Percolation and Rigidity in Disordered Networks

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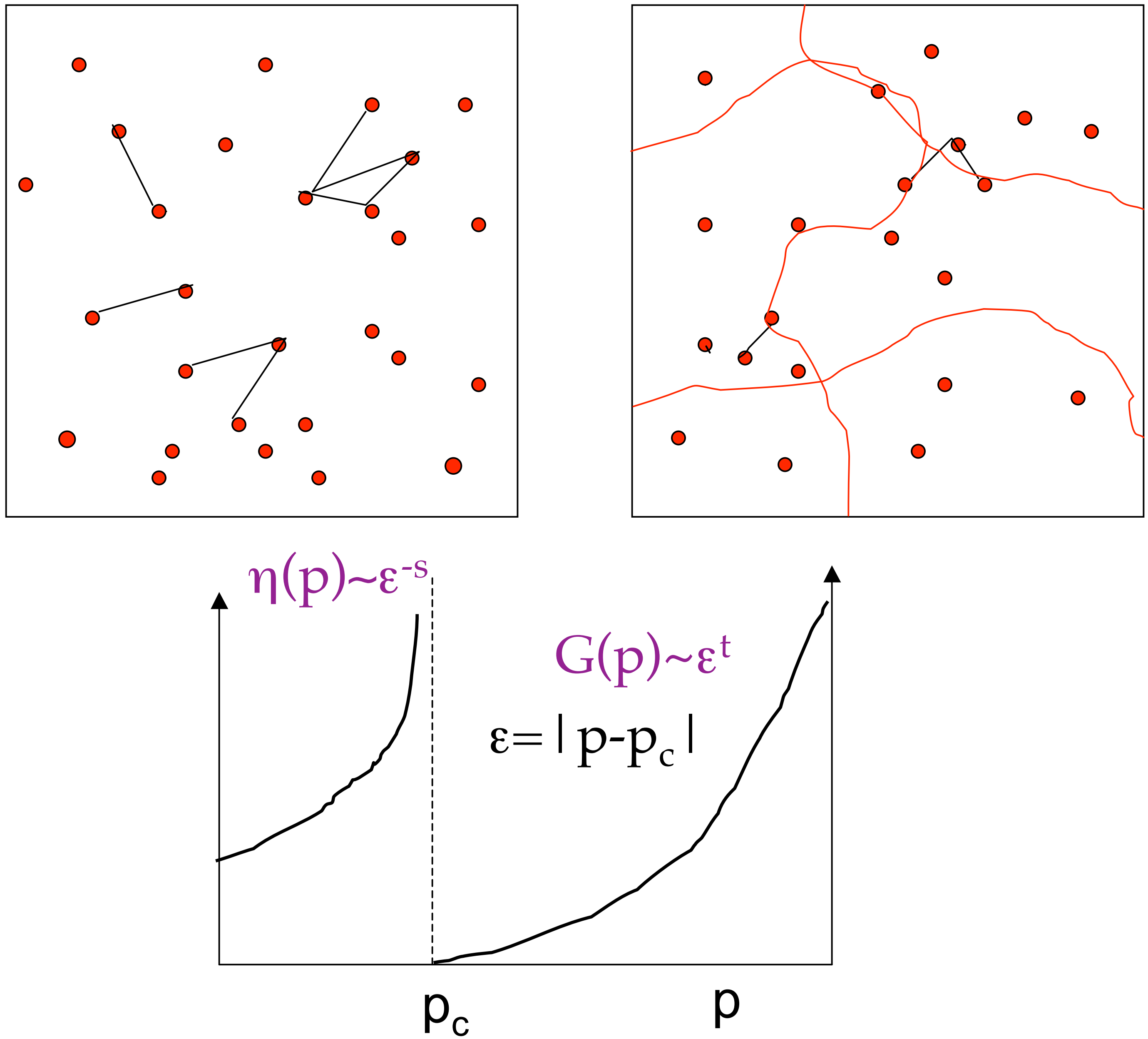
Complex Fluids and Gels

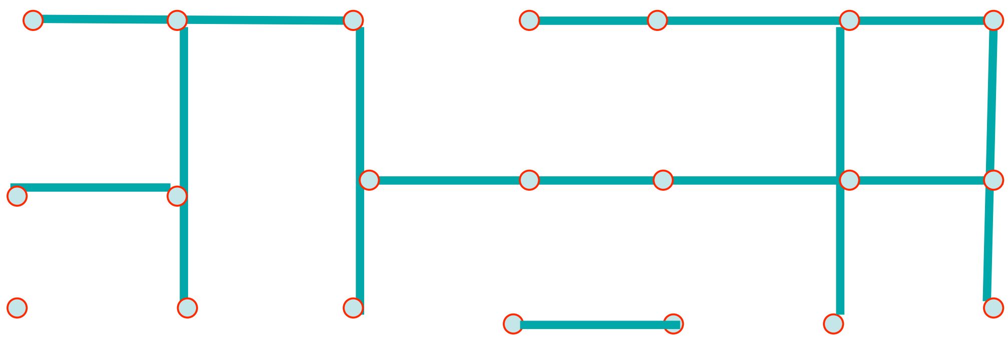


Topics

- Percolation (well understood)
- Rigidity Percolation (T=0) (understood)
- Rigidity at finite T (controversial)

