Graphical Enumeration Techniques: Series Expansions and Animal Problems

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Graphical Enumeration Techniques in Statistical Physics: I: Series expansions and Animal problems

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Abstract

This is a pedagogical introduction to some graphical enumeration problems in statistical physics. I start with the high-temperature and low-temperature expansions of the Ising model. I then discuss enumeration of clusters in the percolation problem, and Martin's algorithm for their enumeration. Exact enumeration of two-dimensional directed animals then described, and extention of this result to the generating function of more general heaps is explained.

The aim of these lecture notes is to introduce the readers to the techniques of graphical enumeration, for solving problems in statistical physics. I assume that you have already had the first course in statistical physics, and basic principles of equilibrium statistical physics are known. In particular, I assume that you have already seen the statistical mechanical treatment of ideal gases (classical monoatomic ideal gases, and the ideal Bose and Fermi gases). The problem of a system of coupled harmonic oscillators reduces to that of non-interacting normal modes, and can be solved similarly. Thus one can calculate the partition function of a system of non-interacting *phonons*, or of photons, and see how the average energy of the system varies as a function of temperature.

1 Ising Model in one dimension

Let us consider a line of N sites, labelled by integers 1 to N. At each site i, we have a spin σ_i, which takes values ± 1. The Hamiltonian of the system is

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \tag{1}$$

There are 2^N distinct configurations. The system is in contact with a heat bath at temperature T, and each configuration $\mathcal{C}$ occurs *in the canonical ensemble*, with a probability $Prob(\mathcal{C}) = exp[-\beta H(\mathcal{C})]/\mathcal{Z}$, where

$$\mathcal{Z} = \sum_C e^{-\beta H(\mathcal{C})} \tag{2}$$

Our first problem is to calculate $\mathcal{Z}(\beta)$.
Method 1: We consider a change of variables. Define Ising variables $\{\tau_i\}$, with $\tau_1 = \sigma_1$, and $\tau_i = \sigma_{i-1}\sigma_i$, for $i > 1$.

Then, we get $H = -J \sum_{i=2}^{N} \tau_i$. The summation over 2^N values of $\{\sigma_i\}$ is same as summation over 2^N values of $\{\tau_i\}$. And we get

$$\mathcal{Z} = 2^N [\cosh \beta J]^{N-1} \tag{3}$$

We can define free energy per site *in the thermodynamical limit* of large N as $f(\beta) = \lim_{N\to\infty} -k_B T(\log \mathcal{Z})/N$. Then we get

$$f(\beta) = -k_B T \log(2 \cosh \beta J) \tag{4}$$

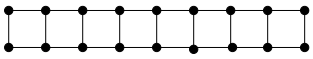

Figure 1: A ladder graph.

Method 2: The Transfer Matrix Method:
Define $Z_n(+)$ = partition function of a chain of n sites with left-most site held fixed $+1$, and sum over the rest. Define $Z_n(-)$ similarly. Then we can write the recursion equation

$$\begin{bmatrix} Z_{n+1}(+) \\ Z_{n+1}(-) \end{bmatrix} = \begin{bmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{bmatrix} \begin{bmatrix} Z_n(+) \\ Z_n(-) \end{bmatrix} \tag{5}$$

Calling the matrix on the right hand side of this equation as the transfer matrix $\mathbf{T}$, we write

$$\begin{bmatrix} Z_{n+1}(+) \\ Z_{n+1}(-) \end{bmatrix} = \mathbf{T} \begin{bmatrix} Z_n(+) \\ Z_n(-) \end{bmatrix}. \tag{6}$$

These recursion equations can be easily solved to give $Z_n(+)$ and $Z_n(-)$ explicitly as functions of n

$$\begin{bmatrix} Z_n(+) \\ Z_n(-) \end{bmatrix} = \mathbf{T}^{n-1} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{7}$$

with

$$Z_n = Z_n(+) + Z_n(-) \tag{8}$$

Let the eigenvalues of T be λ_+ and λ_-, with $\lambda_+ > \lambda_-$. Then, for large N, we get $\mathcal{Z}_N \sim \lambda_+^N$, and $f(\beta)$ is as calculated before.
Exercise 1: Show that the partition function of Ising model on a one-dimensional ring of N sites is $\mathcal{Z}_N = Tr[T^N]$.
Exercise 2: Calculate the partition function of the Ising model on a $2 \times N$ ladder graph (Fig. 1). In this case, the transfer matrix T is a 4×4 matrix.
Excercise 3: Suppose we add an external magnetic field, so that the hamiltonian is $H' = H - h \sum_i \sigma_i$. Extend the treatment above, using the transfer matrix, to calculate the free energy per spin $f(\beta, h)$.

2 High -temperature expansions for Ising systems

We now want to calculate Z for a more non-trivial case. Consider the two-dimensional Ising model. Here we have Ising spins on the vertices of an $L \times M$ square lattice. Each spin has a ferromagnetic coupling to its nearest neighbor of strength J. Let $\sigma_{i,j}$ be the spin at site (i, j). The hamiltonian is now written as

$$H = -J \sum_{i,j} [\sigma_{ij}\sigma_{i+1,j} + \sigma_{i,j}\sigma_{i,j+1}] \tag{9}$$

We want to calculate the partition function

$$Z = \sum_{\{\sigma\}} exp[-\beta H(\{\sigma\})] \tag{10}$$

where $\{\sigma\}$ denotes a configuration of spins on the lattice, and the sum over $\{\sigma\}$ is sum over all spin configurations.

For Ising variables σ and σ', which take only values ± 1, we have the identity

$$exp(\beta J \sigma\sigma') = \cosh(\beta J)[1 + x\sigma\sigma'] \tag{11}$$

where $x = \tanh(\beta J)$.

