STATISTICAL MECHANICS

I Fractals

Structures with no characteristic length (scale-invariant) are known as fractals.

Area of a triangle of side $L$:
$$ A = \frac{\sqrt{3}}{4} L^2 $$

After first step, area of triangular region is:
$$ A(L) = 3 \times A(L/2) = 3^2 A(4L/2^n) = \cdots = 3^n A(L/2^n) $$

Let $b = 2^n$. 
$$ \ln b = \ln 2 \Rightarrow 3^n = e^{\ln 3 \ln b / \ln 2} = b^{\ln 3 / \ln 2} \equiv b^d $$

So
$$ A(L) = b^d \times A(L/b) $$

Let $L/b = a \Rightarrow A(L) = A(a)(L/a)^d \propto L^d$.

Solid triangle scales as $L^2$.

Sierpinski gasket as $L^d$.

Fractal dimension:
$$ d_f = \frac{\ln 3}{\ln 2} \approx 1.58 $$

II Polymer Chain

Consider a chain of bonded monomers. Each step $r_i$ of a random walk represents a bond. Length is fixed: $|r_i| = a$.

End-to-end displacement:
$$ R = \sum r_i $$

The random walk gives the chain a bell shape. Measure size using RMS $\langle R \cdot R \rangle^{1/2}$. Known as radius of gyration $R_g$.

$$ R_g^2 = \langle R \cdot R \rangle = \langle (\sum i r_i) \cdot (\sum j r_j) \rangle = \sum i \langle r_i \cdot r_i \rangle = \sum i < r_i^2 > = Na^2 $$

$$ R_g = \sqrt{Na} $$

much smaller than stretched-out chain for $N \gg 1$

Notice also $\langle R \rangle = 0$

Random walk: many indep. steps following the same distribution.

$\Rightarrow$ invoke Central Limit Theorem

$$ P(R) = \frac{1}{(2\pi Na^2)^{3/2}} \exp \left( -\frac{R^2}{2Na^2} \right) $$

Mass $M$ scales as:
$$ M = Nm = m \left( R_g a \right)^2 $$

$$ M(R) \propto R^2 $$

$d_f = 2$
2.1 Percolation

Large 2D array of square sites, populated with prob. $p$. Joined occupied sites are a **cluster**. A cluster that spans from one edge to the other is a percolating cluster.

Prob. of finding a percolating cluster is vanishingly small below the percolation threshold $P_c$.

2.2 1-D Percolation

- **Probability of spanning cluster**: $p^L$

  But for $p < 1$ and $L \to \infty$, $p^L \to 0$. :: threshold $P_c = 1$

- $n(s, p)$ average # clusters of size $s$ per unit length
  
  $n(s, p) = \frac{1}{L} \times L^2 \times (1-p)^2 p^s = (1-p)^2 p^s$

  Write as $n(s, p) = (1-p)^2 e^{s \ln p} = (1-p)^2 e^{-s \ln 1/p}$

  with $S_\xi = \frac{1}{\ln p}$ **Typical cluster size**

  Clusters at sizes $> S_\xi$ are exponentially hard to find.

As we approach $P_c$, look at $S_\xi$ as a fn. of the distance to the threshold, $s = 1 - p$:

$$\ln p = \ln (1 - S_{\xi(p)})$$

for $S_{\xi(p)} \approx \frac{1}{p}$ as $p \to 1$.

- Another measure of cluster size: mean cluster size $\langle X(p) \rangle$.

  If we simply averaged the sizes of clusters, it would be dominated by small sizes since small clusters are more frequent.

  But each large cluster contains many sites, so weight the cluster size with the number of sites it contains. Weight $w_m = S_m^2$.

  $$X = \frac{\sum S_m w_m}{\sum w_m} = \frac{\sum S_m^2}{p L}$$

  $25m$ is total # of occupied sites which is just $pL$.

