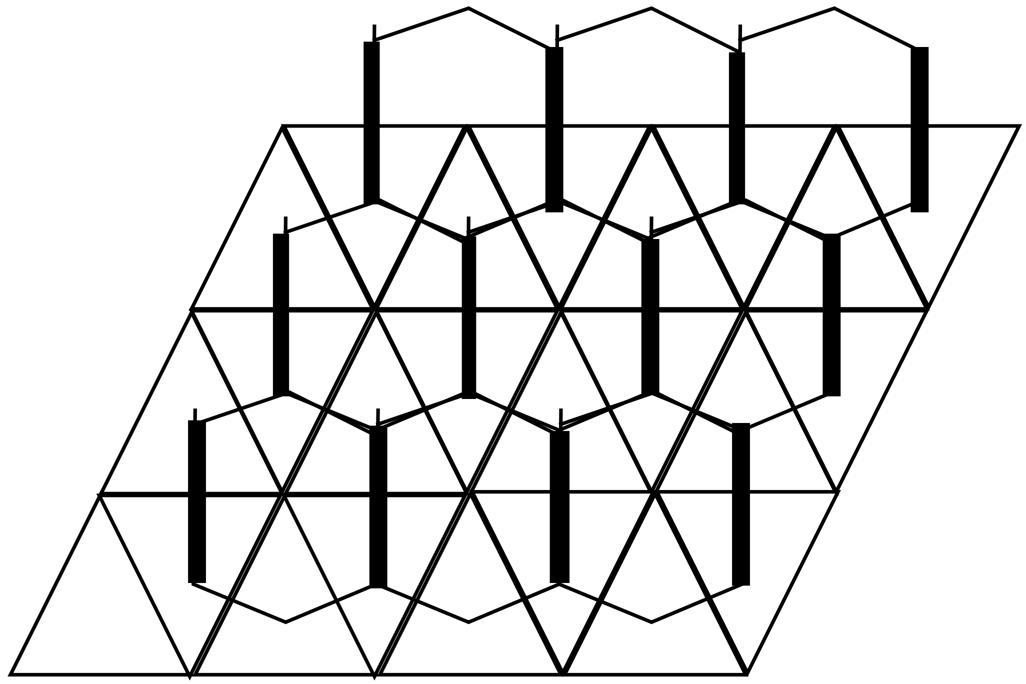
Statistical description in terms of Ensemble of Blocked states (inherent structures)

- Basics of statistical mechanics; fundamental postulates and the ensembles of equilibrium statistical mechanics (We worked these out yesterday)
- Consequences of the Boltzman distribution:
  - Fluctuation-dissipation relations
  - All of Thermodynamics
- Work out consequences of the Edwards' distribution
- Write configurational partition function of a liquid in terms of inherent structures, explore consequences
- Observations in simulations of Lennard-Jones systems
- Introduce a toy model where we can work things out explicitly