Then we get

$$Z = [\cosh \beta J]^{N_B} \sum_{\{\sigma\}} \prod_{B} (1 + x\sigma_B\sigma'_B) \tag{12}$$

where the product over B is over all bonds of the lattice, and σ_B and σ'_B denote two spins at the end of the bond B. N_B is the number of bonds in the graph. Now Z is a polynomial in x (apart from the simple multiplying prefactor). We expand the product, and then first do the summation over $\{\sigma\}$ for each term, and then sum the terms.

Since the number of terms is very large, we need a good way of specifying the different terms. The most convenient scheme that has been found to work is this: we think of the square lattice as specified by its graph, i.e. a set of vertices, with a bond between vertices that are nearest neighbor on the square lattice. After this, we do not worry about the actual distances between vertices, or angles between bonds. Each term in the expansion is associated with a diagram; we draw a bond between two sites for the term

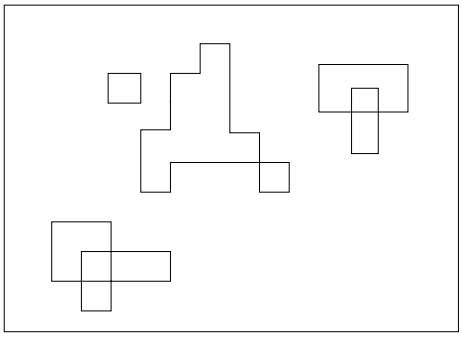

Figure 2: A configuration that contributes to the high temperature expansion for the Ising model

$x\sigma_B\sigma'_B$, and no bond corresponding to the 1 in $(1 + x\sigma_B\sigma'_B)$. Each such diagram has only a subset of bonds of the original graph. There is a one-to-one correspondence between different terms in the expansion, and different diagrams. Then the summation over the 2^{N_B} terms in the expansion Eq.(12) is equivalent to summing over all possible 2^{N_B} diagrams.

Now consider one particular diagram corresponding to specific term. It is easy to sum over $\{\sigma_i\}$, and we get zero, if there is any vertex in the diagram that has an odd number of bonds. If the number is even at all vertices (an example of such a diagram is shown in Fig. 2), then the weight is 2^{N_s}, where N_s is the number of sites in the graph (using $\sigma_{i,j}^2 = 1$).

Then, the partition function Z can be written as $Z = 2^{N_s}[\cosh(\beta J)]^{N_B}\tilde{Z}$, with

$$\tilde{Z} = \sum_{\ell} C(\ell, L, M)x^{\ell} \tag{13}$$

where $C(\ell, L, M)$ is the number of ways one can draw a diagram with ℓ links on the $L \times M$ square lattice , where each vertex has even number of bonds. The problem of determining the partition function of the Ising model has been reduced to the enumeration problem of some kinds of diagrams. For high temperatures (small x), we may keep only terms upto some maximum power of x. Then the result is exact upto that order in x. Hence the name "high temperature expansion".

We note that $C(0, L, M) = 1$. Let us assume periodic boundary conditions for the lattice. For $\ell = 1, 2, 3$, we have $C(\ell, L, M) = 0$. The coefficient $C(4, L, M)$ is the number of ways one can put a small square in different

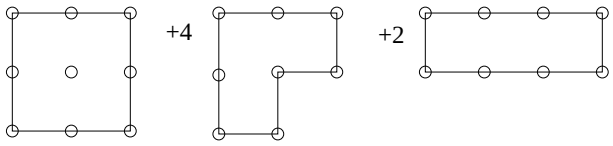

Figure 3: All possible lattice polygons of perimeter 8 on the square lattice.

positions on the lattice. Hence this number is $LM = N_s$. For $\ell = 6$, only diagram possible is a hexagon enclosing two adjacent small squares. Thus, the RHS of Eq.(13) can be written as

$$1 + N_s x^4 + 2N_s x^6 + \mathcal{O}(x^8) \tag{14}$$

The enumeration of terms of order x^8 is more complicated. One can have two small squares, separated from each other, or one can have one simple polygon of perimeter 8. There are $N_s(N_s - 5)/2$ terms of the first type. An exhaustive enumeration of possible lattice octagons (see Fig. 3) shows that the term is $N_s(N_s + 9)x^8/2$.

We define

$$F(x) = \lim_{N_s \to \infty} \frac{1}{N_s} \log \tilde{Z} \tag{15}$$

We assume that $F(x)$ has a Taylor expansion in powers of x :

$$F(x) = F_4 x^4 + F_6 x^6 + F_8 x^8 + \ldots \tag{16}$$

Then clearly $\exp[N_s F(x)]$ has a Taylor expansion in powers of x given by

$$\exp[N_s F(x)] = 1 + N_s F_4 x^4 + N_s F_6 x^6 + [(1/2)F_4^2 N_s^2 + F_8 N_s]x^8 + \mathcal{O}(x^{10}) \tag{17}$$

Comparing with the exact calculated numbers $C(\ell, L, M)$, we see that $F_4 = 1, F_6 = 2$, and $F_8 = 9/2$. So that we have

$$F(x) = x^4 + 2x^6 + \frac{9}{2}x^8 + \ldots \tag{18}$$

We can also write series expansion for $e^{F(x)}$, which is called the partition function per site

$$e^{F(x)} = 1 + x^4 + 2x^6 + 5x^8 + \ldots \tag{19}$$

At higher orders, $C(\ell, L, M)$ would have terms that vary as larger powers of N_s. However, these higher powers cancel out exactly automatically, *if*

we have matched the terms of order N exactly to all lower orders in x. Then, the coefficients F_ℓ are independent of N_s. The fact that terms in the partition function that vary as higher power of N_s than 1 cancel on taking the logarithm, is a consequence of the extensivity of free energy. This important technique is variously called the linked cluster expansion, or the cumulant expansion. For a more general discussion, see [1]. A very readable elementary account of series expansion methods in statistical physics may be found in [2].

