UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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H4.SMR/854-10

College on Computational Physics

15 May - 9 June 1995

Stochastic Simulation Methods

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Research Areas

Phase transitions

Biological molecules

MC Methods

Metropolis

Cluster (SW, Wolff)

Replica MC (spin glass)

Acceptance Ratio Method

Dynamically Optimized MC

Analysis Methods

Points

Single histogram

Umbrella sampling

Multi-stage sampling

Multi-canonical

Multiple histogram

Phase Transitions

Critical Exponents

Magnetism

Liquid - Gas

Melting

Percolation

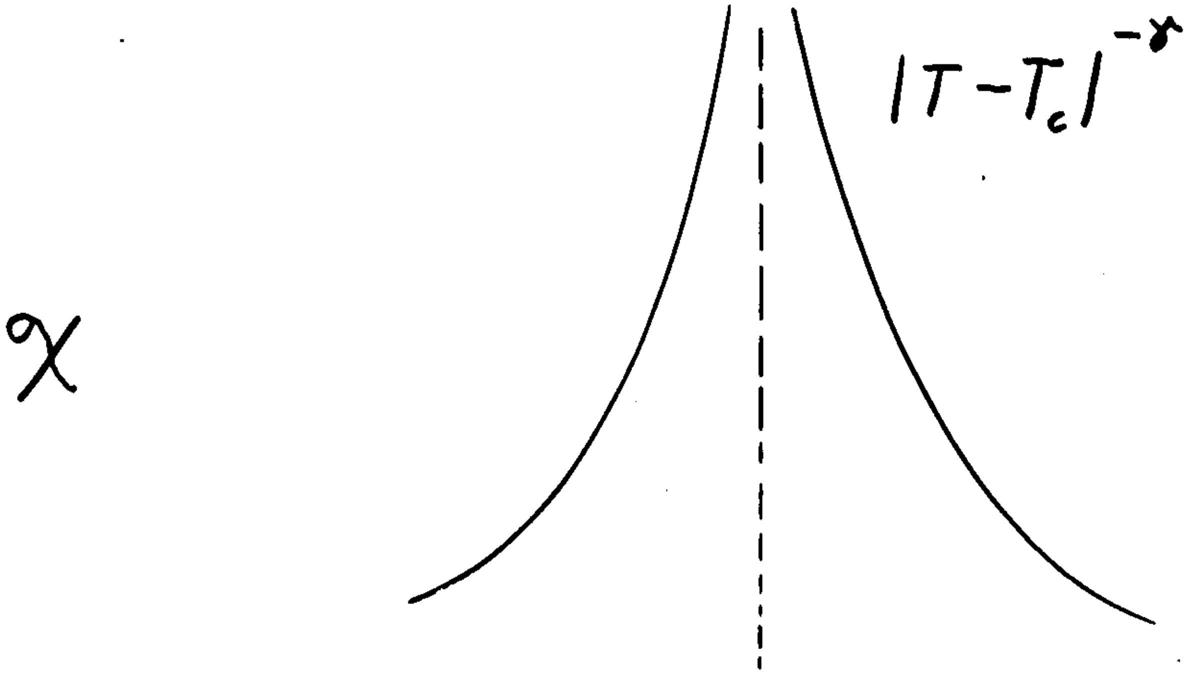
Gelation

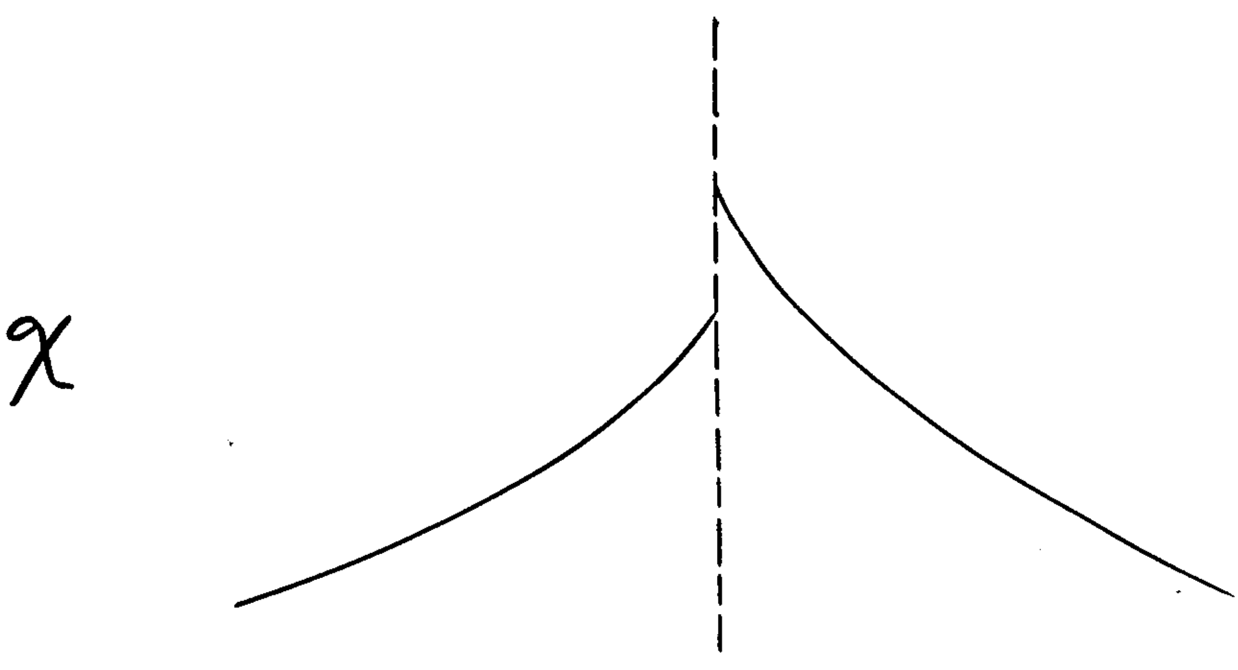
Aggregation

Critical Dynamics

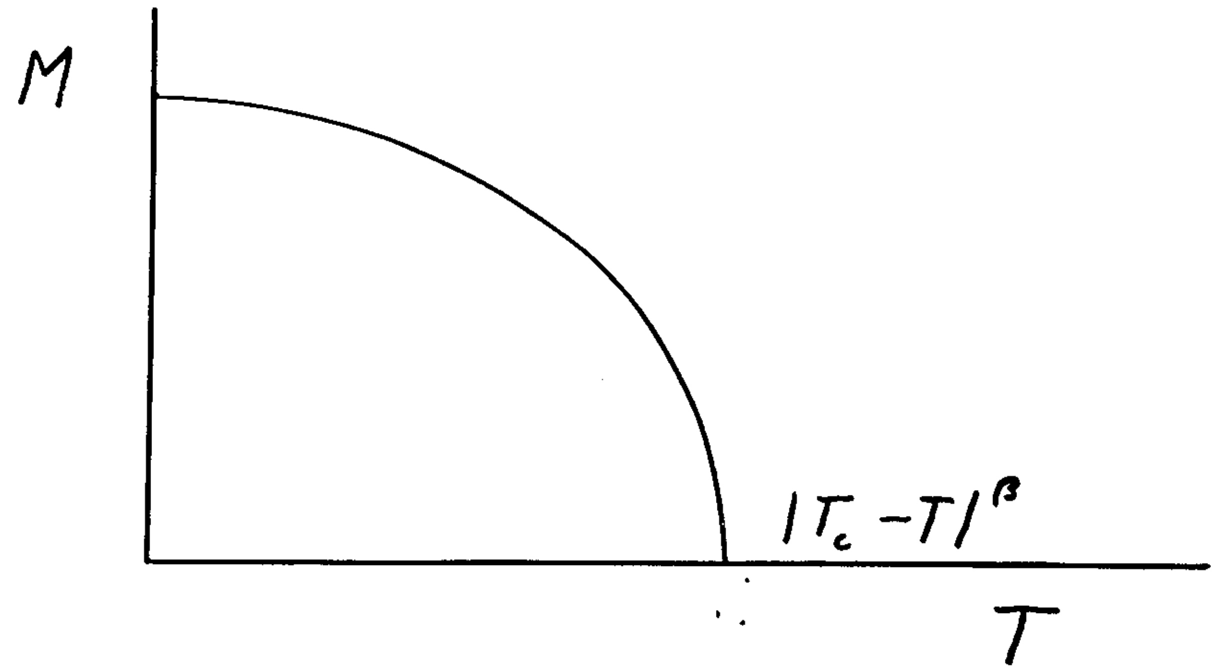
Spin Glasses

Lattice Gauge Theories

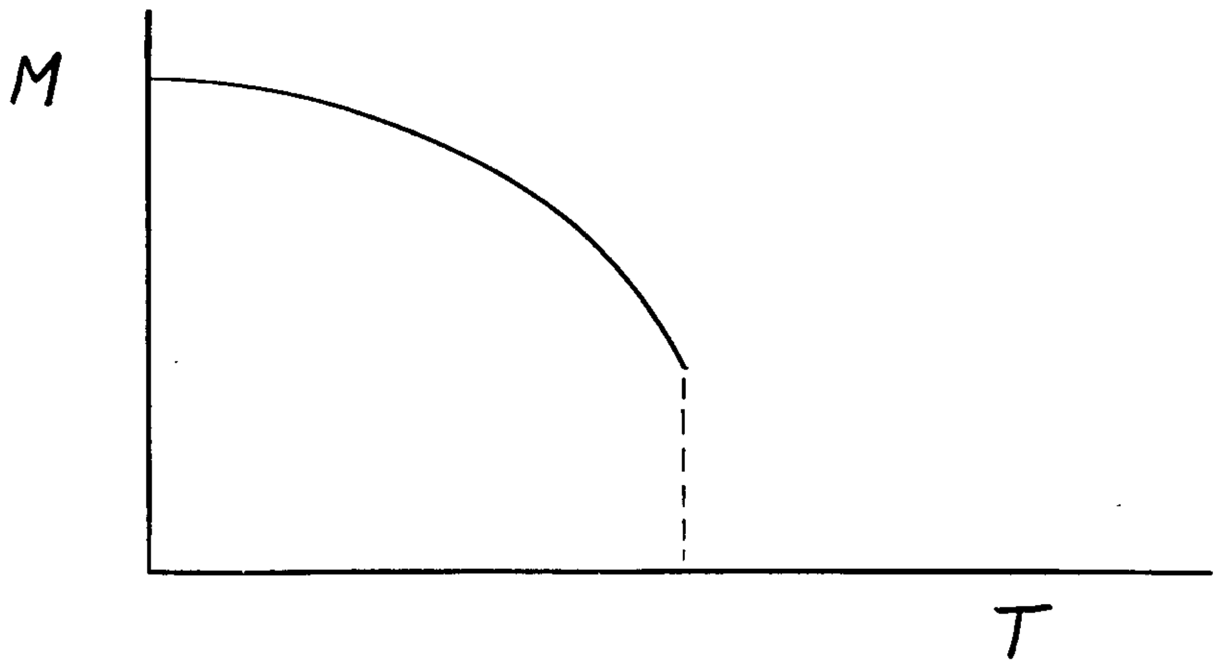

χ
$|T-T_c|^{-\gamma}$


χ

2^{nd} order



1^{st} order



Critical Exponents

Mean Field		
	Specific Heat	
$\alpha = \alpha' = 0$	$C \sim \lvert T - T_c \rvert^{-\alpha}$	$H = 0$
	Magnetization (order parameter)	
$\beta = \frac{1}{2}$	$M \sim (T_c - T)^{\beta}$	$H = 0$
$\delta = 3$	$M \sim H^{1/\delta}$	$T = T_c$
	Susceptibility	
$\gamma = \gamma' = 1$	$\chi \sim \lvert T - T_c \rvert^{-\gamma}$	$H = 0$
	Correlation Length	
$\nu = \frac{1}{2}$	$\xi \sim \lvert T - T_c \rvert^{-\nu}$	$H = 0$
	Correlation Function at T_c	
$\eta = 0$	$\langle \sigma_0 \sigma_r \rangle \sim r^{-(d-2+\eta)}$	$T = T_c$, $H = 0$

