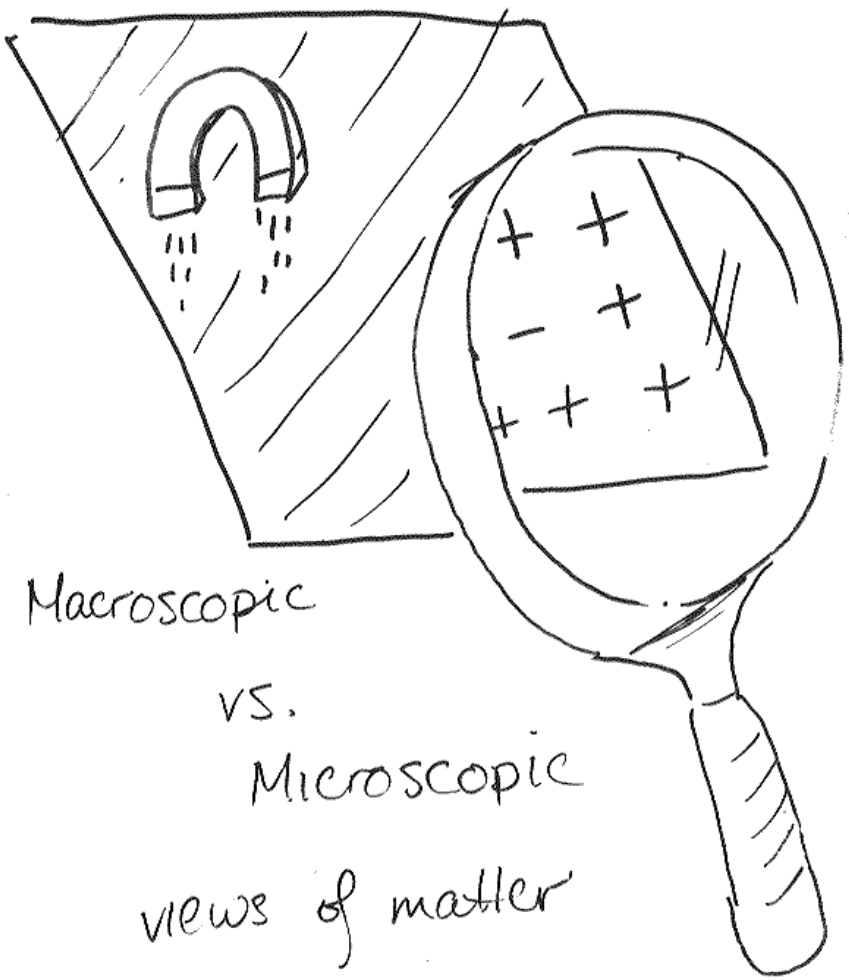
Markov Chain Methods in Physics

Dana Randall
Georgia Tech

Statistical Mechanics:



Macroscopic

vs.

Microscopic

views of matter

The Ising Model

$$\sigma: \begin{array}{cccccc} + & - & - & - & - & + \\ + & + & - & - & + & - \\ + & - & - & + & + & - \\ - & + & - & - & - & - \\ - & + & + & + & - & - \\ + & - & - & + & + & + \end{array}$$

- $$E(\sigma) = -J \sum_{i \sim j} \sigma_i \sigma_j - H \sum_i \sigma_i$$

  $$\Pi(\sigma) = e^{-\beta E(\sigma)} / Z$$ is the <u>Gibbs measure</u>

  where $$Z = \sum_\sigma e^{-\beta E(\sigma)}$$ is the <u>Partition fcn</u>

- <u>Ex:</u>

$$\begin{array}{ccccc} + & + & + & + & + \\ + & + & + & - & - \\ + & + & + & - & - \\ + & + & + & + & - \\ + & + & + & + & - \end{array} \quad \xleftrightarrow{\text{(phase transition)}} \quad \begin{array}{ccccc} + & + & - & - & + \\ + & - & - & + & - \\ - & - & + & - & + \\ + & + & - & + & + \\ + & + & - & + & - \end{array}$$

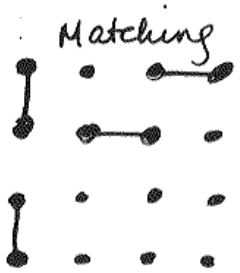
Low temperature ($\beta \to \infty$) High temperature ($\beta \to$

- The Partition fcn $\underline{\underline{Z}}$ determines entropy, free energy, sp. heat, ...