So, now, with the linked cluster expansion theorem, the graphical enumeration problem, for any fixed order ℓ, reduces to a *finite* enumeration problem, where the formal limit $L, M \to \infty$ has been taken already.

Clearly, evaluation of still higher orders requires some practice in graphical enumerations. One can use the enormous power provided by digital computers, to calculate these series to very high orders. For example, for the three dimensional Ising model, the high-temperature series has been extended up to 46th order in x [3]. For many other lattice models, similarly long series expansions have been calculated. For special cases, one can get much longer series. For example, for the directed percolation on the square lattice, the series expansion is known exactly to 171 orders! And this is the best one can do, the exact solution is not known [4]. The series expansion method provides a *systematic* method of making better and better approximations to the exact answer for a problem with no analytical exact solution. Note that, in contrast, most other approximations used in different branches of physics often involve an error that cannot be made "as small as you wish" if you are willing to work harder (e.g. "the effective medium approximation", or the "random phase approximation").

Since one can generate such series to very high orders, the analysis of such series has also become quite sophisticated. For example, in [5], a high order series is used to guess the exact functional form of the answer for counting a type of almost-convex polygons (polygons whose perimeter differs from that of bounding rectangle by at most 4 units), by exact enumeration of the series for perimeter up to $\ell = 110!$. [An exclamation mark, not a factorial sign.]
Excercise 4: Use the high temperature expansion, to show that for the problem in Excercise 1, $Z_N = [2\cosh\beta J]^N(1 + x^N)$.
Excercise 5: Consider the Ising model on the square lattice with 4-spin couplings

$$H_4 = -J \sum_{squares} \sigma_{i,j}\ \sigma_{i,j+1}\ \sigma_{i+1,j}\ \sigma_{i+1,j+1} \tag{20}$$

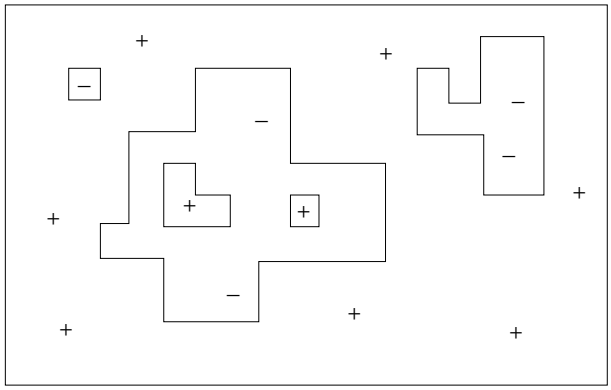

Figure 4: A configuration of the Ising model at low temperatures. The + and − signs denote regions where the spins are + and − respectively.

Show that in the high temperature expansion of this model, all terms except the lowest order are zero.
Excercise 6: Extend the calculation of high temperature series expansion given in Eq.(19) to order x^{10}.

3 Low-temperature expansion of the Ising model and self-duality

One can also develop a low-temperature expansion for the free energy of the Ising model. We note that at low temperatures, a typical configuration would have most spins aligned parallel (say +), and a few − spins interspersed [Fig. 4]. Then, a configuration in which there are ℓ 'bad' bonds has a relative weight $\exp(-2\ell\beta J)$, compared to the ground state. writing this weight as y^ℓ, we see that the partition function looks like

$$Z = e^{2N_s\beta J}[1 + N_s y^4 + 2N_s y^6 + \ldots] \tag{21}$$

These graphs are the same as in the high temperature expansion! We thus get a non-trivial relation between the partion function $Z(\beta)$ and partition function $Z(\beta')$ at a different value β' given by

$$\tanh \beta' J = e^{-2\beta J}, \quad \sinh \beta J \sinh \beta' J = 1 \tag{22}$$

and

$$Z(\beta)\exp(-2N_s\beta J) = Z(\beta')[2\cosh^2\beta' J]^{-N_s} \tag{23}$$

If β is small, β' is large, and vice versa. At one particular value β^* we have $\beta = \beta'$. Then this point must be the common boundary between the high - and low-temperature phases. Thus, we get that the critical temperature for the square lattice Ising model is given by the condition

$$\sinh(J/k_B T_c) = 1 \tag{24}$$

More generally, the high-temperature graphical expansion of the partition function of a lattice model can often be reinterpreted as the low-temperature graphical expansion of some other model. Such models are said to be low-tempearture-high temperature duals of each other. The Ising model on the square lattice is said to be *self-dual*.

4 Percolation and Animal Problems

We will now discuss the use of graphical enumeration technique in percolation and animal problems. The percolation problem is easy to state, and quite nontrivial to study. In particular, it provides a very simple setting for studying phase transitions.

Consider a box full of many small wooden and metal balls, equal in size, and thrown in at random. These will form what is known in literature as a random closed pack structure. We would like to determine the bulk electical conductivity of this mixture, as a function of the relative fraction of metal balls. Call this fraction p. If p is very small, there are few isolated metal balls in a sea of insulating spheres, and the bulk material is an insulator. If p is near 1, the material will be conducting. Also, we note that if we change any ball from insulating to conducting, the conductivity can only increase. Thus, the conductance of this disordered medium is a non-decreasing function of p. And there is some value p_c, such that for $p < p_c$, the conductance is zero, but for $p > p_c$, there are conducting paths between opposite faces of the sample, and the mean bulk conductance is non-zero.