Percolation on a Lattice

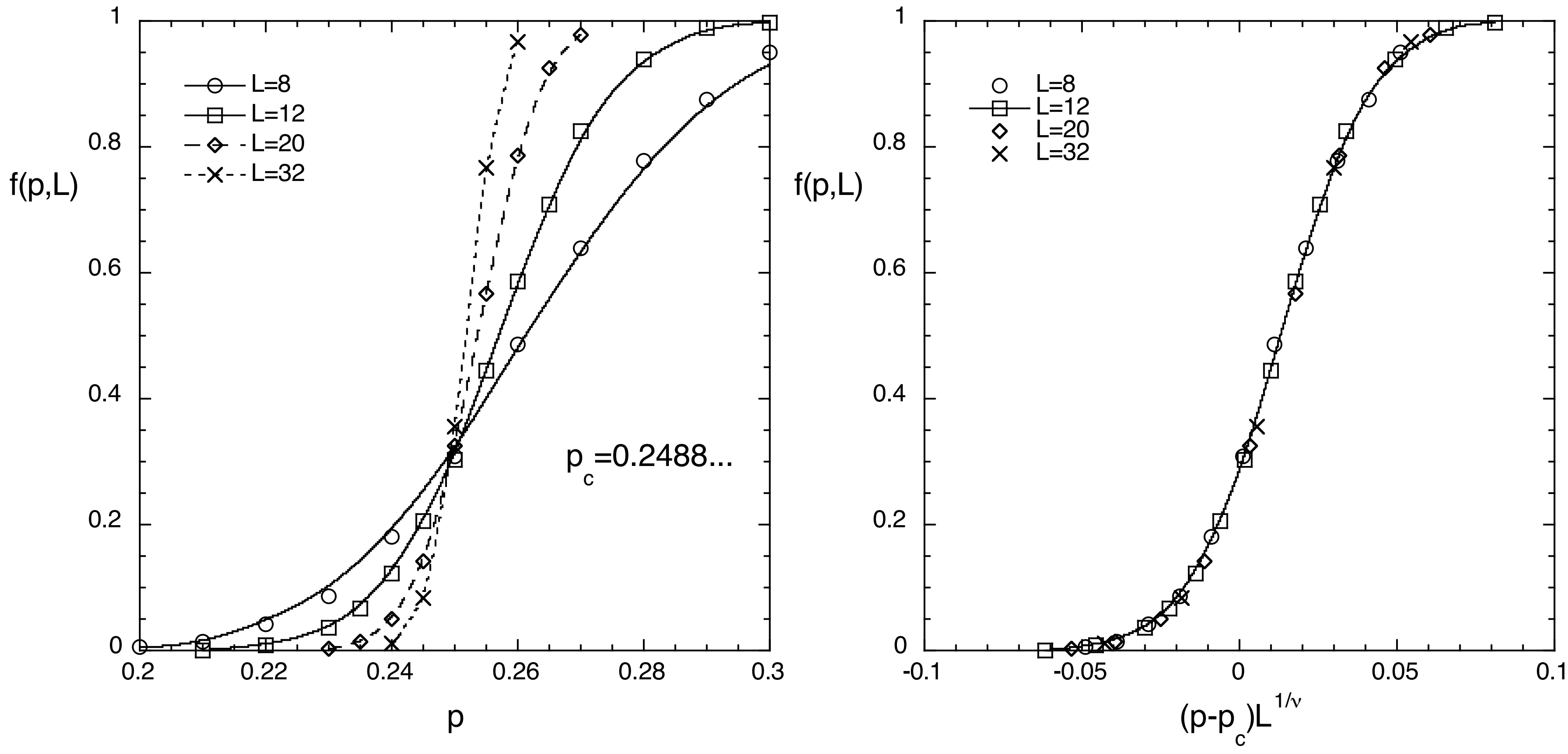
- Nearest-neighbor bonds present with probability p



f(p,L)=probability that a spanning cluster exists at probability p for a lattice of size L

$\xi(p)$=correlation length at probability p for infinite L; $\xi(p) \sim |p - p_c|^{-\nu}$; $P(r,p) \sim \exp(-r/\xi(p))$.

Percolation on Simple Cubic Lattice



$(p-p_c)L^{1/\nu}=g[L/\xi(p)]$

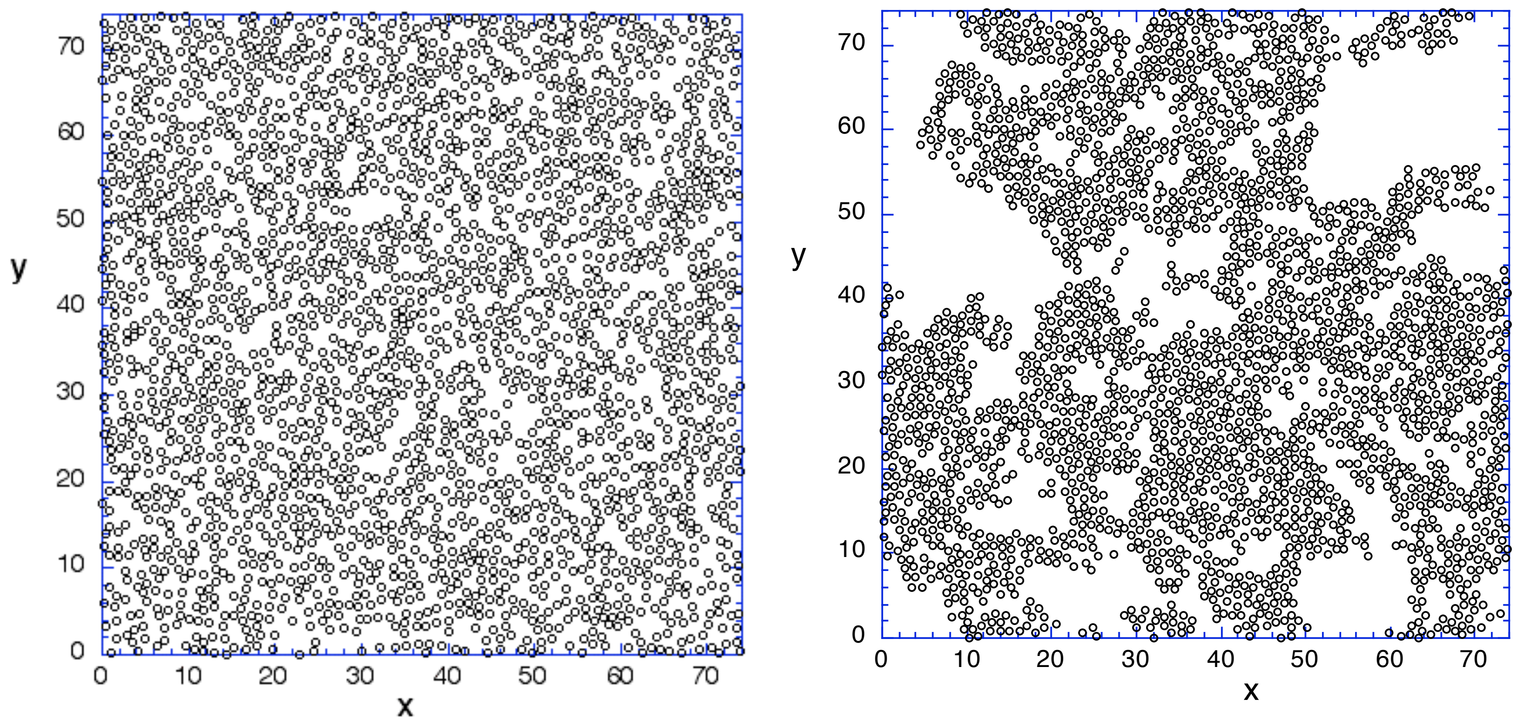
Spanning Cluster, p = 0.502, ε=.002, L =64

