Wang-Landau Sampling in Statistical Physics

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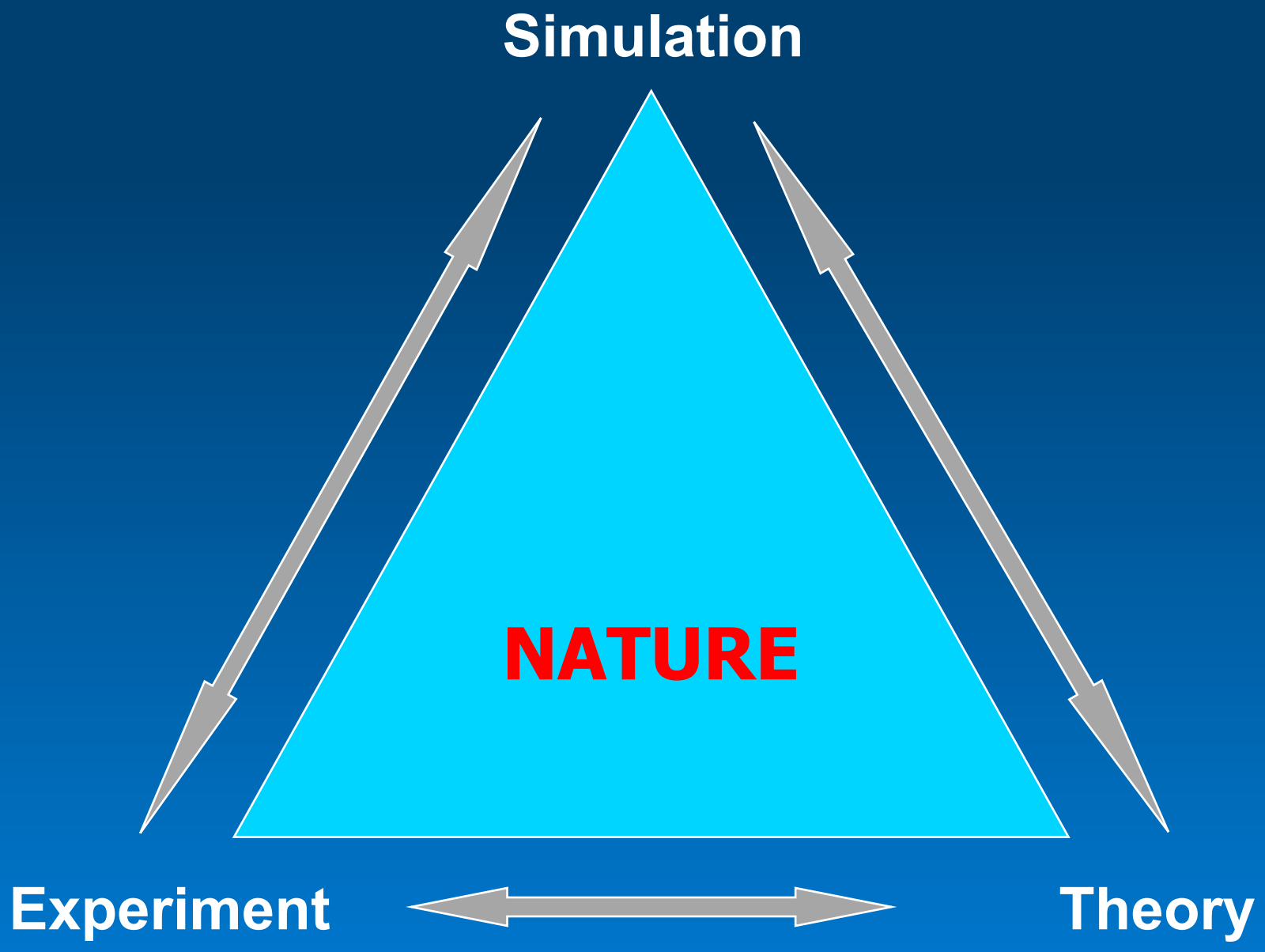
- **Introduction**
- **Basic Method**
- **Simple Applications** *(how well does it work?)*
  - ❑ ***2nd order transitions*** *– 2d Ising model*
  - ❑ ***1st Order transition*** *– 2d Potts Models*
  - ❑ ***Critical endpoint*** *- triangular Ising model*
- **Some Extensions**
- **Conclusions**

Introductory Comments

An understanding of materials behavior at non-zero temperature cannot be obtained solely from knowledge of $T=0$ properties.

For this we need to use statistical mechanics/ thermodynamics coupled with “knowledge” of the interatomic couplings and interactions with any external fields. This can be a very difficult problem!


Simulation
NATURE
Experiment
Theory

Reminder from Statistical Mechanics

The ***Partition function*** contains all thermodynamic information:

$$Z = \sum_{all\ \ states} e^{-\mathcal{H}/k_B T}$$

The probability of the n^{th} state appearing is:

$$P_n = \frac{1}{Z} e^{-\mathcal{H}/k_B T}$$

Thermodynamic properties are then determined from the free energy F where

$$F = -k_B T \ln Z$$

Reminder from Statistical Mechanics

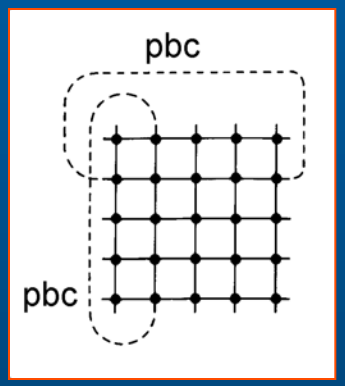
The ***Partition function*** contains all thermodynamic information:

$$Z = \sum_{all\ \ states} e^{-\mathcal{H}/k_B T}$$

Metropolis Monte Carlo approach: sample states via a random walk in probability space

The "fruit fly" of statistical physics: The Ising model

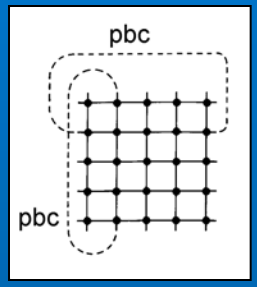
$$\mathcal{H} = -J \sum_{<i,j>} \sigma_i \sigma_j \,, \quad \sigma_i = \pm 1$$

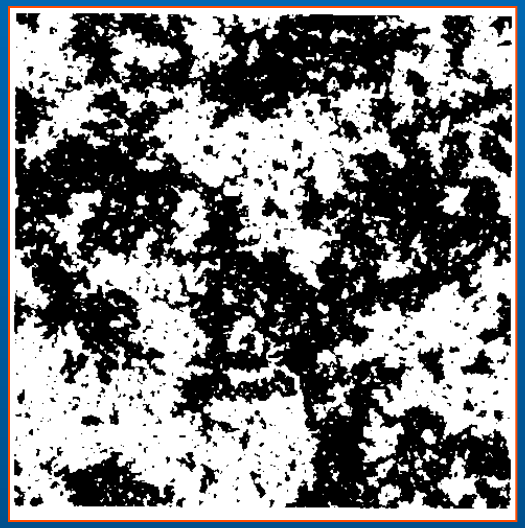


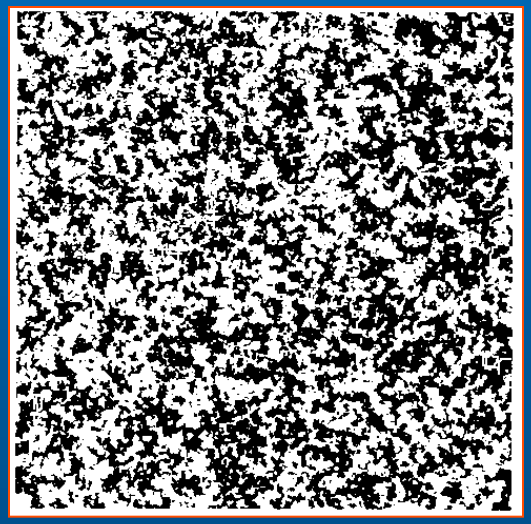
For a system of N spins have 2^N states!

Single Spin-Flip Monte Carlo Method

Typical spin configurations for the Ising square lattice with pbc

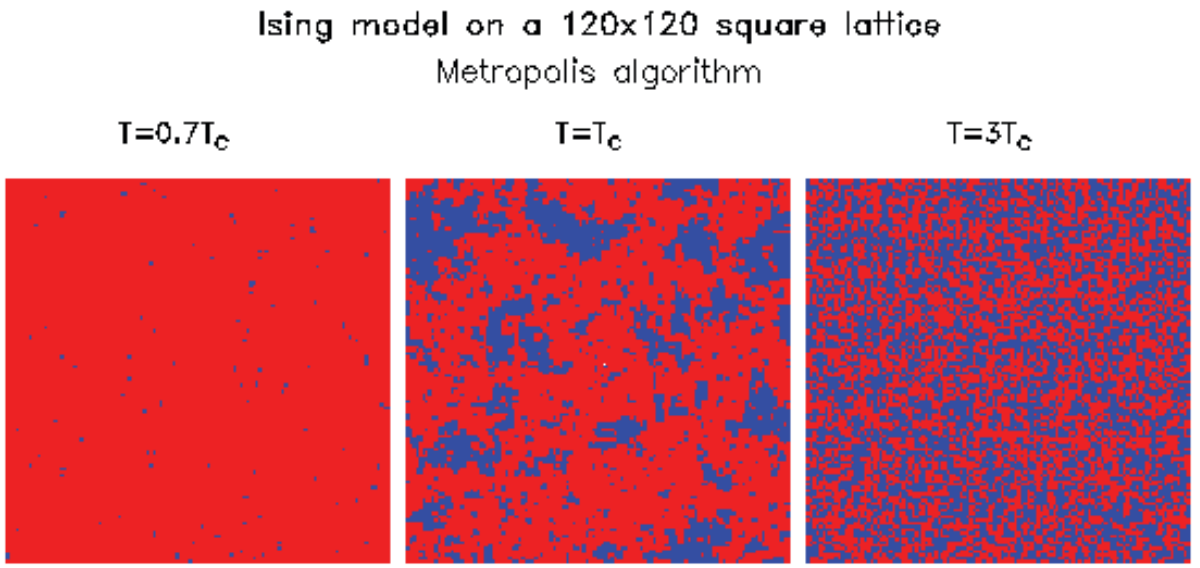






$T << T_c$ $T \sim T_c$ $T >> T_c$

Metropolis Monte Carlo simulations of the 2-dim Ising model



Single spin-flip sampling for the Ising model

Produce the n^{th} state from the m^{th} state … relative probability is $P_n/P_m \rightarrow$ need only the *energy difference*, *i.e.* $\Delta E = (E_n - E_m)$ between the states

Any transition rate that satisfies ***detailed balance*** is acceptable, usually the Metropolis form *(Metropolis et al, 1953).*

$$W(m \rightarrow n) = \tau_o^{-1} \exp(-\Delta E/k_B T), \quad \Delta E > 0$$
$$= \tau_o^{-1}, \quad \Delta E < 0$$

where τ_o *is the time required to attempt a spin-flip.*

Metropolis Recipe:

1. Choose an initial state
2. Choose a site i
3. Calculate the energy change ΔE that results if the spin at site i is overturned
4. Generate a random number r such that $0 < r < 1$
5. If $r < exp(-\Delta E/k_B T)$, flip the spin
6. Go to 2.

This is not a unique solution. An alternative *(Glauber, 1963):*

$$W_{n \to m} = \tau_o^{-1} [1 + \sigma_i \tanh (E_i / k_B T)],$$

where $\sigma_i E_i$ is the energy of the i^{th} spin in state n.

Both Glauber and Metropolis algorithms are special cases of a general transition rate *(Müller-Krumbhaar and Binder, 1973)*

Correlation times

Define an equilibrium relaxation function $\phi(t)$

$$\phi_{MM}(t) = \frac{<(M(0)M(t)> - <M>^2}{<M^2> - <M>^2}$$

$$\xrightarrow[t\to\infty]{} e^{-t/\tau}$$

and

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

i.e. τ ***diverges*** at T_c !

Problems and Challenges

Statics: **Monte Carlo methods are valuable, but near T_c**

$\Rightarrow$ ***critical slowing down*** **for** 2^{nd} ***order*** **transitions**

$\Rightarrow$ ***metastability*** **for** 1^{st} ***order*** **transitions**

$\therefore$ ***Try to reduce characteristic time scales or circumvent them***

"Dynamics": **stochastic vs deterministic**

Multicanonical Sampling

The canonical probability $P(E)$ may contain multiple maxima, widely spaced in configuration space (e.g. *1st order phase transition, etc.*)

$\Rightarrow$ Standard methods become "trapped" near one maximum; infrequent transitions between maxima leads to poor relative weights of the maxima and the minima of $P(E)$.

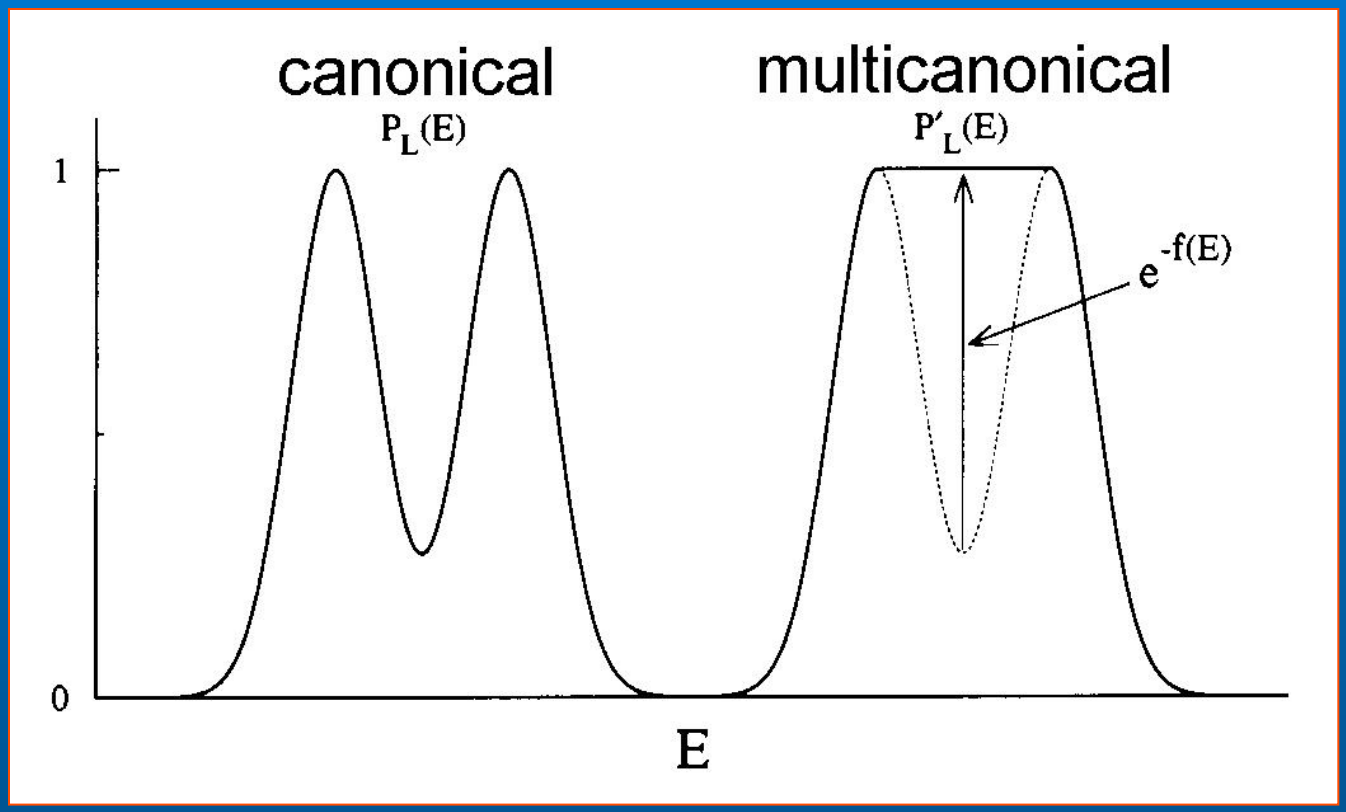
$\therefore$ modify the single spin flip probability to enhance the probability of the "unlikely" states between the maxima $\Rightarrow$ accelerates effective sampling!

