8.334 Statistical Mechanics II: Statistical Physics of Fields Spring 2008

For information about citing these materials or our Terms of Use, visit: <u>http://ocw.mit.edu/terms</u>.

VI.F Summing over Phantom Loops

The high temperature series can be *approximately* summed so as to reproduce the Gaussian model. This correspondence provides a better understanding of why Gaussian behavior is applicable in high dimensions, and also prepares the way for the exact summation of the series in two dimensions in the next section. The high temperature series for the partition function of the Ising model on a d-dimensional hypercubic lattice is obtained from

$$Z = \sum_{\{\sigma_i\}} e^{K \sum_{\langle ij \rangle} \sigma_i \sigma_j} = 2^N \cosh^{dN} K \times S, \qquad (\text{VI.35})$$

where S is the sum over all allowed graphs on the lattice, each weighted by $t \equiv \tanh K$ raised to the power of the number of bonds in the graph. The allowed graphs have an even number of bonds per site. The simplest graphs have the topology of a single closed loop. There are also graphs composed of *disconnected* closed loops. Keeping in mind the cumulant expansion, we can set

$$\Xi = \text{sum over contribution of all graphs with one loop},$$
 (VI.36)

and introduce another sum,

$$S' = \exp(\Xi) = 1 + \Xi + \frac{1}{2} (\Xi)^2 + \frac{1}{6} (\Xi)^3 + \cdots$$

=1 + (1 loop graphs) + (2 loop graphs) + (3 loop graphs) + \cdots. (VI.37)

Despite their similarities, the sums S and S' are not identical: There are ambiguities associated with loops that intersect at a single site, which will be discussed more fully in the next section. More importantly, S' includes additional graphs where a particular bond contributes more than once, while in the original sum S, each lattice bond contributes a factor of 1 or t. This arises because after raising Ξ to a power ℓ , a particular bond may contribute up to ℓ times for a factor of t^{ℓ} . In the spirit of the approximation that includes multiple appearances of a bond, we shall allow additional closed paths in Ξ , in which a particular bond is traversed more than once in completing the loop. Qualitatively, S is the partition function of a gas of *self-avoiding* polymer loops with a monomer fugacity of t. The self-avoiding constraint is left out in the partition function S', which thus corresponds to a gas of *phantom* polymer loops, which may pass through each other with impunity. Loops of various shapes can be constructed from closed random walks on the lattice, and the corresponding free energy of phantom loops is

$$\ln S' = \sum \text{ all closed random walks on the lattice} \times t^{\text{length of walk}}$$
$$= N \sum_{\ell} \frac{t^{\ell}}{\ell} \text{ (number of closed walks of } \ell \text{ steps starting and ending at } \mathbf{0}\text{).}$$
(VI.38)

Note that extensivity is guaranteed since (up to boundary effects) the same loop can be started from any point on the lattice. The overall factor of $1/\ell$ accounts for the ℓ possible starting points for a loop of length ℓ .

A transfer matrix method can be used to count all possible (phantom) random walks on the lattice. Let us introduce a set of $N \times N$ matrices,

$$\langle \mathbf{i}|W(\ell)|\mathbf{j}\rangle \equiv \text{number of walks from } \mathbf{j} \text{ to } \mathbf{i} \text{ in } \ell \text{ steps},$$
 (VI.39)

in terms of which eq.(VI.38) becomes

$$\frac{\ln S'}{N} = \frac{1}{2} \sum_{\ell} \frac{t^{\ell}}{\ell} \langle \mathbf{0} | W(\ell) | \mathbf{0} \rangle.$$
(VI.40)

The additional factor of 2 arises since the same loop can be traversed by two random walks moving in opposite directions. Similarly, the spin–spin correlation function

$$\langle \sigma(\mathbf{0})\sigma(\mathbf{r})\rangle = \frac{1}{Z} \sum_{\{\sigma_i\}} \sigma(\mathbf{0})\sigma(\mathbf{r}) \prod_{\langle ij\rangle} (1 + t\sigma_i\sigma_j), \qquad (\text{VI.41})$$

is related to the sum over all paths connecting the points $\mathbf{0}$ and \mathbf{r} on the lattice. In addition to the simple paths that directly connect the two points, there are *disconnected* graphs that contain additional closed loops. In the same approximation of allowing all intersections between paths, the partition function S' can be factored out of the numerator and denominator of eq.(VI.41), and

$$\langle \sigma(\mathbf{0})\sigma(\mathbf{r}) \approx \sum_{\ell} t^{\ell} \langle \mathbf{r} | W(\ell) | \mathbf{0} \rangle.$$
 (VI.42)