Thus, we have a phase transition from an insulating to a conducting phase, as p is increased above p_c. Perhaps this is *the* simplest example of a phase transition. It is a geometrical phase transition, and the phase transition occurs as a function of the concentration p. Temperature does not play any role.

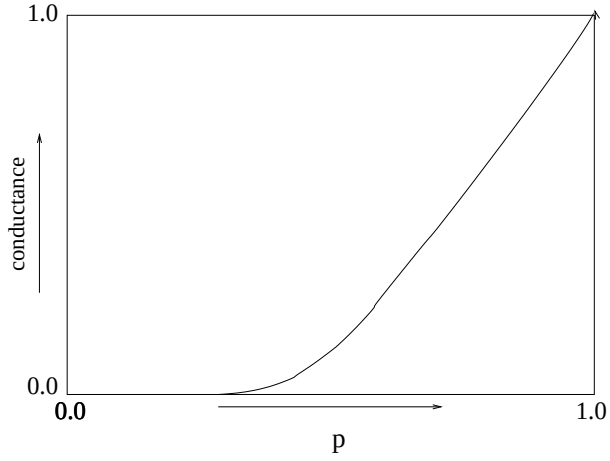

Figure 5: Schematic dependence of the normalized conductance of a medium containing insulating and conducting beads, on the concentration p of conducting beads

One can define a lattice model of percolation, instead of the continuum model defined above, which is simpler to study. In our mixed bead example, we imagine that the beads are packed in a regular closed packed lattice structure. In the site percolation model, we have a lattice, say a hypercubical lattice in d dimensions, and each site is occupied or empty, independent of other sites, with probability p or $(1-p)$ respectively. In the bond-percolation model, all sites are present, but links between nearest neighbor sites may be present or absent, again independent of other links, with probability p and $(1-p)$ respectively. In Fig. 6, we have shown a realization of site percolation on a square lattice for different p.

In fact, the percolation transition is one of the simplest examples of a *continuous* phase transition. As p tends to p_c from below, The mean size of a *connected cluster* diverges as $|p_c - p|^{-\nu}$. The mean number of sites in the cluster to which a randomly chosen site belongs, diverges as $|p_c - p|^{-\gamma}$. For $p > p_c$, the mean fraction of sites in the infinite cluster increases as $(p - p_c)^{\beta}$.

These exponents ν, γ, and β are similar to the exponents defined in other critical phase transitions. In fact, the relationship of percolation model to Ising model is quite deep. One can define a more general model, called the q-state Potts model, for which $q = 1$ is the percolation problem, and $q = 2$ corresponds to the Ising model [6]. Constraints of time and space do not

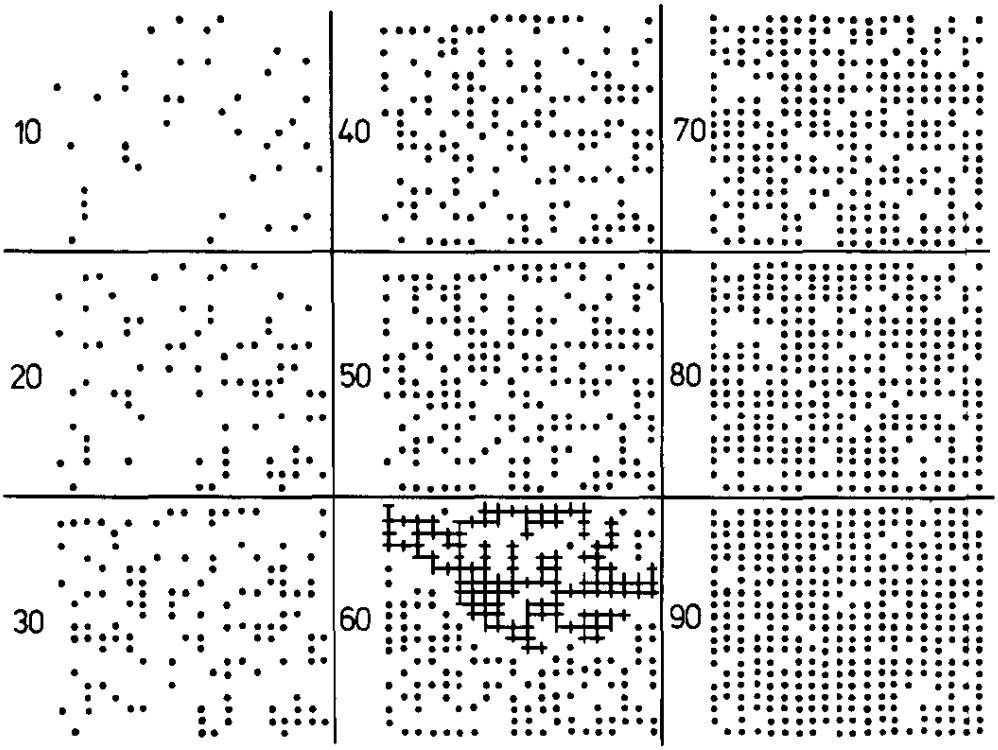

Figure 6: Site percolation on a square lattice. some typical configurations as a function of density of occupied sites. The number in each panel gives the density in percent. A spanning cluster is indicated for $p = 0.60$. Figure taken from [7].

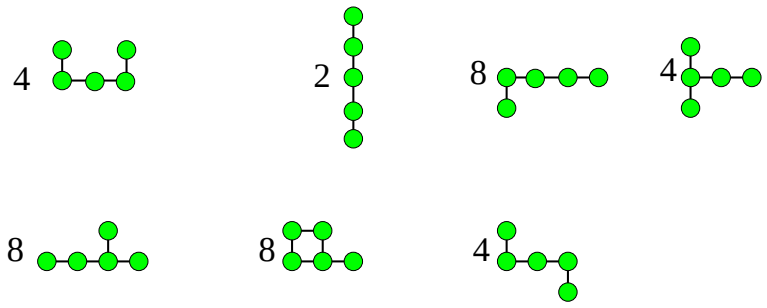

Figure 7: Different unrooted clusters with 5 sites on the square lattice.

permit us to pursue this direction here.