Toy model

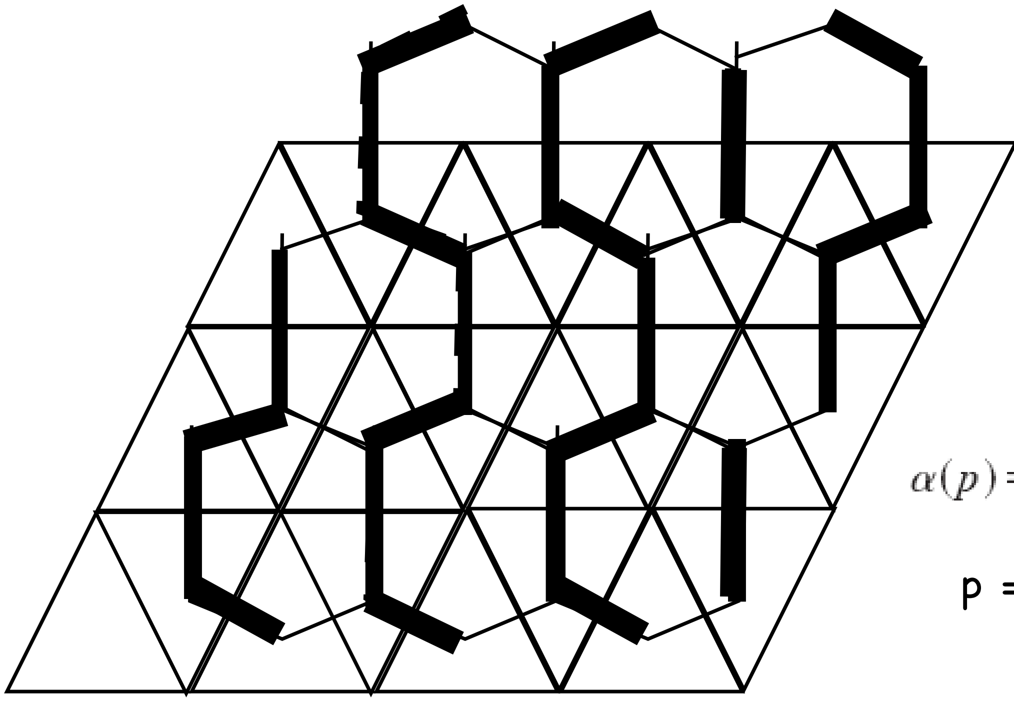
- Triangular-lattice Ising antiferromagnet (interaction strength J)
- Frustrated system wit exponentially large # of ground states
- Making the lattice compressible or introducing a staggered field lifts degeneracy and picks out a globally stable state
- Think in terms of the inherent structures of this model (setting J to infinity analogous to hard sphere/rod constraint)

Inherent structures are dimer coverings of the honeycomb lattice



- This one is the completely ordered state and has no local excitations

Conserved quantities: strings



The ``green" state has 4 strings

Can divide inherent structures into string sectors.

States belonging to same string sector are connected by local dynamics

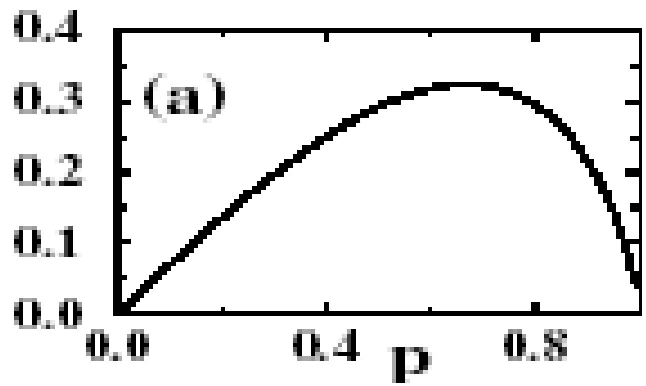
Count # of states in a string sector which gives us S(# of strings)

$$S(p) = L^2 \alpha(p)$$

$$\alpha(p) = p \ln 2 + \frac{2}{\pi} \int_0^{\pi p/2} dx \ln[\cos(x)]$$

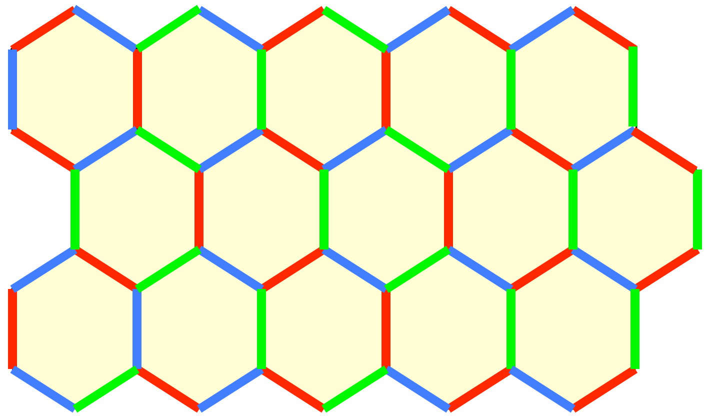
A. Dhar et al , PRB 61, 6227 (1999)