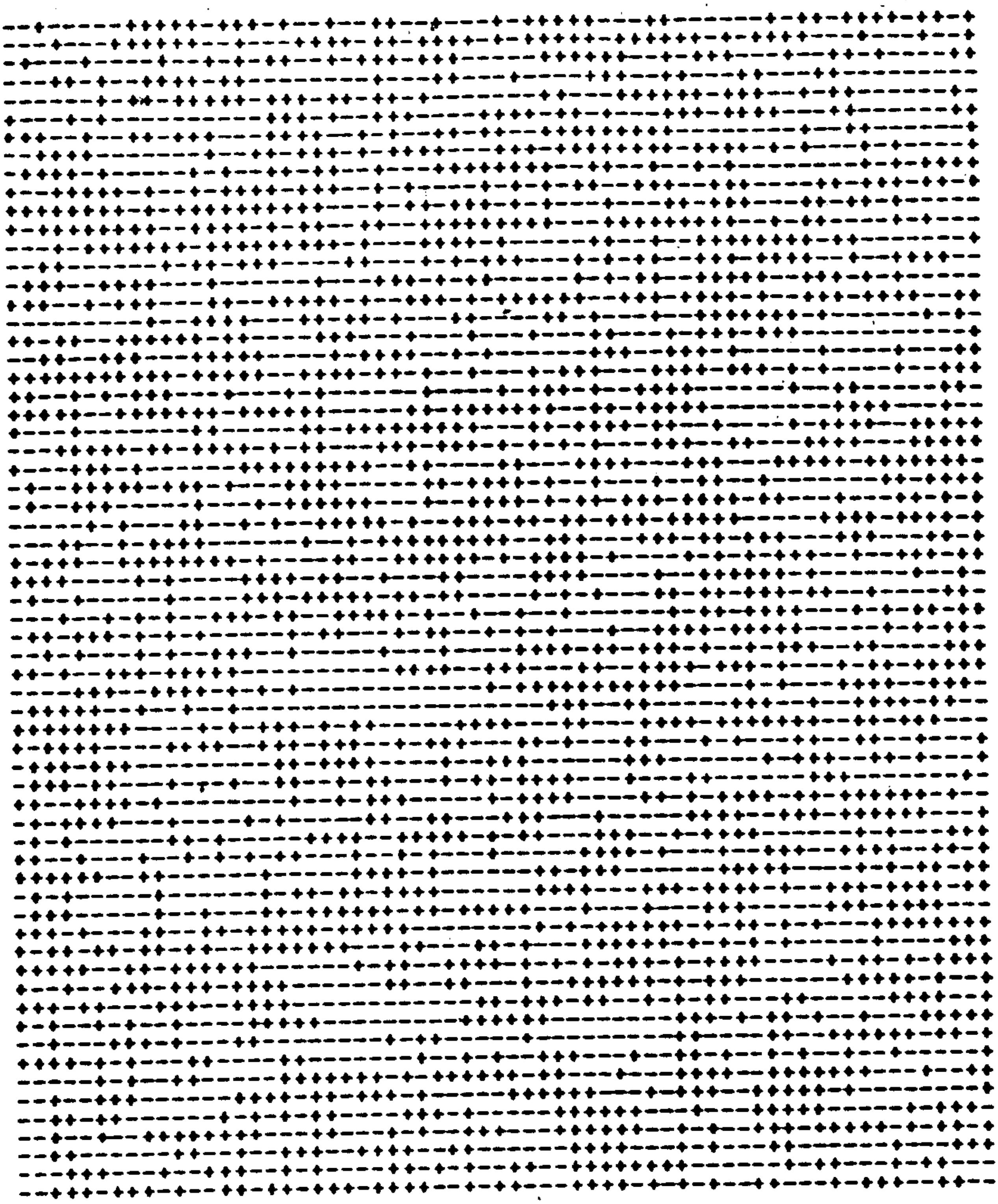
ISING MODEL

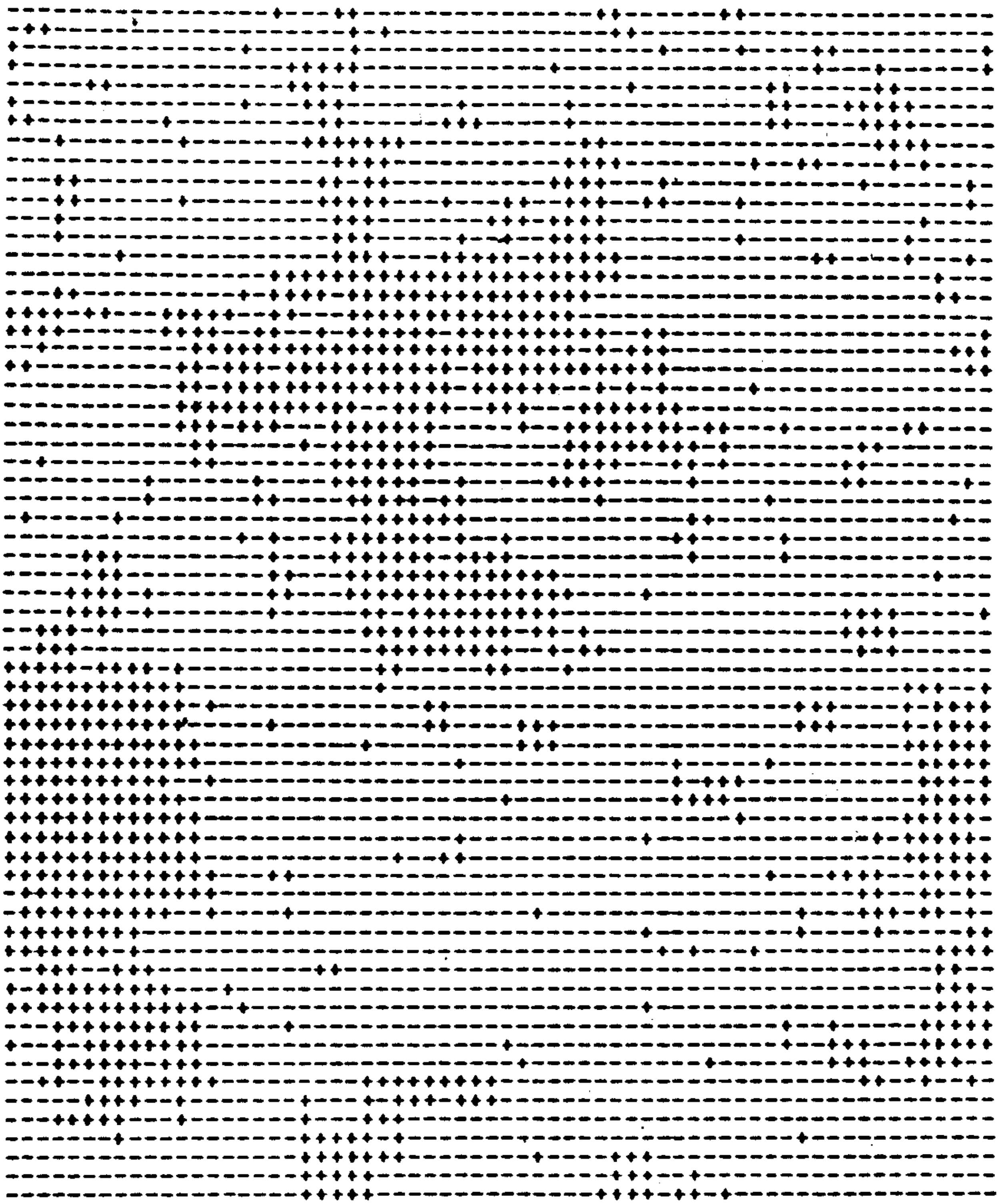
"Spins" σ_i on lattice sites

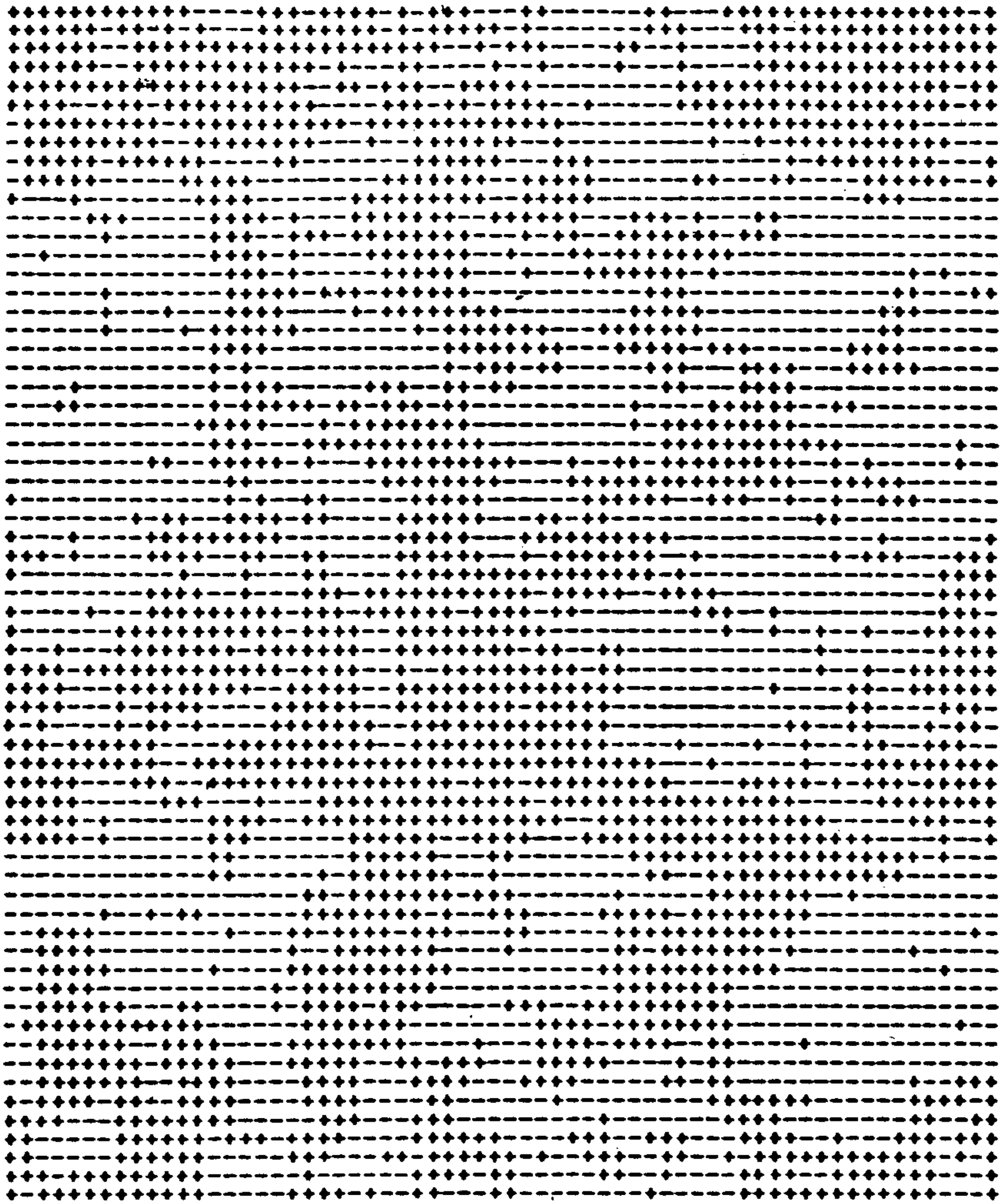
$$\sigma_i = +1 \quad \text{or} \quad -1$$