Consider site-percolation on the square lattice. Define $\mathrm{Prob_p(s)}$ as the probability that the origin belongs to a connected cluster of exactly s occupied sites. This is independent of the size of the lattice, so long as the boundaries are far enough, and the largest s-site cluster cannot reach the boundary.

It is easy to see that $\mathrm{Prob_p(s=0) = q}$, $\mathrm{Prob_p(s=1) = pq^4}$, and $\mathrm{Prob_p(s=2) = 4p^2q^6}$. Here $q = 1 - p$. For larger s, one has to consider all possible different clusters that can occur having s sites. For a cluster having s sites, and t perimeter sites (nearest neighbor of sites in cluster, but not part of cluster), the probability weight is $p^s q^t$. In general, we have

$$\mathrm{Prob_p(s) = \sum_t N(s,t) p^s q^t} \tag{25}$$

We would like to determine $N(s,t)$ for different s and t, and for different lattices. In Fig. 7, we have shown all the different types of clusters with 5 sites. The number in front of the cluster is the total number of distinct clusters obtainable from it by reflections or rotations. Also, the clusters shown are unrooted. The number of rooted clusters is larger than this by a factor 5, as in any cluster, there are 5 ways of marking which site is the origin.

5 Algorithm for enumerating clusters

While, in principle, for any finite s, there is a finite number of possible clusters, which can be put into a finite list, producing such a list becomes

quite nontrivial, even for $s = 6$. One has to ensure that no cluster is omitted, and there is no double counting. One needs an algorithm to organize such a list. Then the actual tedious enumeration can be done by a computer. One such algorithm is called the Martin's algorithm. It allows us to encode a complicated branched structure of the cluster by a finite binary sequence $10011001 \ldots 1$.

Given a cluster of s sites on the square lattice, Martin's algorithm assigns a label $1, 2, 3...$ to the sites of the cluster, and its perimeter sites. Let us denote the ith entry of the list as $S(i)$, which is the site with label i. We define the occupation number $N(i) = 1$, if $S(i)$ is occupied, and 0 otherwise. Since in this process we assign labels to all occupied sites, and their neighbors, the number of labels used when the above process stops is greater than s. Let the number be r. Then the cluster is coded by an r-bit binary sequence $10011100101 \ldots$, where the i-th bit in the sequence gives the value of $N(i)$.

The algorithm proceeds to generate the labeling of sites as follows:
1. We first choose a priority ordering of neighbors for each site of the lattice. This rule can be different at different sites, but will remain the same for all clusters. For example, on the square lattice, we may choose the ordering $N > E > W > S$ for all sites.
2. The root is labelled as site 1. Clearly, $N(1) = 1$.
3. At this point, there is only 1 entry in the list S, i.e. the root.
4. Go to the first unvisited occupied site in the list.
5. Assign labels to all unassigned neighbors of this site consecutively, using the chosen priority rule, and add them to the list.
6. If there are no occupied sites without assigned labels, stop. Else, go to step 4.

Clearly, the algorithm will produce a unique binary sequence $N(i)$ for any given cluster. But, a little bit of thought shows that given the sequence $N(i)$, and the known priority rule for neighbors at each site, one can reconstruct the cluster completely.

As an example, for the left-most cluster in Fig. 7 in the lower row, if the root site is the left-most occupied site, the corresponding binary sequence is 101000101100000. Also, there is no valid cluster corresponding to the binary sequence 100001.

A cluster with s sites will have a binary sequence with s ones. The number of zeroes in the sequence will be different for different clusters, but it is $\leq 2s+2$ for the square lattice. Then, one can produce all binary sequences

with s ones, and at most $2s+2$ zeroes, list the sequences that correspond to valid connected clusters in (say) the dictionary order. This can be done efficiently on the computer using the backtracking strategy. A very elegant and short computer program in Fortran that implements this for a general translationally invariant lattice, using less than 40 lines of program, is given in [8].

6 The Animal Problem

The solution of the percolation problem, then, involves determination of the cluster numbers $N(s,t)$, for different s, t, and for different lattices. In particular, we are interested in studying how these numbers vary when s and t are much greater than 1. This is usually a difficult problem, and has been solved exactly only in a few lucky cases.

One can define the two-variable generating function for $N(s,t)$ as

$$\tilde{N}(x,y) = \sum_{s=1}^{\infty}\sum_{t=1}^{\infty} N(s,t)x^s y^t \tag{26}$$

For the original percolation problem, $y = 1-x$. A simpler case of the problem corresponds to setting $y = 1$. This was given the catchy name "the Animal problem" by Harary, where one imagines all possible shapes an animal with s cells, living on a lattice, can have, with the only constraint being the connectivity constraint that all cells must be connected. We define $A(s)$ as the number of animals of s sites. Then

$$A(s) = \sum_{t=1}^{\infty} N(s,t) \tag{27}$$

and the corresponding generating function

$$\tilde{A}(x) = \sum_{s=1}^{\infty} A(s)x^s = \tilde{N}(x, y=1) \tag{28}$$

Let us first prove that $A(s)$ increases at most exponentially with s. We note that on a lattice with coordination number z, a cluster of s sites, will have at most zs perimeter sites. Then the corresponding binary sequence will be at most of length $(z+1)s$. This number is $\leq 2^{(z+1)s}$. Not all of binary sequences correspond to connected clusters. Hence