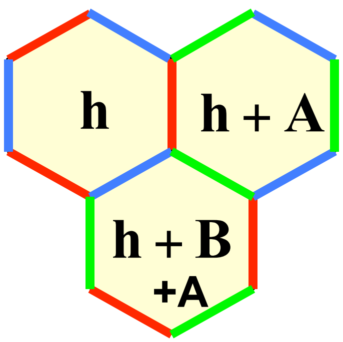
p = # of strings/unit length

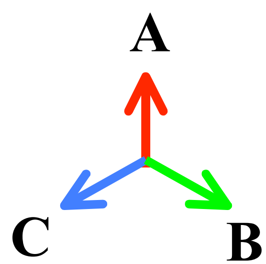


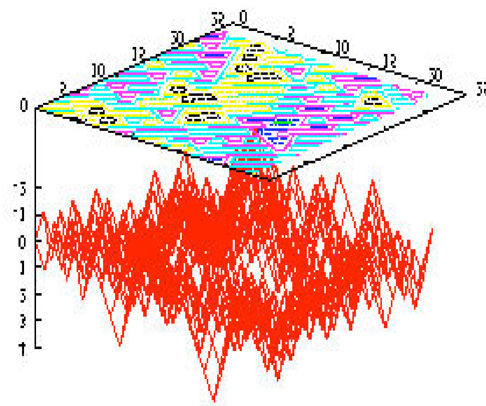
S goes to zero linearly !

Three-coloring model

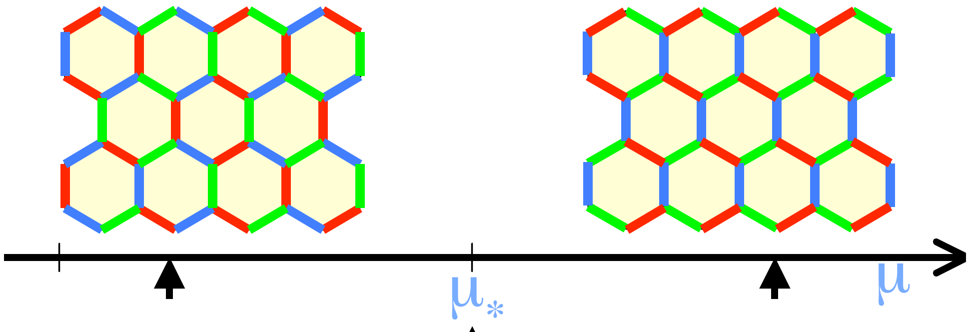


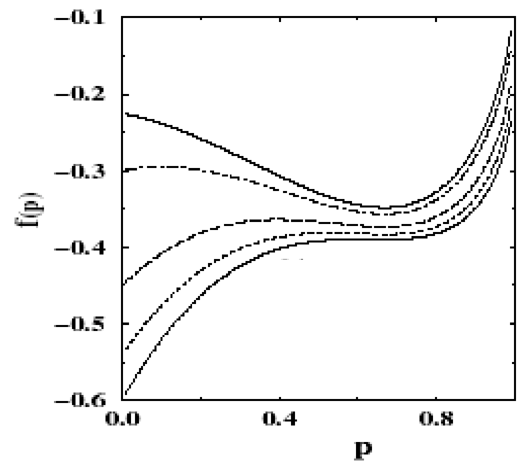






Equilibrium transition





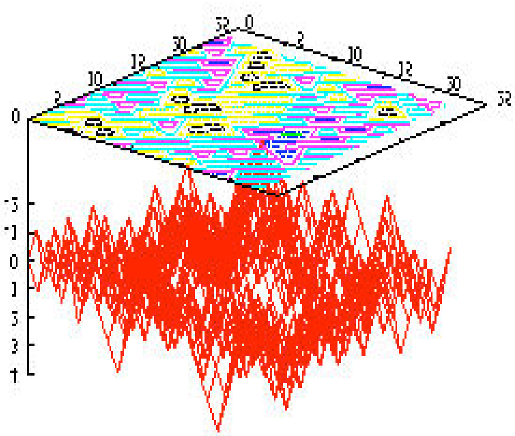
Disordered

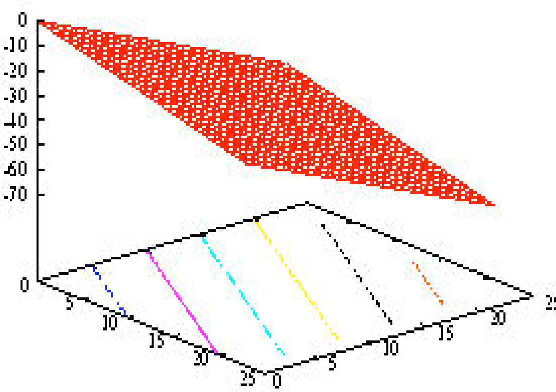
(liquid-like)