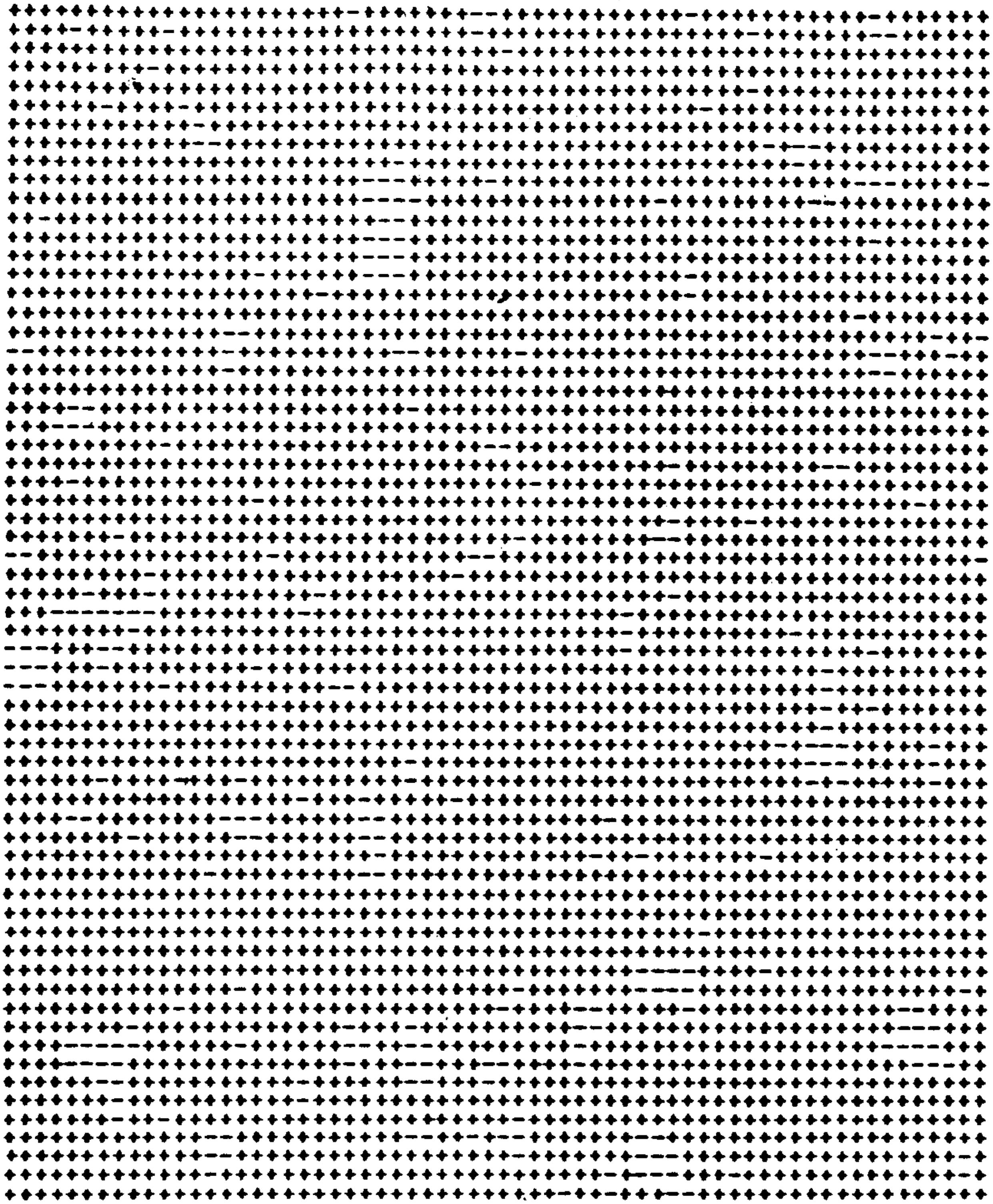
$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

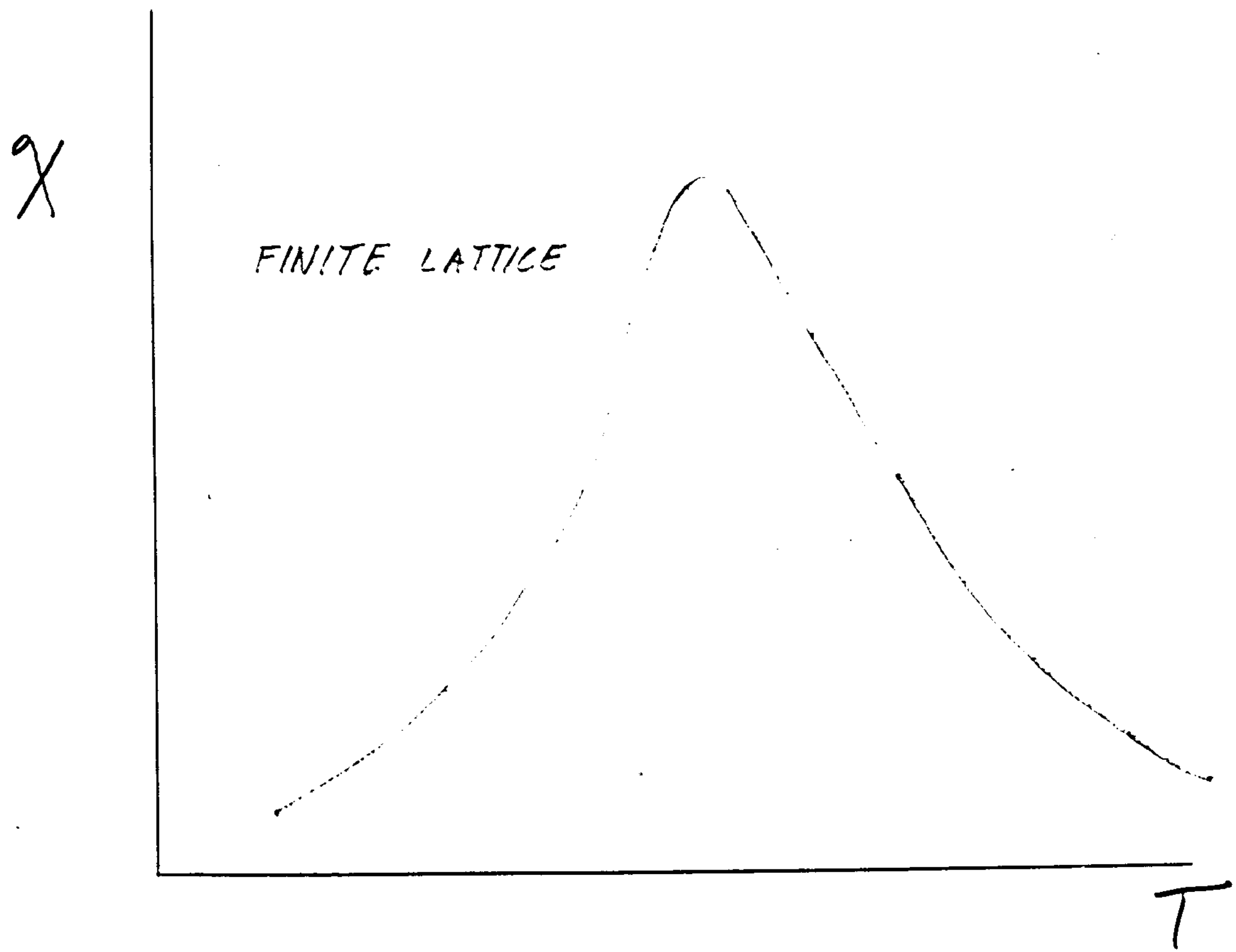
Neighbors	Energy
$+\,+$ or $-\,-$	$-J$
$+\,-$ or $-\,+$	$+J$