Other Models:

- **Monomer-Dimer**

$$Z = \sum_{M \text{ matching}} \lambda^{|M|}$$



- **Hard-Core model (Ind Sets)**

$$Z = \sum_{I \text{ ind set}} \lambda^{|I|}$$

- **Ice Model (6 vtx Model)**

Z = # of Eulerian Orientations

- **Potts Model** $\sigma_i \in \{1, \dots, q\}$

$$E(\sigma) = -J \sum_{i \sim j} \delta(\sigma_i, \sigma_j)$$

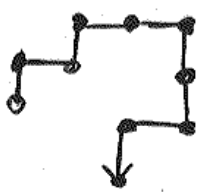
$$Z = \sum_{\sigma} e^{-\beta E(\sigma)}$$

zero temp: k-Coloring

1	2	4	1
3	4	3	2
1	3	1	3

- **Self-Avoiding Walks**

$$Z = \sum_{\omega} \beta^{|\omega|}$$



Can we calculate Z (in general)?

Hardness results!!

Monomer-Dimer: large λ → Counting Matchings

Hard-Core: Counting max ind. sets

Potts Model: Zero temp: k-colorings

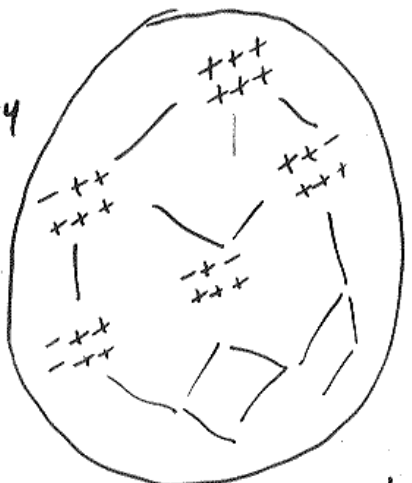
Self-Avoiding Walks:

large λ → Counting Hamiltonian cycles

Approximation Algs : Markov Chain Monte Carlo

(Ω, P, π)

- Ω: state space
- P: transition probs.
- π: stationary dist.



Metropolis alg defines transition probabilities P

$$P(\sigma, \tau) = \min\left(1, \frac{\pi(\tau)}{\pi(\sigma)}\right)$$

Fact P irreducible, aperiodic

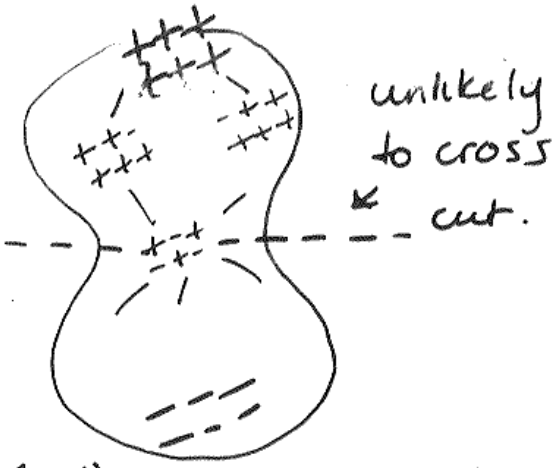
$\Rightarrow P^t$ converges to π as $t \to \infty$.

use to
- sample from Gibbs measure π
- Estimate Z

[Jerrum, Valiant Vazirani]

Mixing Rates:

low temperature —



Def: $$\Phi_S = \frac{\sum_{\substack{s \in S \\ s' \in \bar{S}}} \pi(s) P(s,s')}{\sum_{s \in S} \pi(s)},$$

$$\Phi = \min_{S : \pi(S) \leq \frac{1}{2}} \Phi_S .$$

Thm: [Jerrum, Sinclair]
A M.C. is rapidly mixing iff $\Phi \geq \frac{1}{\text{poly}}$.