No fluid

Finite clusters removed, $d_f = \frac{91}{48}$

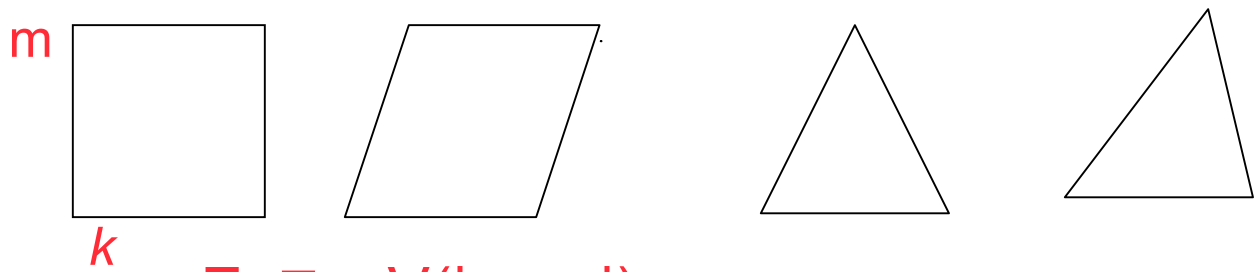
Fluid present

Backbone fractal, $d_f \approx 1.65$



M.P. Phys. Rev. E, (2006)

Rigidity Percolation, Central Forces



$$E=\Sigma_{k,m}V(|\mathbf{r}_k-\mathbf{r}_m|)$$

Mean Field Argument (Feng and Sen, 1984)

N=# of sites, z=# of nearest neighbors,

p=probability that a nearest neighbor bond exists

N_c= total number of constraints =$pNz/2$

N_f=# of degrees of freedom = dN

At p_r, $N_f = N_c$ or $p_r = 2d/z$

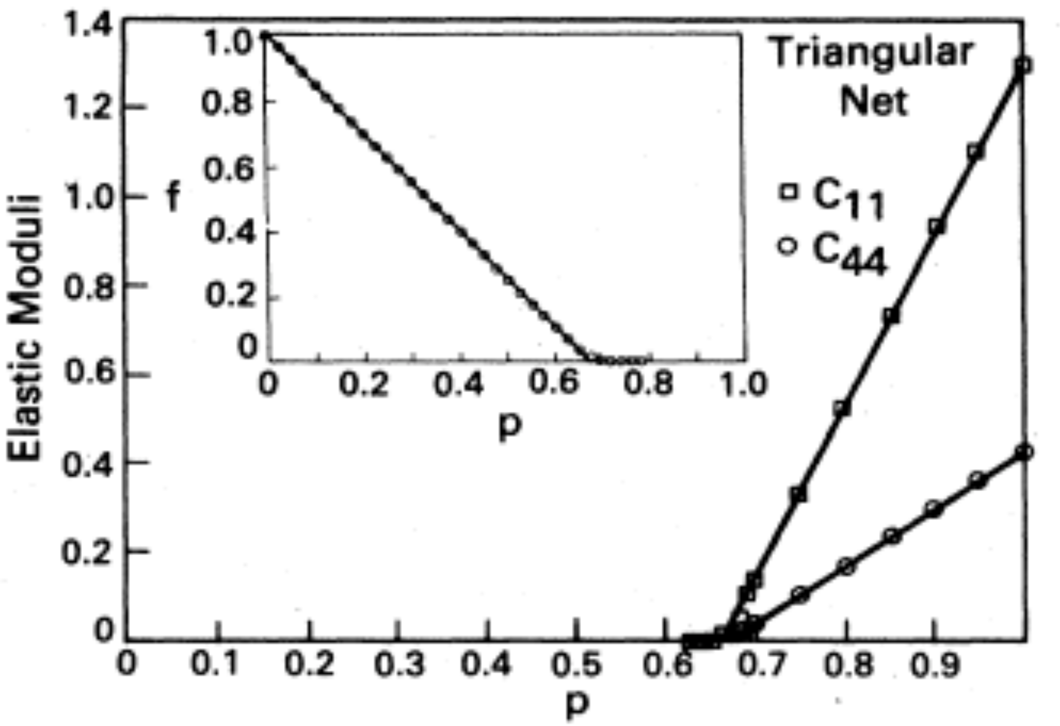
Square lattice: $p_r = 1.0$, $p_c = 0.5$

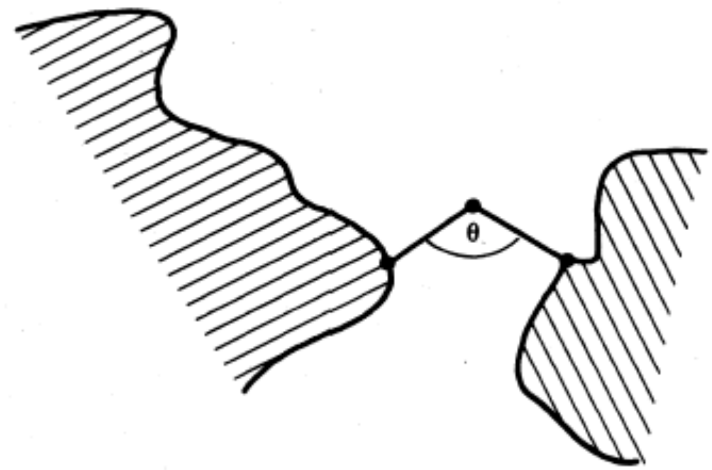
Triangular lattice: $p_r = 2/3$, $p_c = 0.34$

Simulations: p_r=0.6602

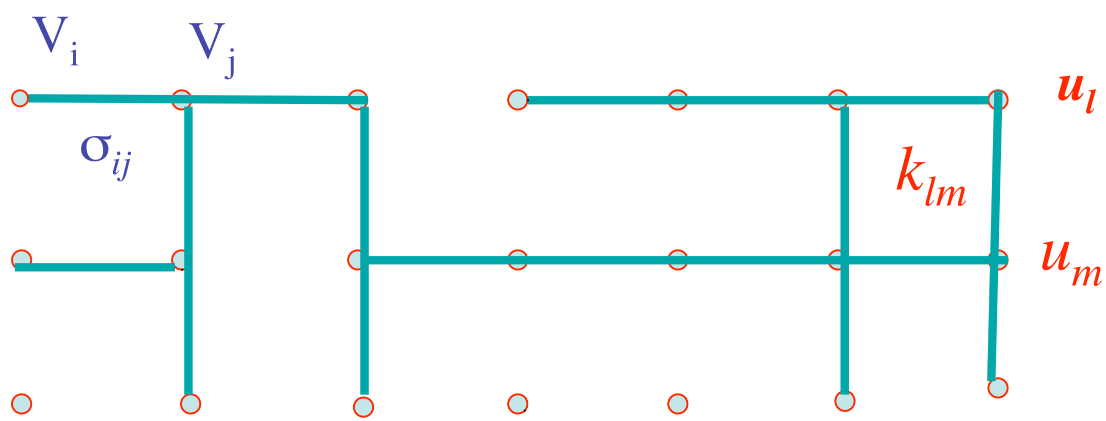
Rigidity Percolation, Triangular Lattice

Feng et al. Phys. Rev. (1984)