Reformulate the problem $\Rightarrow$ an effective Hamiltonian

$$\mathcal{H}_{eff}(\sigma) = \mathcal{H}_{eff}(\beta\,\mathcal{H}(\sigma))$$

Berg and Neuhaus (1991)

Compare ensembles:

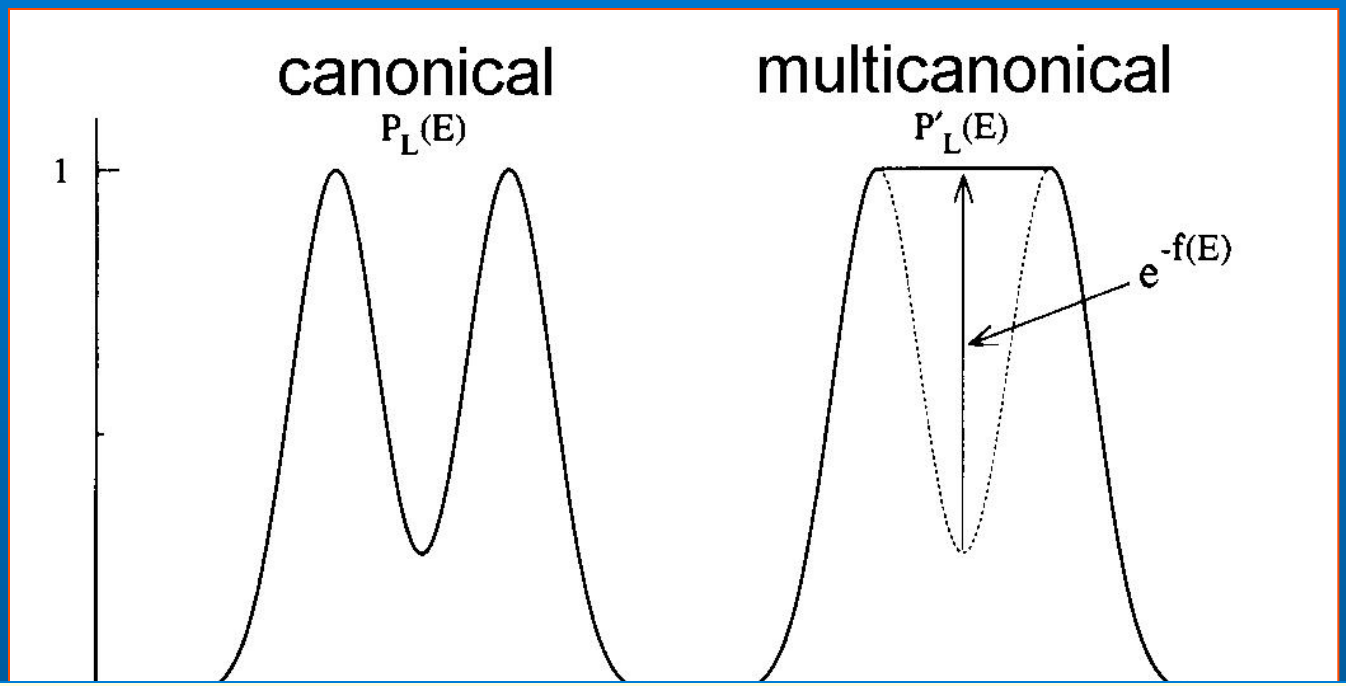


Then,

$$\langle A \rangle_\beta = \frac{\langle A \exp(\mathcal{H}_{eff} - \mathcal{H}) \rangle}{\langle \exp(\mathcal{H}_{eff} - \mathcal{H}) \rangle}$$

Thermodynamic variable

Compare ensembles:



But, finding $\mathcal{H}_{eff}$ isn't easy

Then,

$$\langle A \rangle_\beta = \frac{\langle A \exp(\mathcal{H}_{eff} - \mathcal{H}) \rangle}{\langle \exp(\mathcal{H}_{eff} - \mathcal{H}) \rangle}$$

Thermodynamic variable

Parallel tempering (replica exchange)

Create multiple systems at different T_i

T_1 T_2 T_3 T_4 T_5 . . .

Define $\beta_i = 1/T_i$

Hukushima and Nemoto (1996); Swendsen and Wang (1986)

Parallel tempering (replica exchange)

Create multiple systems at different T_i

T_1 T_2 T_3 T_4 T_5 . . .

Define $\beta_i = 1/T_i$

- Simulate all systems simultaneously

Hukushima and Nemoto (1996); Swendsen and Wang (1986)

Parallel tempering (replica exchange)

Create multiple systems at different T_i

Define $\beta_i = 1/\mathrm{T}_i$

- Simulate all systems simultaneously
- At regular intervals interchange configurations at neighboring T with probability P given by:

$$P = \exp\left[\left(\beta_i - \beta_{i-1}\right)\left(E_i - E_{i-1}\right)\right]$$

Energy of state i

Parallel tempering (replica exchange)

Create multiple systems at different T_i

Define $\beta_i = 1/\mathrm{T}_i$

But, the T_i must be chosen carefully

neighboring T with probability P given by:

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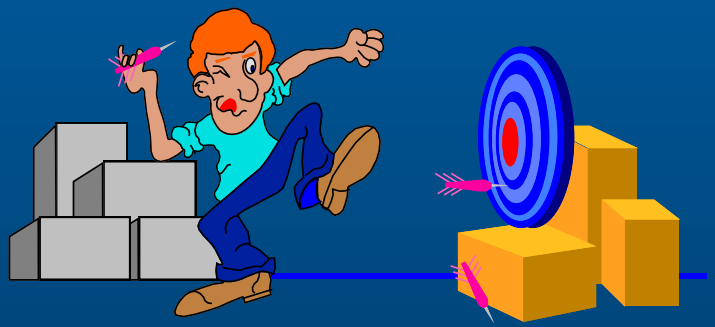
Energy of state i

Types of Computer Simulations

Deterministic methods . . . (Molecular dynamics)

Stochastic methods . . . (*Monte Carlo*)



Perspective:

Monte Carlo for the masses

REPRINTED FROM RISK JUNE 2000

Can a mathematical modelling technique first introduced to finance by derivatives traders make a difference to retail investors? Two recent initiatives, one by JP Morgan and the other by start-up venture Financial Engines, are the latest wave in a growing movement to popularise Monte Carlo, which was invented by the American atom bomb scientist John von Neumann during World War II.

JP Morgan's Morgan Online is the more "upmarket" of the two initiatives. According to co-head of Morgan Advice Lab Ashvin Chhabra, it is aimed at tech-literate new economy employees with $1 million in assets – a level of wealth that excludes them from traditional private banking services. Clients are charged $2,500 a year, and in addition to portfolio modelling, they can access JP Morgan research reports and use the firm's brokerage services.

Morgan Online's "expert system" quizzes users on different goals such as retirement, children's education and luxury expenditure, then uses multi-variate Monte Carlo to optimise these goals simultaneously over time. Clients see the results in terms of a wealth projection over time, together with the probability of meeting their goals.

Morgan Online says it will try to ensure that client goals are achieved by dispensing buy and sell asset allocation recommendations via e-mail. But what if a client's chosen goal resembled the payout of an option contract? Chhabra concedes that in this case, his system's buy and sell recommendations could potentially amount to a delta hedging strategy that replicated that contract.

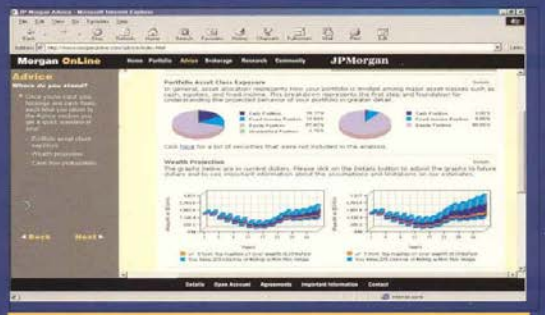
This closely resembles the so-called life options idea of Harvard economist Robert Merton, whereby complex long-term financial needs of individuals would be met by tailored derivatives contracts. Merton – who has an exclusive consulting relationship with JP Morgan – is now helping Chhabra develop this idea.

Silicon Valley-based Financial Engines says that it wants to cater for US citizens with a savings account or mutual fund. Fees are $15 a quarter for the advice-only service, which is the brainchild of Stanford University economist Bill Sharpe. Once users enter their details, they are treated to an animated graphic depicting the Monte Carlo process for their portfolio, creating a probability distribution for their retirement income.

Monte Carlo was introduced to finance by the University of Waterloo's Phelim Boyle, who wrote an influential paper on option pricing in 1977. Boyle proposed using a randomly generated sample of asset price histories to calculate options value. His idea was not immediately adopted, because using a computer to do simulations was very time-consuming. Today, Monte Carlo is the standard tool for options pricing desks worldwide.

During the 1990s, Monte Carlo was adapted by institutional asset managers to model investment portfolios and high net worth individual accounts. More recently, software packages have been developed that allow independent financial advisers to use it as well. ■

Nicholas Dunbar



Above: A screenshot of the Morgan Online Web site, showing Monte Carlo–generated wealth projection charts.

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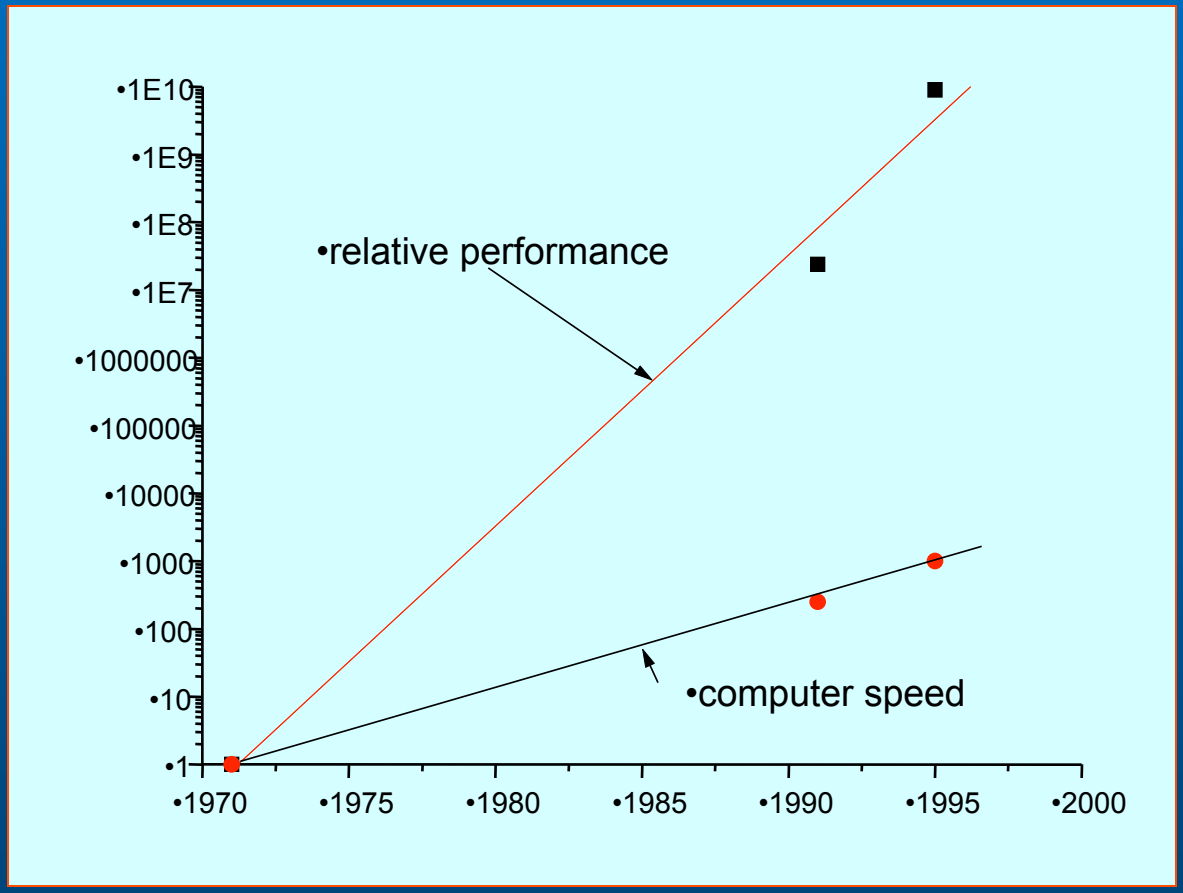
JUNE 2000

Improvements in Performance (Ising model):

- Computer speed
- Algorithmic advances - cluster flipping, reweighting . . .



The "Random Walk in Energy Space with a Flat Histogram" method

or

"Wang-Landau sampling"

A Quite Different Approach

Random Walk in Energy Space with a Flat Histogram

Reminder:

$$Z = \sum_{\substack{all \\ states}} e^{-\mathcal{H}/k_B T} \equiv \sum_{\substack{all \\ energies}} g(E)\, e^{-\mathcal{H}/k_B T}$$

Estimate the *density of states* $g(E)$ directly — how?

1. Set $g(E)=1$; choose a modification factor (e.g. $f_0 = e^1$)
2. Randomly flip a spin with probability: $p(E_1 \rightarrow E_2) = \min\left(\frac{g(E_1)}{g(E_2)}, 1\right)$
3. Set $g(E_i) \rightarrow g(E_i) * f$
   $H(E) \rightarrow H(E)+1$ (histogram)
4. Continue until the histogram is "flat"; decrease f, e.g. $f_{i+1} = f^{1/2}$
5. Repeat steps 2 - 4 until $f = f_{min} \sim \exp(10^{-8})$
6. Calculate properties using final density of states $g(E)$

How can we test the method?