* First provably efficient algo for:
- Monomer-Dimer Models [Jerrum Sinclair]
- Ice [Mihail, Winkler]
- Ising Model [J, S]

"Goals":

Physics	CS
lattice graphs	general graphs
"Glauber dynamics"	sophisticated algs
Very fast ($O(n \log n)$)	"Efficient"
heuristics	rigorous algs.

Thm: [L, V] $\lambda \leq \frac{1}{\Delta - 3} \Rightarrow$ mixing time $= O(n^3 \lg \frac{1}{\epsilon})$

(for the M.C. with edge moves)

Cor: Glauber dynamics are rapidly mixing.

Proof based on <u>coupling</u>.

Define M.C. on $\Omega \times \Omega$ s.t.

correlate random coin flips!!)

- viewed separately, just see transitions ☺
- States w. agreement stay together

Coupling time $= \max_{x,y} E[$time for states to agree starting at $x, y]$

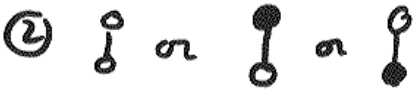
Thm: Coupling time < poly $\Rightarrow$ rapid mixing

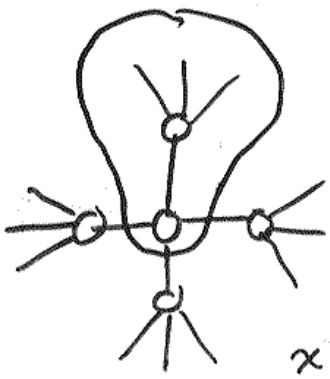
PATH COUPLING

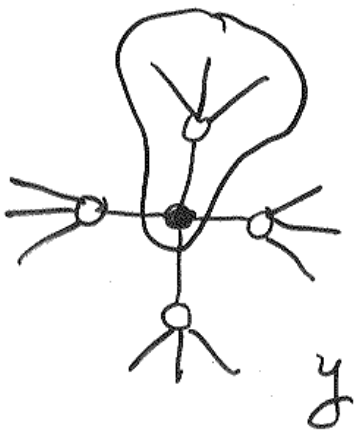
Thm: [Bubley, Dyer] On a metric space Φ

it suffices to show $E[\Delta \Phi(x,y)] \leq 0$ for $x \sim y$

To couple pick ① same edge

② 

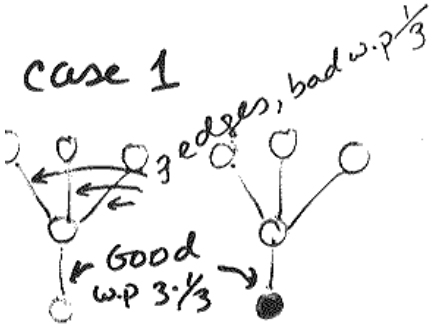




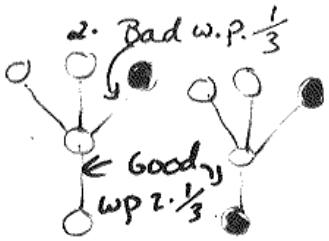
Show $E[\Delta \Phi] \leq 0$

(let $\lambda = 1$)

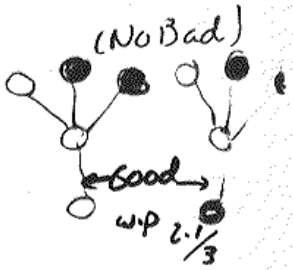
case 1



case 2



case 3



$\Rightarrow$

$E[\Delta \Phi] \sim (\#\text{bad} - \#\text{good}) \leq 0$

Independent Sets (Hard-core Model)

For $\lambda > 0$.

