surface is smooth.

### Renormalization of the Sine-Gordon model

To learn more about the phase transition, we need to perform an explicit RG calculation. The good news about the SG model is that we can do so using the standard Wilson RG momentum shell approach. Since this approach is already familiar, we only outline the main steps.

1) We treat the Gaussian part of the Action

$$S_o = \frac{1}{2\tilde{g}} \int d\mathbf{x} (\nabla\varphi(\mathbf{x}))^2$$

as the reference system, and treat

$$S_\lambda = -\lambda \int d\mathbf{x} \cos \varphi(\mathbf{x})$$

as a perturbation. This is a valid approach, since we shall see that  $\lambda$  remains infinitesimally small near the transition (i.e. the RG fixed point is at  $\lambda = 0$ ).

2) As usual, we break up the fields into long wavelength and short wavelength components

$$\varphi(\mathbf{k}) = \varphi_{long}(\mathbf{k}) + \varphi_{short}(\mathbf{k}),$$

and then we integrate out  $\varphi_{short}(\mathbf{k})$  through a cumulant expansion in the interaction  $S_\lambda$ . To lowest order, the renormalized Action takes the form

$$\tilde{S}[\varphi_{long}] = \tilde{S}_o[\varphi_{long}] + \delta\tilde{S}[\varphi_{long}],$$

with

$$\delta\tilde{S}[\varphi_{long}] = \langle S_\lambda[\varphi_{long} + \varphi_{short}] \rangle_{S_o[\varphi_{short}]} + O(\lambda^2).$$

To get the full RG description, we need to actually include both first and second order terms in  $\lambda$ , but we will only do the first term here as an illustration, and just quote the result of the full calculation.

Explicitly, the first order term is

$$\begin{aligned} \delta\tilde{S}^{(1)}[\varphi_{long}] &= \langle S_\lambda[\varphi_{long} + \varphi_{short}] \rangle_{S_o[\varphi_{short}]} \\ &= -\lambda \int d\mathbf{x} \langle \cos[\varphi_{long}(\mathbf{x}) + \varphi_{short}(\mathbf{x})] \rangle_{S_o[\varphi_{short}]} \\ &= -\frac{\lambda}{2} \text{Re} \int d\mathbf{x} \langle \exp[i\varphi_{long}(\mathbf{x}) + i\varphi_{short}(\mathbf{x})] \rangle_{S_o[\varphi_{short}]} \\ &= -\lambda \int d\mathbf{x} \cos(\varphi_{long}(\mathbf{x})) \exp\left\{-\frac{1}{2} \langle \varphi_{short}^2(\mathbf{x}) \rangle\right\}. \end{aligned}$$

Since

$$\langle \varphi \rangle_{short}^2(\mathbf{x}) = \frac{\tilde{g}}{2\pi} \int_{\Lambda/b}^{\Lambda} \frac{dk}{k^2} = \frac{\tilde{g}}{2\pi} \ln b,$$

we find that the Action preserves its form under renormalization, while the coupling constant  $\lambda$  is rescaled as

$$\lambda \longrightarrow b^{-\tilde{g}/4\pi} \lambda.$$

3) The last step, as usual, is to restore the old ultraviolet cutoff by length rescaling  $\Lambda/b \longrightarrow \Lambda$ . Note that the usual field renormalization  $\varphi_{long}(\mathbf{x}) \longrightarrow b^{1-d/2}\varphi(\mathbf{x})$ , which leaves the Gaussian part of the same form as before, in  $d = 2$  cancels out. However, the  $\lambda$ -term picks up (similarly as the  $r$ -term in the  $\varphi^4$  theory) another factor of  $b^2$ , due to the rescaling of the integration measure  $d^2\mathbf{k}$ . Finally

$$\lambda(b) = b^{2-\tilde{g}/4\pi} \lambda,$$

or in differential form ( $b = e^\ell$ )

$$\frac{d\lambda}{d\ell} = \left(2 - \frac{\tilde{g}}{4\pi}\right) \lambda.$$

As we can see from this equation, the nonlinear coupling  $\lambda \rightarrow 0$  for  $\tilde{g} > \tilde{g}^*$ . In this high temperature phase of the surface roughening (SG) model, the behavior reduces to that of a free massless theory. In this regime, the surface height fluctuations

$$\langle h^2(\mathbf{x}) \rangle \sim G_o(x=0) = \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{\tilde{g}}{k^2} \sim \ln(L/a),$$

and the surface is “rough”, as we predicted from the Coulomb gas analogy. In the opposite low temperature ( $\tilde{g} < \tilde{g}^*$ ) limit,  $\lambda$  grows, and the behavior is dominated by the nonlinear term. The field  $\varphi(\mathbf{x}) \approx \varphi_n = 2\pi n$ , i.e. the surface height  $h \approx nd$ . The field is “locked” near one of the minima of the periodic potential. To calculate the fluctuations (which are small), we can now expand the nonlinear term

$$\cos \varphi(\mathbf{x}) \approx 1 - \frac{1}{2} \varphi^2(\mathbf{x}),$$

and the Action takes the form

$$S[\varphi(\mathbf{x})] \approx \frac{1}{2\tilde{g}} \int d\mathbf{x} [(\nabla \varphi(\mathbf{x}))^2 + \lambda \varphi^2(\mathbf{x})] + O(\varphi^4).$$

The propagator is now “massive”

$$G(k) \approx \frac{\tilde{g}}{\lambda + k^2},$$

and the height fluctuations

$$\langle h^2(\mathbf{x}) \rangle \sim G(x=0) = \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{\tilde{g}}{\lambda + k^2} \sim \ln \lambda$$

are finite, and the surface is “smooth”.

To actually calculate the renormalized value of  $\lambda$  as a function of temperature, we need to examine the renormalization of the coupling constant  $\tilde{g}$  as well. To do this, the calculation has to be extended to  $O(\lambda^2)$ . As in the case of the  $\phi^4$  theory, we evaluate the renormalized couplings by keeping only the appropriate lowest order terms in the external momenta, since terms with extra powers of the momentum prove irrelevant by power counting. One finds that the RG equation for  $\lambda$  acquires a correction of order  $\lambda^2$ , but this term proves

subleading near the fixed point, and can be ignored. However,  $\tilde{g}$  now acquires a nontrivial renormalization that contributes to leading order, which takes the form

$$\frac{d}{d\ell}\tilde{g}^{-1} = \frac{\pi}{4}a^8\lambda^2.$$

We will do this in the next lecture, where we perform the full analysis of the Kosterlitz RG equations. Since in real space the propagator is  $G(\mathbf{x}) \sim \exp - \{|\mathbf{x}|/\xi\}$ , with  $\xi = \lambda^{-1/2}$ , we really need to calculate the temperature-dependent correlation length  $\xi$ .