For a *2nd order* transition, study the 2-dim Ising model:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j , \quad \sigma_i = \pm 1$$

- T_c is known for an infinite system *(Onsager)*
- Bulk properties are known
- $g(E)$ is known exactly for small systems

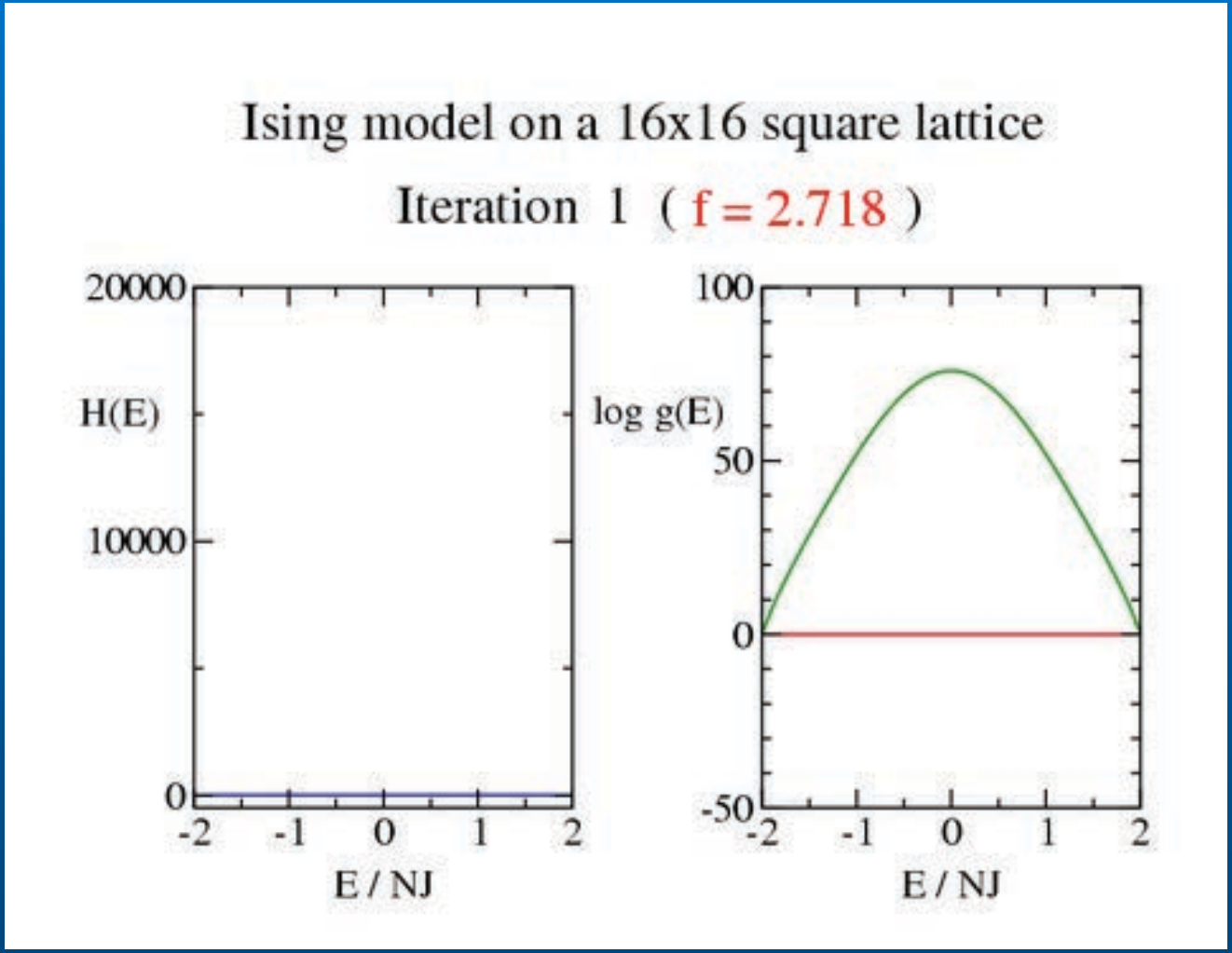
For a *1st order* transition, study the 2-dim Potts model:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j} , \quad \sigma_i = 1, \ldots, q$$

for $q=10$

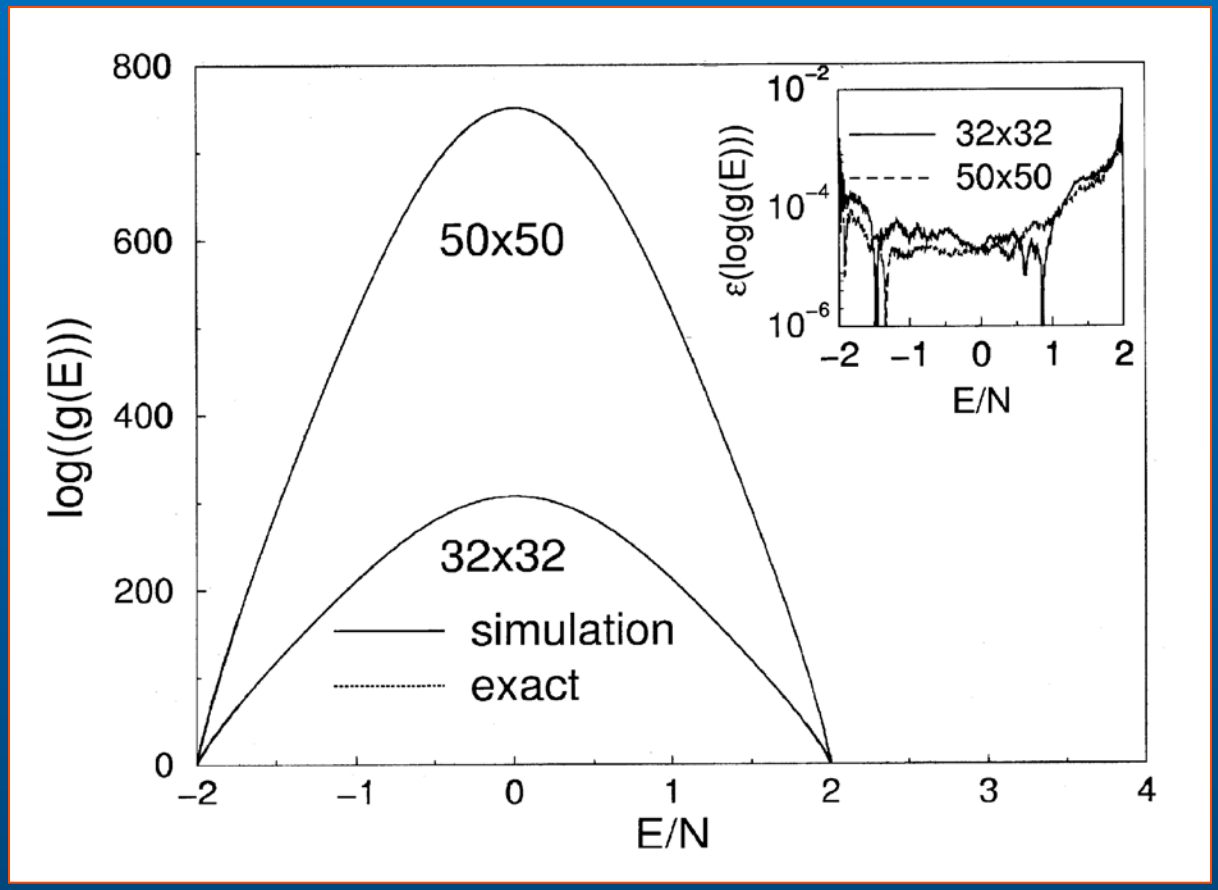
- T_c is known for an infinite system *(duality)*
- Good numerical values exist for many quantities

Demo: Wang-Landau Sampling for the 2-dim Ising model



Density of States for the 2-dim Ising model

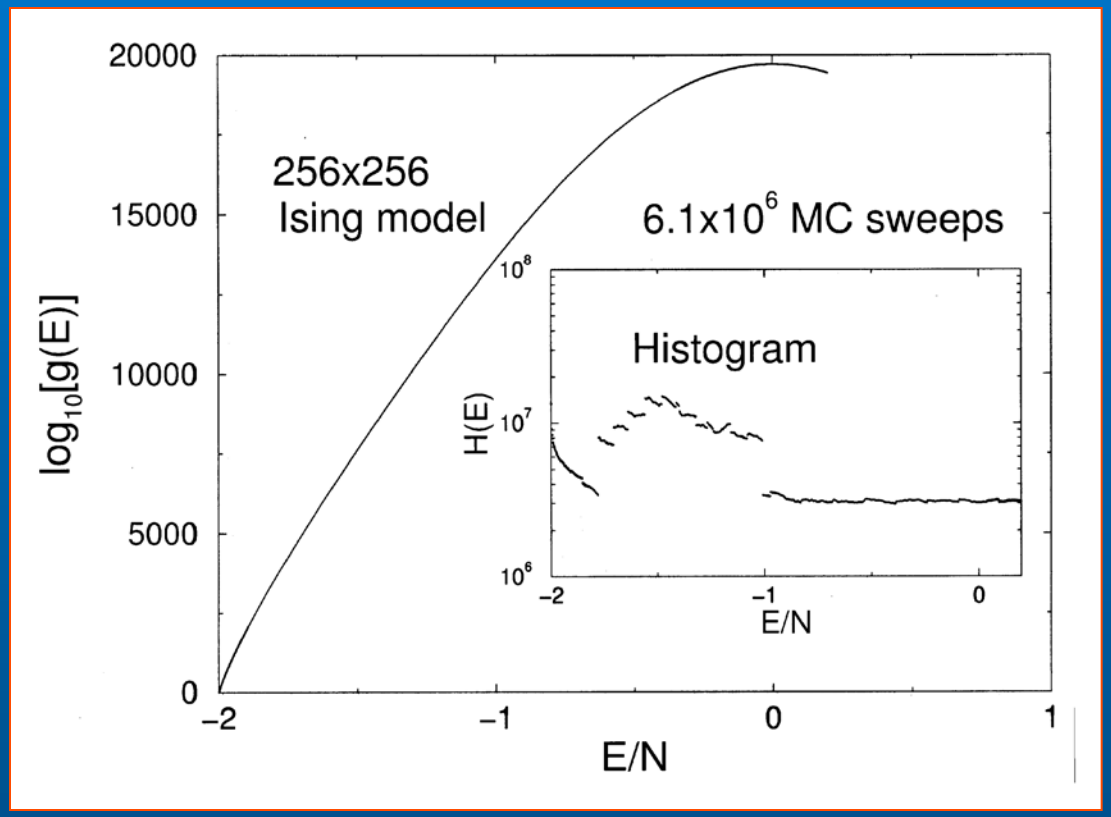
Compare exact results with data from random walks in energy space: *L× L lattices with periodic boundaries*



ε = relative error (*exact solution is known for L≤ 64*)

Density of States: Large 2-dim Ising Model

➢ *use a parallel, multi-range random walk*

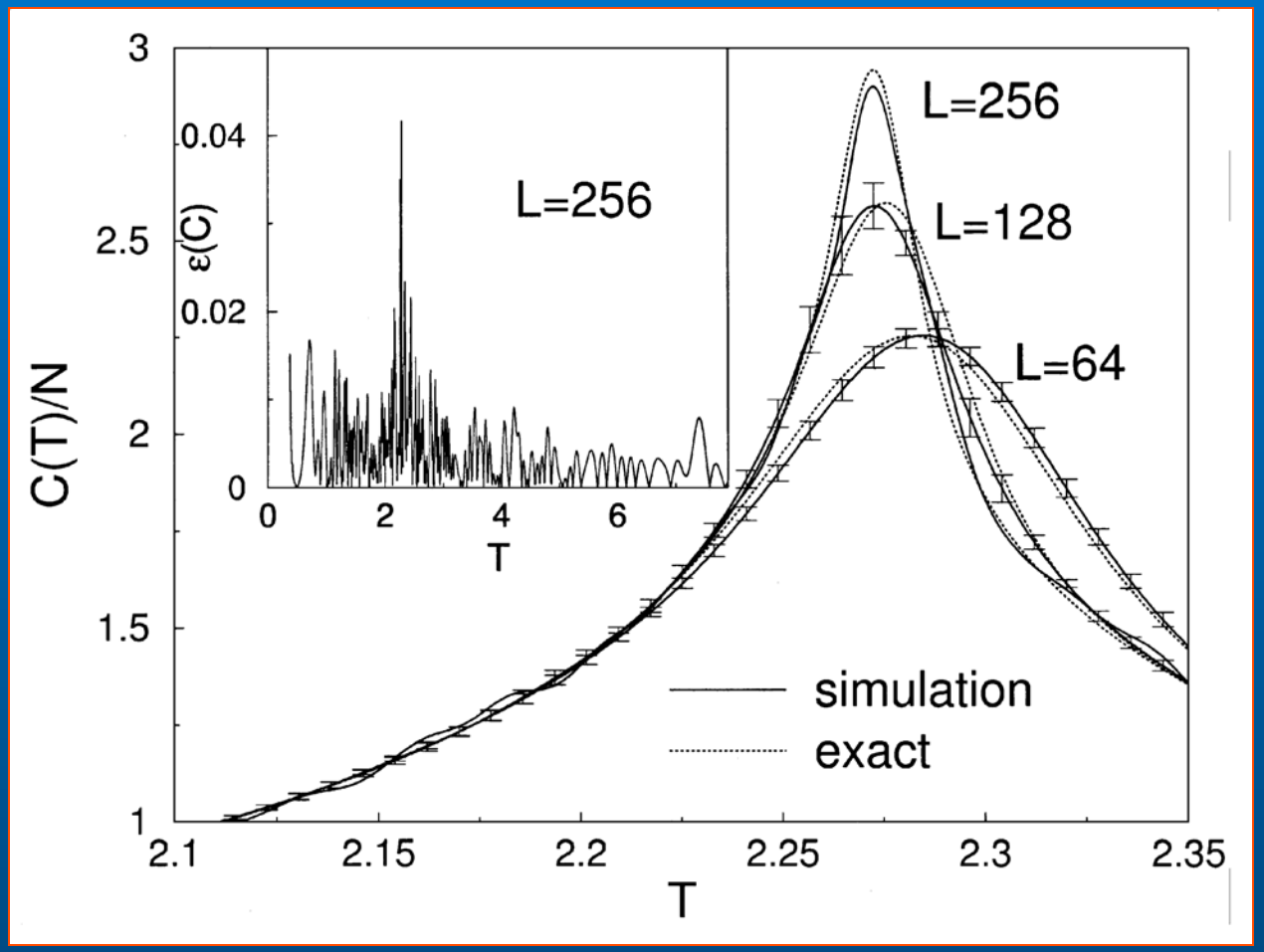


NO exact solution is available for comparison!