There are $L \times n(s, p)$ cluster with the same size $s$,
Note can also interpret $X(p)$ as: pick random site, ask what is the size of the cluster it belongs to, average over many trials

$$X = \frac{1}{pL} \sum_{s=1}^{L} s^2 \text{L} \times n(s,p) = \frac{\sum s^2 n(s,p)}{p}$$

Using form of $n(s,p)$:

$$X(p) = \frac{(1-p)^2}{p} \sum_{s} s^2 p^s = \frac{1+p}{1-p}$$

4. If site $i$ is occupied, what is the prob. that $j$ is in the same cluster?

$$g(i,j) = p \times \frac{1-i-j-1}{s} = p |i-j|$$

prob $j$ is prob all sites are occupied.

$$g(i,j) = e^{-|i-j|/\xi} \text{ where } \xi(p) = \frac{1}{\ln p} = \xi \text{ correlation length}$$

5. Measures:

<table>
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<th>R</th>
<th>Typical cluster size</th>
<th>$S_\xi = \frac{1}{\ln p}$</th>
<th>$\propto \frac{1}{1-p}$</th>
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<td>Correlation length</td>
<td>$\xi = \frac{1}{\ln p}$</td>
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III BETHE LATTICE

Bethe lattices have no loops. Each site has 2 neighbors. ($t=1$)

Focus on a particular site ($h=0$). It has 2 direct neighbors which have $2(2-1)$ direct neighbors ($l=2$)

Can also see $l=0$ as parent with $2$ branches

Percolation problem: is $l=0$ connected to sites at $l=\infty$ via occupied sites?

1. Build up a cluster starting from $l=0$.

On average, $2^p$ occupied $l=1$ sites.

Next step: expect $(2^p) \times p$ occupied $l=2$ sites.

Carry on, and if we can continue indefinitely then there's a spanning cluster.

Need $(2-1)p \geq 1$ \[ \Rightarrow p_c = \frac{1}{2-1} \]

(which also guarantees)

For $t=2$, $p_c = 1$ i.e. 1-D chain.
2) \( \lambda(p) \), mean cluster size: expected size of a cluster to which any particular site would belong.

\[ \lambda(p) = 1 + 2pB \]

\( l \geq 0 \) -> average size of sub-branches

Look at \( B \). All sub-branches are equivalent. Each branch at generation \( l > 0 \) has an occupied site and, on avg., \((2-1)p\) direct occupied neighbours.

\[ \Rightarrow B = 1 + (2-1)pB \Rightarrow B = \frac{1}{1-(2-1)p} \]

This breaks for infinite clusters.

Substitute: \( \lambda(p) = \frac{1+p}{1-(2-1)p} = \frac{p_c(1+p)}{p_c - p} \) for \( p < p_c \)

As \( p \to p_c \), \( \lambda(p) \approx \frac{1}{(p_c - p)} \)

3) \( b_{ij} \): distance (# steps) between \( i \) and \( j \).

- treating \( i \) as \( l=0 \), \( j \) is of generation \( b_{ij} \):

\[ N(i,l) \]: expected number of sites at generation \( l \) of cluster with root \( i \).

\[ N(i,l) = \sum_{b_{ij} = l} p^{b_{ij}} = p^l \times (\# \text{sites at generation } l') = 2(2-1)^{l-1}p^l \]

Probability of neighbours at generation \( l \) to be in the same cluster as \( i \):

\[ = \frac{l}{2-1} \cdot \frac{l}{(2-1)p} \cdot \frac{l}{2-1} \cdot e^{-l/b_{eq}} \]

with \( b_{eq}(p) = \frac{1}{\ln(2-1)p} = \frac{1}{\ln p_c} \).

As \( p \to p_c \), \( b_{eq} \approx \frac{1}{p - p_c} \)

Correlation length (infinite)

4) Cluster size distribution \( n(s,p) = \frac{p_s}{s(1-p)}t(s)g(s,z) \)

- \( t(s) \): if we add an extra site to a cluster, we gain \((2-1)\) empty sites but lose a previously unoccupied perimeter site.

\( \Rightarrow t(s+1) = t(s) + (2-2) \)

Since \( t(s=1) = 2 \Rightarrow t(s) = (2-2)s + 2 \)
\[ n(s,p) = p^s (1-p)^{(\ell-2)s+2} \]

\( g(s,\ell) \) is hard to calculate. However, notice it doesn't depend on \( p \).