Connection with Random Resistor Networks



$\Sigma_j \sigma_{ij}(V_i - V_j) = 0$

$\sigma(p) \sim (p - p_c)^t$

$\Sigma_m k_{lm}(\boldsymbol{u}_l - \boldsymbol{u}_m) = 0$

$G(p) \sim (p - p_c)^t$

Works for $E = kr^2$ but <u>not</u> $E = k(r - r_0)^2$

de Gennes, 1976

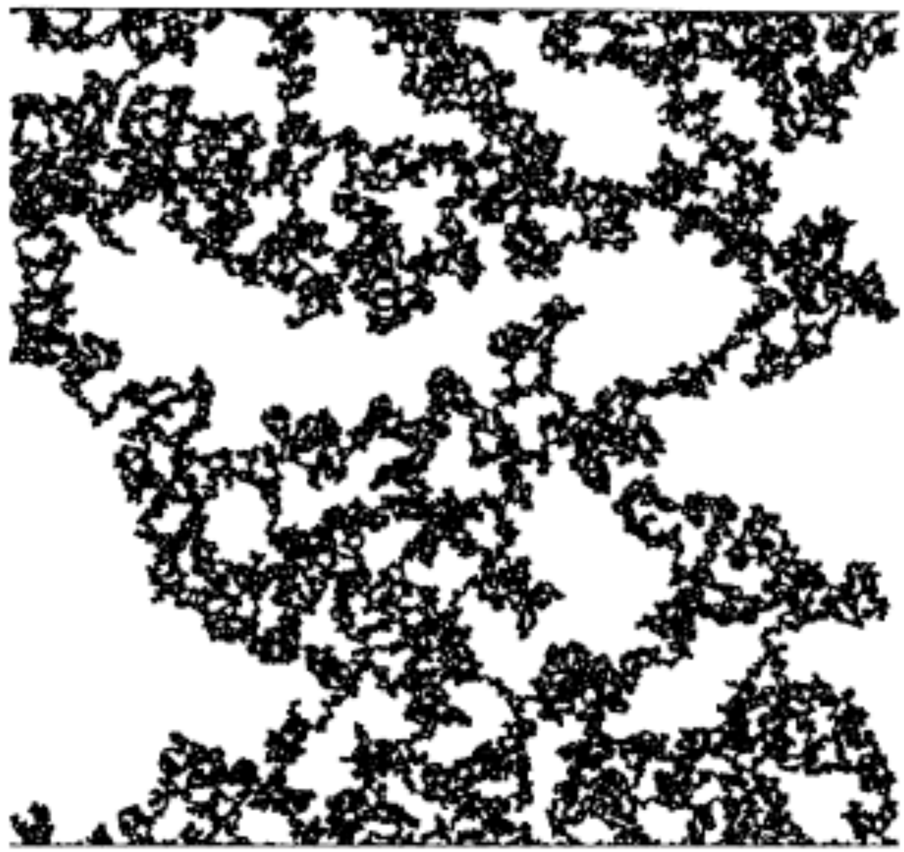
<u>But:</u> Rigidity Percolation, $p_r \neq p_c$, exponents are in general different

Candidate Values of t

d	deGennes	Rigidity Percolation CF	Rigidity Percolation BB	Scaling/RG (Xing *et. al.* PRL, 2004) $t = d\nu$
2	1.3	3.48	3.97	8/3
3	1.9	1.76	3.8	2.64

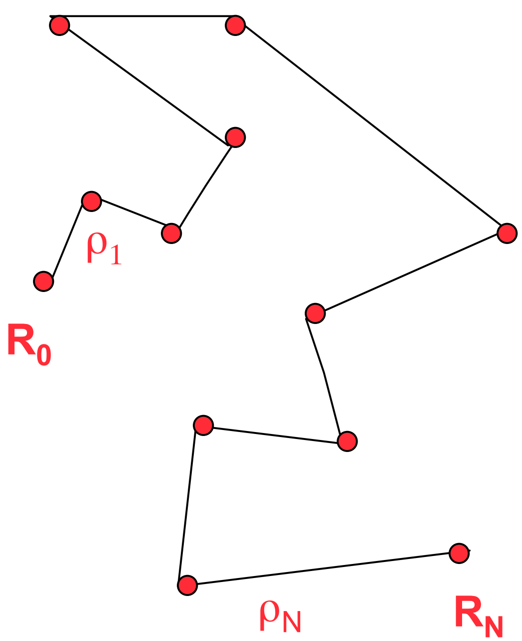
Backbone of Spanning Cluster at p_c

Moukarzel and Duxbury, Phys. Rev. Lett. (1995)



Polymer Entropy

Freely jointed chain, links of length *a*



$$\mathbf{R} = \mathbf{R_N} - \mathbf{R}_0$$

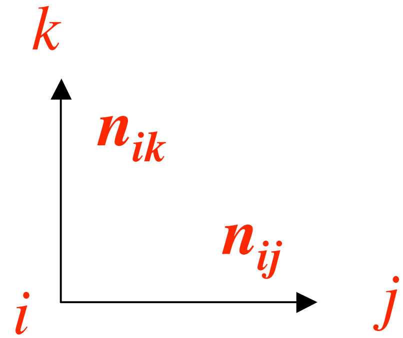
$$S(\mathbf{R}) = k_B \prod_i \int d^3\rho_i \delta(|\rho_i| - a)\delta(\mathbf{R} - \rho_1 - \ldots\rho_N)$$

$$= \frac{(4\pi a^2)^N}{(2\pi)^3} \int d^3k e^{-i\mathbf{k}\bullet\mathbf{r} - Nk^2a^2}$$

$$\propto e^{-3R^2/2Na^2}$$

Model

- $H = H_{bond} + H_{SA} + H_{BB}$
- $H_{bond} = 0.5k_{ij}(r_{ij} - r_0)^2$ between crosslinked particles
- $H_{SA}(i,j) = \varepsilon(\sigma/r_{ij})^{36}$, between all particles, “hard core”
- $H_{BB}(i,j,k) = 0.5v_{ang}(\mathbf{n}_{ij}\cdot\mathbf{n}_{ik})^2$, three-body bond-bending force