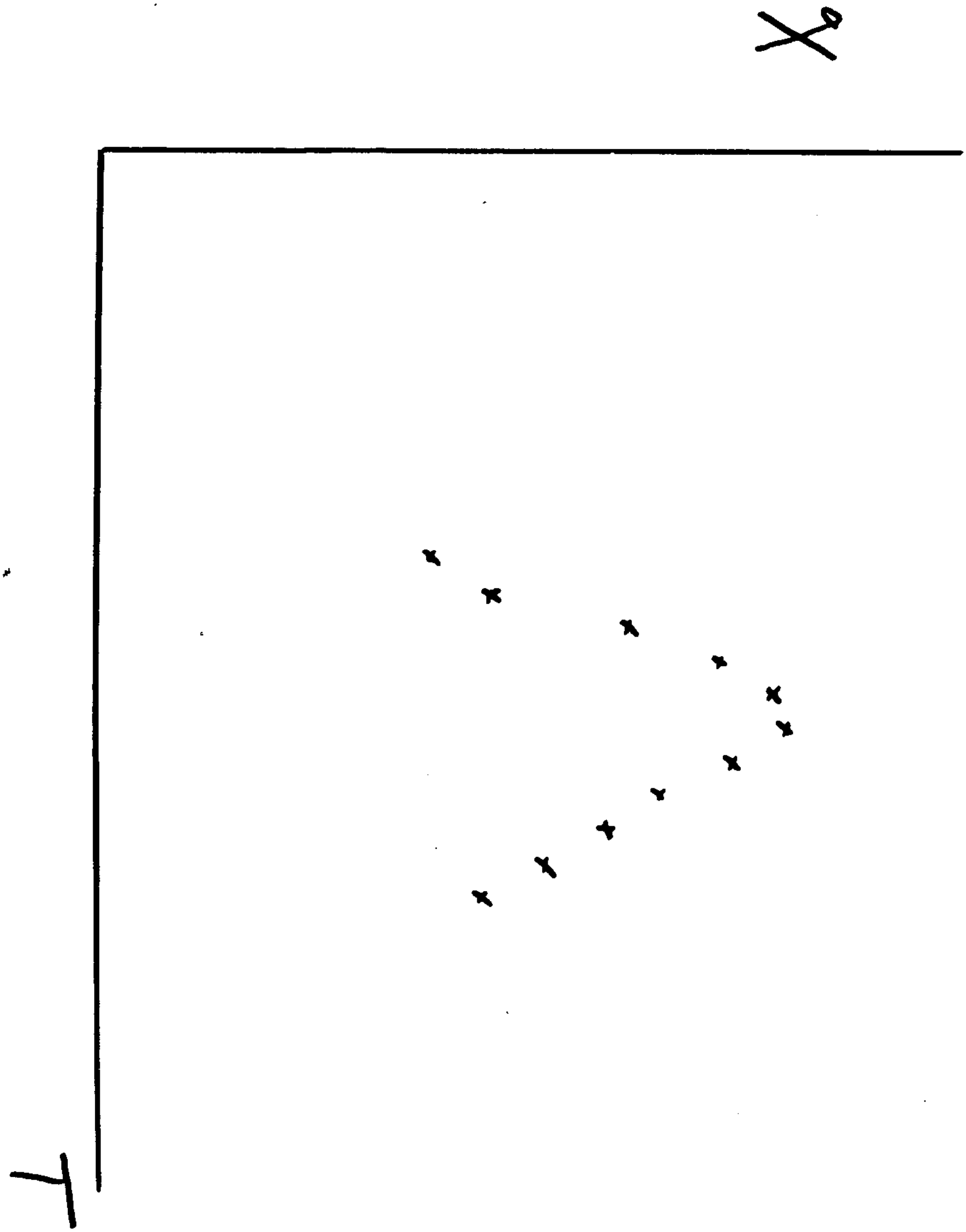


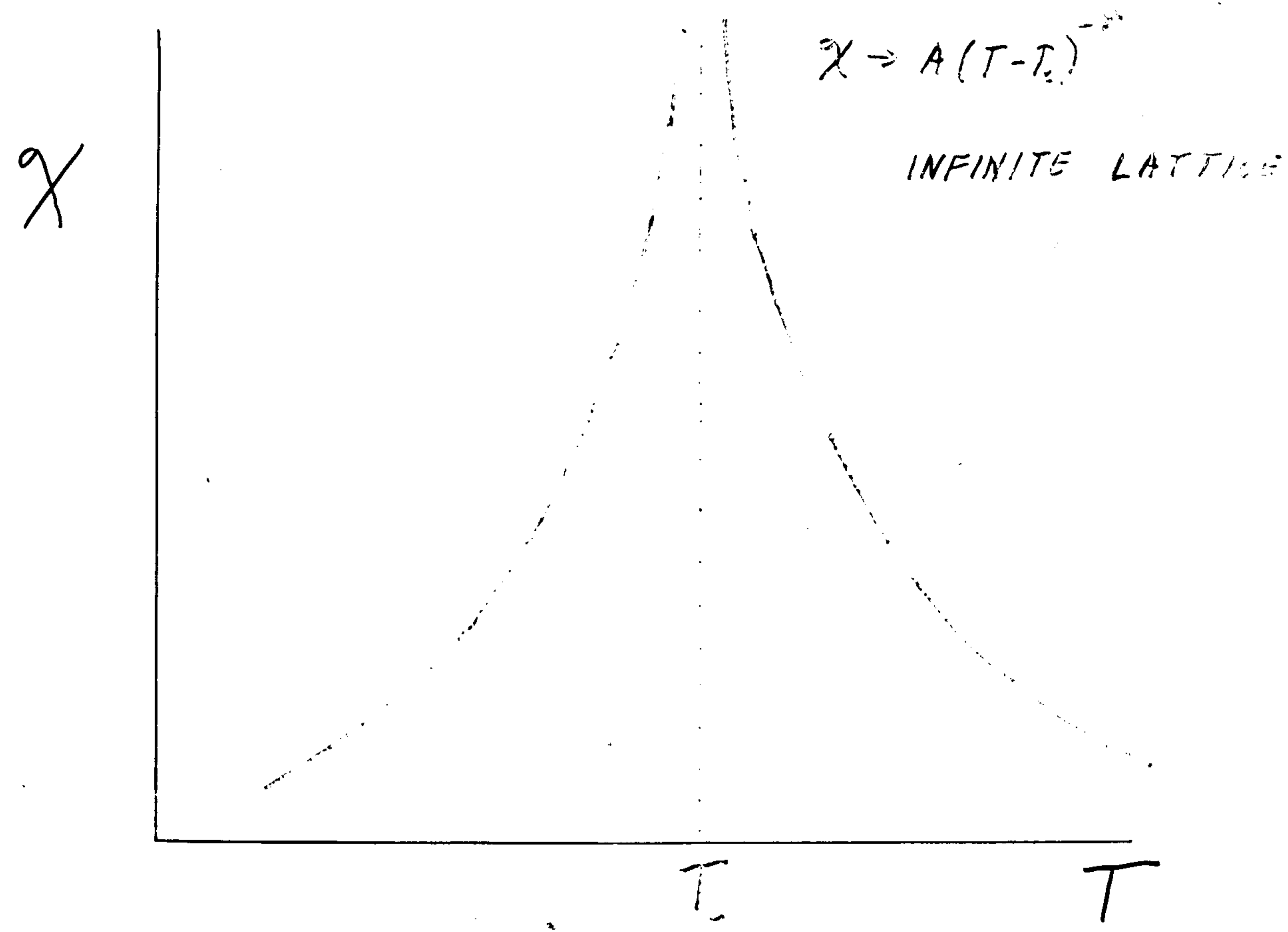






χ
FINITE LATTICE
T




$\chi \rightarrow A(T-T_c)^{-\gamma}$
INFINITE LATTICE
χ
T_c
T

Finite-size scaling

$$\chi \sim t^{-\gamma}$$

In a finite system of length L,
no fluctuations are larger than L.

$\Rightarrow$ At the peak

$$\chi \sim L^{\gamma/\nu}$$

Critical Slowing Down

$$\tau \sim \xi^{z} \qquad\qquad z \approx 2$$

$$\xi \sim |T - T_c|^{-\nu}$$

$$\tau \sim |T - T_c|^{-z\nu}$$

For finite L, as $T \to T_c$, the largest clusters grow until $\xi \approx L$

$\Rightarrow$ At T_c

$$\tau \sim L^{z}$$

Finite-size scaling

Near T_c, the only important lengths are

$$L \quad \text{and} \quad \xi \sim t^{-\nu}$$

$$L/\xi \qquad L t^{\nu} \qquad t L^{1/\nu}$$

$$M = L^{-\beta/\nu} f_M (t L^{1/\nu})$$

Monte Carlo

Computer Simulations

Advantages

- Simplicity
- General applicability
- Systematically improvable
- Errors can be calculated

Disadvantages

- Long relaxation times near T_c
- Finite-size rounding of critical singularities
- Time consuming to calculate phase diagram

Markov Process

Master Equation:

Equilibrium Probability Density

$$P_{eq}(\sigma) = \frac{1}{Z} \exp\left[-E(\sigma)/k_B T\right]$$

$$Z = \underset{\sigma}{\mathrm{Tr}} \exp\left[-E(\sigma)/k_B T\right]$$

$$\langle E \rangle = \underset{\sigma}{\mathrm{Tr}}\, E(\sigma)\, P_{eq}(\sigma)$$

[illegible]

[illegible]

Necessary condition for $P(\sigma, t) \longrightarrow P_{eq}(\sigma)$

[illegible]

- Stronger condition

  Detailed Balance

$$W(\sigma' \to \sigma)\, P_{eq}(\sigma') = W(\sigma \to \sigma')\, P_{eq}(\sigma)$$

Detailed Balance

$$W(\sigma' \to \sigma)\, P_{eq}(\sigma') = W(\sigma \to \sigma')\, P_{eq}(\sigma)$$

$$\frac{W(\sigma' \to \sigma)}{W(\sigma \to \sigma')} = \exp\left[\left(E(\sigma') - E(\sigma)\right)/kT\right]$$

Theorem for Markov Processes

IF:

1) For any two states, σ_A and σ_B, there exists a sequence of states, $\sigma_1 \dots \sigma_n$, such that

$$W(\sigma_A \to \sigma_1)\, W(\sigma_1 \to \sigma_2) \dots W(\sigma_n \to \sigma_B) \neq 0$$

and

2) Detailed Balance

THEN:

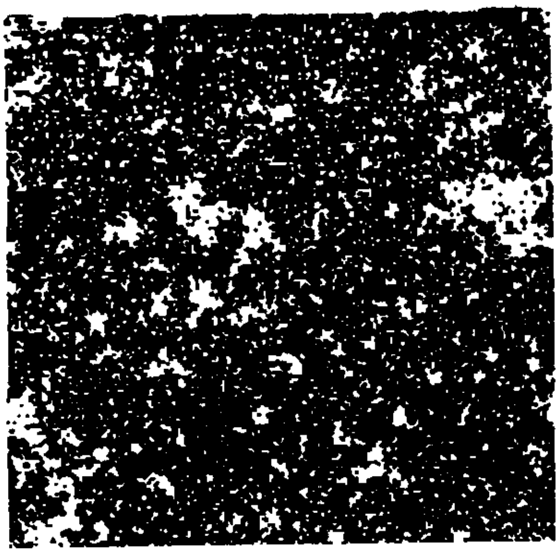
$$P(\sigma, t) \xrightarrow[t \to \infty]{} P_{eq}(\sigma)$$

+	−	+	−	+
−	+	+	−	−
+	+	+	−	−
+	+	+	+	+
−	−	+	+	−

MC

$T = T_c$

256×256



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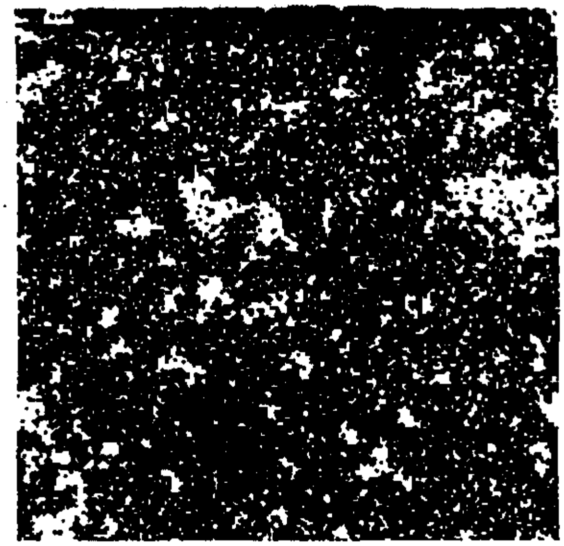

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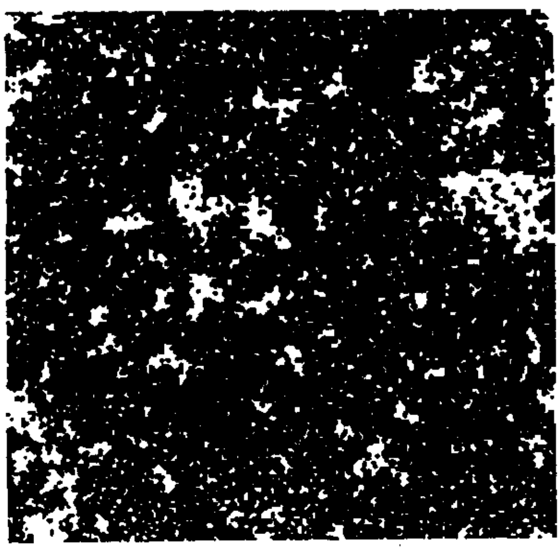

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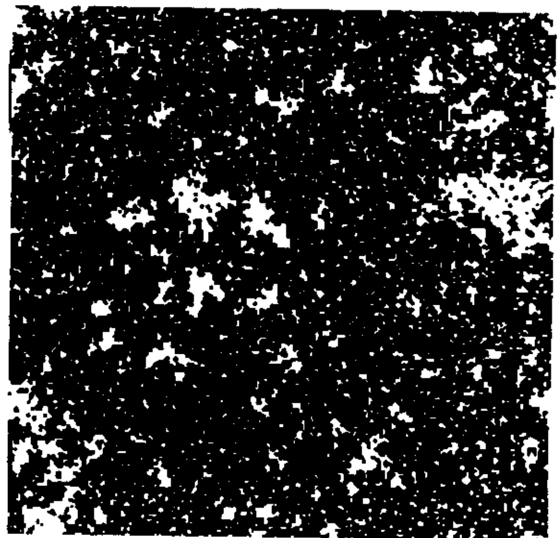

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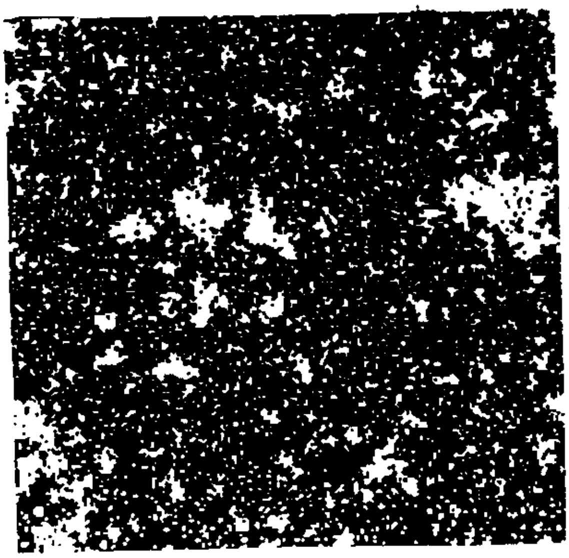