Question:

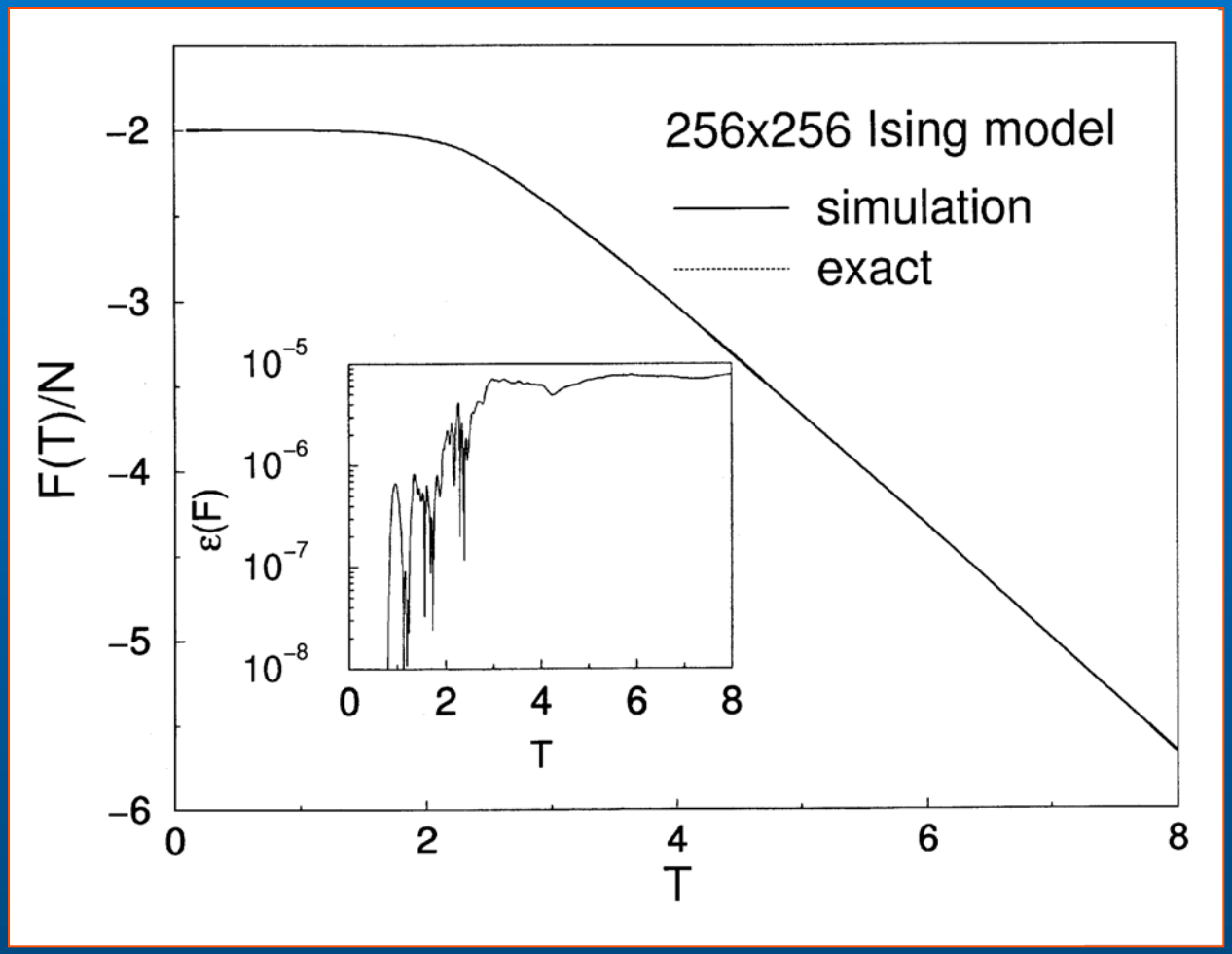
- Need to perform a random walk over ALL energies?

Specific Heat of the 2-dim Ising Model



ε = relative error

Free Energy of the 2-dim Ising Model



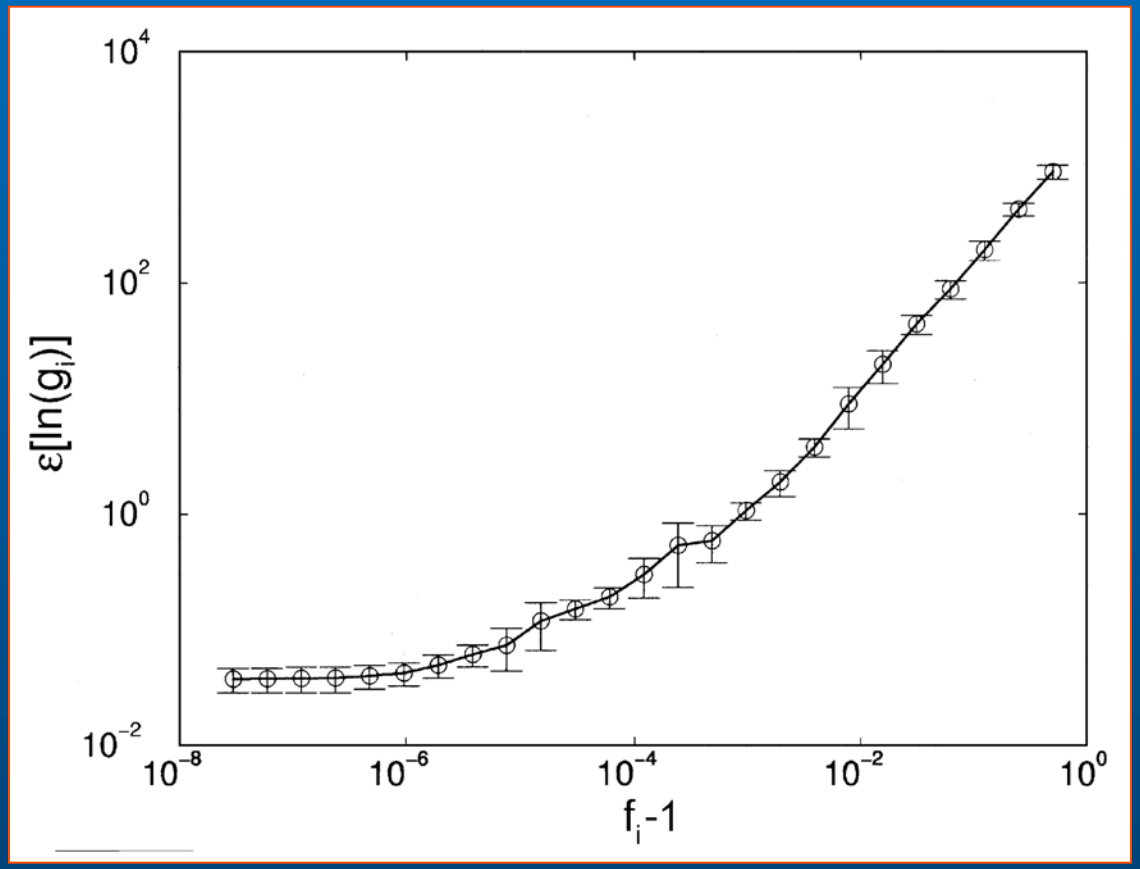
ε = relative error

How Does f_i Affect the Accuracy?

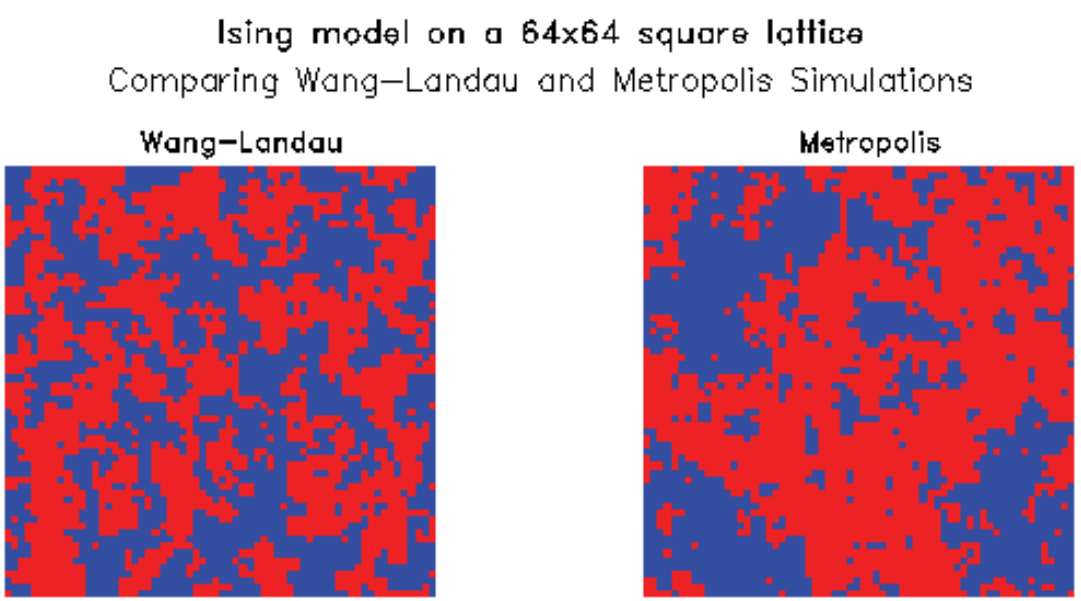
Data for *L*=32:

$$\varepsilon\left[\ln\left(g_i\right)\right] = \frac{1}{N_E}\sum_E \left|\ln\left[g_i(E)\right] - \ln\left[g^{exact}(E)\right]\right|$$

error



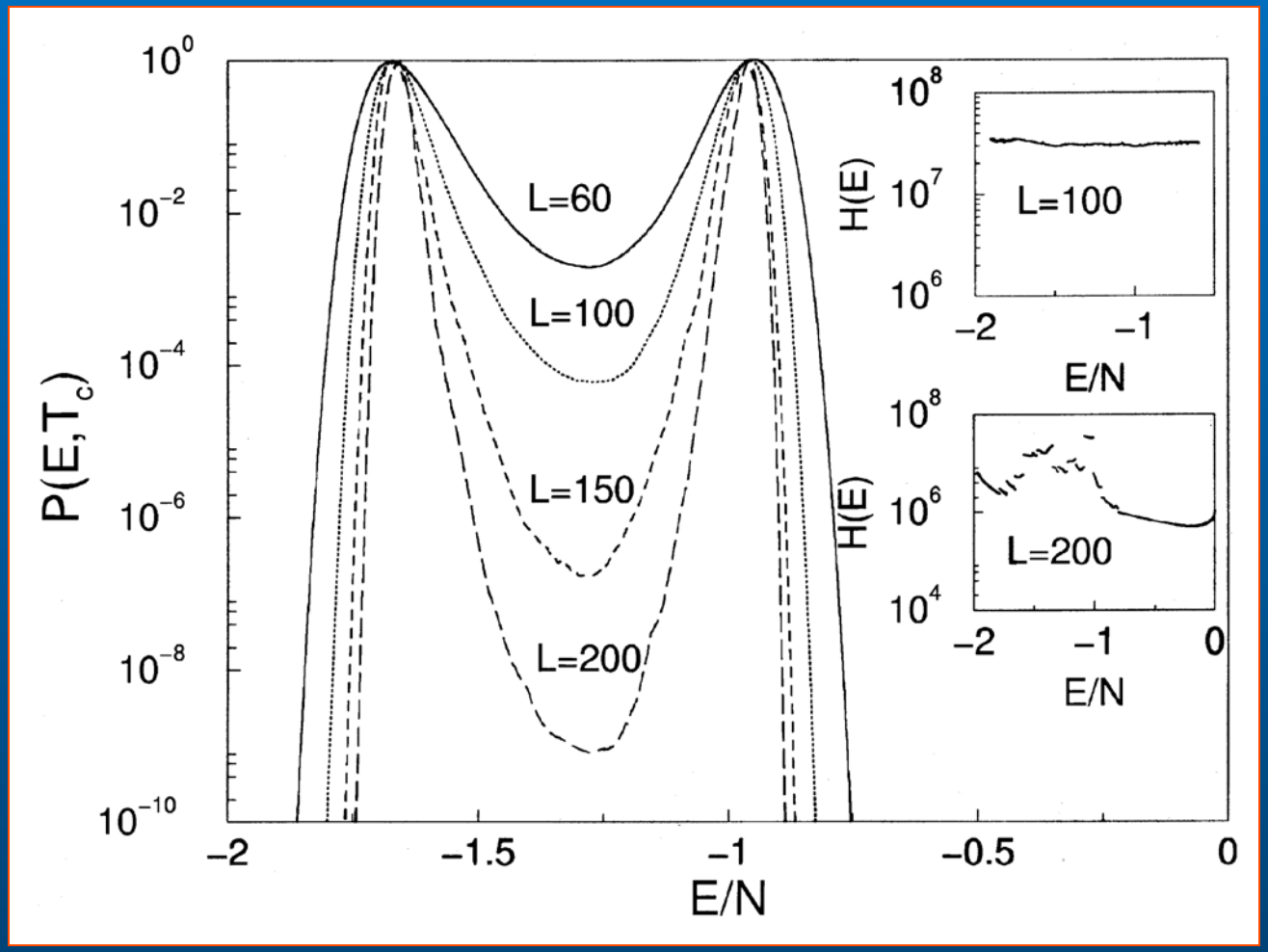
Compare Sampling in the 2-dim Ising Model



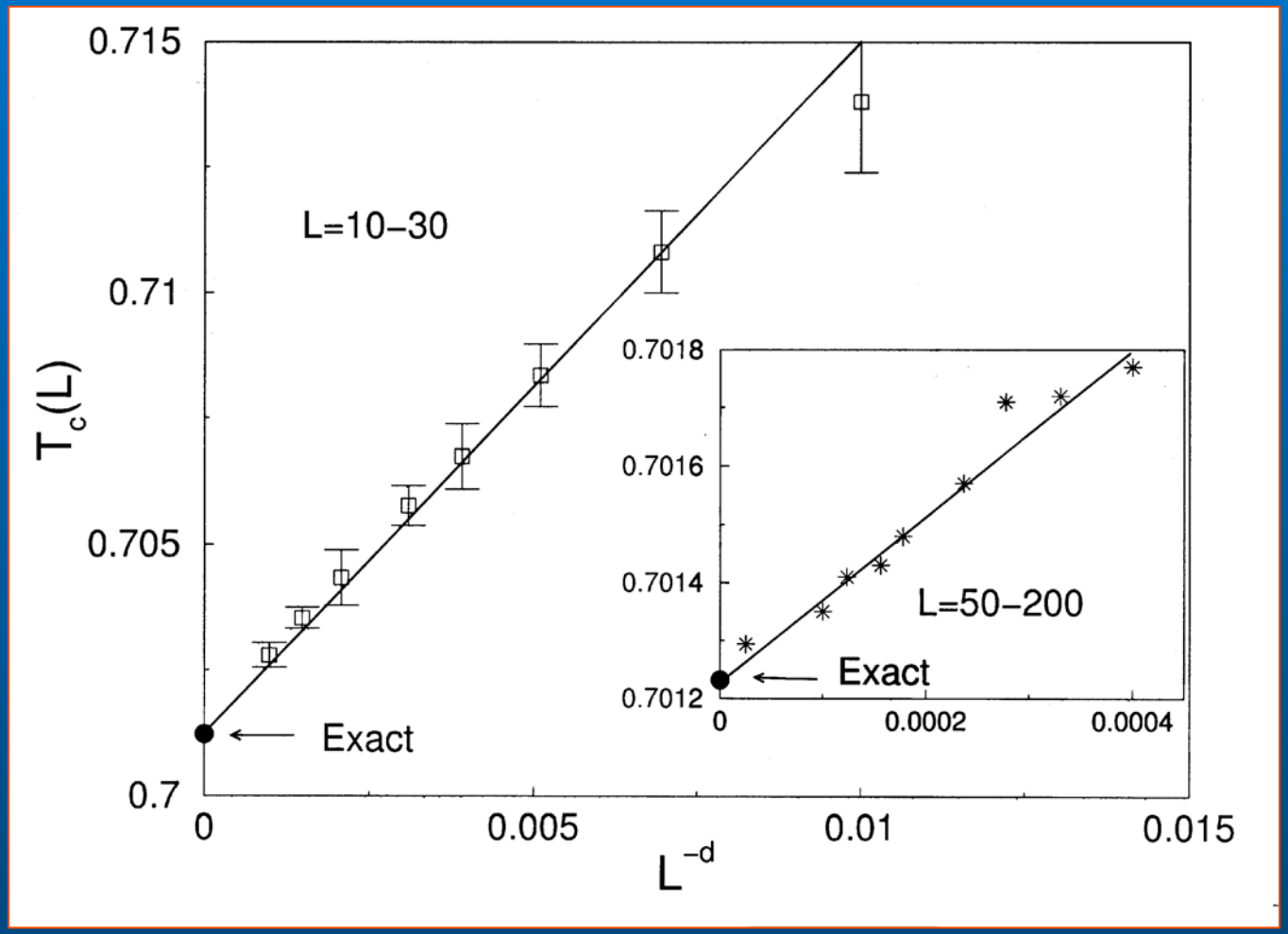
What About a 1st Order Transition?