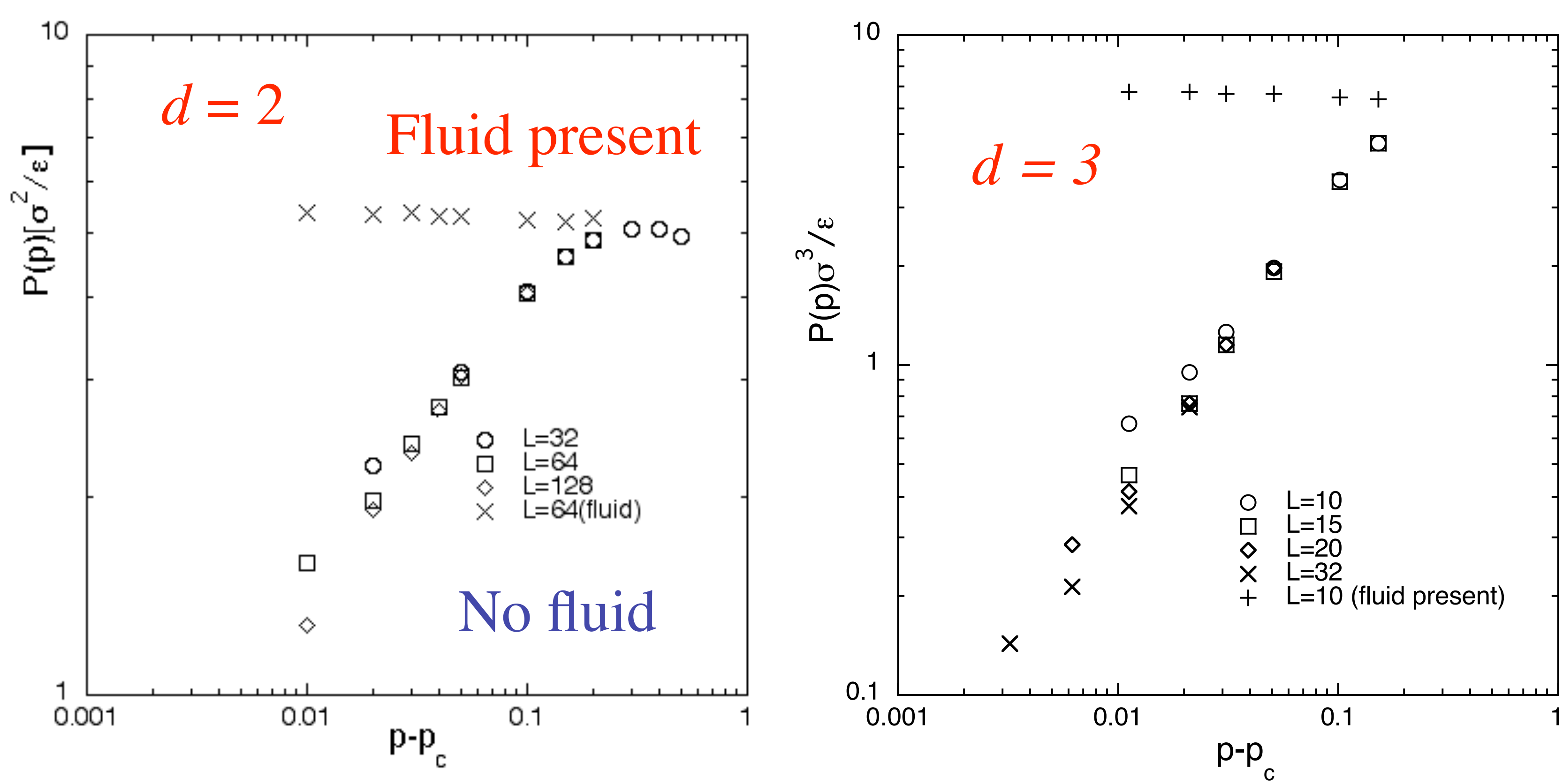
Technical Points

Particles initially on a lattice, nearest neighbor bonds inserted with probability p; Brownian dynamics at $k_BT=\varepsilon$ in $d=2$ ($N=L^2$ particles, $L \leq 128$), $d=3$ ($N=L^3$ particles, $L \leq 32$) for

(i) only the spanning cluster and (ii) spanning cluster + fluid.

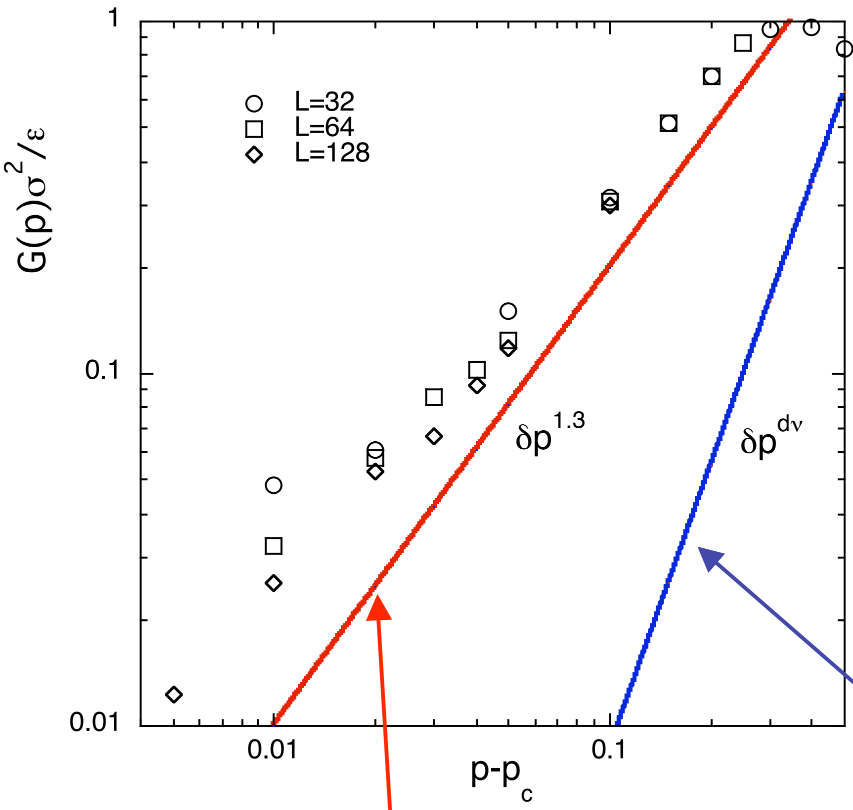
Quantities calculated: stress tensor, $\sigma_{\alpha\beta}(p)$, shear modulus, G.