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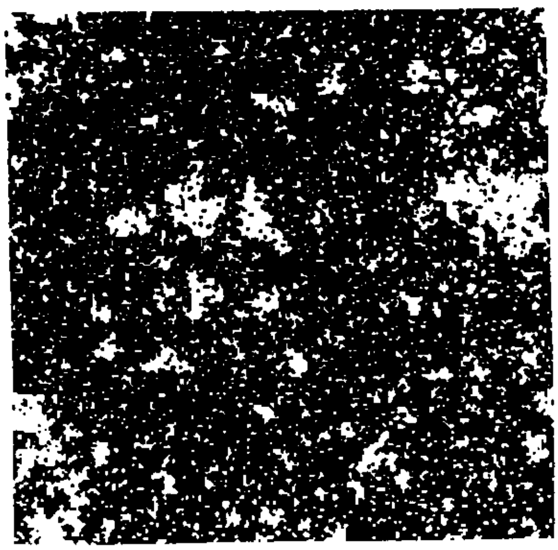
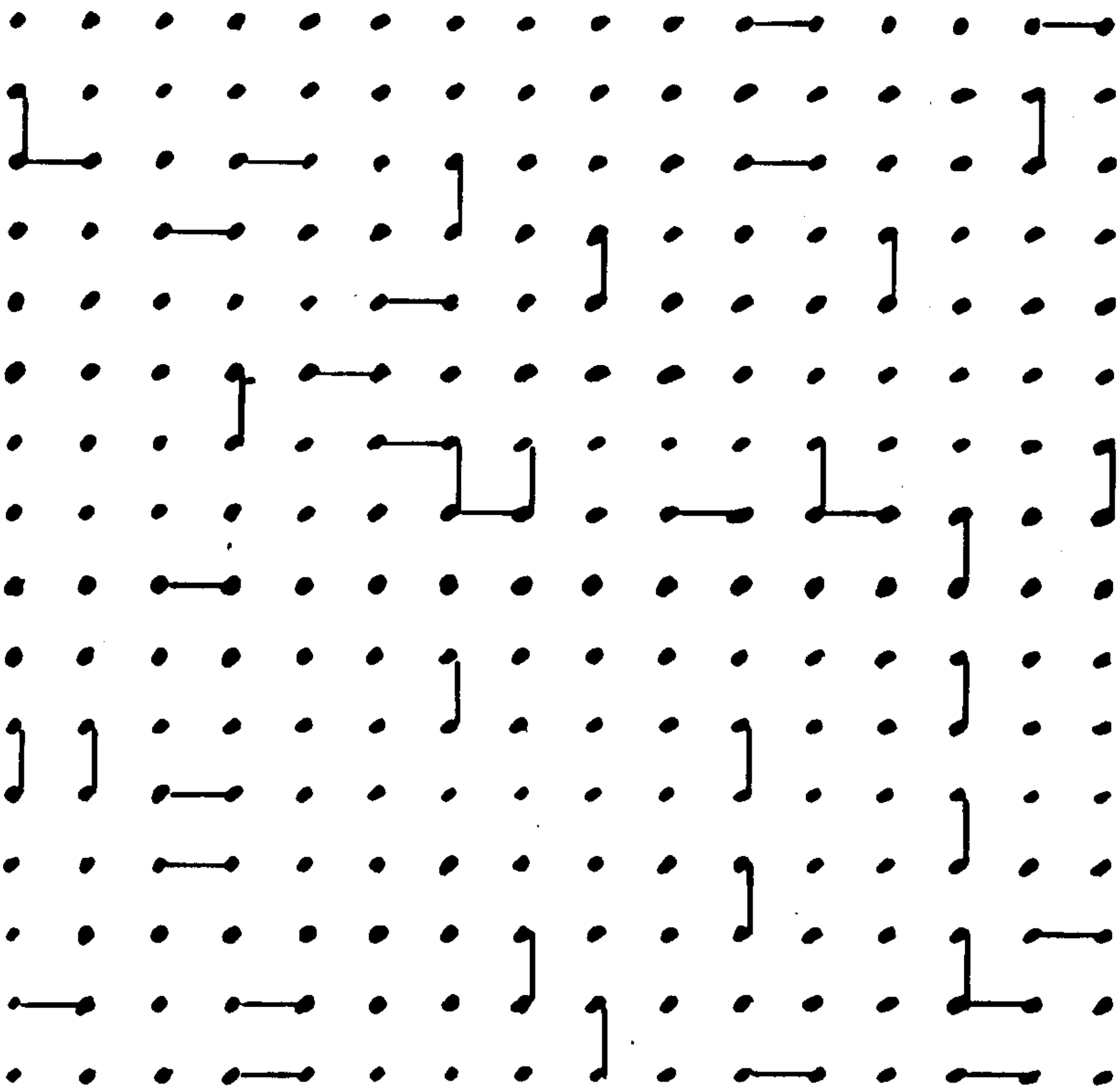
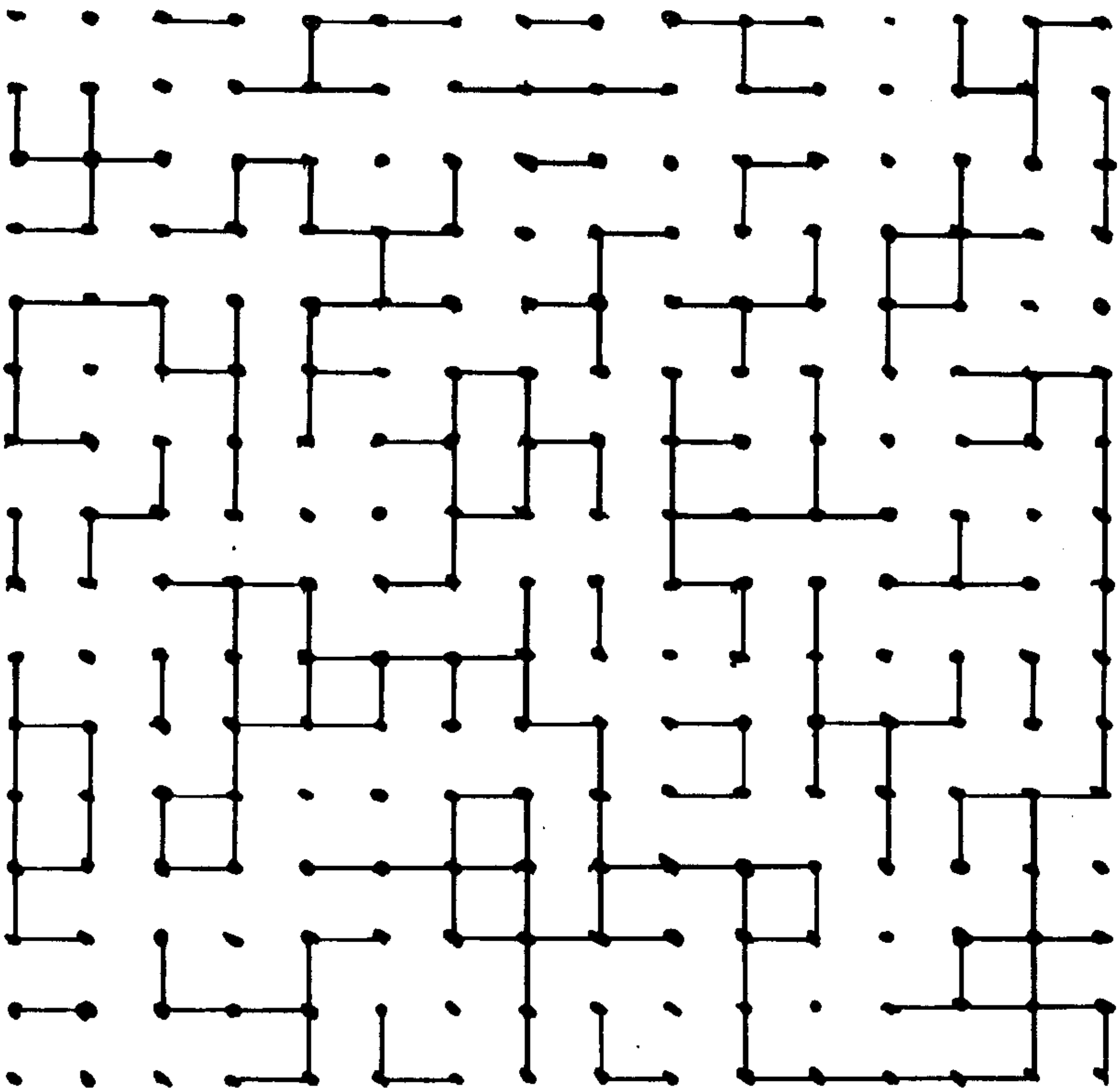