$$A(s) \leq 2^{(z+1)s}. \tag{29}$$

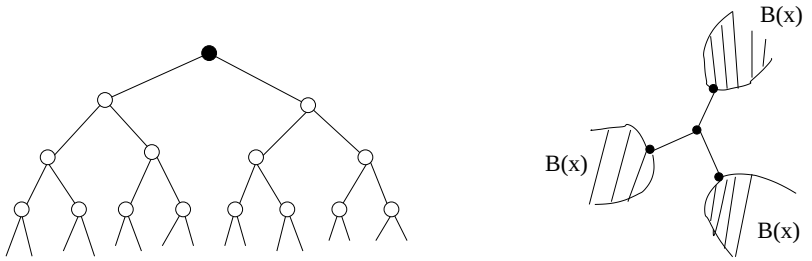

Figure 8: (a) A binary tree. The root site is denoted by a filled circle. (b) Generating function for enumerating animals on the 3-coordinated Bethe lattice. Here $B(x)$ denotes sum over all animals on the binary tree with that root.

Exercise 7: Improve the bound (29).

Also, it is easy to see that $A(s) > 2^s$. Thus, it grows exponentially with s, for large s. In fact, one finds that

$$A(s) \sim C\lambda^s s^{-\theta} \tag{30}$$

where C and λ are constants, and θ is some exponent, that is found to be independent of the details of the lattice, and only depends on dimension.

In the original percolation problem, for $p < p_c$, the probability that a randomly chosen site belongs to a cluster of size varies as $D_p e^{-C_p s} s^{-\theta}$, where C_p and D_p are p-dependent functions, for $C_p s \gg 1$. The exponent θ is independent of p. It can thus be considered as an off-critical exponent of the percolation problem. Thus, while the "critical exponents" of percolation can only be seen only very near the critical point, the "off-critical exponent" θ is seen in the entire low-density phase of percolation theory. For a discussion of other off-critical exponents of the percolation theory, see [9].

6.1 The Bethe lattice

One simple case where the function $\tilde{A}(x)$ can be determined exactly is for a Bethe lattice with coordination number z. We will consider here the case $z = 3$. We define $\tilde{A}(x)$ as the sum over all animals containing the origin, with the weight of an animal of size s being x^s. Let $B(x)$ be the generating function of all animals rooted to the vertex of an infinite binary tree (see

Fig. 8). Then, clearly, we have

$$B(x) = x[1 + B(x)]^2 \tag{31}$$

This quadratic equation can be solved for $B(x)$, giving

$$B(x) = \frac{1}{2x}[1 - 2x - \sqrt{1 - 4x}] \tag{32}$$

Which can be Taylor expanded to give

$$B(x) = x + 2x^2 + 5x^3 + \ldots \tag{33}$$

Finally, the generating function $\tilde{A}(x)$ is given by

$$\tilde{A}(x) = x[1 + B(x)]^3 \tag{34}$$

Which then gives

$$\tilde{A}(x) = x + 3x^2 + 9x^3 + 28x^4 + \ldots \tag{35}$$

The singularity closest to origin of $\tilde{A}(x)$ in the complex x-plane occurs at $x = 1/4$, and from Eq. (31) and (33), it is easy to see that $\tilde{A}(x = 1/4 - \epsilon) \sim 2 - 12\sqrt{\epsilon}$ to leading order in ϵ, for small ϵ. This implies that $A_n \sim 4^n n^{-3/2}$, for large n.

6.2 Directed Animals

One can also obtain the exact animal generating function for a variant of the animal problem for a regular two dimensional graph. We consider a directed square lattice, where all bonds are directed right or up. A directed animal is a connected cluster of sites where each site belonging to the cluster is either the origin, or has a downward or leftward neighbor that also belongs to the cluster. An example is shown in Fig. 9.

The directed animal problem turns out to be much simpler than the corresponding undirected problem, as the allowed configurations of animals for $x + y > T$ depend on the sites occupied on the line $x + y = T$ and not on the configuration of the animal below this line. In fact, one can think of T as a "time" coordinate, and then the directed animal becomes the space-time plot of a process where a particle can move one step left or right, divide into two, or die.

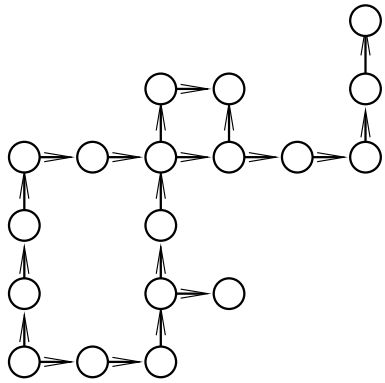

Figure 9: A directed animal on a square lattice.

Let A_n be the number of animals with n sites on the square lattice. We define $A(x) = \sum_n A_n x^n$. Then it is easily seen that

$$A(x) = x[1 + 2A(x) + A_{11}(x)] \tag{36}$$

where $A_{11}(x)$ is the generating function for all directed animals that have a source at two adjacent point along the line $x + y = 1$, say $(1, 0)$ and $(0, 1)$. Similarly, we can write $A_{11}(x)$ in terms of more complicated functions

$$A_{11}(x) = x^2[1 + 3A(x) + 2A_{11}(x) + A_{101}(x) + A_{111}(x)] \tag{37}$$

Here $A_{101}(x)$ and $A_{111}(x)$ are generating function for animal with source 101 and 111 along a constant -T line (in a fairly self-explanatory notation).

