

# An Introduction to Percolation Theory -III

Deepak Dhar

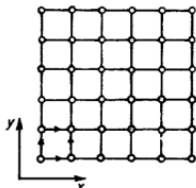
I.C.T.S., T.I.F.R., Bengaluru

Bengaluru School in Statistical Physics XV, Sep 3-20, 2024

## Directed Animals

For the undirected animals enumeration problem, exact analysis has not been possible in any nontrivial case so far. The situation is better in the directed case.

Consider a directed square lattice. A directed animal is a set of sites connected to the origin by directed bonds.



Let  $A_n$  be number of directed animals of  $s$  sites, besides the origin.

Then it is easy to see that for  $s = 1, 2, 3, 4, \dots$

$$A_s = 1, 2, 5, 13, \dots$$

Define  $A(x) = \sum_{s=1}^{\infty} A_s x^s$ .

$A(x)$  is the generating function, sum over all animal configurations, the weight of a configuration of  $s$  sites being  $x^s$ .

Then using the directedness property, we can set up a recursion relation

$$A(x) = x[1 + 2xA(x) + x^2 A_{11}],$$

where  $A_{11}$  is the generating function for animals starting with two neighboring sites along a constant  $t = (x + y)$  line.

Thus  $A(x)$  can be expressed in terms of  $A_{11}(x)$ . There is a recursion relation for  $A_{11}(x)$

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

Note also that  $A_{111} = xA_{101}$ .

More generally, consider a general source  $C$ , specified by its binary string of the form 11000101..., we denote the generating function by  $A_C(x)$ .

Then  $A_C(x)$  satisfies the recursion relation

$$A_C(x) = x^{|C|} \left[ \sum_{C'} A_{C'}(x) \right],$$

where the sum is over all possible allowed occupation states of the next layer  $C'$  after  $C$ .

These are called recursion relations, as if we know these functions as a power series to some order  $x^n$ , then using the series, we can determine the coefficients of the series expansion of order  $x^{n+1}$ , and so on.

The full hierarchy can be truncated at any level, and all coefficients of lower order are exactly determined.

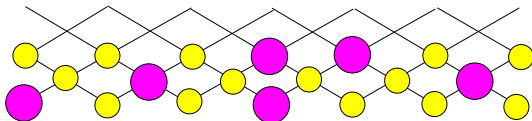
In fact, we used such recursion relations, along with the Martin's algorithm, in 1982, we managed to produce a longish series

Square
1
2
5
13
35
96
267
750
2 123
6 046
17 303
49 721
143 365
414 584
1 201 917
3 492 117
10 165 779
29 643 870
86 574 831
253 188 111
741 365 049
2 173 243 128
6 377 181 825
18 730 782 252
55 062 586 341
161 995 031 226
476 941 691 177
1 405 155 255 055
4 142 457 992 363
12 219 350 698 880
36 064 309 311 811
106 495 542 464 222
314 626 865 716 275

## A model of growing mixed crystals

We consider a model of growth of a crystal from a supersaturated solution of mixture of NaCl and KCl.

The growth in the model occurs layer by layer, Each 'odd' site may be occupied by K or Na. This occurs with different probabilities. Denote K atom by 1 ( large magenta spheres), and Na atom by 0 (small yellow spheres).



The rule for growth: A potential site may be occupied by K, only if both sites below are Na, and then only with a probability  $p$ . Else, it occupied by Na.

If the system grows for a long time, it forgets the memory of initial state. Then there is a fractional density of  $K$  sites in this state,  $\rho(p)$  that depends on  $p$ .

This Markovian evolution has an explicit directed structure. One can write an equation for  $\rho(p)$ :

$$\text{Prob}(1) = p[\text{Prob}(00)],$$

and using inclusion-exclusion principle, this may be written as

$$= p[1 - 2\text{Prob}(1) + \text{Prob}(11)],$$

More generally, we denote by  $\text{Prob}(1100101)$  the probability that we get a **local** configuration 1100101 in the steady state. Then we get, for a general string  $C$

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

where the sum over  $C'$  is over all possible occupations of sites that are **predecessors** of occupied sites in  $C$ .