To extract typical size \( s_k \), consider ratio:

\[ \frac{n(s,p)}{n(s,pc)} = p^s (1-p)^{(\ell-2)s+2} \Rightarrow n(s,p) = n(s,pc) (1-p)^{2} \left( \frac{(1-p)^{s+2} p}{(1-p)^{s+2} pc} \right)^S \]

Typical cluster size:

\[ s_k = -\frac{1}{\ln \left[ \frac{(1-p)^{s+2} p}{(1-p)^{s+2} pc} \right]} \]

We assumed \( n(s,pc) \) doesn't decay exponentially.

\[ p = \sum_s s n(s,p) \]

At \( p = pc \), must diverge but if \( \int ds s^2 n(s,pc) \) is \( \int ds s^2 e^{-s/s_k} \), it would converge: \( n(s,pc) \) doesn't decay exponentially.

For large \( s \), \( n(s,pc) \sim \frac{1}{s^{s/2}} \Rightarrow \) cluster is fractal.

As \( p \to pc^- \), \( s_k(p) \sim \frac{1}{(pc-p)^2} \), \( n(s,p) \sim \frac{1}{s^{s/2}} \left( e^{-s/s_k(p)} \right) \) \([s_k(p) \to 0] \)

3. Can explore what happens above the percolation threshold:

**Strength of the infinite cluster** \( P_0(p) \): prob. that a site belongs to the percolating cluster, or equivalently, the fraction of lattice sites taken up by the percolating cluster.

\[ P_0 = P \left[ 1 - (\text{prob. that no branch}) \right] = P \left[ 1 - Q^\ell \right] \]

where \( Q \): prob. a branch is not connected to \( \infty \)

\( Q = \left( \text{prob. that } \ell = 1 \text{ branch} \right) = (1-p) + p \left( \text{prob. that no } \ell = 2 \right) \)

\[ \Rightarrow Q = (1-p) + p Q^{\ell-1} \]

For \( \ell = 3 \) it's just a quadratic, \( Q = \left( \frac{1}{p-1} \right) \left( \text{between 0 and 1 only} \right) \)

\[ P_0(\rho, \rho_c = \frac{1}{2}) = P \left( 1 - Q^{\ell=3} \right) = P \left( 1 - \frac{(1-p)^3}{p^3} \right) \sim 6 (p-p_c) \]

Many of the results above are independent of \( \ell \) near \( pc \).

This is known as **universality**.
3.1 Scaling Hypothesis

In 3 and more dimensions there are few analytic results, but power laws appear again for singular quantities near the threshold. Scaling hypothesis of percolation near threshold:

(i) Singular properties of the system near threshold are described by a single characteristic length scale.
(ii) The characteristic length scale diverges at the transition as a power law in the distance to \( p_c \).
(iii) The system is fractal at all scales below the characteristic length scale. It's scale invariant at \( p_c \).

For site percolation: characteristic length scale = typical cluster size \( \xi \)

The main results for power laws are independent of the details of the lattice near criticality — universality.

3.2 Cluster Strength and Size Distribution

The order parameter for percolation is \( P \propto (p_c - p)^\beta \) as \( p \to p_c^+ \).

Note \( p_c \) is not a universal quantity.

Can extend \( X(p) \) above \( p_c \) ignoring \( 0 \) clusters. \( X(p) \propto (p-p_c)^\gamma \) as \( p \to p_c^- \).

Power law only works in a range not too close and not too far from \( p_c \): at \( p_c \), very large clusters appear which might reach the size of the system.

Cluster size distribution \( n(s, p) \propto G(s/\xi) \) as \( p \to p_c \).

\[ G(k) = \begin{cases} \frac{d!}{2\pi} \sum_{n=0}^\infty \sqrt{\frac{2}{\pi n}} (nk)^d e^{-nk} & d=1 \\ e^{-x} \sin(x) & d=\infty(\text{Dirichlet}) \end{cases} \]

\( S \propto \frac{1}{(p-p_c)^{1/\nu}} \) as \( p \to p_c \).

Provided \( G(0) \) is non-zero, \( n(s, p_c) \) should be a power law:

\[ \Rightarrow \text{scale-invariant at criticality} \]

This graph suggests the system appears scale-invariant up to a certain scale \( (s_\xi) \) as captured by

\[ n(s, p) \propto s^{-\tau} G(s/\xi) \] as \( p \to p_c \).
We expect $S_n(s,p)$ to be a function of $G$ of just the variable $\frac{S}{S^*}$.

Hence the plot to the left for different $p$ is just the same curve rescaled.

Can discuss cluster sizes in terms of how large they are $\rightarrow \xi$.

Correlation length.