6

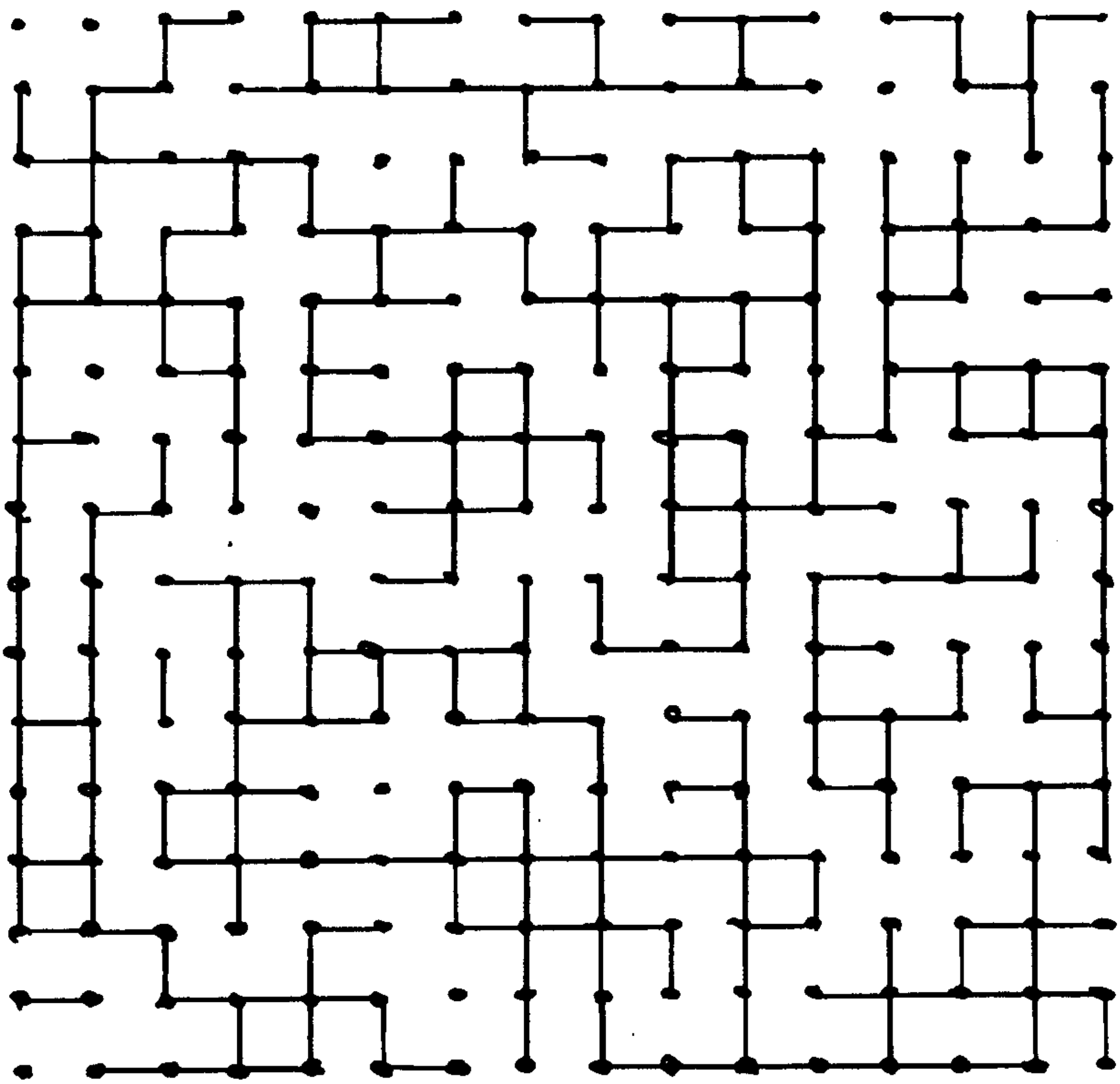
$p = 0.10$



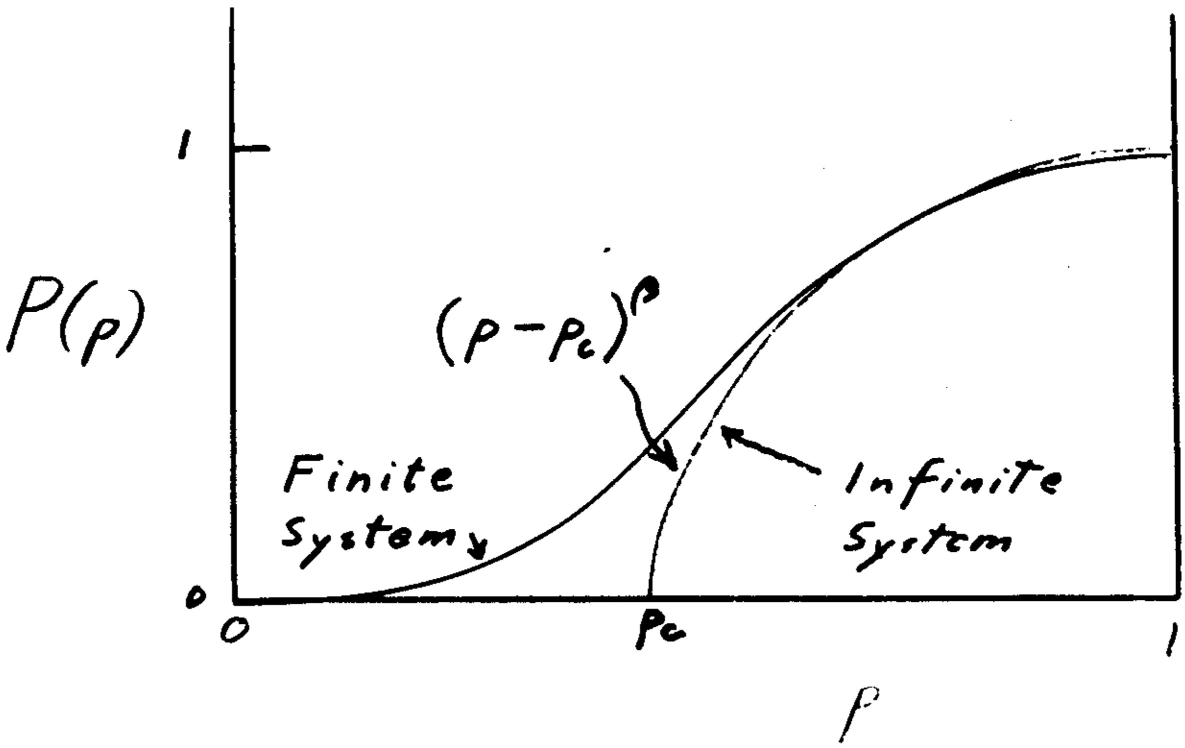
$p = 0.40$



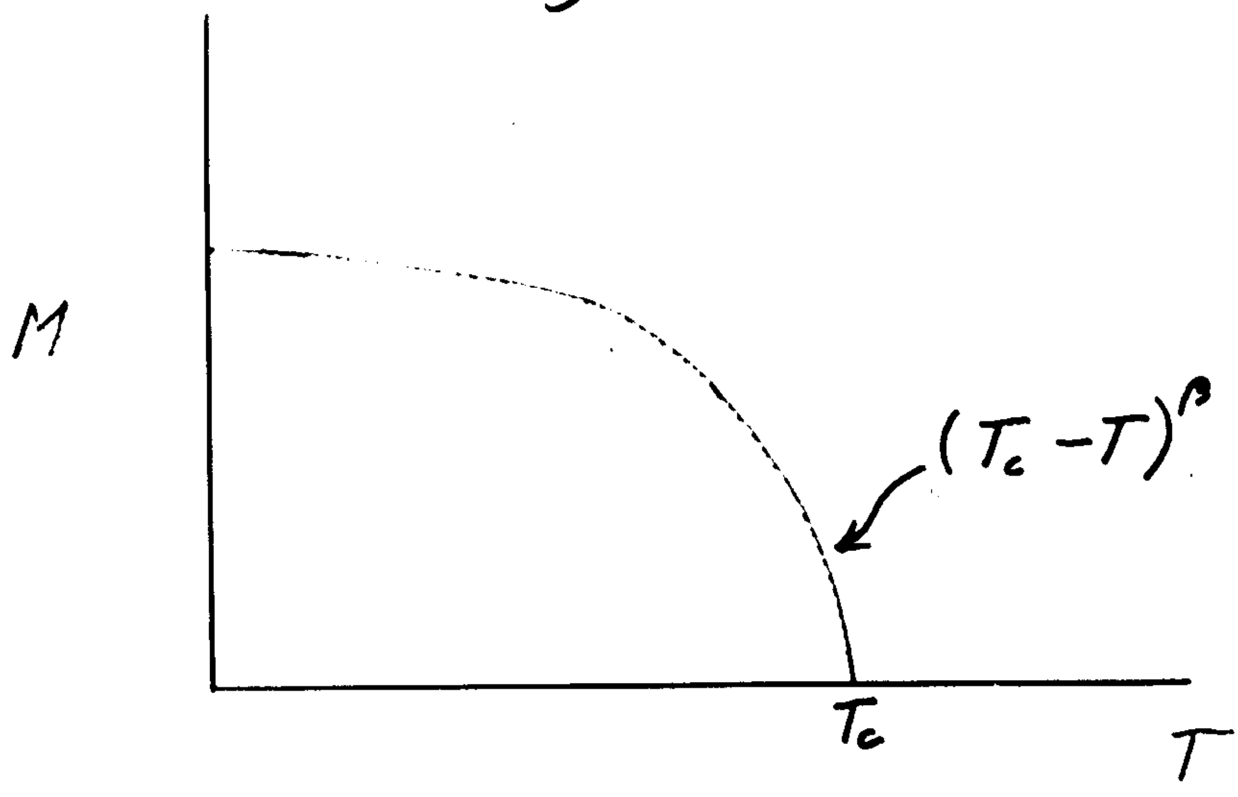
$p = 0.55$



Percolation



Magnetization



Ising Model

$$H = K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j}$$

$\sigma_i = +1$ or -1

or

$\sigma_i = 1$ or 2.

Potts Model

$\sigma_i = 1, 2, 3, \ldots q$

Potts $\rightarrow$ Percolation

$$H = K \sum_{\langle ij \rangle} (\delta_{\sigma_i, \sigma_j} - 1)$$

$$Z = \operatorname*{Tr}_{\sigma} e^{H}$$

$$H_{\langle \ell m \rangle} = K \sum_{\substack{\langle ij \rangle \\ \neq \langle \ell m \rangle}} (\delta_{\sigma_i, \sigma_j} - 1)$$

$$Z^{same}_{\langle \ell m \rangle} \equiv \operatorname*{Tr}_{\sigma} e^{H_{\langle \ell m \rangle}} \delta_{\sigma_\ell, \sigma_m}$$

$$Z^{diff}_{\langle \ell m \rangle} \equiv \operatorname*{Tr}_{\sigma} e^{H_{\langle \ell m \rangle}} (1 - \delta_{\sigma_\ell, \sigma_m})$$

$$Z = Z^{same}_{\langle \ell m \rangle} + e^{-K} Z^{diff}_{\langle \ell m \rangle}$$

Potts $\rightarrow$ Percolation

$$Z = Z^{same}_{\langle \ell m \rangle} + e^{-K} Z^{diff}_{\langle \ell m \rangle}$$

$$Z^{indep}_{\langle \ell m \rangle} \equiv \operatorname*{Tr}_{\sigma} e^{H_{\langle \ell m \rangle}}$$

$$Z^{indep}_{\langle \ell m \rangle} = Z^{same}_{\langle \ell m \rangle} + Z^{diff}_{\langle \ell m \rangle}$$

$$Z = \underbrace{(1 - e^{-K})}_{p} Z^{same}_{\langle \ell m \rangle} + \underbrace{e^{-K}}_{(1-p)} Z^{indep}_{\langle \ell m \rangle}$$

Potts → Percolation

$$Z = p\, Z^{same}_{\langle \ell m \rangle} + (1-p)\, Z^{indep}_{\langle \ell m \rangle}$$

$$p = 1 - e^{-K}$$

$$Z = \underset{\{links\}}{Tr}\; p^{b}\,(1-p)^{\bar{b}}\; s^{N_c}$$

$$Z = \left\langle s^{N_c} \right\rangle_{\{links\}}$$

$$\langle N_c \rangle = \lim_{s \to 1} \left[\frac{\partial}{\partial s} \ln Z \right]$$

Kasteleyn + Fortuin, 1969

Order Parameter

Ising Ferromaget

$M =$ [illegible]

$$= \lim_{H \to 0^+} \lim_{L \to \infty} L^{-d} \left\langle \sum_n C_n \sigma_n \right\rangle$$

$\uparrow$ sum on clusters

$$M = \lim_{H \to 0^+} \lim_{L \to \infty} L^{-d} \left\langle C_{largest} \right\rangle$$

Magnetic Susceptibility

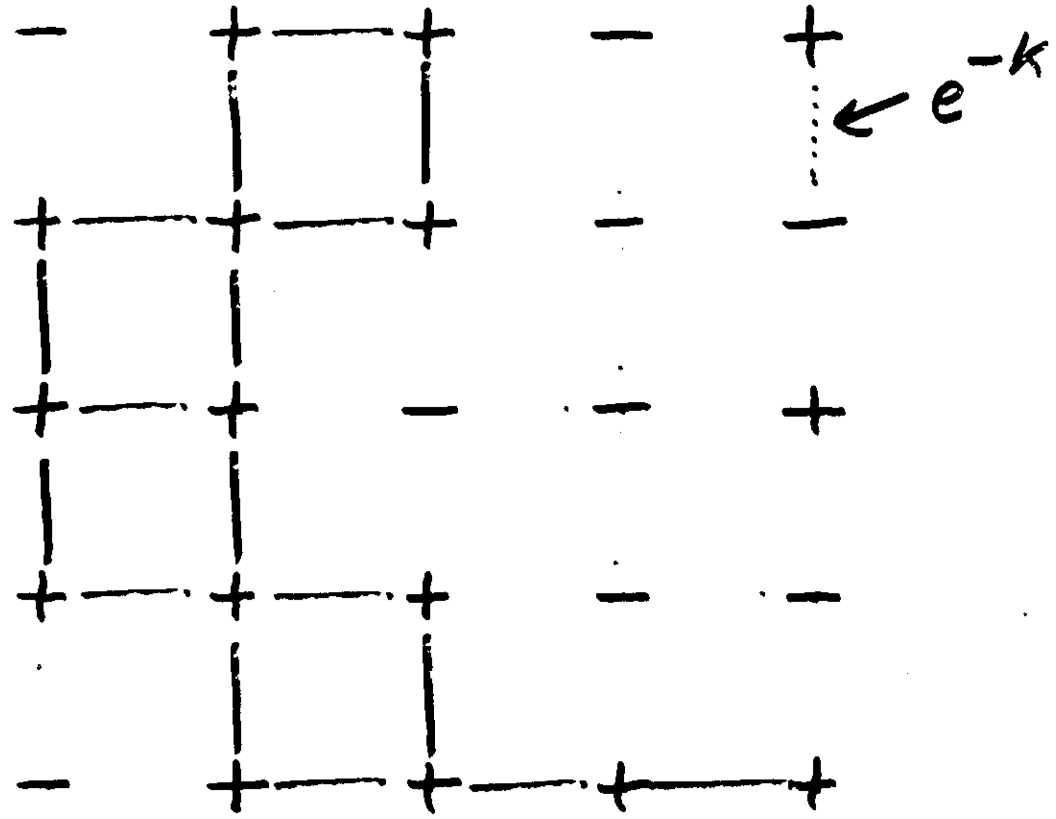
$$\chi = L^{-d} \left\langle \sum_{n,m} c_n c_m \sigma_n \sigma_m \right\rangle$$