The counting of phantom paths on a lattice is easily accomplished by taking advantage of their *Markovian* property. This is the property that each step of a random walk proceeds from its last location and is independent of its previous steps. Hence, the number of walks can be calculated *recursively*. First, note that the any walk from **0** to **r** in ℓ steps can be accomplished as a walk from 0 to some other point \mathbf{r}' in $\ell - 1$ steps, followed by a single step from \mathbf{r}' to \mathbf{r} . Summing over all possible locations of the intermediate point leads to

$$\langle \mathbf{r} | W(\ell) | \mathbf{0} \rangle = \sum_{\mathbf{r}'} \langle \mathbf{r} | W(1) | \mathbf{r}' \rangle \times \langle \mathbf{r}' | W(\ell - 1) | \mathbf{0} \rangle$$

= $\langle \mathbf{r} | TW(\ell - 1) | \mathbf{0} \rangle$, (VI.43)

where the sum corresponds to the product of two matrices, and we have defined $T \equiv W(1)$. The recursion process can be continued and

$$W(\ell) = TW(\ell - 1) = T^2 W(\ell - 2)^2 = \dots = T^{\ell}.$$
 (VI.44)

Thus all lattice random walks are generated by the transfer matrix T, whose elements are

$$\langle \mathbf{r} | T | \mathbf{r}' \rangle = \begin{cases} 1 & \text{if } \mathbf{r} \text{ and } \mathbf{r}' \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$
(VI.45)

(It is also called the *adjacency*, or *connectivity* matrix.) For example in d = 2,

$$\langle x, y | T | x', y' \rangle = \delta_{y,y'} \left(\delta_{x,x'+1} + \delta_{x,x'-1} \right) + \delta_{x,x'} \left(\delta_{y,y'+1} + \delta_{y,y'-1} \right), \qquad (VI.46)$$

and successive actions of T on a walker starting at the origin $|x, y\rangle = \delta_{x,0} \delta_{y,0}$, generate the patterns

The value at each site is the number of walks ending at that point after ℓ steps.

Various properties of random walks can be deduced from diagonalizing the matrix T. Due to the translational symmetry of the lattice, this is achieved in the Fourier basis $\langle \mathbf{r} | \mathbf{q} \rangle = e^{i\mathbf{q}\cdot\mathbf{r}}/\sqrt{N}$. For example in d = 2, starting from eq(VI.46), it can be checked that

$$\langle x, y | T | q_x, q_y \rangle = \sum_{x', y'} \langle x, y | T | x', y' \rangle \langle x', y' | q_x, q_y \rangle$$

$$= \frac{1}{\sqrt{N}} \left[e^{iq_y y} \left(e^{iq_x (x+1)} + e^{iq_x (x-1)} \right) + e^{iq_x x} \left(e^{iq_y (y+1)} + e^{iq_y (y-1)} \right) \right]$$

$$= \frac{1}{\sqrt{N}} e^{i(q_x x + q_y y)} \left[2\cos q_x + 2\cos q_y \right] = T(q_x, q_y) \langle x, y | q_x, q_y \rangle .$$
(VI.47)

The generalized eigenvalue for a d-dimensional hypercubic lattice is

$$T(\mathbf{q}) = 2\sum_{\alpha=1}^{d} \cos q_{\alpha} \,. \tag{VI.48}$$

The correlation function in eq. (VI.42) is now evaluated as

$$\begin{aligned} \langle \sigma(\mathbf{r})\sigma(\mathbf{0}) \rangle &\approx \sum_{\ell}^{\infty} t^{\ell} \langle \mathbf{r} | W(\ell) | \mathbf{0} \rangle = \sum_{\ell}^{\infty} \langle \mathbf{r} | (tT)^{\ell} | \mathbf{0} \rangle \\ &= \left\langle \mathbf{r} \left| \frac{1}{1 - tT} \right| \mathbf{0} \right\rangle = \sum_{\mathbf{q}} \langle \mathbf{r} | \mathbf{q} \rangle \frac{1}{1 - tT(\mathbf{q})} \langle \mathbf{q} | \mathbf{0} \rangle \\ &= N \int \frac{d^{d}\mathbf{q}}{(2\pi)^{d}} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{N} \frac{1}{1 - 2t \sum_{\alpha=1}^{d} \cos q_{\alpha}} = \int \frac{d^{d}\mathbf{q}}{(2\pi)^{d}} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{1 - 2t \sum_{\alpha} \cos q_{\alpha}} \,. \end{aligned}$$
(VI.49)