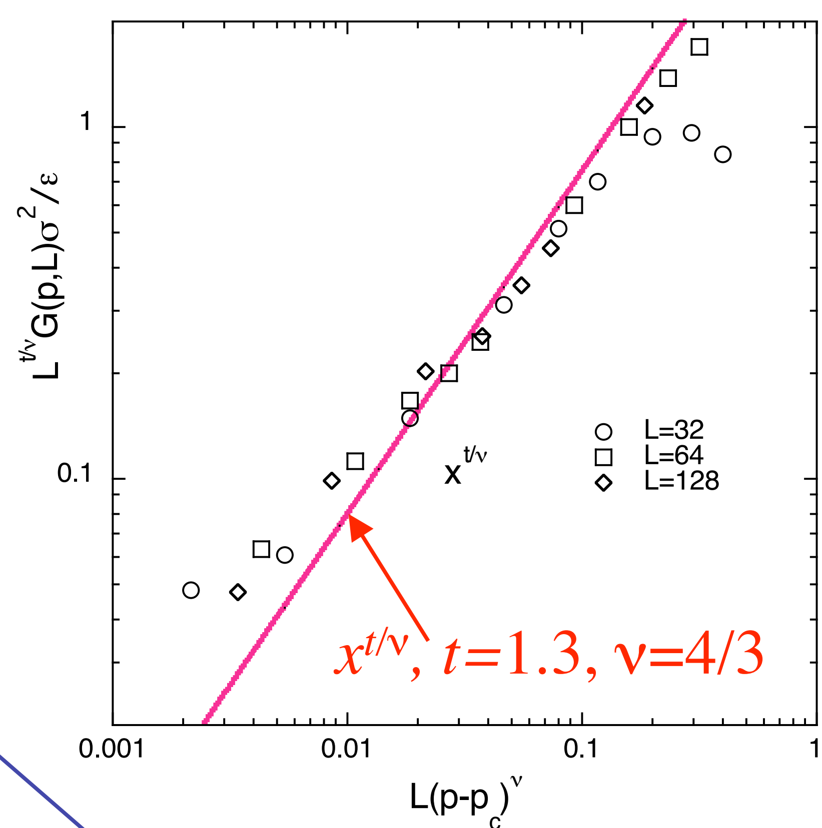
Pressure in two and three dimensions



Shear Modulus in d = 2

$G(p,L) = L^{-t/\nu}\Phi(L/\xi(p))$





$x^{t/\nu}$, t=1.3, ν=4/3

de Gennes prediction, t = 1.3

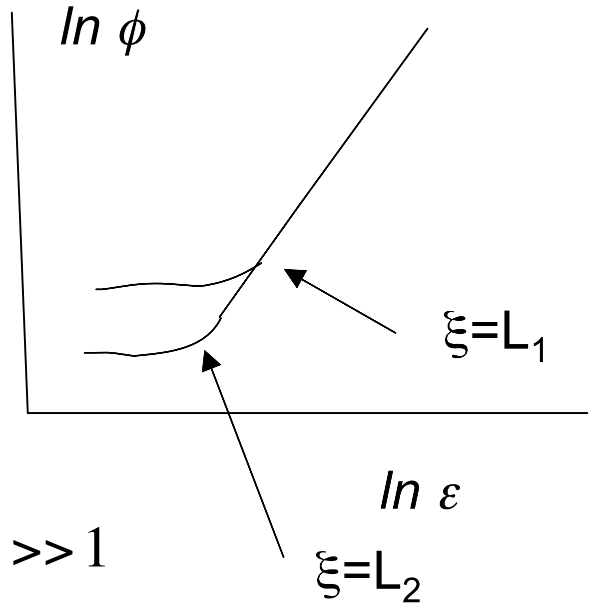
Scaling/RG

Finite Size Scaling

- Suppose $\phi(\varepsilon, L=\infty) \sim \varepsilon^{\Delta}; \quad \xi(\varepsilon, L=\infty) \sim \varepsilon^{-\nu} \quad \varepsilon << 1$
- Then $\xi(\varepsilon, L) \sim \begin{matrix} \varepsilon^{-\nu} & \xi < L \\ L & \xi \geq L \end{matrix}$

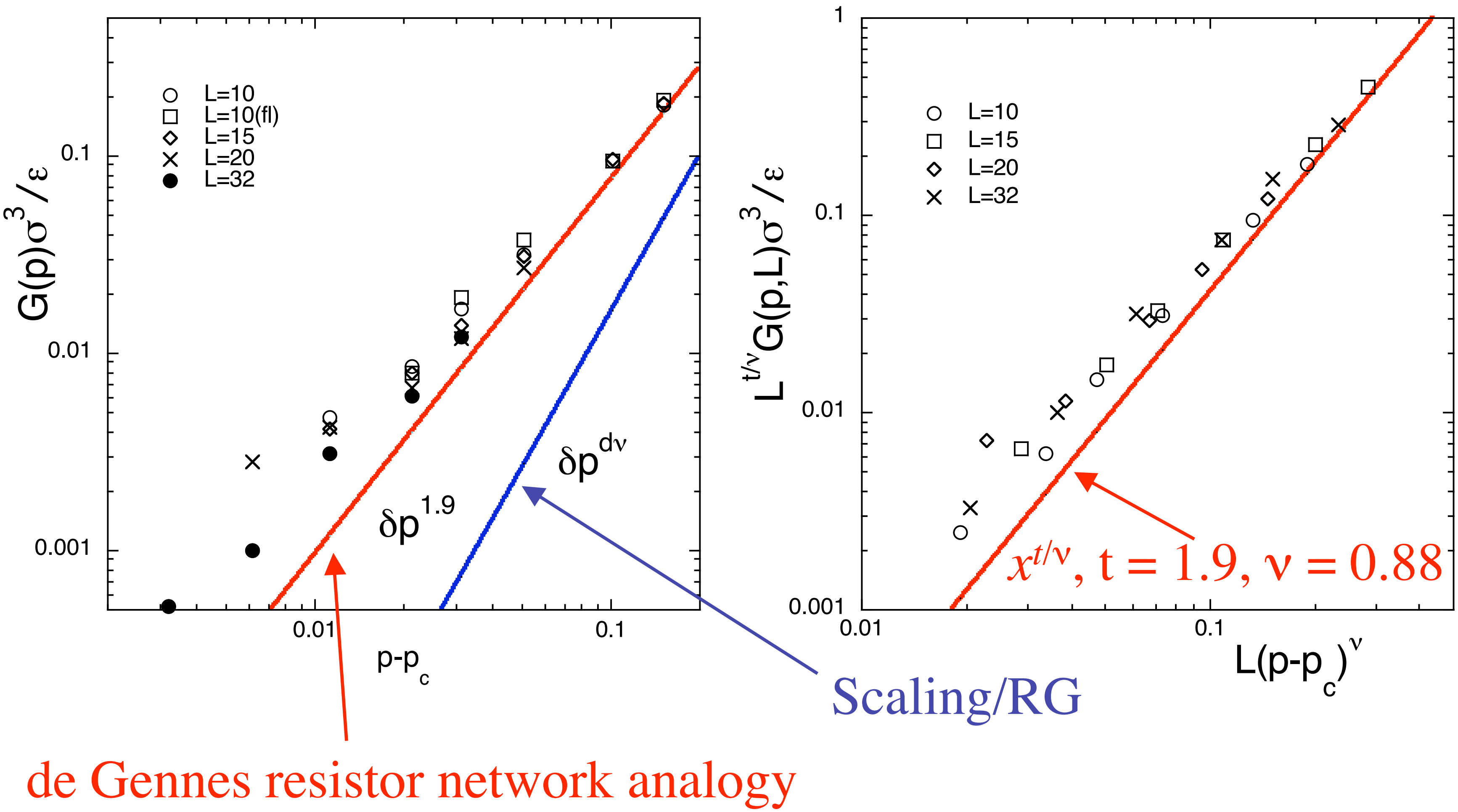
$$\varepsilon_{sat} \sim L^{-1/\nu}, \quad \phi_{sat} \sim L^{-\Delta/\nu}$$

$$\phi(\varepsilon, L) \sim \begin{matrix} \xi^{-\Delta/\nu} & \xi < L \\ L^{-\Delta/\nu} & \xi \geq L \end{matrix}$$