$$\langle \sigma_n \sigma_m \rangle = \delta_{n,m}$$

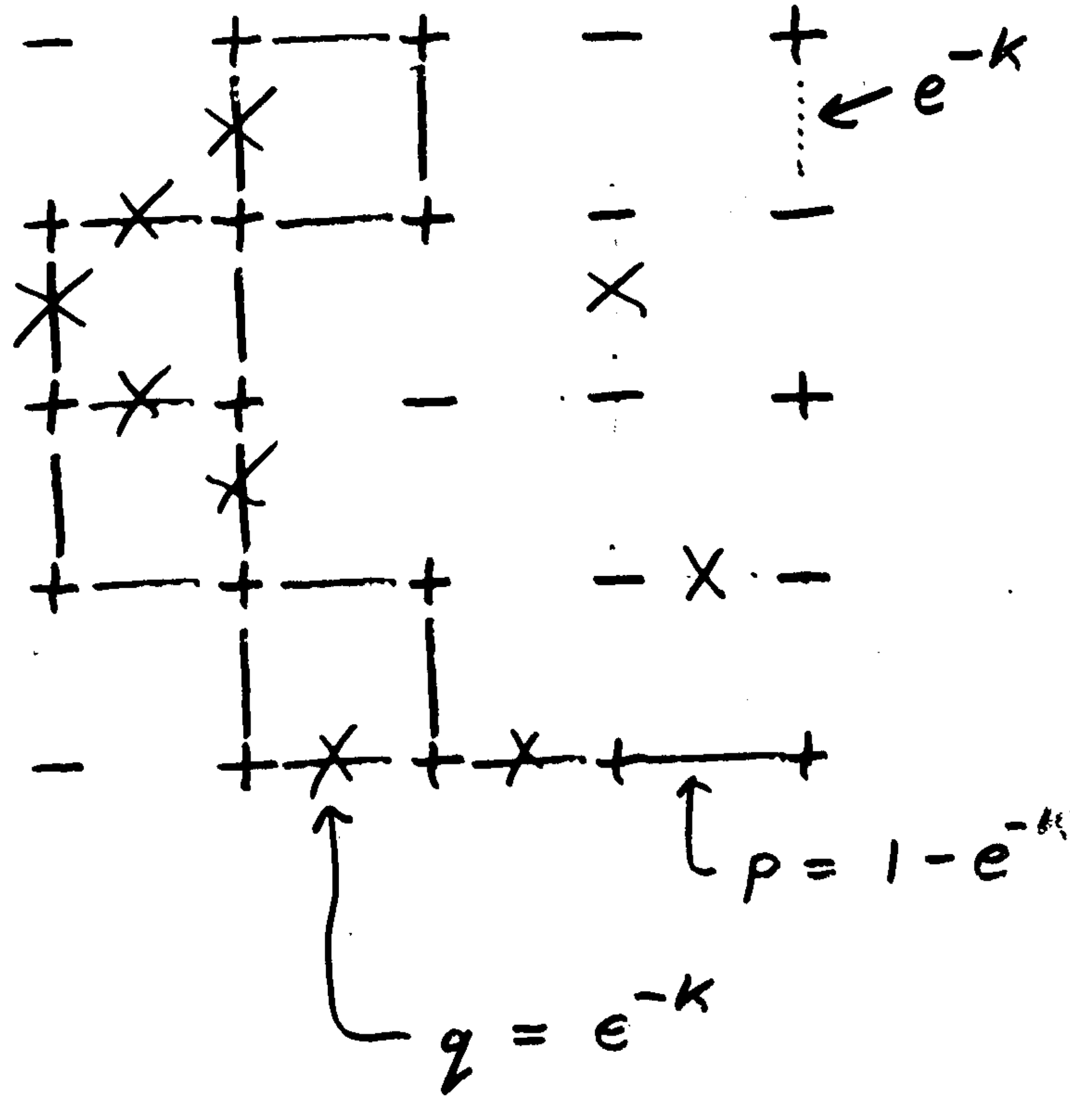
$$\chi = L^{-d} \left\langle \sum_n c_n^2 \right\rangle$$