For $t \to 0$, the shortest path costs least energy and $\langle \sigma(\mathbf{0})\sigma(\mathbf{r}) \rangle \sim t^{|\mathbf{r}|}$. As t increases, larger paths dominate the sum because they are more numerous (i.e. entropically favored). Eventually, there is a singularity for $1 - tT(\mathbf{0}) = 0$, i.e. at $2d \times t_c = 1$, when arbitrarily long paths become important. For $t < t_c$, the partition function is dominated by small loops, and a polymer connecting two far away points is stretched by its line tension. When the fugacity exceeds t_c , the line tension vanishes and loops of arbitrary size are generated. Clearly the neglect of intersections (which stabilizes the system at a finite density) is no longer justified in this limit. This transition is the manifestation of Ising ordering in the language of paths representing the high temperature series. On approaching the transition from the high temperature side, the sums are dominated by very long paths. Accordingly, the denominator of eq.(VI.49) can be expanded for small \mathbf{q} as

$$1 - tT(\mathbf{q}) = 1 - 2t \sum_{\alpha=1}^{d} \cos q_{\alpha} \simeq (1 - 2dt) + tq^2 + \mathcal{O}(q^4) \approx t_c(\xi^{-2} + q^2 + \mathcal{O}(q^4)), \quad (\text{VI.50})$$

where

$$\xi \equiv \left(\frac{1-2dt}{t_c}\right)^{-1/2}.$$
 (VI.51)

The resulting correlation functions, $\langle \sigma(\mathbf{0})\sigma(\mathbf{r})\rangle \propto \int \frac{d^d \mathbf{q}}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{r}}/(q^2+\xi^{-2})$, are identical to those obtained from the Gaussian model, and

$$\langle \sigma(\mathbf{0})\sigma(\mathbf{r})\rangle \propto \begin{cases} \frac{1}{r^{d-2}} & \text{for } r < \xi \qquad (\eta = 0)\\ \frac{e^{-r/\xi}}{r^{(d-1)/2}} & \text{for } r > \xi \end{cases}$$
(VI.52)

The correlation length in eq.(VI.51) diverges as $\xi \sim (t_c - t)^{-1/2}$, i.e. with the Gaussian exponent of $\nu = 1/2$.

We can also calculate the free energy in eq. (VI.40) as

$$\frac{\ln S'}{N} = \frac{1}{2} \sum_{\ell}^{\infty} \frac{t^{\ell}}{\ell} \langle \mathbf{0} | W(\ell) | \mathbf{0} \rangle = \frac{1}{2} \left\langle \mathbf{0} \left| \frac{t^{\ell} T^{\ell}}{\ell} \right| \mathbf{0} \right\rangle$$
$$= -\frac{1}{2} \left\langle \mathbf{0} | \ln(1 - tT) | \mathbf{0} \right\rangle = -\frac{N}{2} \int \frac{d^{d} \mathbf{q}}{(2\pi)^{d}} \left\langle \mathbf{0} | \mathbf{q} \right\rangle \ln\left(1 - tT(\mathbf{q})\right) \left\langle \mathbf{q} | \mathbf{0} \right\rangle$$
(VI.53)
$$= -\frac{1}{2} \int \frac{d^{d} \mathbf{q}}{(2\pi)^{d}} \ln\left(1 - 2t \sum_{\alpha=1}^{d} \cos q_{\alpha}\right).$$

In the vicinity of the critical point at $t_c = 1/(2d)$, the argument of the logarithm is proportional to $(q^2 + \xi^{-2})$ from eq.(VI.50). This is precisely as in the Gaussian model, and as discussed earlier the singular part of the free energy scales as

$$f_{\rm sing} \propto \xi^{-d} \propto (t_c - t)^{d/2}.$$
 (VI.54)

The singular part of the heat capacity, obtained after taking two derivatives, is governed by the exponent $\alpha = 2 - d/2$. Note that in evaluating the sums appearing in eqs.(VI.49) and (VI.53), the lower limit for ℓ is not treated very carefully. The series in eq.(VI.49) is assumed to start from $\ell = 0$, and that of eq.(VI.53) from $\ell = 1$. In fact the first few terms of both series may be zero because the number of steps is not sufficient to reach **0** from **r**, or to from a closed loop. This is not a serious omission, in that the *singular* behavior of a series is not effected by its first few terms. Treating the first few terms properly can only add analytic corrections to the singular forms calculated in eqs.(VI.49) and (VI.53).