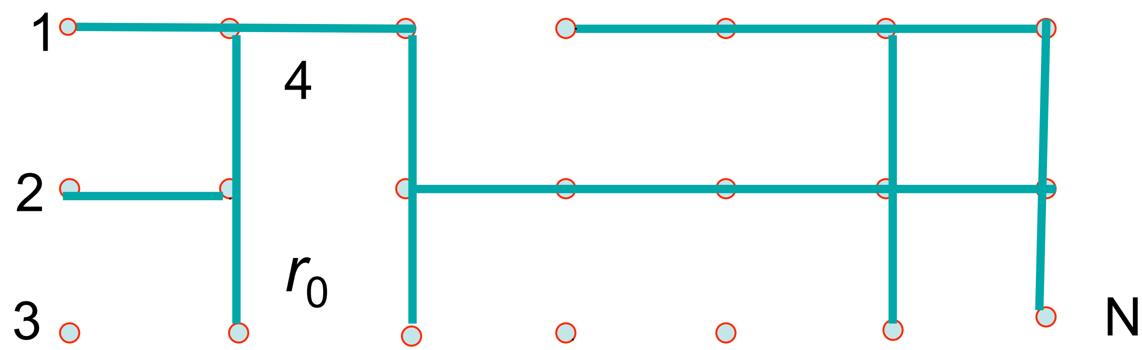


$$L^{\Delta/\nu}\phi(\varepsilon, L) = f(L/\xi) = f(x) \sim \begin{matrix} x^{\Delta/\nu} & x >> 1 \\ C & x \leq 1 \end{matrix}$$

Shear modulus, *d* = 3



Renormalization Group Transformation



$$H(N,k,r_0) = \sum_{i,j} k(r_{ij} - r_0)^2$$

$$Z(N,k,r_0) = \int d^3r_1 d^3r_2 \ldots d^3r_N e^{-H(N,k,r_0)/k_BT} = e^{-F/k_BT}$$

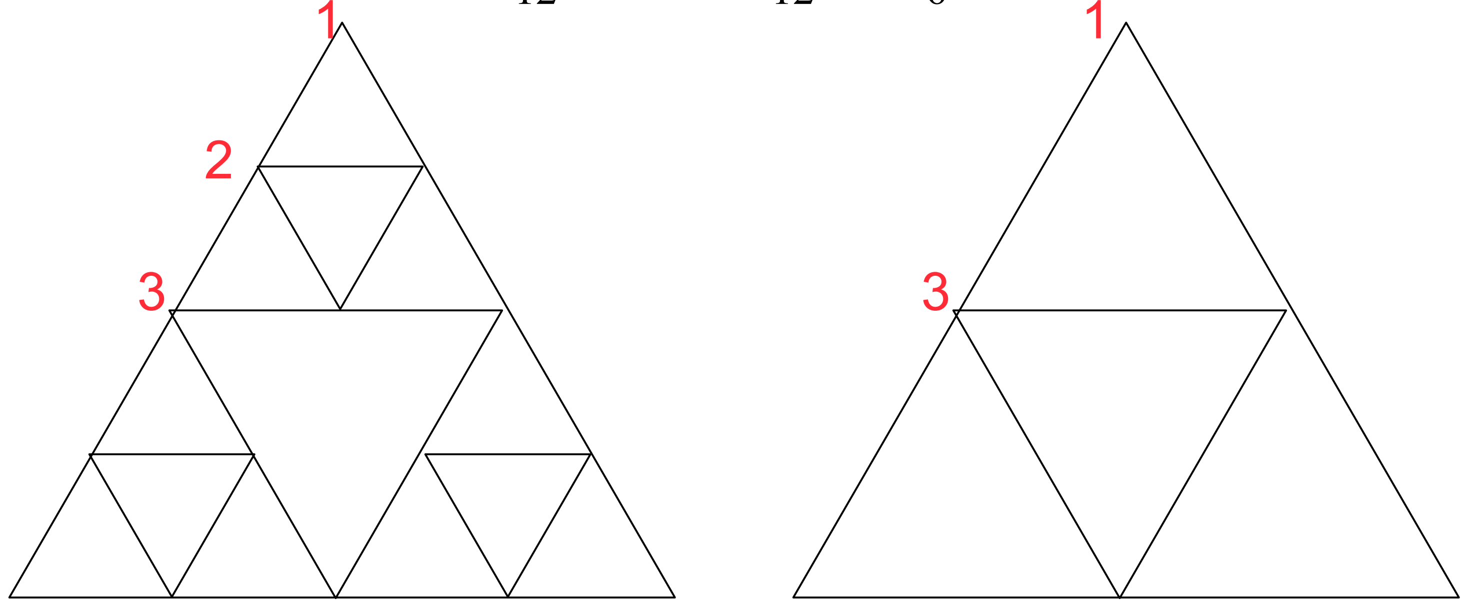
$$e^{-H'(N/2,k',2r_0)/k_BT} \stackrel{?}{=} \int d^3r_2 d^3r_4 \ldots d^3r_N e^{-H(N,k,r_0)/k_BT}$$

$$H(N,k,r_0) \to H'(N/2,k',2r_0) \to H''(N/4,k'',4r_0)\ldots$$

Renormalization Group: Hierarchical Lattices

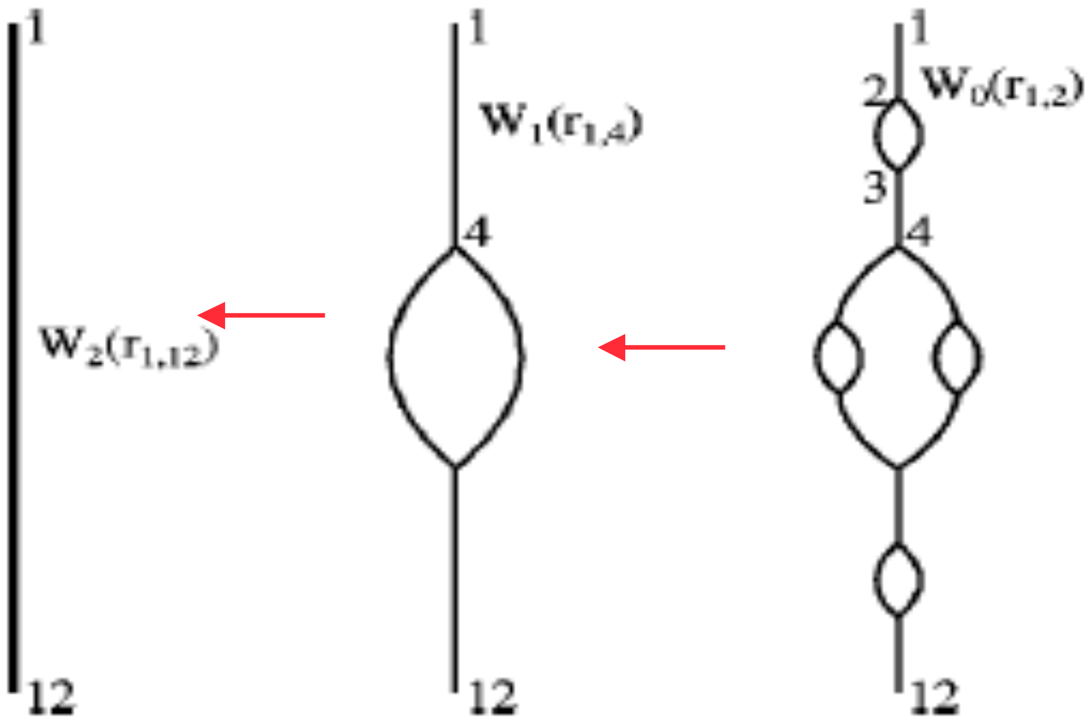
$$\int d\mathbf{r}_2 e^{-\beta H(\mathbf{r}_{12})} e^{-\beta H(\mathbf{r}_{23})} \equiv \int d\mathbf{r}_2 W(\mathbf{r}_{12}) W(\mathbf{r}_{23}) = W'(\mathbf{r}_{13})$$