Critical point

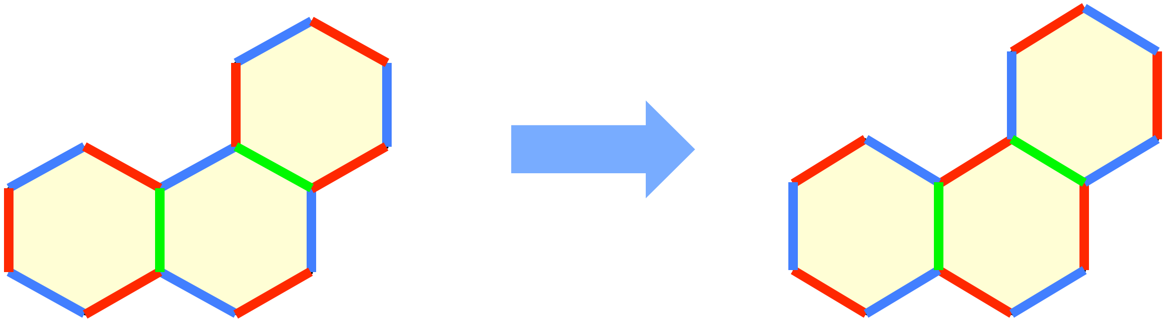
Ordered

(solid-like)