Look at the q=10 Potts model in 2-dim

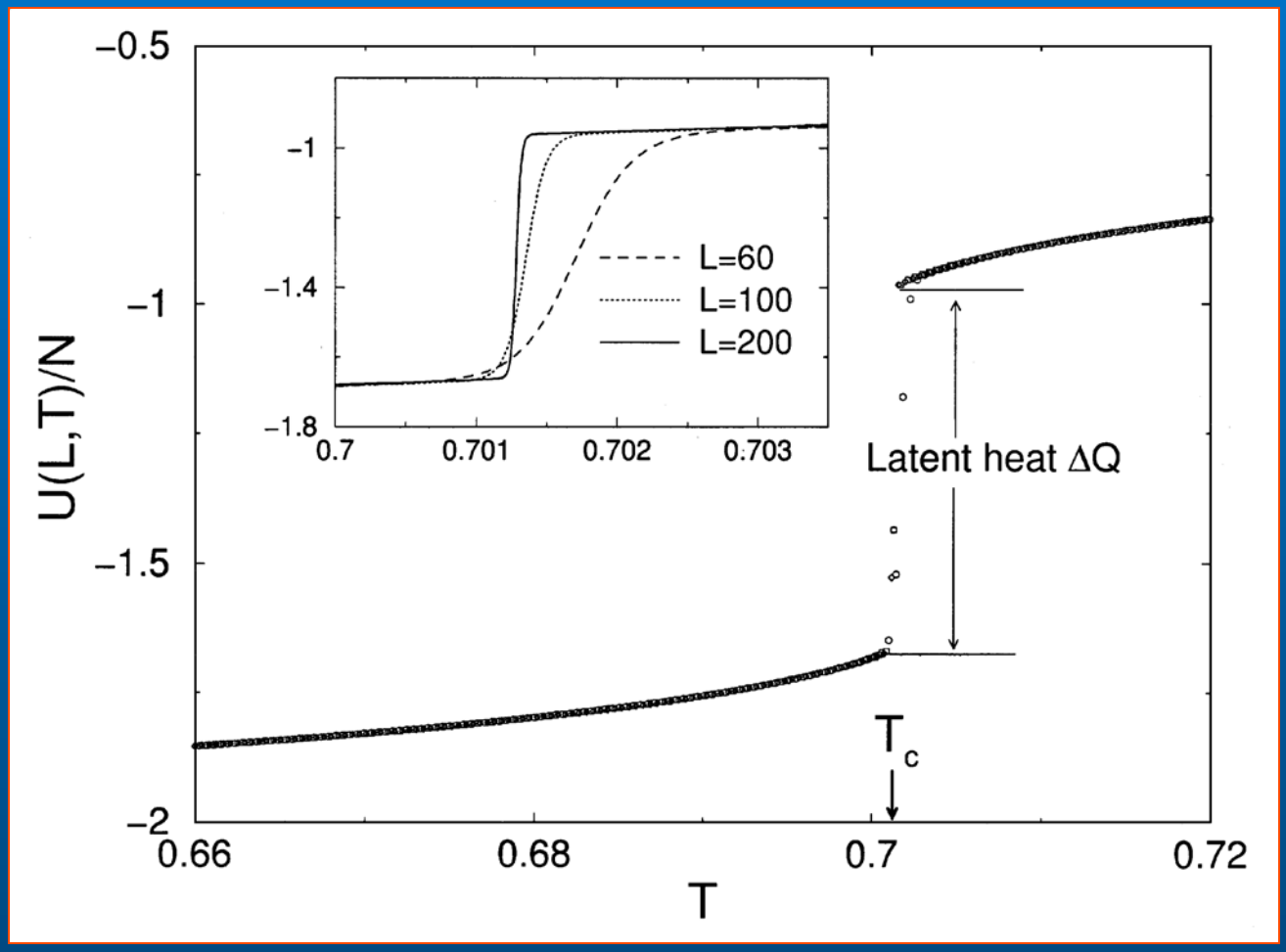
At T_c *coexisting states* are separated by an energy barrier



q=10 Potts Model: Determine T_c



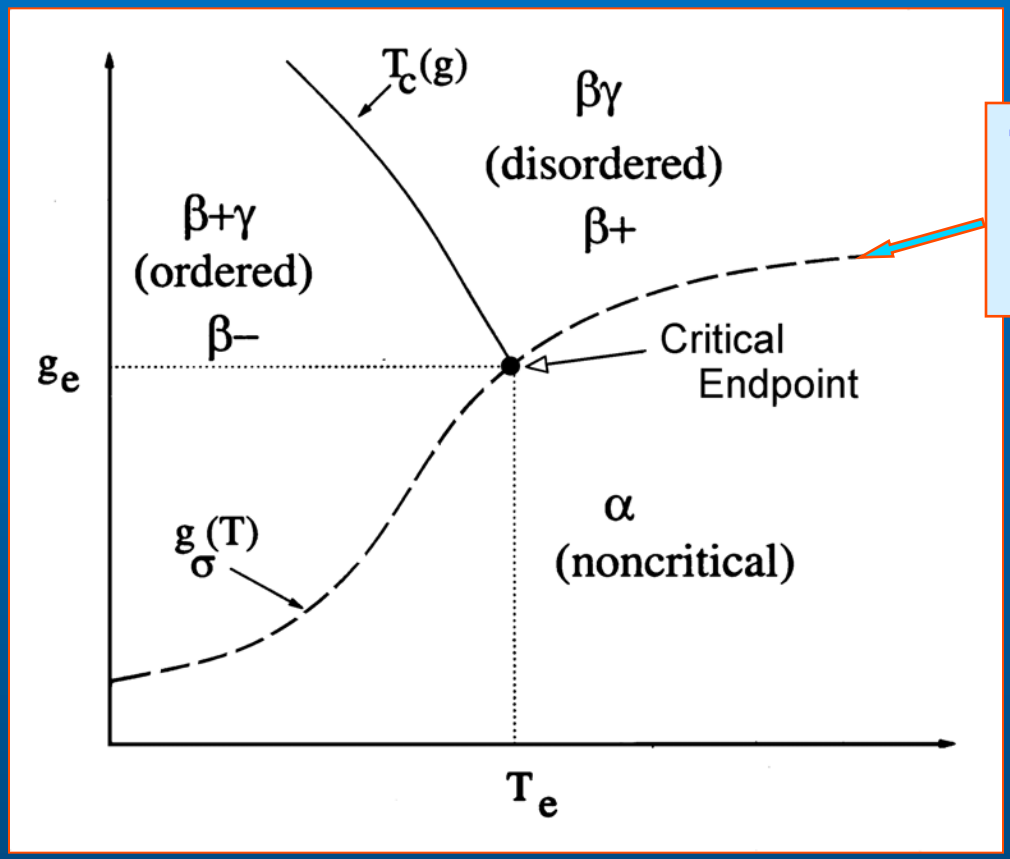
q=10 Potts Model: Internal Energy



A "new" old problem: A Critical Endpoint*

A schematic view: T is temperature; g is a non-ordering field

Theory predicts new singularities at (g_e, T_e) (Fisher and Upton, 1990)



*Historical note, this behavior was described but not given a name in:
H. W. B. Roozeboom and E. H. Büchner, Proceedings of the Koninklijke Academie der Wetenschappen (1905); The Collected Works of J. W. Gibbs (1906).

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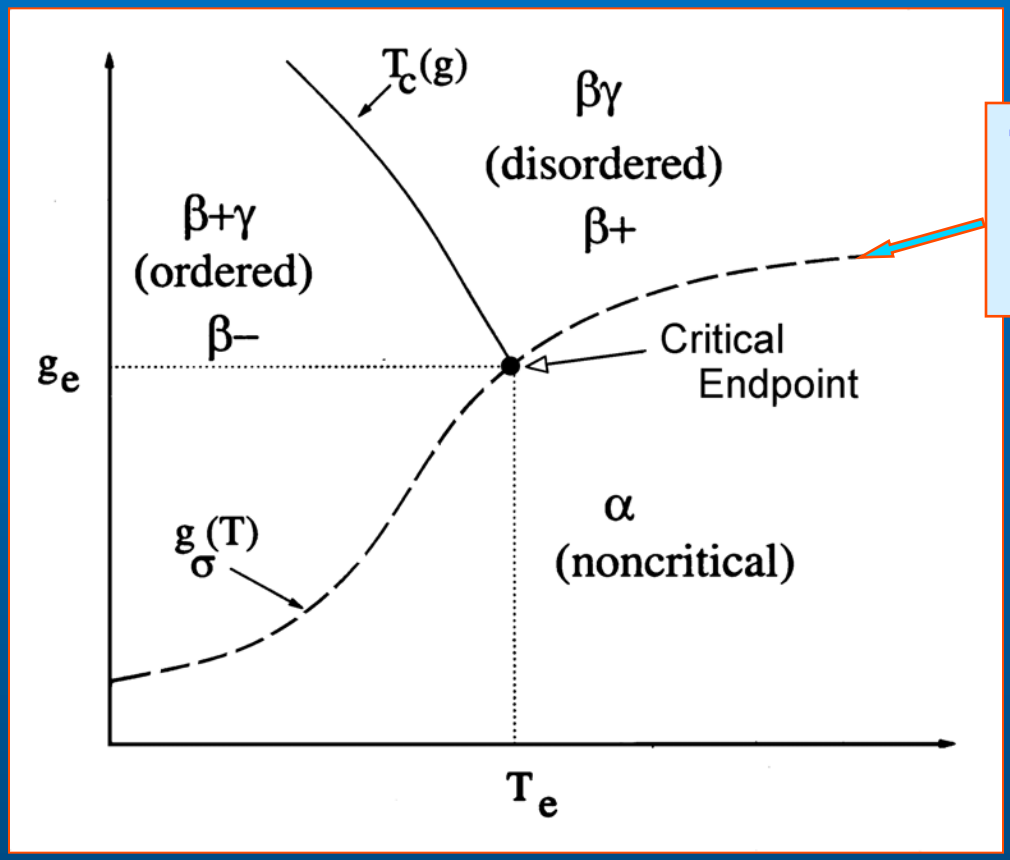


"Spectator" phase boundary

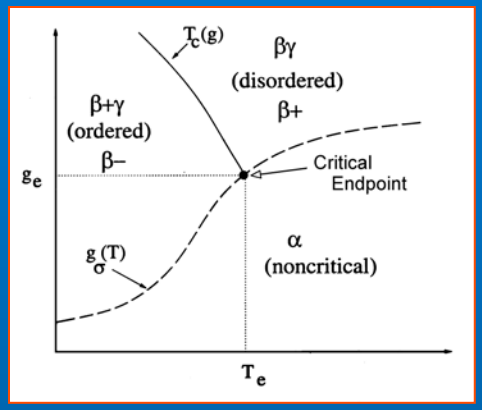
*Kritische Endpunkt: *Büchner, Zeit. Phys. Chem.* ***56*** *(1906) 257; van der Waals and Kohnstamm, "Lehrbuch der Thermodynamik," Part 2 (1912).*

Critical Endpoint: "New" singularities

The phase boundary:

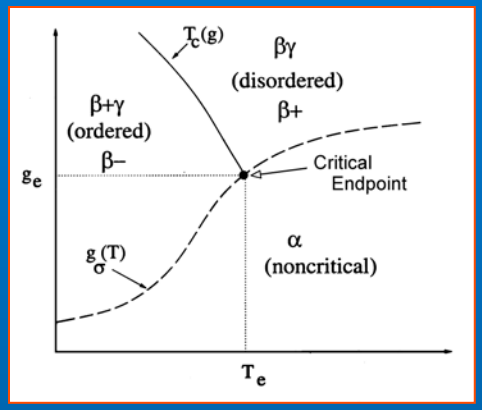
$$t = \left| \frac{T - T_{ce}}{T_{ce}} \right|$$

$$g_\sigma(T) - g_o(T) \approx -X_\pm |t|^{2-\alpha} \qquad as\ T \to T_{ce}$$



(Fisher and Upton, 1990)

Critical Endpoint: "New" singularities



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$$g_\sigma(T) - g_o(T) \approx -X_\pm |t|^{2-\alpha} \quad as\ T \to T_{ce}$$

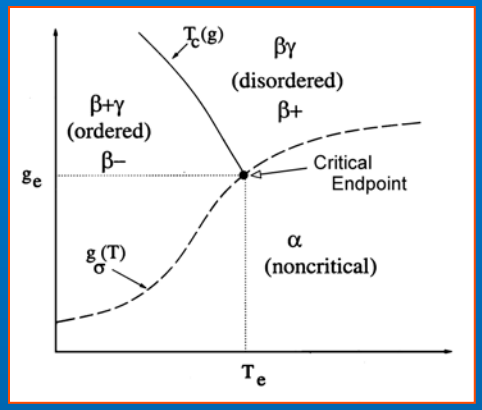
(Fisher and Upton, 1990)

The coexistence density:

$$\rho_d(T) = -U_\pm |t|^{1-\alpha} - V_\pm |t|^{\beta} + terms\ analytic\ at\ T_{ce}$$

(Wilding, 1997)

Critical Endpoint: "New" singularities



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(Fisher and Upton, 1990)