I : an independent set in G

$$\mu(I) = \frac{\lambda^{|I|}}{\sum_{I: \text{ind set}} \lambda^{|I|}} = \frac{\lambda^{|I|}}{Z}$$

← partition function

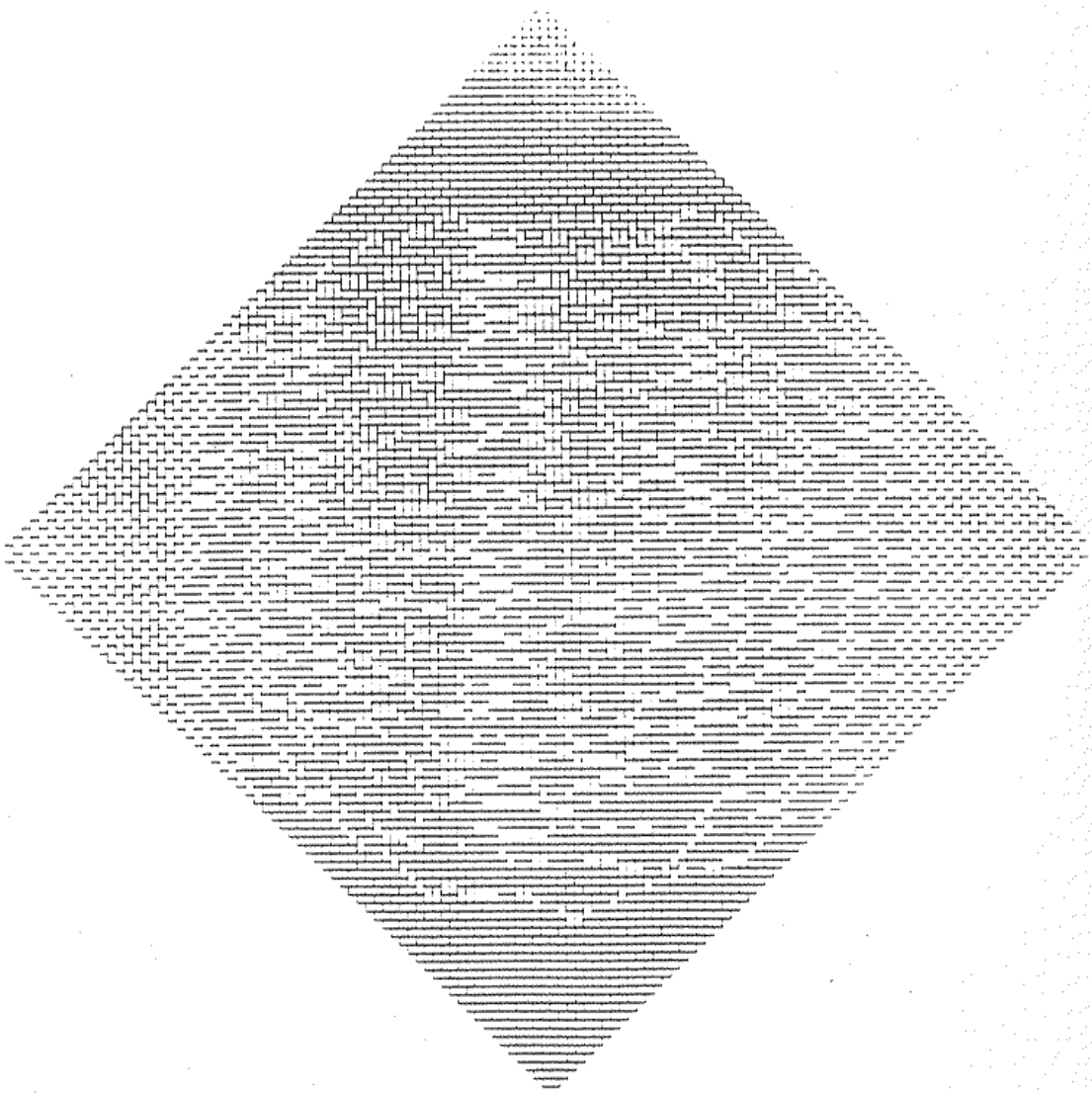
(Note: $\lambda = 1$ is the uniform case!)