One can similarly write recursion equations for $A_{101}(x)$ etc. More generally, let C be a configuration of occupied sites on a line of constant time $x + y = T$. Then $A_C(x)$ is the generating gunction of all directed animals with starting from a point in C. Then it is easy to see that $A_C(x)$ satisfies the recursion equation

$$A_C(x) = x^{|C|} \left[1 + \sum_{C'} A_{C'}(x)\right] \tag{38}$$

where C' is a possible nonempty configuration of occupied sites on the line $x+y = T+1$, and the sum over C' is over all such sources. $|C|$ is the number of sites in C.

One can use such recursion relations to generate the series expansions for $A_C(x)$ to very high orders [10].

We can use these recursion relations to establish the equivalence of the $1+1$-dimensional directed animal problem to that of time evolution of a one dimensional lattice gas with nearest neighbor exclusion, and no particle conservation. This then gives us a very simple example of the important phenomena of *dimensional reduction*, where the calculation of properties of some d-dimensional system reduces to that of a different lower -dimensional problem (here lower by 1). This is very useful, as the lower dimensional problems are usually easier to solve [11].

Let us consider time evolution of a lattice gas on a line. Assume that evolution is discrete time, Markovian, with odd-even parallel update with the following evolution rule: A site x at time t is occupied with probability p, if at time $t-1$ both sites $x-1$ and $x+1$ were empty, and is unoccupied otherwise, irrespective of its earlier value. It is easy to see that these rules satisfy detailed balance condition corresponding to the hamiltonian

$$H = +\infty \sum_i n_i n_{i+1} - \mu \sum_i n_i \tag{39}$$

The somewhat non-standard notation is a short hand for interaction strength J, in the limit J tends to infinity. In the long time steady state of the Markov chain, the probabilities of different configurations are same as in the Boltzmann-Gibbs measure corresponding to H. In the latter, one can easily determine the average density $\rho(z)$ of the gas corresponding to the activity $z = \exp(\beta\mu)$. We have

$$\rho(z) = \frac{1}{2}\left[1 - \frac{1}{\sqrt{1+4z}}\right] \tag{40}$$

We can now ask what is the probability that in the steady state of this Markov process, if we observe at a particular time T, the set of sites C will be all occupied. Denote this by $Prob(C)$. Clearly, $Prob(C)$ is equal to the probability that each of the sites was vailable of occupation, and it was occupied. The latter probability is $p^{|C|}$. the former is the probability that each of the neighbors of sites in C was *not occupied*. This is easily determined using the inclusion -exclusion principle. Thus, $Prob(C)$ satisfies the recursion equation

$$Prob(C) = p^{|C|}\left[1 + \sum_{C'}(-1)^{|C'|} Prob(C')\right] \tag{41}$$

Here the sum over C' is over all proper subsets of set of neighbors of C. Comparing with the eq. (34), we can make the identification

$$A_C(x = -p) = (-1)^{|C|} Prob(C) \tag{42}$$

In particular, the mean density of this Markovian evolving gas gives us the generating function of the 2-d site animals. We note that the activity of the gas in terms of p is $z = p/(1-p) = -x/(1+x)$. This gives

$$A(x) = -\rho(z = \frac{-x}{1+x}) \tag{43}$$

Eq. (40) then gives

$$A(x) = \frac{1}{2}\left[\sqrt{\frac{1+x}{1-3x}} - 1\right] \tag{44}$$

From this it is easily seen that for large n, A_n increases as $3^n n^{-1/2}$.

Note that the singularity of $A(x)$ closest to the origin occurs for $x = 1/3$. This corresponds to the Markovian evolution of the 1-dimensional lattice gas, but with $p = -1/3$ [12]. Negative values of p, of course, are unphysical. One has to think of the Markov matrix (whose matrix elements are simple polynomial functions of p), and analytically continue this matrix to negative values of p. Equivalently, one can think of the stochastically evolving lattice -gas as a particular kinetic Ising model, where the spins are evolving in the presence of a field, and then take the analytical continuation to magnetic fields that are imaginary. Then this problem becomes equivalent to the *critical dynamics of Ising model near the Lee-Yang Edge singularity*. The study of Lee-Yang edge singularity is an important problem in statistical physics, as it relates to the analytical structure of singuraities of equation of state of hard core gases (see [13] for a longer discussion of this point). But it is difficult to study, as the corresponding Boltzmann weights are non-positive, and usual thermodynamic convexity relations do not hold. The directed animals problem gives us a realization of the Lee-Yang problem with positive weights.

This relationship between equilibrium statistics of a d-dimensional nearest neighbor exclusion gas to the $d+1$-dimensional directed animal is valid for arbitrary d. In particular, one can use the known exact solution of the hard hexagon lattice gas by Baxter [14] to determine the exact number of 3-dimensional directed animals [15]. One can also relate correlation functions of the lattice gas to those of the animals problem [16].

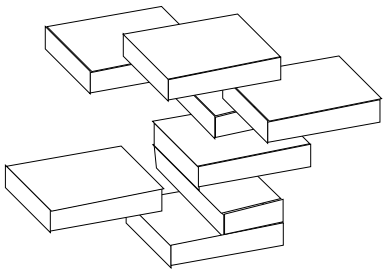

Figure 10: A heap in three dimensions, made of two different types of horizontal rectangular pieces.

7 Heaps

The problem of directed animals has a very elegant, and nontrivial generalization to heaps [17]. Informally, heaps are like directed animals, but are made up of different types of "pieces". In Fig. 10, we have shown a 3-dimensional heap made of two types of rectangles. The heap is made up of different layers of tiles. In each layer, the tiles are non-overlapping, and each tile is "supported" from below, i.e. it can not fall down to the lower layer under gravity, as at least one site below is already occupied by another tile in the lower layer.