−	+	+	−	+
+	+	+	−	−
+	+	−	−	+
+	+	+	−	−
−	+	+	+	+

Potts Clusters

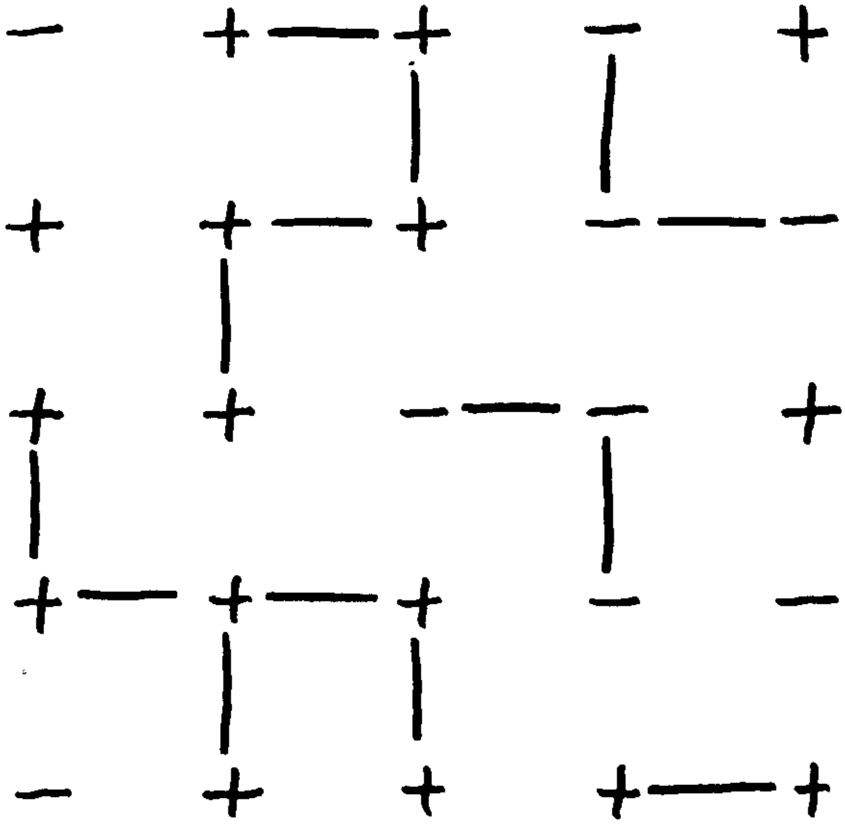


Potts Clusters

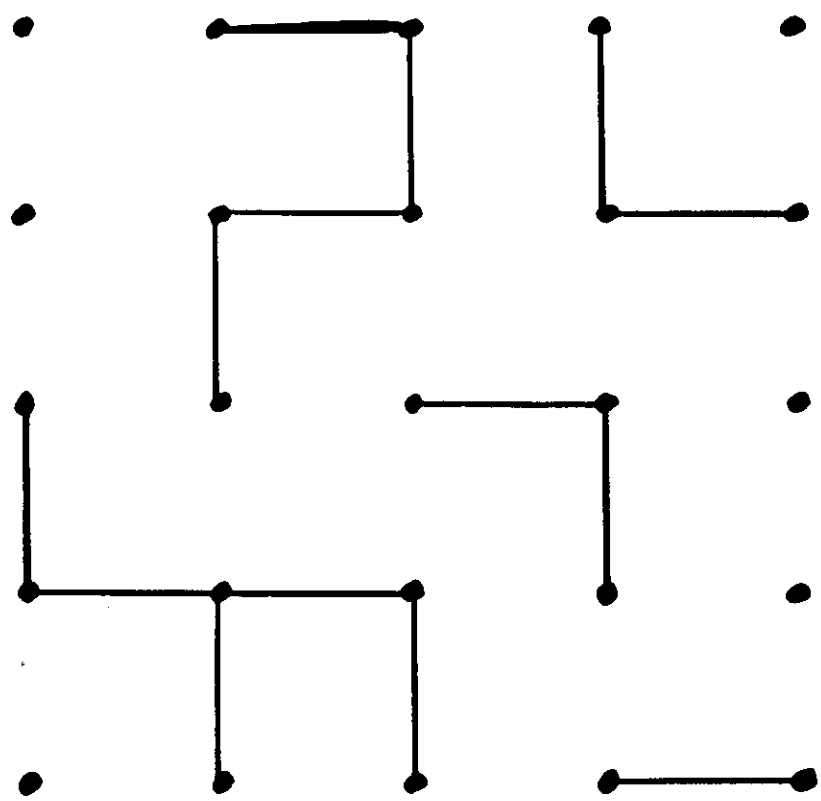


Site - Bond

Correlated Percolation



Percolation Clusters

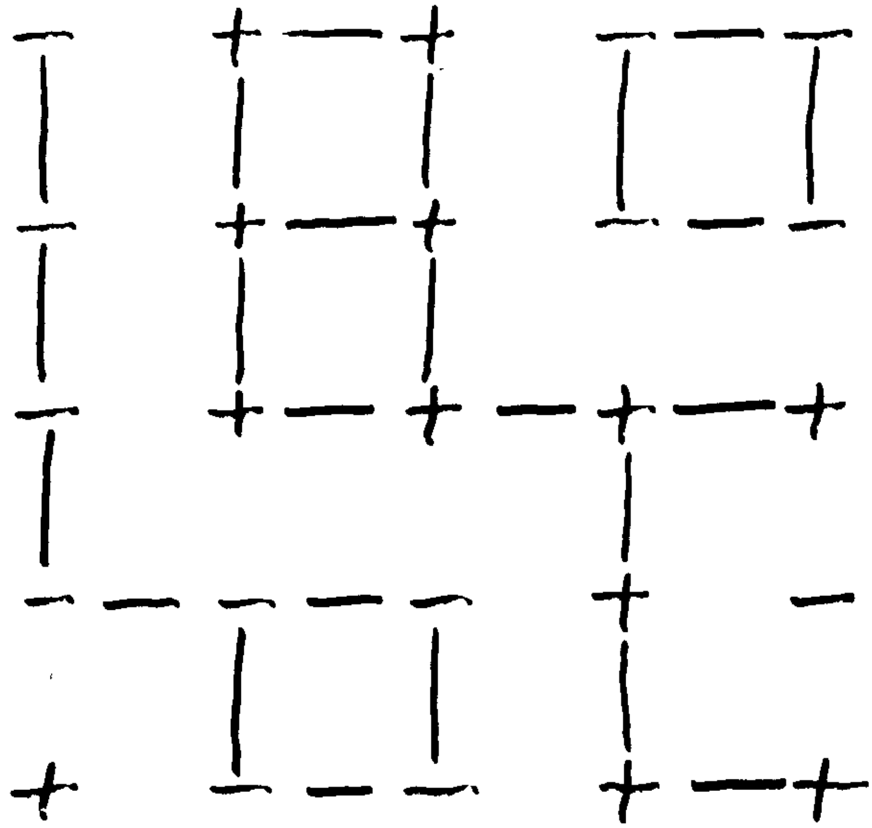


S = # of Potts states

$q = e^{-K} = 1 - p$

−	+	+	−	−
−	+	+	−	−
−	+	+	+	+
−	−	−	+	−
+	−	−	+	+

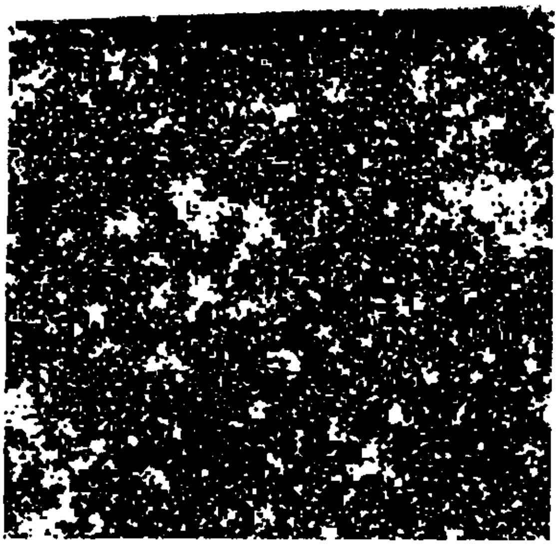
New Potts Clusters



Potts-
Percolation

256 x 256

$T = T_c$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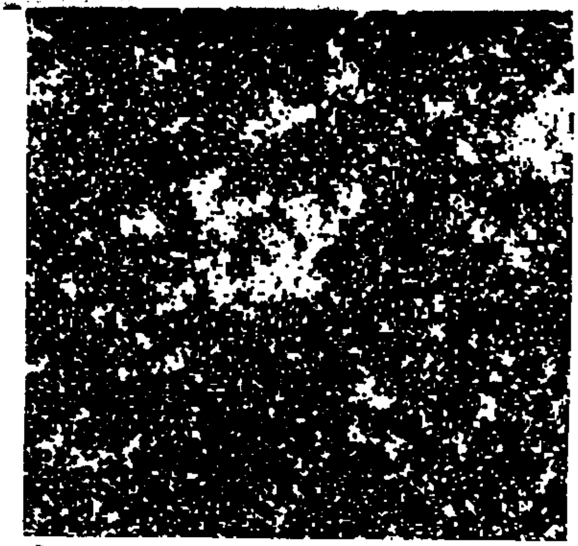
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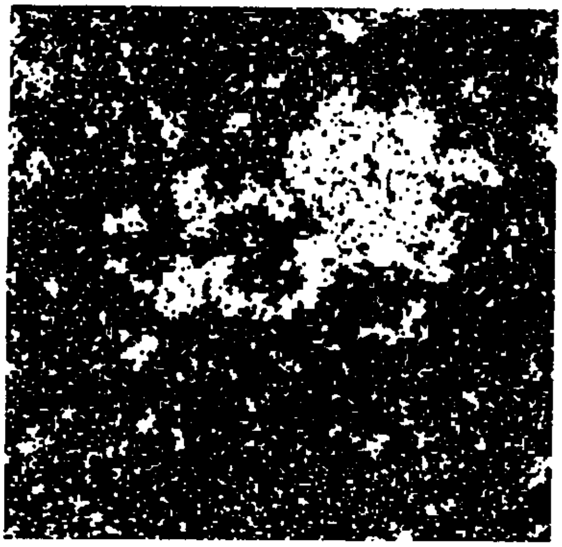
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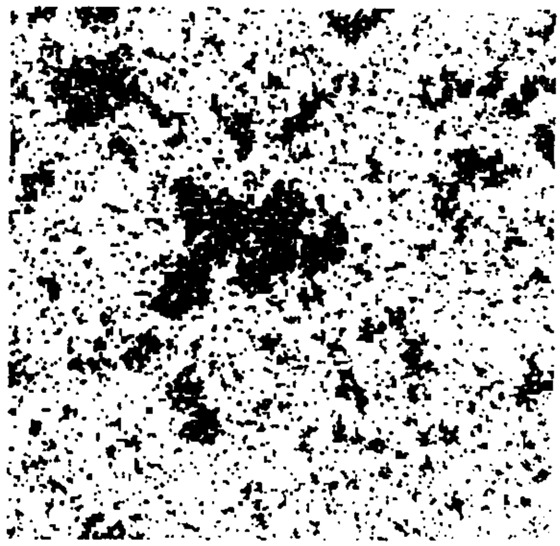
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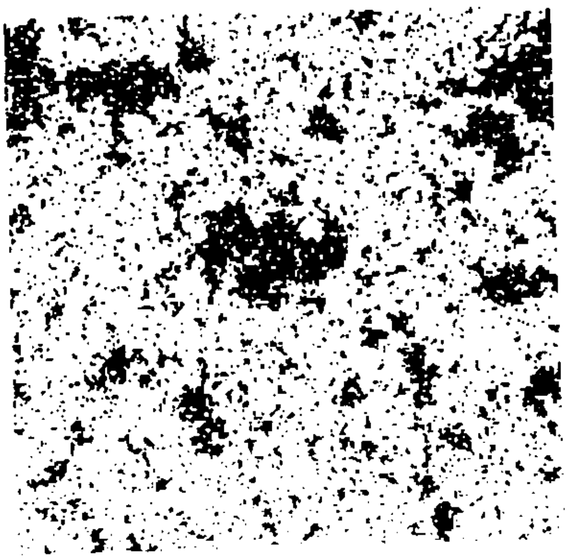
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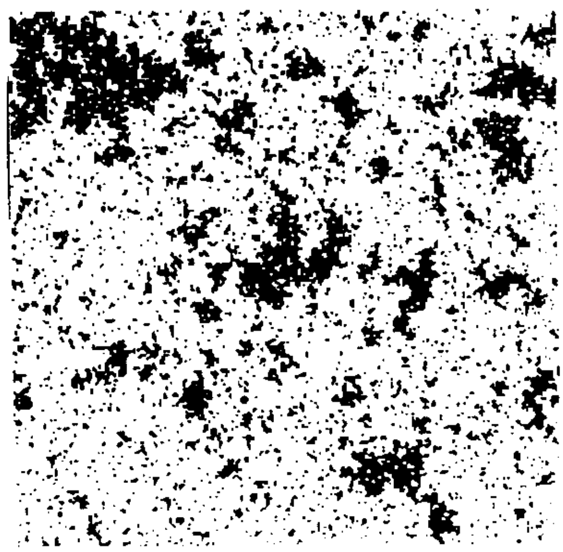
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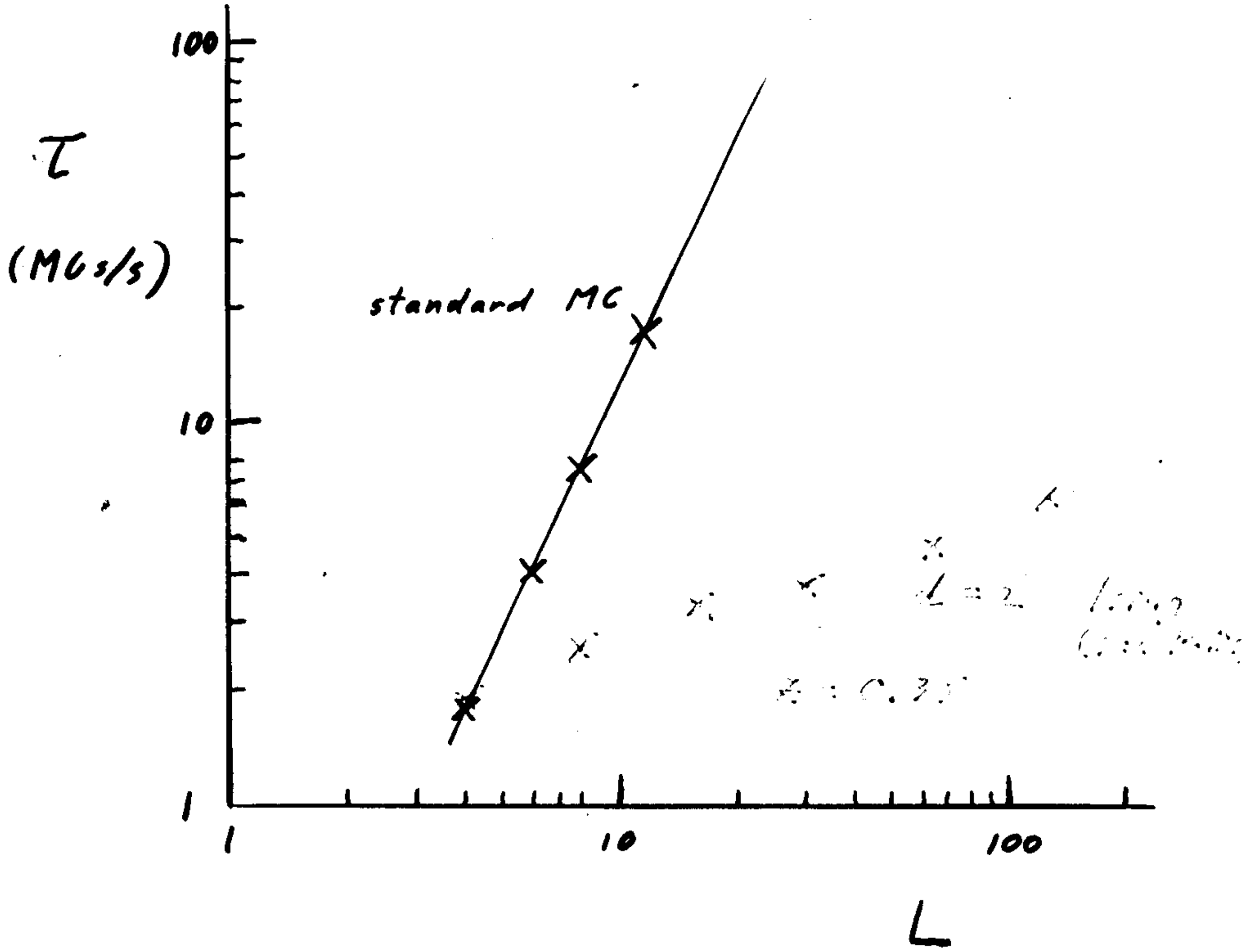
Critical Slowing Down

$$\tau \sim \xi^{z}$$

- For finite L, at $T = T_c$

$$\tau \sim L^{z}$$

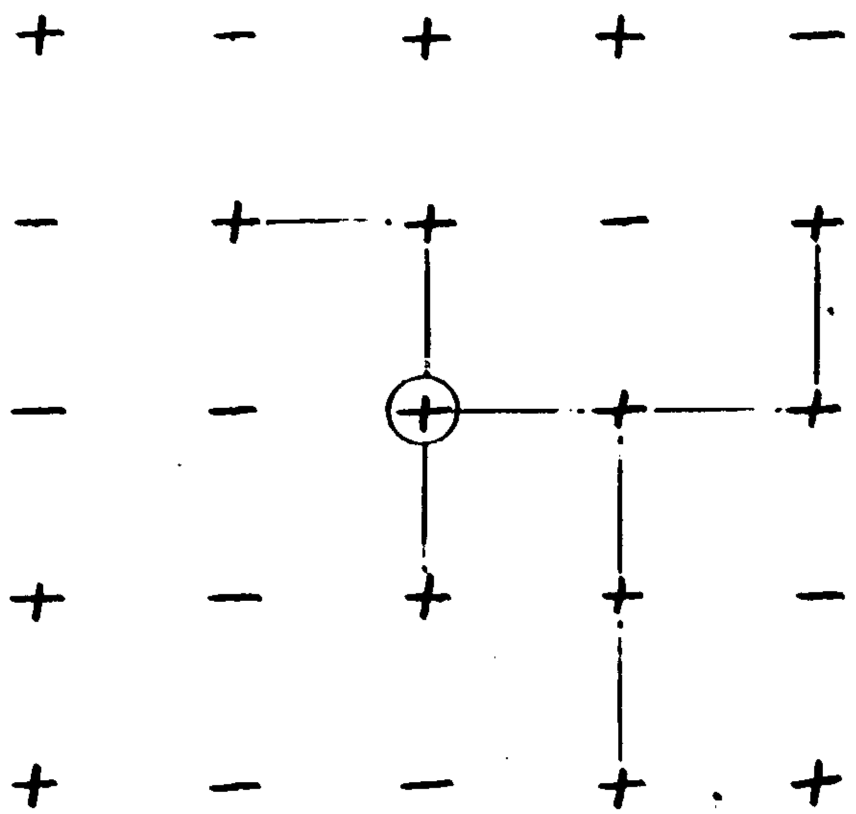
Correlation time vs. size



$N = L^d$

Single-Cluster Algorithm

U. Wolff

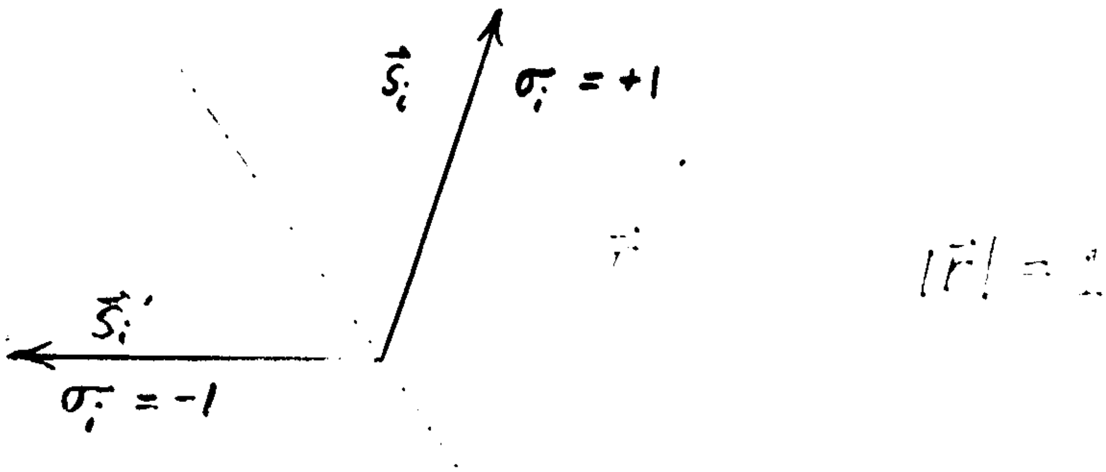


Embedded Ising Variables

U. Wolff

For O(n) models

Example: $\vec{s}_i = (s_{ix}, s_{iy})$, $|\vec{s}_i| = 1$



$$\vec{s}_i\,' = \vec{s}_i + (\sigma_i - 1)\,(\vec{r}\cdot\vec{s}_i)\,\vec{r}$$

Application to

Anti ferromagnet

$K < 0$

PROBLEM:

$$p = 1 - e^{-K} < 0$$

$$q = e^{-K} > 1$$

Ising Antiferromagnet

$$K < 0$$

$$e^{K} Z = \underset{\substack{\uparrow \\ p}}{(1 - e^{K})} Z^{\text{diff}}_{\langle \ell m \rangle} + \underset{\substack{\uparrow \\ 1-p}}{e^{K}} Z^{\text{IND}}_{\langle \ell m \rangle}$$

$1 - e^{K}$ = Probability of antibond

$\Rightarrow$ Anticlusters