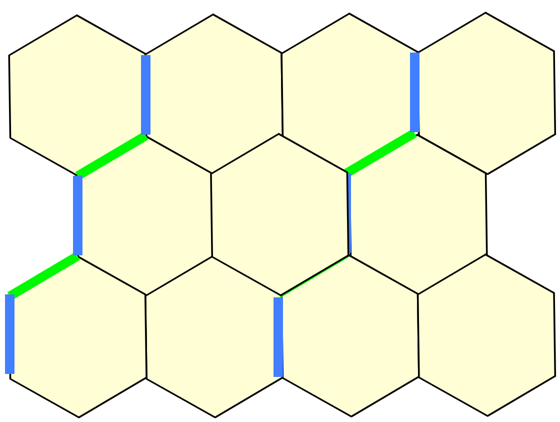




Constraints ➔ Loop dynamics



Loops of all sizes get updated



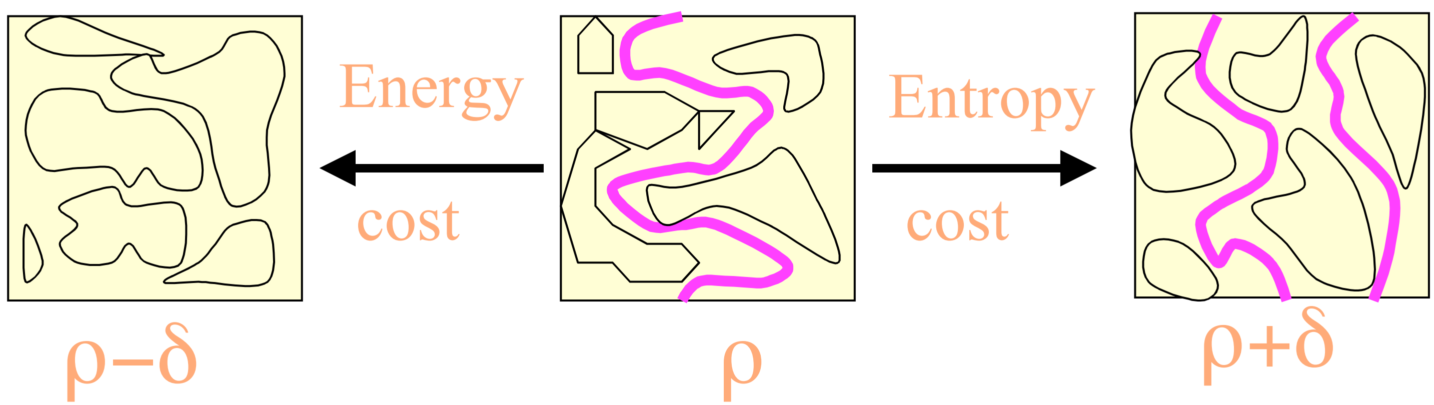
Loops with non-zero winding numbers

Necessary to update these to change the tilt

Transition Rates

$$W_{L\rho \rightarrow L\rho-1} \sim \exp[-\Delta E]$$

$$W_{L\rho-1 \rightarrow L\rho} \sim \exp[-\Delta S]$$



Master Equation

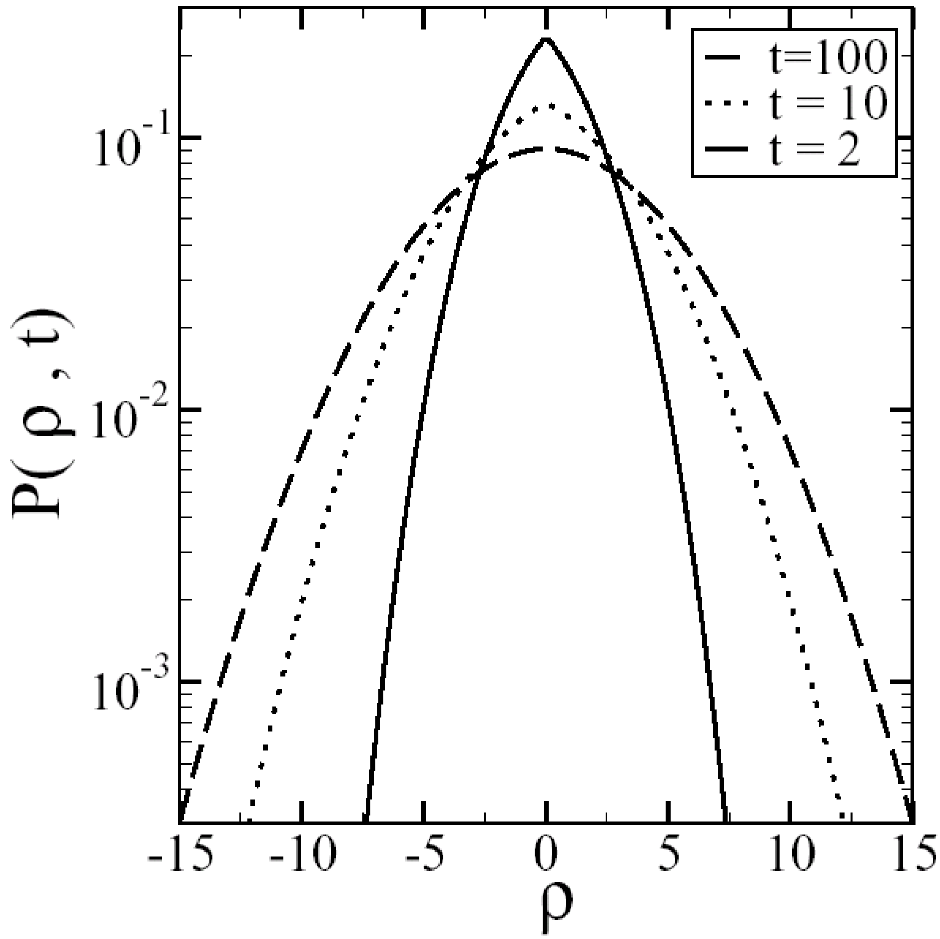
$$\frac{\partial P(\rho)}{\partial t} = -(W_{\rho\to\rho-1} + W_{\rho\to\rho+1})P(\rho) + W_{\rho-1,\rho}P(\rho-1) + W_{\rho+1\to\rho}P(\rho+1)$$

Continuum limit

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial \rho}[\epsilon\rho e^{-\mu^*|\rho|}P + 2De^{-\mu^*|\rho|}\frac{\partial P}{\partial \rho}]$$

Without these factors, this equation would lead to usual Langevin equation for ρ

P(ρ,t) away from critical point



$$l_1 \simeq \log t/\mu^*$$

distance from critical point

$$l_2 = \sqrt{\frac{2D}{\lambda}}$$

Crossover time:

$$\tau_c = e^{2\mu^*\sqrt{D/\lambda}}$$

Also shows log-normal distribution of hopping times