We consider heaps defined on a discrete space. The "base" is the lowermost layer, and consists of a finite number of sites. Each higher layer is an exact copy of the base placed "vertically above" it. Each tile covers a finite number of sites in one layer. We assume we have a finite number of different types of tiles. We associate activity $z_1, z_2, z_3 \ldots$, with tiles of type $1, 2, 3 \ldots$. The weight of a heap $\mathcal{H}$ containing n_i tiles of type i is $z^{\mathcal{H}} = \prod_i z_i^{n_i}$. We define the heap generating function

$$H(\{z_i\}) = \sum_{\mathcal{H}} z^{\mathcal{H}} \tag{45}$$

Let $D(\{z_i\})$ be the grand partition function of the gas of non-overlapping tiles placed on the base space. This is just all possible heaps with tiles only in the first layer. i.e.

$$D(\{z_i\}) = \sum_{\mathcal{H}_1} z^{\mathcal{H}_1} \tag{46}$$

Example: Consider a base space consisting of only four sites forming a 2×2

square. There are two types of tiles : dimers that occupy two adjacent sites, and have activity z_1, and triangular pieces that occupy three sites, and have activity z_2. Then clearly, $D(z_1, z_2)$ is a finite polynomial in z_1, z_2, given by

$$D(z_1, z_2) = 1 + 4z_1 + 2z_1^2 + 4z_2 \tag{47}$$

Here $H(z_1, z_2)$ is the formal infinite series, which starts as

$$H(z_1, z_2) = 1 + 4z_1 + 4z_2 + 14z_1^2 + 8z_1z_2 + 16z_2^2 + \ldots \tag{48}$$

Then, with H and D defined by Eqs. (45) and (46), we have the remarkable general result

$$H(\{z_i\}) = 1/D(\{-z_i\}) \tag{49}$$

where $D(\{-z_i\})$ is the polynomial obtained by replacing z_i by $-z_i$, for all i in $D(\{z_i\})$. Note that the result is valid independent of the number and shape of tiles. In fact, the structure of the base space also does not come into picture. It shows the dimensional reduction, by expressing that the partition function of "3-dimensional" heaps in terms of the "two-dimensional" partition function D.

Proof: We define a tile in a heap to be maximal, if there is no tile above it, i.e. it can be removed from top without encountering other obstructing tiles. We can write Eq.(49) as

$$H(\{z_i\})D(\{-z_i\}) = \sum_{\mathcal{H},\mathcal{H}_1} (-1)^{|\mathcal{H}_1|} z^{\mathcal{H}} z^{\mathcal{H}_1} = 1 \tag{50}$$

The proof of relation follows by showing different terms in the expansion corresponding to configurations having at least one tile can be paired in way that each pair adds up to zero. Then the total sum is equal to the only unpaired term in the summation, which corresponds to the trivial configuration with no tiles.

Given the heaps $\mathcal{H}$ and $\mathcal{H}_1$, we define a set of tiles $\mathcal{T}$, which contains tiles in $\mathcal{H}_1$, and those maximal tiles in $\mathcal{H}$ that do not overlap with any tile in $\mathcal{H}_1$. Now, the sum over $\mathcal{H}, \mathcal{H}_1$ in Eq.(50) can be written as sum over different possible $\mathcal{T}$, and $\mathcal{H}'$, the remainder of $\mathcal{H}$ on removing the maximal pieces. Now, consider the summation over $\mathcal{T}$, for a fixed $\mathcal{H}'$. In this summation, each allowed $\mathcal{T}$ contains non-overlapping tiles. Any one tile may come from $\mathcal{H}$, or from $\mathcal{H}_1$. If the tile i is allowed in this sum, and comes from $\mathcal{H}$, it contributes a factor z_i, but if it comes from $\mathcal{H}_1$, it contributes a factor $(-z_i)$.

These factors cancel exactly, and the only nonvanishing term in the sum in Eq.(50) comes from the term where $\mathcal{H}$ and $\mathcal{H}_1$ are both empty sets. This contribution is exactly 1, proving the claim.

Note that the theorem remains valid, if we make the weights of pieces space-dependent and associate activities $z_i(\{\vec{x}\})$ for the tile i at positions $\vec{x}$ along the base. Then differentiating the logarithm of the grand partition function $D(\{z_i\})$ with respect to $z_i(\vec{x})$ gives the probability that tile i will be present at position $\vec{x}$ in the ensemble. Interestingly, this has a direct combinatorial interpretation, which is a generalization of the Eq.(43). The analogue a single directed animal in the heaps is called a 'pyramid', that is a heap with a single maximal piece (one should think of the inverted pyramid as a heap supported at base by only one tile). The generating function of a pyramid with maximal piece M is given by $P_M(\{z_i\}) = N(\{z_i\})/D(\{z_i\})$ where

$$N\{z_i\}) = \sum_{\mathcal{H}_1'}(-1)^{\mathcal{H}_1} z^{\mathcal{H}_1'} \tag{51}$$

where the prime over summation indicates that the summation in which the tile M is not used. The proof of this proposition is very similar to the earlier proof, and is omitted here [17].

The heaps were first discussed in the context of applications in computer science. One thinks of distributed computing, where there are N different processors, and several jobs to be executed. Let us consider for simplicity the case where each job takes one unit of time. Each job corresponds to a tile and may occupy more than one processor. There is a time ordering of jobs on any one processor, but no necessary relative time order between jobs that do not involve common processors. Then, in the optimal scheduling, the space-time-history of computation is a heap, where occupied/unocupied sites denote which processors are busy /idle at what times [18].

More recently, heaps have been used in modelling random space -time stuctures involved in theories of quantum gravity. Unfortunately, details of this very interesting subject are outside the scope of these lectures. The interested reader may consult [19].

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