The equivalence of these results to the Gaussian model is a manifestation of field– particle duality. In a field theoretical description, (imaginary) time appears as an additional dimension, and the two point correlations describe the probability of propagating a particle from one point in space–time to another. In a wave description, this probability is calculated by evolving the wave function using the Schrödinger equation. Alternatively, the probability can be calculated as the sum over all (Feynman) paths connecting the two points, each path weighted with the correct action. The second sum is similar to the above calculation of $\langle \sigma(\mathbf{r})\sigma(\mathbf{0}) \rangle$.

This approach provides an interesting geometrical interpretation of the phase transition. The establishment of long range order implies that all parts of the system have selected the same state. This information is carried by the bonds connecting nearest neighbors, and can be passed from the origin to a point \mathbf{r} , through all paths connecting these two points. The fugacity t is a measure of the reliability of information transfer between neighboring sites. Along a one dimensional chain, unless t = 1, the transferred information decays at large distances and it is impossible to establish long range order. In higher dimensions there are many more paths, and by accumulating the information from all paths it is possible to establish order at $t_c < 1$. Since the number of paths of length ℓ grows as $(2d)^{\ell}$ while their information content decays as t^{ℓ} , the transition occurs at $t_c = 1/(2d)$. (A better approximation is obtained by including some of the constraints by noting that the random walk cannot back track. In this case the number of walks grows as $(2d-1)^{\ell}$.) The total information from paths of length ℓ is weighted by $(2dt)^{\ell}$, and decays exponentially for $t < t_c$. The characteristic path length, $\overline{\ell} = -1/\ln(2dt)$, diverges as $(t_c - t)^{-1}$ on approaching the transition. For paths of size $\ell \ll \overline{\ell}$ there is very good information transfer. Such paths execute random walks on the lattice and cover a distance $\xi \approx \overline{\ell}^{1/2}$. The divergence of ν with an exponent of 1/2 is thus a consequence of the random walk nature of the paths.

Why does the classical picture fail for $d \leq 4$? Let us focus on the dominant paths close to the phase transition. Is it justified to ignore the intersections of such paths? Random walks can be regarded as geometrical entities of fractal (Hausdorf) dimension $d_f = 2$. This follows from the general definition of dimension relating the mass and extent of an object by $M \propto R^{d_f}$, and the observation that the size of a random walk $(R \propto \xi)$ is the square root of its length $(M \propto \ell)$. Two geometrical entities of dimensions d_1 and d_2 will generally intersect in d-dimensional space if $d_1 + d_2 \ge d$. Thus our random walkers are unlikely to intersect in $d \ge d_u = 2 + 2 = 4$, and the above (Gaussian) results obtained by neglecting the intersections are asymptotically valid. Below the upper critical dimension of 4, random walks have frequent encounters and their intersections must be treated correctly. The diagrams obtained in the perturbative calculation of the propagator with um^4 correspond precisely to taking into account the intersections of paths. (Each factor of u corresponds to one intersection.) It is now clear that the constraint of self-avoidance will swell the paths beyond their random walk size leading to an increase in the exponent ν . Below the transition the length of paths grows without bound and the self-avoiding constraint is necessary to ensure the stability of the system.

The loop expansion is easily generalized to *n*-component spins. The only difference is that each closed loop now contributes a factor of *n*. In the phantom limit, where intersections are ignored, the free energy (eq.(VI.53)) is simply multiplied by *n*, while the correlation function is left unchanged (precisely as in the Gaussian model). Corrections due to intersections, which modify critical behavior in d < 4, now depend on n. For example, in correcting the two point correlation function, we have to subtract contributions from the self-intersection of the random walk, as well as from contacts with loops (which have a fugacity of n). The correspondence with the perturbative series of the propagator with a nonlinearity $u(\vec{m} \cdot \vec{m})^2$, is again apparent.