In 1-D we found $\xi \sim S_\xi$ near the threshold. We can't simply say $S_\xi = \xi^d$ since clusters may be fractal and full of holes.

Power law in $n(s,p)$ suggests that fractality holds up to size $S_\xi$ away from $p_c$. If so, we expect that a region of linear size $l \leq S_\xi$ contains $\sim l^D$ occupied sites, with $D$: fractal dimension.

Define characteristic length scale $\xi$ as the linear size of the cluster at its characteristic size $S_\xi$.$$
S_\xi \sim \xi^D \quad (D\leq d) \quad \text{as} \quad p \rightarrow p_c$$

As $p \rightarrow p_c$, expect $\xi \sim \frac{1}{(p-p_c)^\nu}$. Also have $S_\xi \sim \frac{1}{(p-p_c)^\nu}$ as $p \rightarrow p_c$

$\Rightarrow D = \frac{1}{\nu}$

How to estimate $\nu$? Make use of finite size effects.

For a finite cluster of size $L$, $P_\infty(p,L)$ can be nonzero even if $P_\infty(p,L=\infty) = 0$ at $p < p_c$. This is because any cluster of size $> L$ would be counted as percolating.

$\Rightarrow$ expect to start finding percolating clusters when $\xi \sim L$.

The smaller $L$, the higher the chance of percolating through $L$. 
scaling hypothesis — near $p_c$, singular properties of the system are controlled by $\xi(p)$ and $L$. Note that for finite size, $\chi(p)$, $P_\infty$ etc. are smooth functions.

For $L=\infty$ system, $P_\infty(p, L=\infty) \sim (1-p_c) \sim \xi^{-\beta/\nu}$ as $p \to p_c^-$.

This also applies to finite system if $L >> \xi$

$$P_\infty(p, L >> \xi) \sim \xi^{-\beta/\nu} \quad \text{as } p \to p_c^-$$

($P_\infty$ will deviate if we reduce $L$ or get closer to $p_c$ since that increases $\xi$)

**Finite scaling hypothesis:** if no other scales control $P_\infty$, it's only their relative magnitudes that matter ($L/\xi$). Postulate:

$$P_\infty(p, L) \sim \xi^{-\beta/\nu} f(\xi/L) \quad \text{as } p \to p_c^-$$

Require:

- $f(0)=1$ to agree with infinite case
- $\xi^{-\beta/\nu}$ should cancel for $L \ll \xi$ since in that case $P_\infty$ shouldn't have information on $\xi$ (only a function of $L$)

$\Rightarrow$ asymptotic behaviour:

$$f(\xi/L) \sim \begin{cases} \text{const} & \text{as } \xi/L \to 0 \\ (\xi/L)^{\beta/\nu} & \text{as } \xi/L \to \infty \end{cases}$$

$\Rightarrow P_\infty(p, L) = \begin{cases} \xi^{-\beta/\nu} & L \gg \xi \\ L^{-\beta/\nu} & L \ll \xi \end{cases}$

The form of $P_\infty$ for $L \ll \xi$ allows us to extract $\beta/\nu$. It applies best to $P_\infty(p_c, L)$ since $\xi \to \infty$ at $p_c$.

We already know that below $S_\xi$, $n(s, p) \sim s^{-T}$. Expect similar behaviour for $P_\infty$.

We have shown that below $S_\xi$, the number of occupied sites in a cluster spanning the window of size $L$ is $\sim L^D$. Since the volume is $L^d$, we expect the density of occupied sites to be $P_\infty \sim \frac{L^D}{L^d} = L^{D-d}$ for $L \ll \xi$

Comparing with expression for $P_\infty(p_c, L)$ above: $D = d - 1/\nu$.
As we zoom out:

- At $p = p_c$ we have a fractal cluster. The statistical properties are indistinguishable as we zoom out.
- At $p < p_c$ we get a similar picture as long as the scale $\ll \xi$. If the scale $\gg \xi$ we lose self-similarity:
  - clusters are at most of size $\sim \xi$, and are visually shrinking as we zoom out.
  - clusters that looked infinite in a smaller window are finite.
  - we lose resolution on the small islands of occupied sites, so clusters appear more and more disconnected
  \[ \Rightarrow \] $p_c$ appears to be decreasing as we zoom out.
- At $p > p_c$ there is a percolating cluster
  - clusters that didn't look connected in a smaller window might be connected
  - we lose resolution on the small vacancies, so the infinite cluster appears denser and denser
  \[ \Rightarrow \] $p_c$ appears to be increasing as we zoom out.