It is very interesting that the structure of these equations is the same as in the directed animals problem. In fact, we see that the equations transform into each other under the identification

$$\text{Prob}(C) = (-1)^{|C|} A_C(x = -\rho).$$

Then the problem of determining  $A(x)$  reduces to that of determining the asymptotic density of  $K$  atoms in the CGM.

But the same picture of CGM may be thought of as a plot of [the history of a 1-dimensional lattice gas undergoing parallel update even odd evolution](#) with the following transition probabilities:

010  $\rightarrow$  000, with probability  $(1 - \rho)$ ,

000  $\rightarrow$  010, with probability  $\rho$ .



But these transition rates satisfy the **detailed balance condition** corresponding to the **1-dimensional nearest -neighbor exclusion lattice gas** with the Hamiltonian

$$H_{nne} = +\infty \sum_i n_i n_{i+1} - \mu \sum_i n_i,$$

with activity  $z = \exp(\beta\mu) = p/(1 - p)$ .

Then in the long -time steady state of CGM, probabilities of different configurations on a constant time slice correspond to the equilibrium measure of the Hamiltonian  $H_{nne}$ .

cc

In this case, it is easy to see that the Landau free energy per site is

$$\omega(z) = \log \left[ \frac{1 + \sqrt{1 + 4z}}{2} \right],$$

Then the density is given by the  $\rho(z) = z \frac{d}{dz} \omega$ , giving

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

Then converting this result to the generating function for animal numbers, we get

$$A(x) = \left[ \sqrt{\frac{1-x}{1-3x}} - 1 \right] / 2.$$

This agrees exactly with all the series coefficients calculated numerically earlier.

More importantly, the arguments are easily extended to higher dimensions. Consider the directed bcc lattice in  $d$ -dimensions.



Fig: The directed bcc lattice in 3 dimensions.

In this case, we get the generating function for directed animals in  $d$  dimensions equal to the density of the nearest exclusion gas in  $(d - 1)$ -dimensions with activity  $z$  denoted by  $\rho_{(d-1)}(z)$  as

$$A_{d,bcc}(x) = -\rho_{(d-1)}(z = -x/(1-x)).$$

The directed animals problem shows **dimensional reduction**, in that the solution of a  $d$ -dimensional problem reduces to the solution of a (usually easier)  $(d - 1)$ -dimensional problem.

Unfortunately, the nearest -neighbor exclusion gas on a square lattice is not exactly solved, and so, this does not yield an explicit determination of  $A_{3,bcc}$ .

But we can construct a directed cubic lattice, with directed bonds to first and second nearest neighbors. In this case, the generating function reduces to the solution of another hard core lattice gas model: hard hexagons, for which the exact solution was obtained by Baxter in 1972.



The directed cubic lattice with next nearest bonds.

Then using Baxter's expression for the density of the hard hexagon gas a function of activity, we get for this lattice, the exact generating function. Unfortunately, the expression is a bit complicated.

Set

$$g(x) = \prod_{n=1}^{\infty} \frac{(1-x^{5n-4})(1-x^{5n-1})}{(1-x^{3n-3})(1-x^{5n-2})} \quad (2)$$

0305-4470/80/030061+10\$01.00 © 1980 The Institute of Physics

L61

#### L62 Letter to the Editor

Let  $z$  be the activity and  $\kappa = Z^{1/N}$  the partition function per site. Then, for  $z$  less than some critical value  $z_c$ ,

$$z = -x[g(x)]^5, \quad (3)$$

$$\kappa = \prod_{n=1}^{\infty} \frac{(1-x^{6n-4})(1-x^{6n-3})^2(1-x^{6n-2})(1-x^{5n-4})^2(1-x^{5n-1})^2(1-x^{5n})^2}{(1-x^{6n-3})(1-x^{6n-1})(1-x^{6n})^2(1-x^{5n-3})^3(1-x^{5n-2})^3}; \quad (4)$$

while for  $z > z_c$

$$z^{-1} = x[g(x)]^5, \quad (5)$$

$$\kappa = x^{-1/3} \prod_{n=1}^{\infty} \frac{(1-x^{3n-2})(1-x^{3n-1})(1-x^{2n-3})^2(1-x^{2n-2})^2(1-x^{5n})^2}{(1-x^{3n})^2(1-x^{5n-4})^3(1-x^{5n-1})^3}. \quad (6)$$

The number of animals of  $s$  sites, for large  $s$  grows as  $C\lambda^s s^{-\theta}$ , where  $\lambda = (9 + 5\sqrt{5})/2$ ,  $\theta = 5/6$ .