The coexistence density:

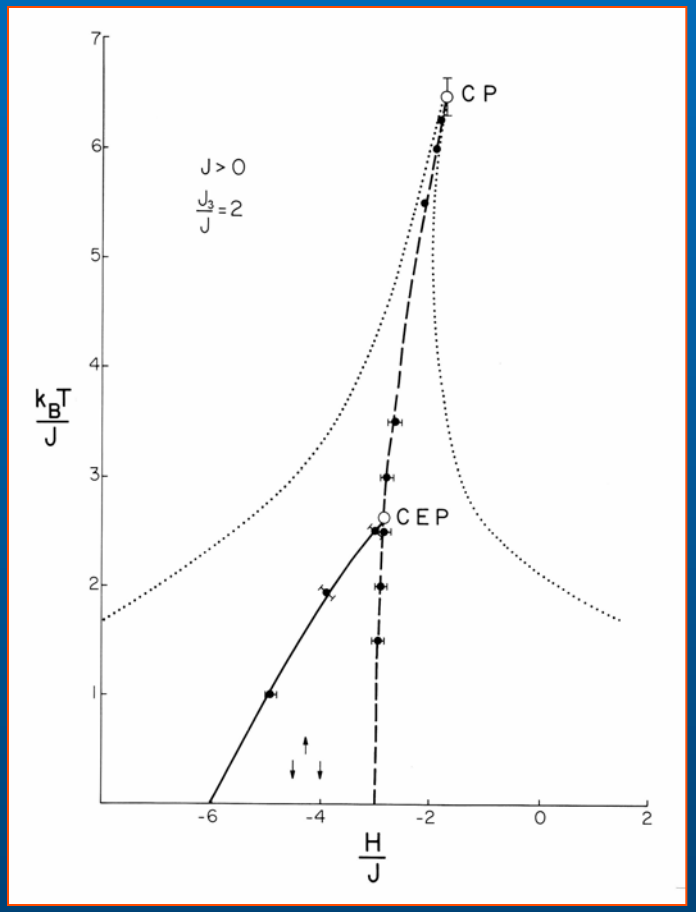
$$\rho_d(T) = -U_\pm |t|^{1-\alpha}$$

For the symmetric case

(Wilding, 1997)

Triangular Ising Model with Two-Body and Three-Body Interactions

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J_3 \sum_{\langle i,j,k \rangle} \sigma_i \sigma_j \sigma_k - H \sum_i \sigma_i , \qquad \sigma_i = \pm 1$$

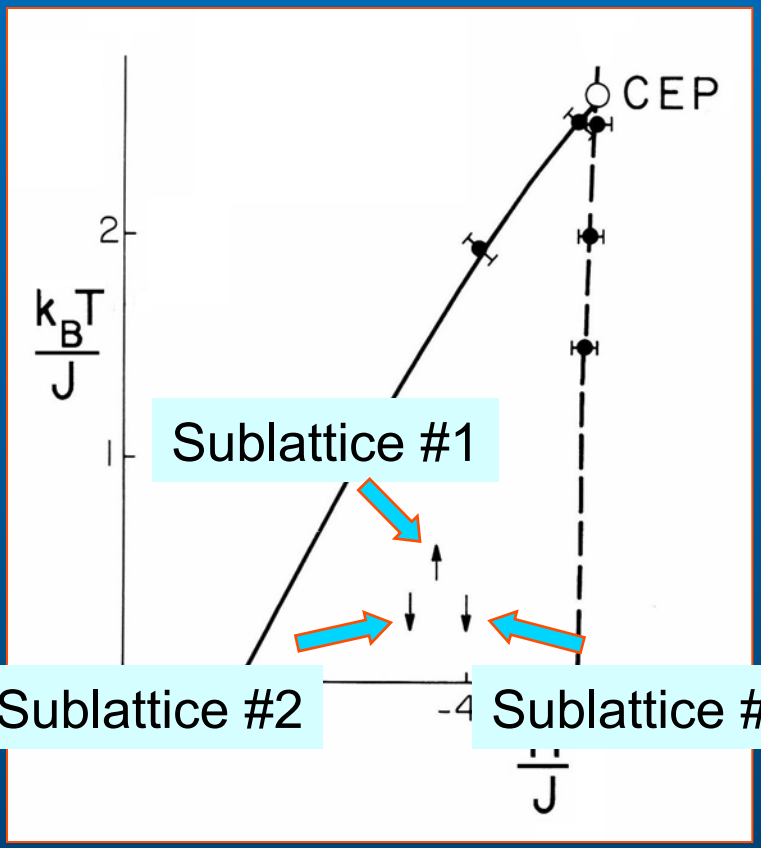


∴ Must search for the critical endpoint (CEP) in (H,T) space!

(after Chin and Landau, 1987)

Triangular Ising Model with Two-Body and Three-Body Interactions

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J_3 \sum_{\langle i,j,k \rangle} \sigma_i \sigma_j \sigma_k - H \sum_i \sigma_i , \qquad \sigma_i = \pm 1$$



Order parameter

$$P_1 = \frac{1}{2}\left(M_1 - \frac{M_2 + M_3}{2} \right)$$

$$P_2 = \frac{\sqrt{3}}{4}\left(M_2 - M_3 \right)$$

$$P = \sqrt{p_1^2 + P_2^2}$$

(after Chin and Landau, 1987)

Triangular Ising Model with Two-Body and Three-Body Interactions

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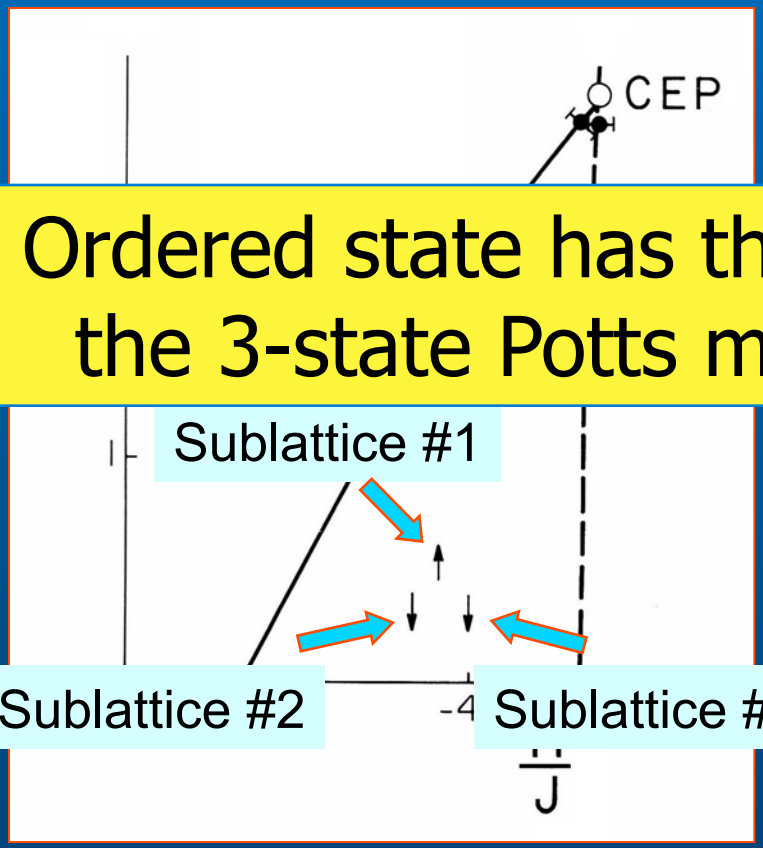


Order parameter

$$P = \sqrt{p_1^2 + P_2^2}$$

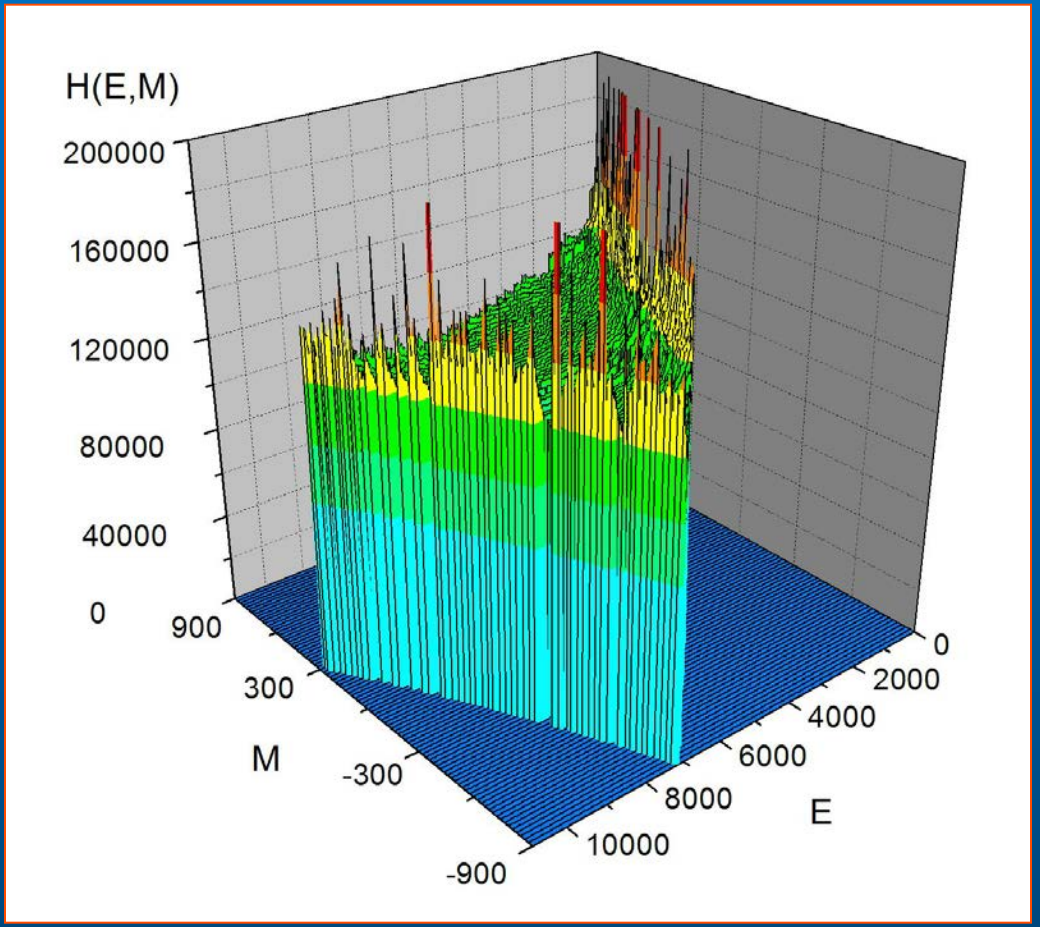
Ordered state has the same symmetry as the 3-state Potts model

(after Chin and Landau, 1987)

Triangular Ising Model with Two-Body and Three-Body Interactions

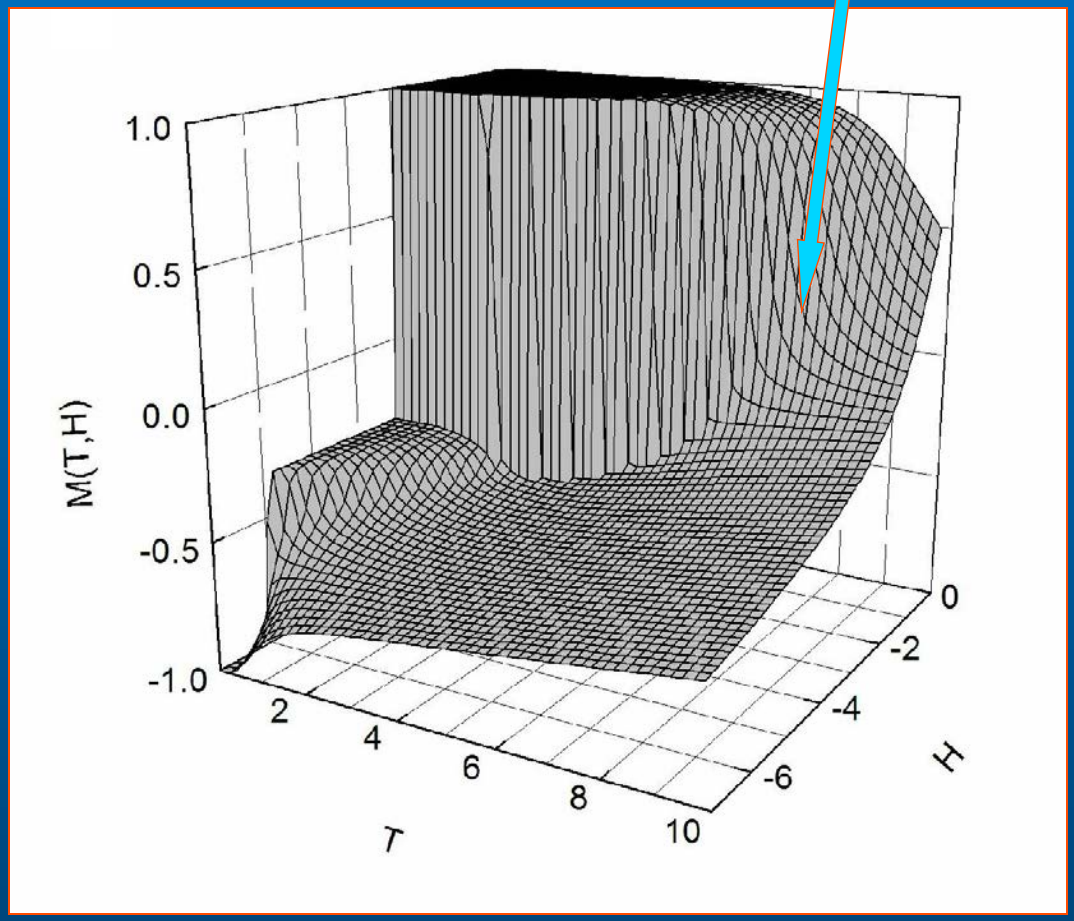
W-L sampling:

Generate a 2-dim histogram in E-M space ⇒ use to determine g(E,M)