Glauber Dyn:

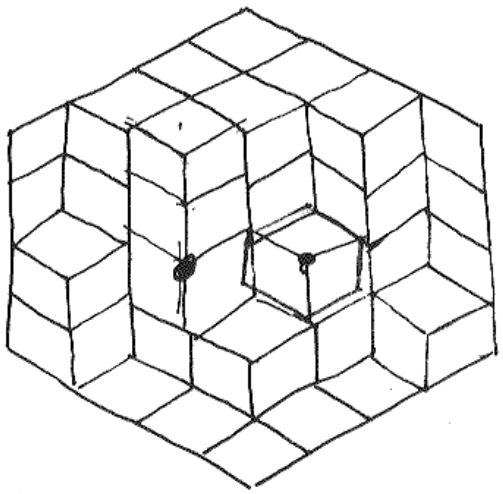
Repeat
- choose $v \in_u V$
- if $v \in$ Ind set
  remove w.p. $\frac{1}{1+\lambda}$
- if $v \notin$ Ind set
  add (if possible)
  w.p. $\frac{\lambda}{1+\lambda}$

Edge Moves: [Luby Vigoda

Repeat
- choose $e = \{u, v\} \in_u E$
- $J = \begin{cases} I \setminus \{u, v\} & \text{w.p. } \frac{1}{1+2\lambda} \\ I \setminus \{u\} \cup \{v\} & \text{w.p. } \frac{\lambda}{1+2\lambda} \\ I \setminus \{v\} \cup \{u\} & \text{w.p. } \frac{\lambda}{1+2\lambda} \end{cases}$
- Move to J if J is an ind. set.



③ Lozenge tilings (Cube packings)

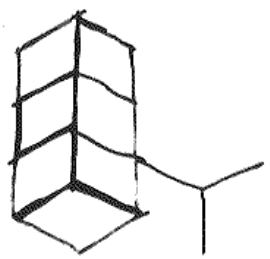


MC 102

- Start with any tiling
- Repeat:
  - Pick a hexagonal window u.a.r.
  - add/remove "cube" w.p. 1/2 if possible.

alt MC tower

· If base of a tower of ht h add/remove tower wp $\frac{1}{2h}$



Tower moves:

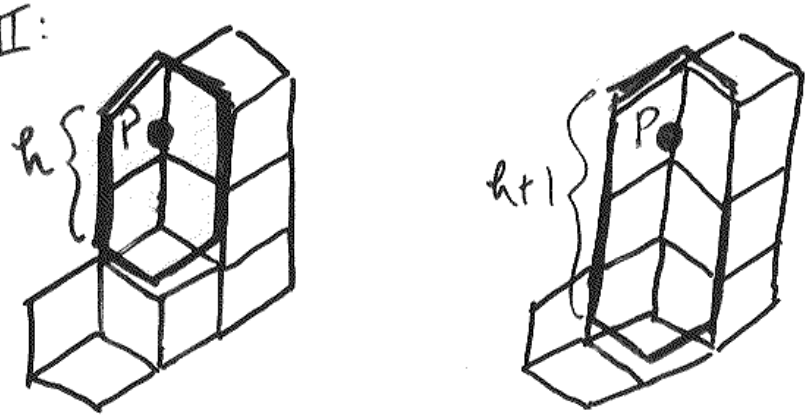
- pick $\underline{v}$ u.a.r.
- if v starts/ends a vertical tower of ht h, remove/add it w.p. $1/2h$.

Thm: [LRS]
The tower chain is rapidly mixing

"Pf:" There is a coupling s.t. $E[\Delta d(\omega_1, \omega_2)] \leq 0$

Pf of mixing w/ tower moves [Luby, R, Sinclair]