## The Lee-Yang theory of phase transitions

Consider the grand partition function of molecules with a hard core, and also longer rang attractive interactions, in a box of volume  $V$ .

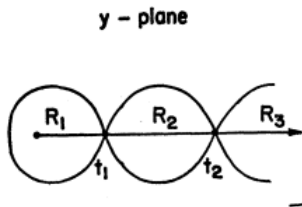
$$\Omega_V(z) = \sum_{n=0}^{n_{max}} \mathcal{Z}_n(V, T) z^n$$

This is a polynomial in  $z$  of degree  $n_{max} \approx 1.V$ . Then it has exactly  $n_{max}$  zeros in the complex  $z$ -plane.

The partition function is analytically extended in the whole complex plane. The log of the partition function is like the potential due to unit charges at the placed at the zeros of  $\Omega$ .

In the limit of large  $V$ , the zeroes have a limiting continuous distribution. Lee and Yang showed that in some cases, there are lines of zeroes with a continuous line-density.

As we change temperature, the zeroes move. If the zeroes pinch in on the real axis, it gives singularities in the partition function per molecule.



**Figure:** Figure from Lee and Yang's paper, showing lines on zeros in the complex  $z$ -plane (called  $y$ -plane here), showing two phase transitions.

## The universal Yang-Lee edge singularities

M E Fisher noted that the radius of convergence of the Mayer series for density as a function of the activity  $z$  is governed by the singularity closest to the origin in the complex  $z$  -plane.

It turns out that this is usually on the negative real- $z$  axis. The position varies with temperature, but the qualitative nature of singularity is the same for different fluids; Hard spheres, ferromagnetic/ antiferromagnetic Ising models, Lennard-Jones fluids ...

The value of the exponent depends only on the dimension. Near this point, the analytically continued correlation length diverges, and this is a genuine critical point, where the analytically continued free energy has a singularity. Now called the Yang-Lee edge singularity.



At the YL- edge singularity, there is only one independent critical exponent.

At the end-points of lines of zeros, the density of zeros has a power-law singularity  $\sim \epsilon^{\phi-1}$ , where the exponent  $\phi$  is **universal, independent of temperature, and depends only on dimension.**

Thus, if we analytically continue the equation for  $P(z)$  to complex values of  $z$ , the closest singularity to the origin is on the negative  $z$ , and should have this singularity.

There is an even more amazing dimensional reduction, and it is shown that the undirected animals enumeration problem in  $(d + 1)$ -dimensions can also be related to the Lee-Yang edge singularity in  $(d - 1)$  dimensions.

Unfortunately, this argument is rather subtle, using supersymmetry, and not fully understood by me [Brydges and Imbrie, *Annals of Mathematics*, 158 (2003), 1019–1039].

In the end, we get this relation between the critical exponents :

$$\theta_{directed}[d] = \sigma_{YL}[d - 1] + 1 = \theta_{undirected}[d + 1] - 1.$$

The value of  $\sigma_{YL}[d]$  is known exactly for  $d = 0, 1, 2$ , and  $d \geq 6$ . It is  $-1, -1/2, -1/6$  and  $1/2$ . In other cases, only estimates from series expansions, or  $\epsilon$ -expansion with Borel - resummation, are available.

## Exercises:

1. Use the expression for  $A(x)$  for directed 2-d animals to deduce the asymptotic behavior of  $A_s$  for large  $s$ .
2. From the exact solution of the hard hexagon gas, it is known that it undergoes a phase transition at a critical value of the activity  $z$ . What constraints does it place on the density of zeroes in the complex plane?