Triangular Ising Model with Two-Body and Three-Body Interactions

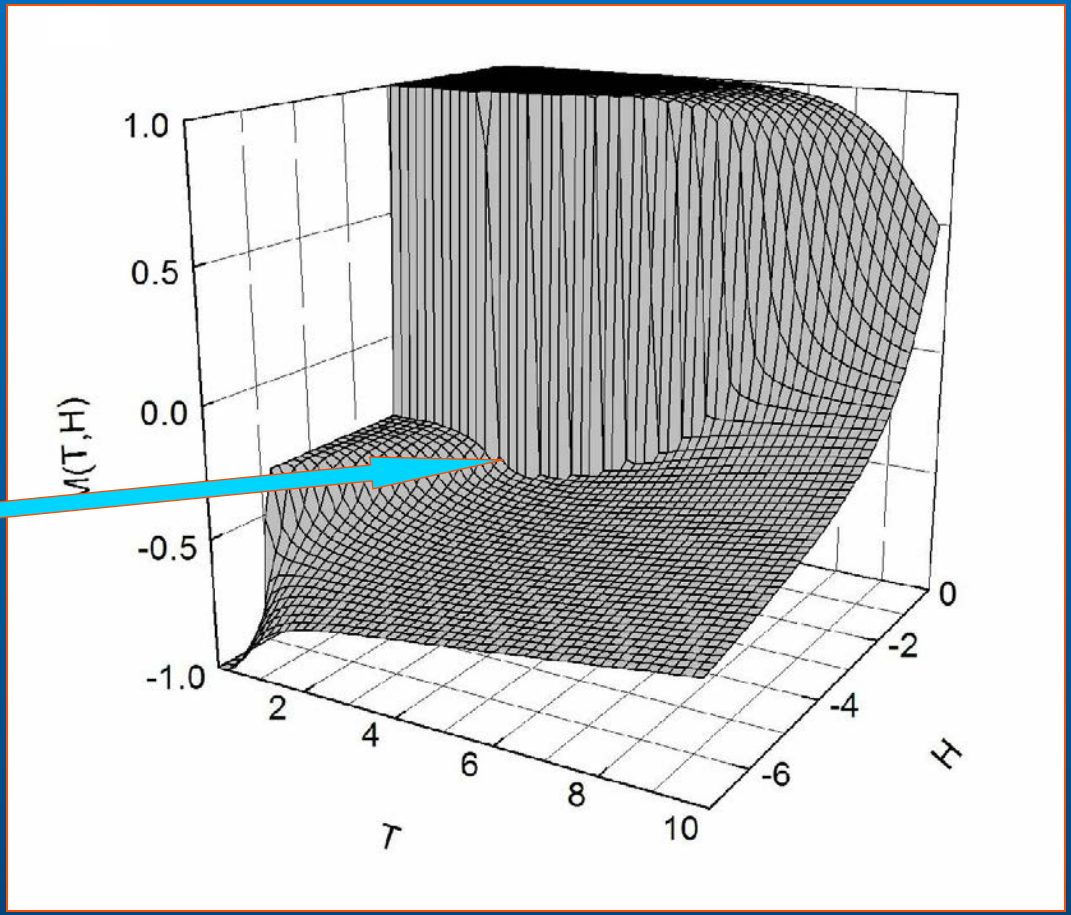
Magnetization as a function of both temperature and magnetic field



Triangular Ising Model with Two-Body and Three-Body Interactions

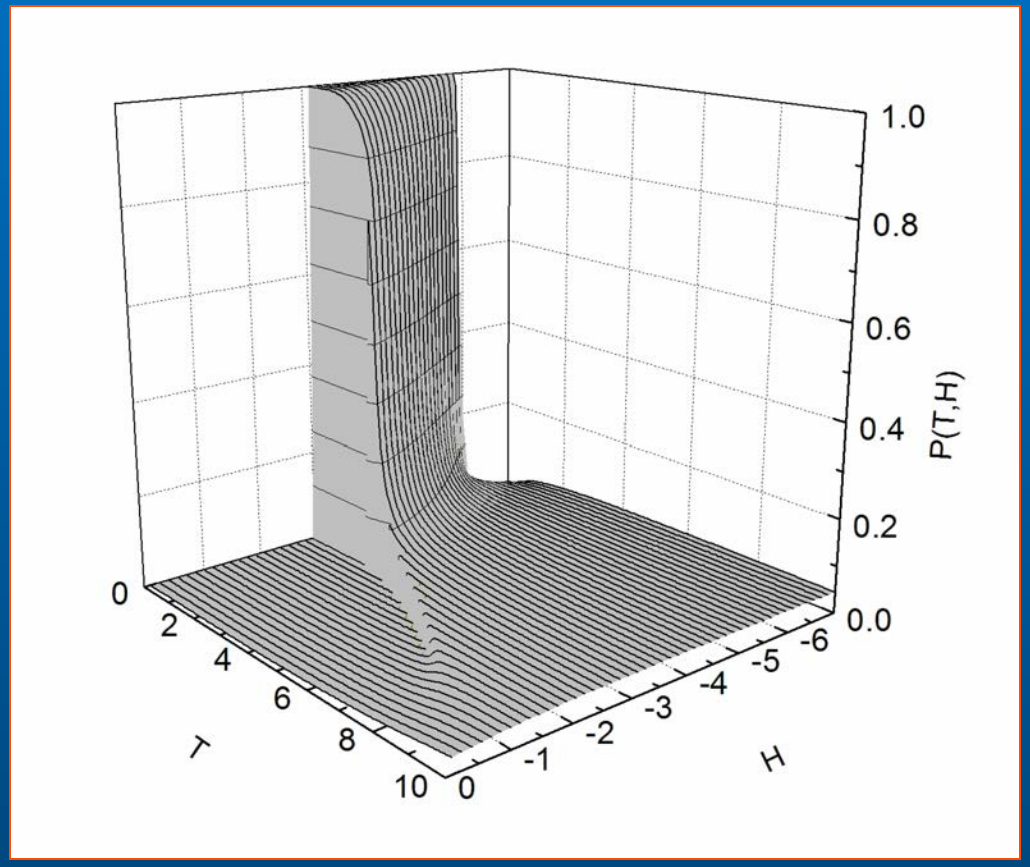
Magnetization as a function of both temperature and magnetic field

Critical endpoint



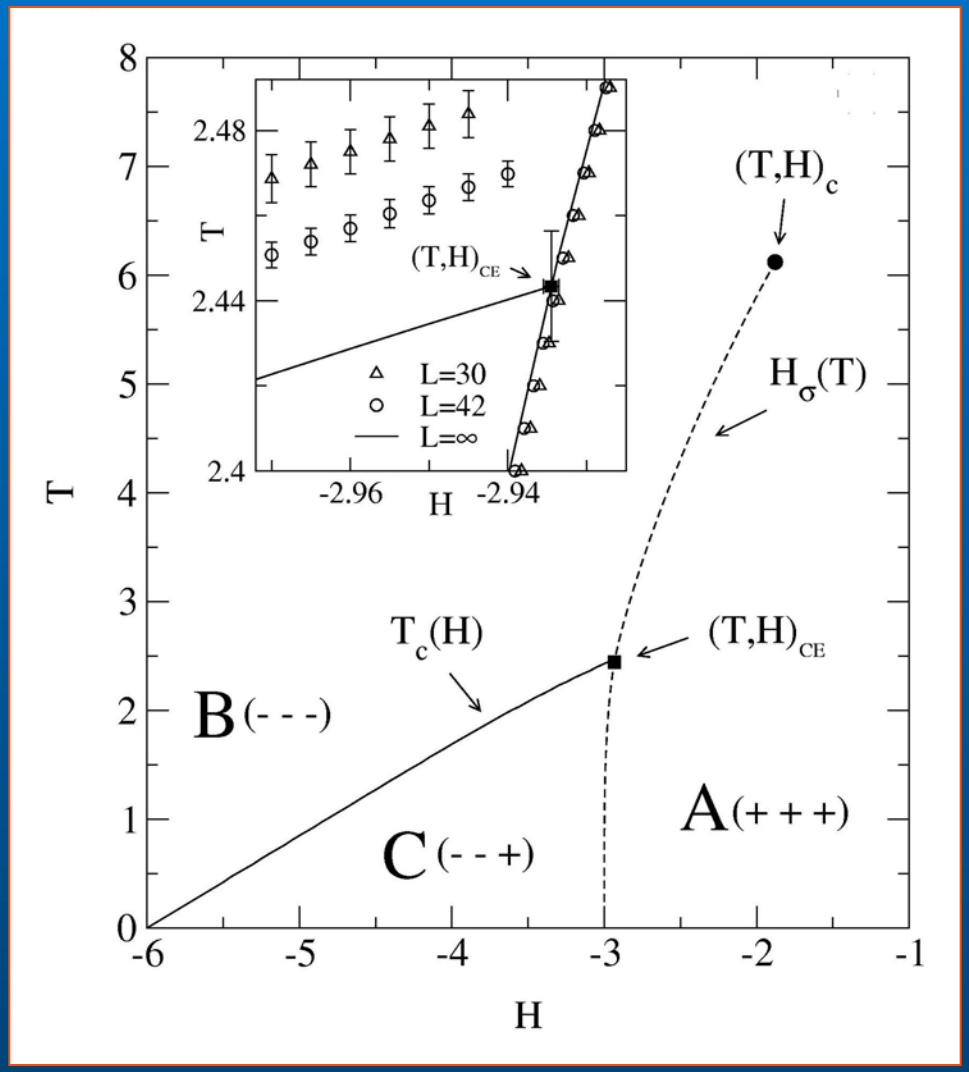
Triangular Ising Model with Two-Body and Three-Body Interactions

Order parameter as a function of both temperature and magnetic field



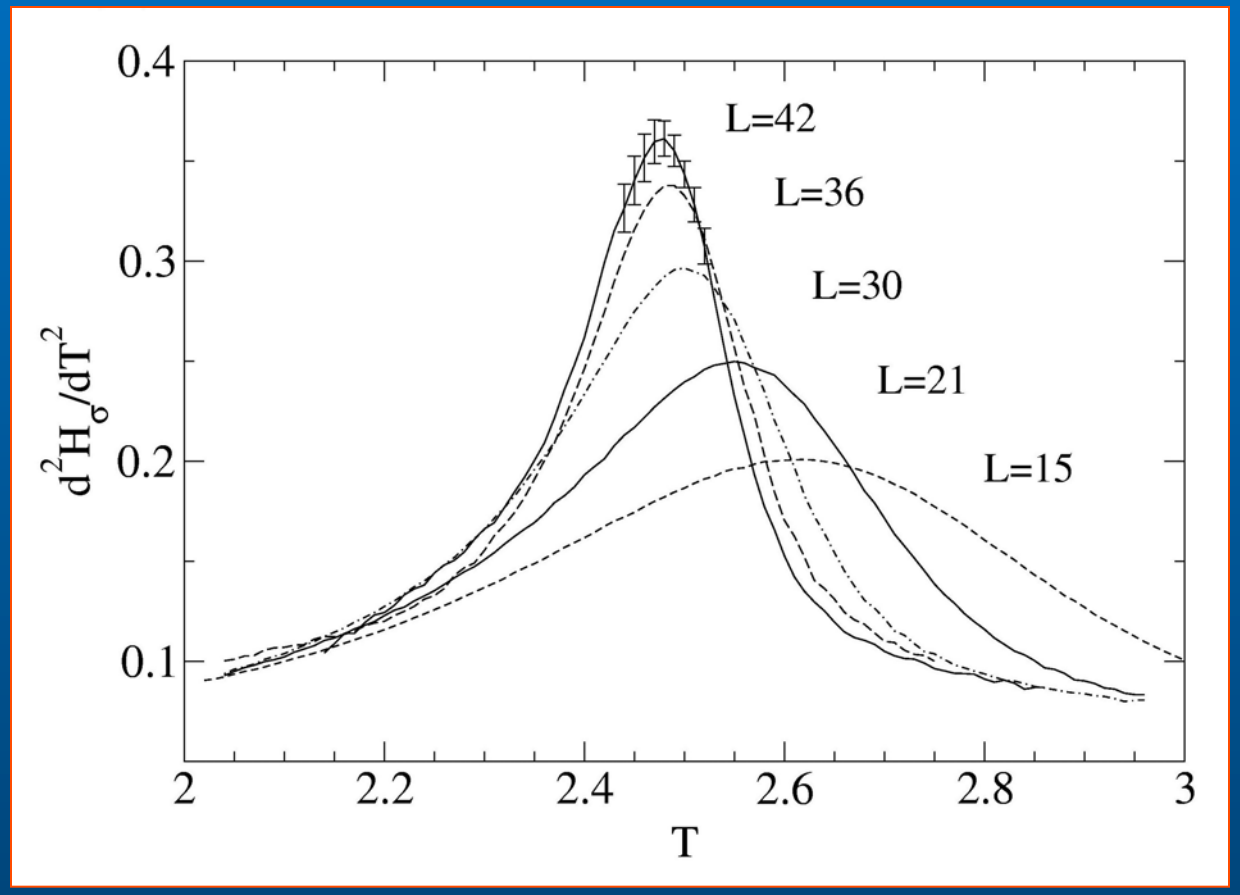
Triangular Ising Model with Two-Body and Three-Body Interactions

Phase diagram in temperature-magnetic field space: Finite size effects ⇒ locate the **critical endpoint**



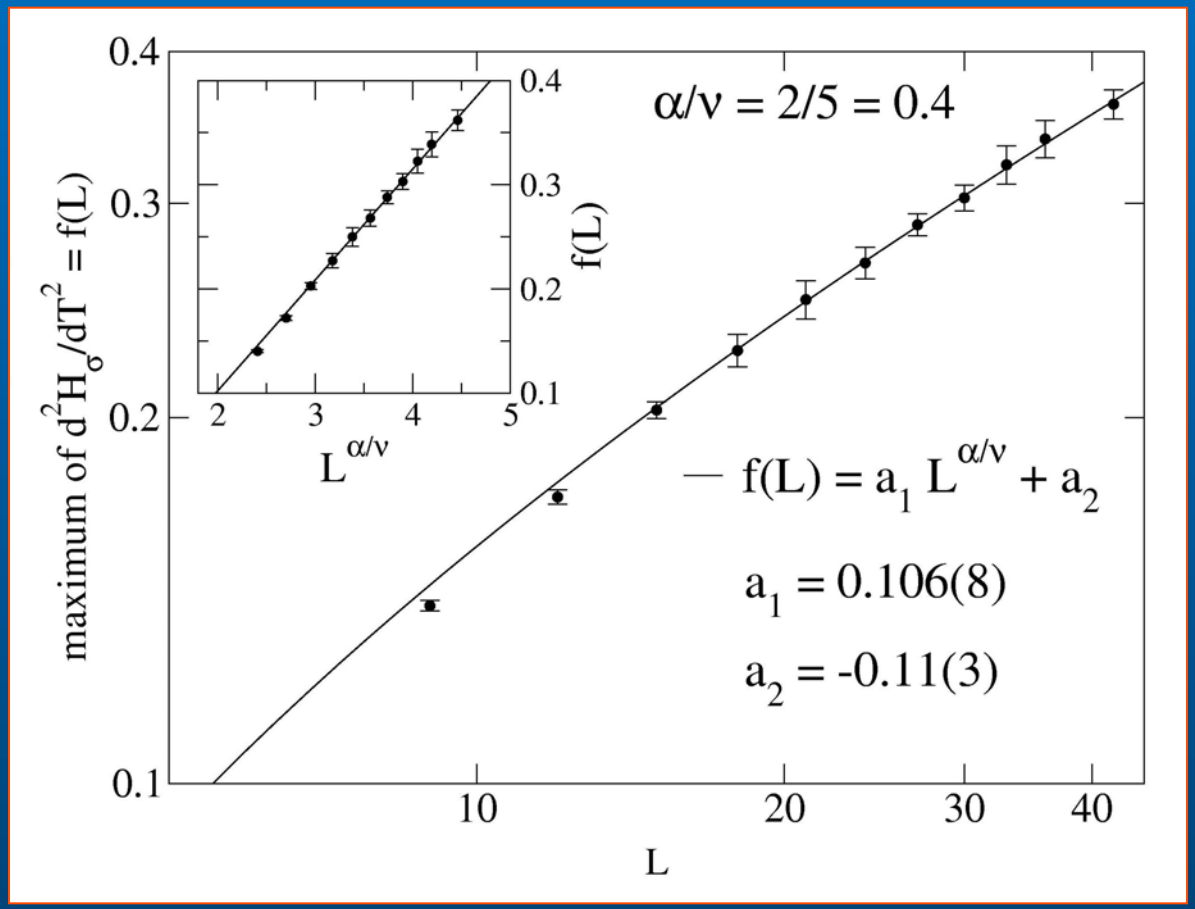
Triangular Ising Model with Two-Body and Three-Body Interactions