$$H(\mathbf{r}_{12}) = k[|\mathbf{r}_{12}| - r_0]^2$$

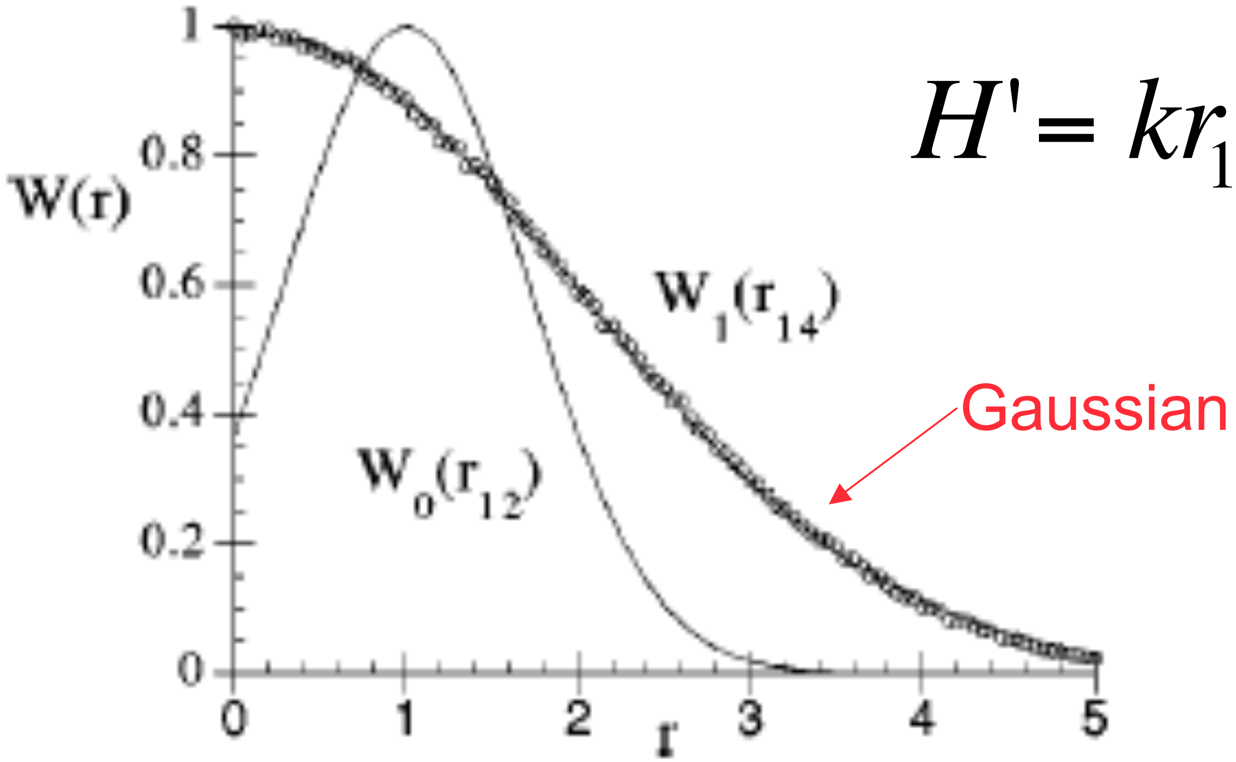


Sierpinski gasket

Another Hierarchical Structure



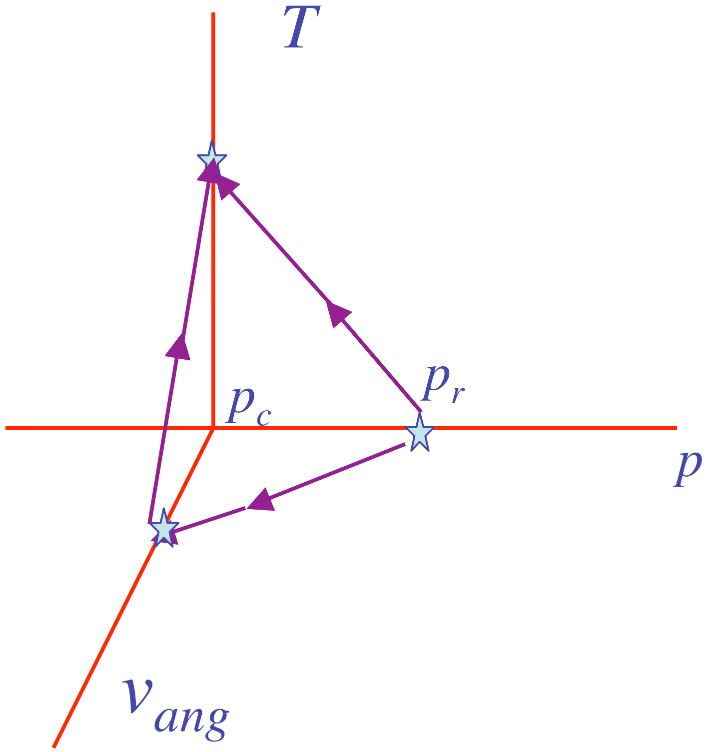
One Renormalization Step



$$H' = kr_{14}^2$$

Summary

Fixed Points and Flow



Experimental Results

Adam *et. al*. (1985) t=2.1±0.3
Axelos and Kolb (1990) t=1.93 ±0.08
Adam and Aime (1991) t =1.9 ±0.1
Takahashi *et al*. (1994) t=2.05 ±0.05
Borchard *et al*. (2001) t≈1.9

but

Martin *et al*. (1993) t = 2.8 ±0.2
Lusignan *et al*. (1995) t = 2.7 ± 0.3