- Below the threshold, as we zoom out the system appears more disconnected, corresponding to a picture at small $p$.
- Above the threshold, everything begins to look connected, corresponding to a picture at $p \sim 1$.
- At the threshold, the system is scale invariant.

View this procedure of examining the system at larger and larger scales as a renormalization of the parameters of the system ($p$).

Zoom out at $p < p_c$ --- reduction in $p$ (probability flows to the left, towards $p = 0$)

Zoom out at $p > p_c$ --- increase in $p$ (probability flows towards $p = 1$)

$p = p_c$ doesn't get renormalized, but a small deviation from $p_c$ will...
4.2 Renormalisation Scheme

$R_b(p)$ for square lattice

- For $p < p_c$, $R_b(p) < p$
- For $p > p_c$, $R_b(p) > p$
- For $p = p_c$, $R_b(p) = p$

We should be able to deduce information about the system near the threshold from the system far away from percolation, where the situation is simpler. (in particular about $\xi(p)$)

$p' = R_b(p) \Rightarrow p'' = R_b(p') \Rightarrow \ldots \Rightarrow \xi(p) = \frac{\xi(p_0)}{b^n}$

$\xi(p)$ diverges as $p \to p_c$ 

So even though at each step $\xi$ changes by $\frac{1}{b}$, the renormalisation factor can be very small.

$\Rightarrow$ For $p$ close to $p_c$, approximate $p' = R_b(p)$ by Taylor expansion around $p_c$:

$p' = R_b(p) \approx R_b(p_c) + \frac{dR_b}{dp} \bigg|_{p_c} (p - p_c) = p_c + \frac{dR_b}{dp} \bigg|_{p_c} (p - p_c)$

rearrange:

$\Rightarrow (p' - p_c) = \lambda(b) (p - p_c)$

Also have $\xi = |p - p_c|^{-\nu}$, $\xi' = \xi(p') = \frac{\xi(p)}{b}$

$|p' - p_c|^{-\nu} = |\lambda(b)(p - p_c)|^{-\nu} \Rightarrow |p - p_c|^{-\nu} = \lambda(b) = b^\nu$

So $p' - p_c = \lambda(b)(p - p_c) = b^\nu (p - p_c) \Rightarrow \nu = \frac{\ln b}{\ln \left( \frac{dR_b}{dp} \bigg|_{p_c} \right)}$

Note $\frac{dR_b}{dp}$ is continuous across $p_c$ \Rightarrow $\xi(p)$ diverges with the same $\nu$ on either side of the threshold.
Microstate: a state of the system defined by a complete microscopic configuration (e.g., position, momenta, spins of all particles).

Macrostate: thermodynamic state of the system described by macroscopic state variables (e.g., temperature, volume...)

Ensembles

Take many replicas of one system, each in a different microstate.
Postulate: the avg. of a physical quantity over an ensemble of replicas gives the same result as the time-avg. of one single system.

Microcanonical ensemble: select replicas with same energy and # particles. All members give the same value for all conserved quantities.

Postulate: given an isolated system in equilibrium, all microstates have the same statistical weight.

Ergodicity → the system visits all the possible microstates. (might be over-optimistic, phase space can be very large).

Canonical ensemble: allow energy exchange with reservoir at temp. T. Different members of the ensemble have different energies, weight them according to it.

\[ p_i = \frac{1}{\mathcal{Z}} e^{-\beta E_i}, \quad \mathcal{Z} = \sum_i e^{-\beta E_i} \]

Partition function

Grand canonical ensemble: allow particle exchange with the reservoir.

\[ p_i = \frac{1}{\mathcal{G}} e^{-\beta (E_i - \mu N_i)}, \quad \mathcal{G} = \sum_i e^{-\beta (E_i - \mu N_i)} \]

Grand partition function

Entropy & Boltzmann weight

For the microcanonical ensemble, macrostates have fixed \( U, V, N \). Suppose there are \( \Omega \) microstates at a given energy.

\[ S^*(U,V,N) = k \ln \Omega(U,V,N) \]

More microstates \( \Rightarrow \) more entropy → measures "lack of knowledge" generally:

\[ S = -k \sum p_i \ln p_i \]