Type III:



$$E[\Delta\Phi \mid \text{point } p \text{ chosen}]$$

$$= \frac{1}{h+1}(-1) + \left(\frac{1}{h} - \frac{1}{h+1}\right)(h)$$

$$= 0$$

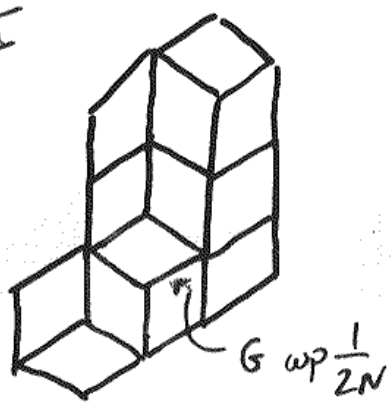
So

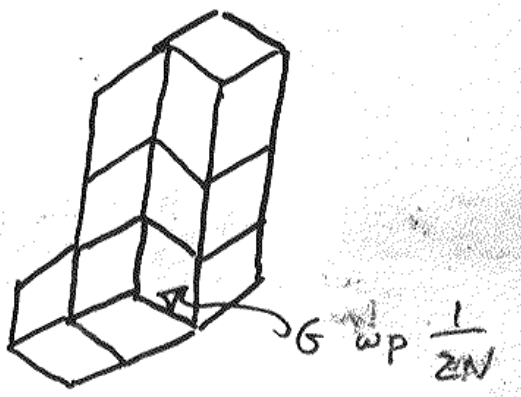
$$E[\Delta\Phi] \leq \underbrace{-\frac{1}{N}}_{\text{Type I}} + \underbrace{\frac{1}{N}}_{\text{Type II}} + \underbrace{0}_{\text{Type III}} \leq 0.$$

Thm [R, Tetali] MC_{TOWER} mixing $\Rightarrow$ $MC^{\text{mix}}_{\text{GLAUBER}}$

Pf of mixing w/ tower moves [Luby, R, Sinclair]

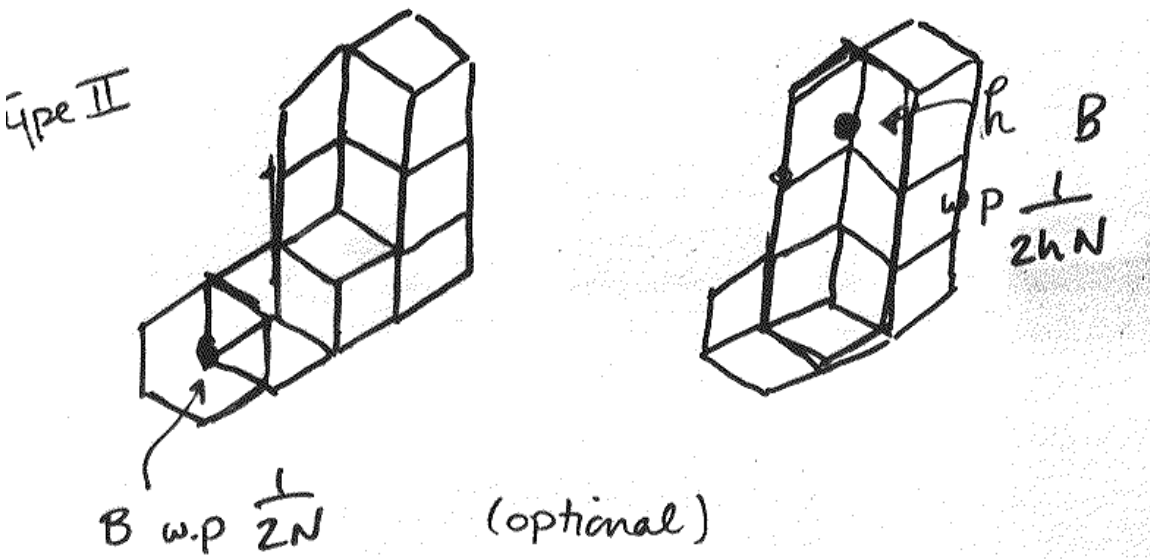
Type I





$$E(\Delta\Phi) = \underset{\text{Type I}}{-2 \cdot \frac{1}{2N}} + \dots$$

Pf of mixing w/ tower moves [Luby, R, Sinclair]



$$E[\Delta\Phi] \leq \underbrace{-2 \cdot \frac{1}{2N}}_{\text{Type I}} + \frac{1}{2N} + \underbrace{h \cdot \frac{1}{2hN}}_{\text{Type II}} + \dots$$