Curvature of the 1st order phase boundary near the critical endpoint



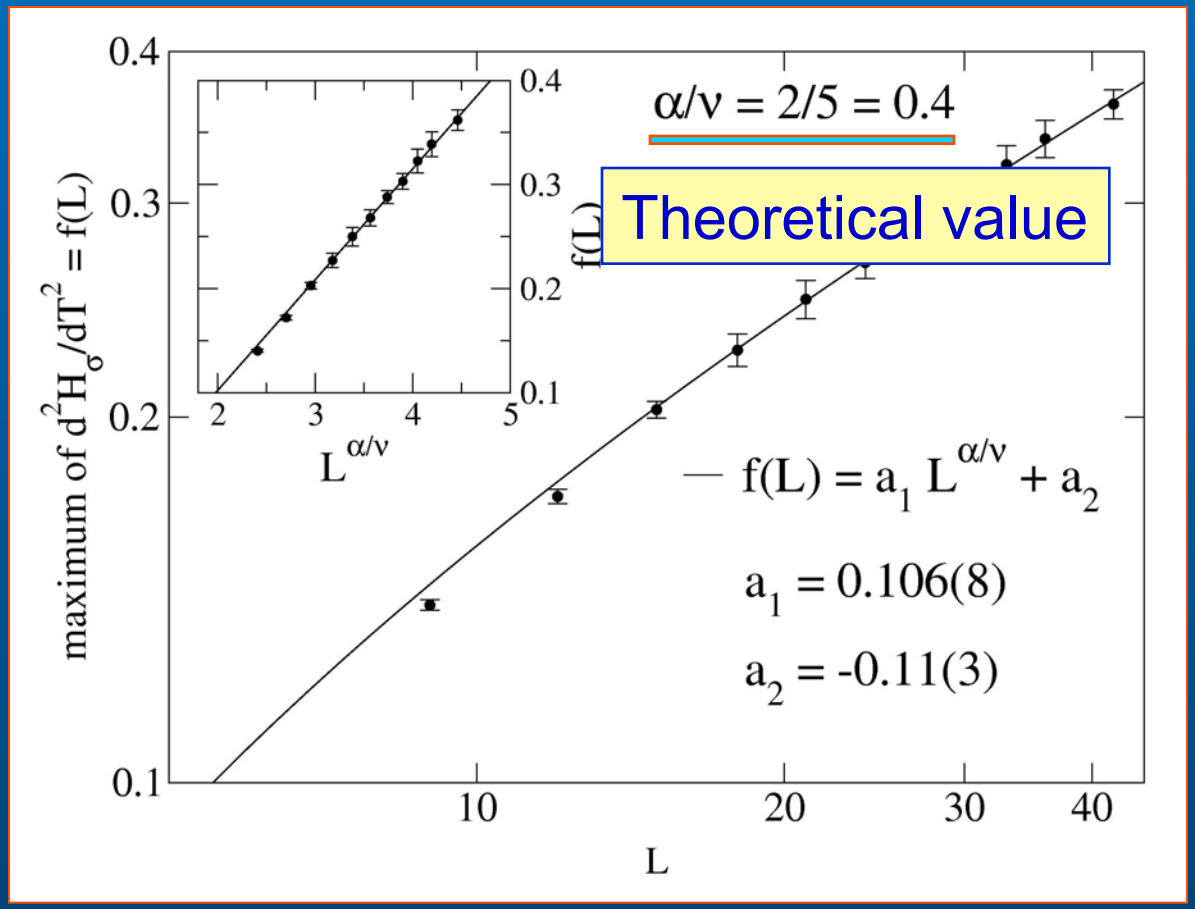
Triangular Ising Model with Two-Body and Three-Body Interactions

Finite size scaling of the maximum in curvature

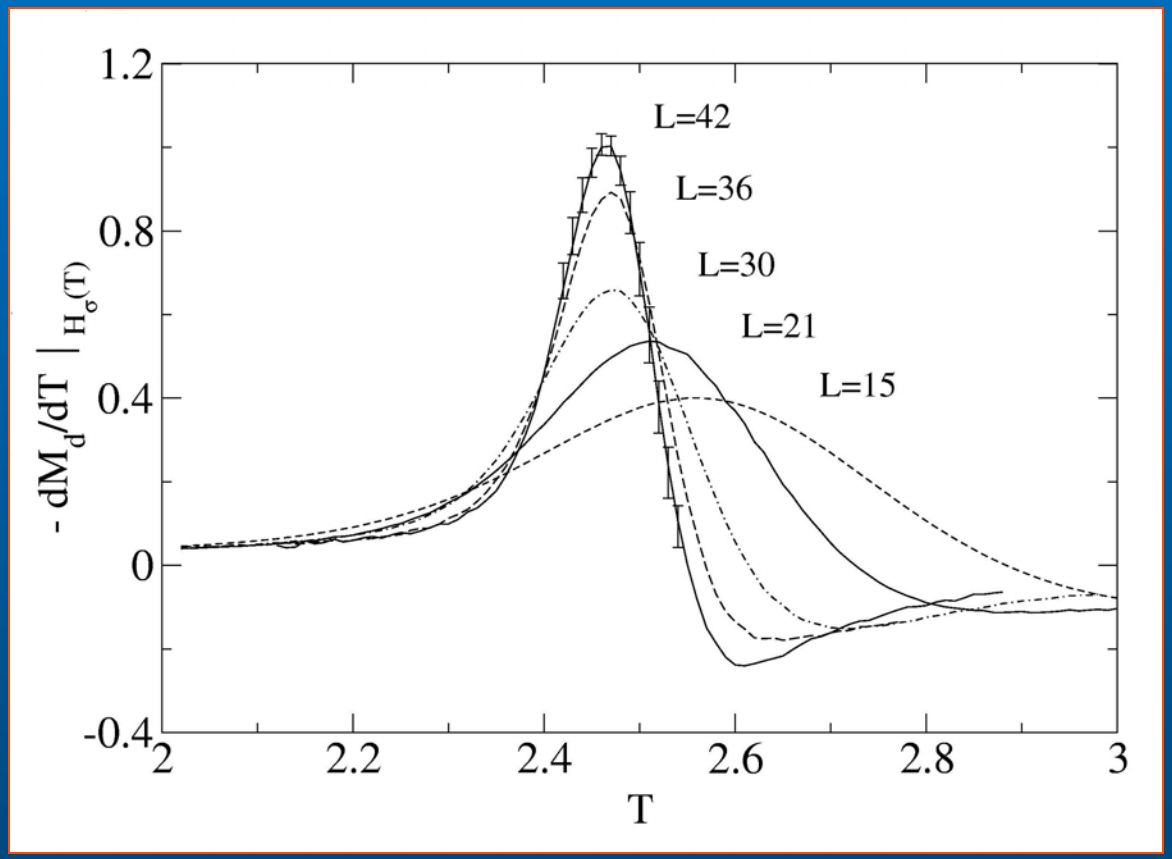


Triangular Ising Model with Two-Body and Three-Body Interactions

Finite size scaling of the maximum in curvature

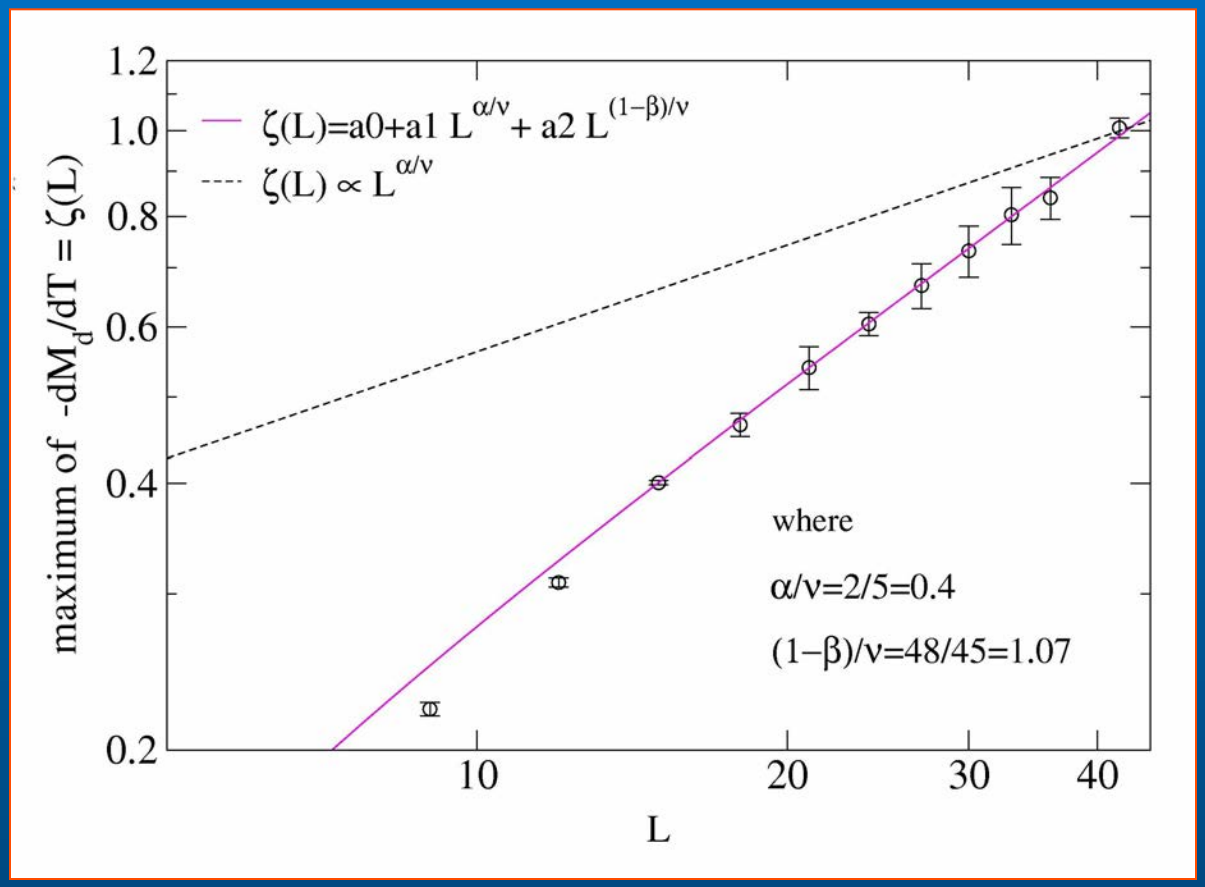


Triangular Ising Model with Two-Body and Three-Body Interactions



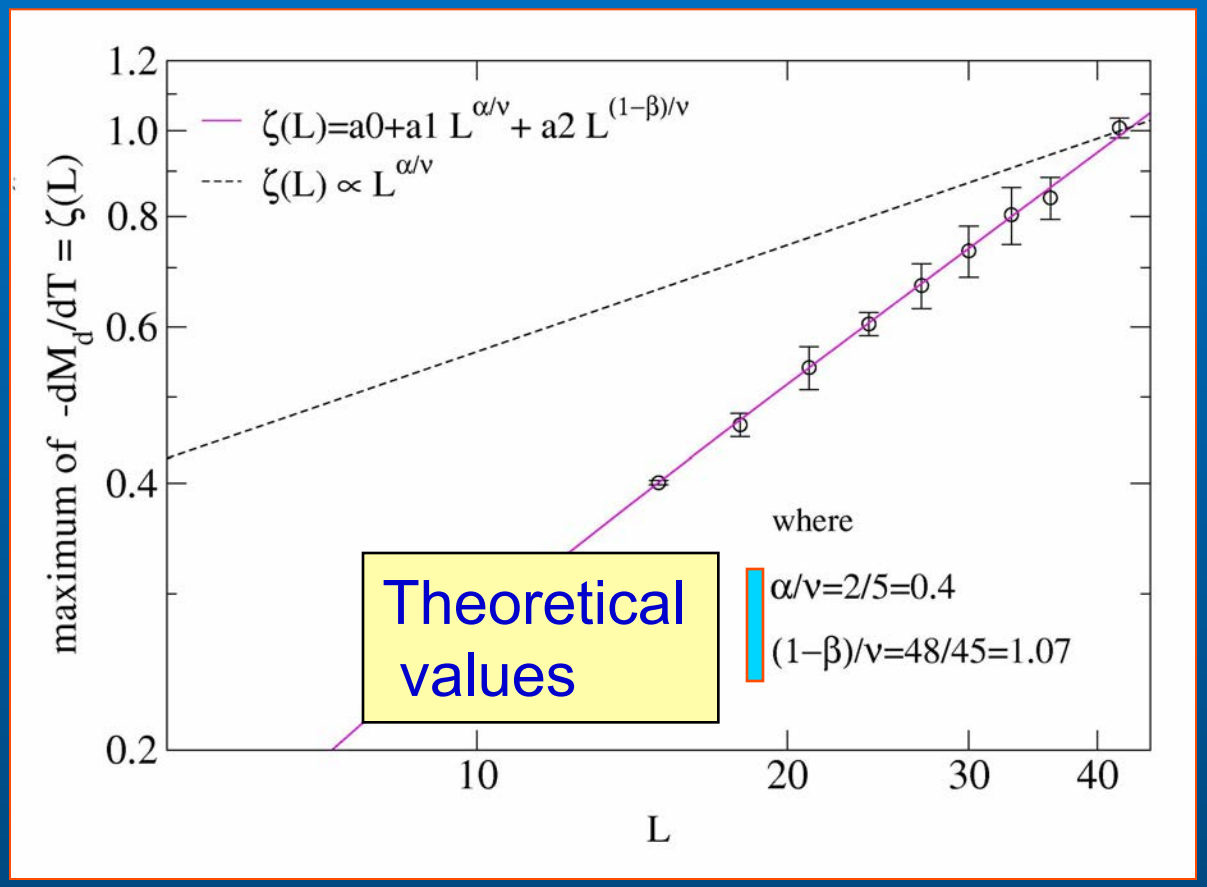
Derivative of the magnetization coexistence diameter at the transition as a function of temperature

Triangular Ising Model with Two-Body and Three-Body Interactions



Maximum of the derivative of the magnetization coexistence diameter

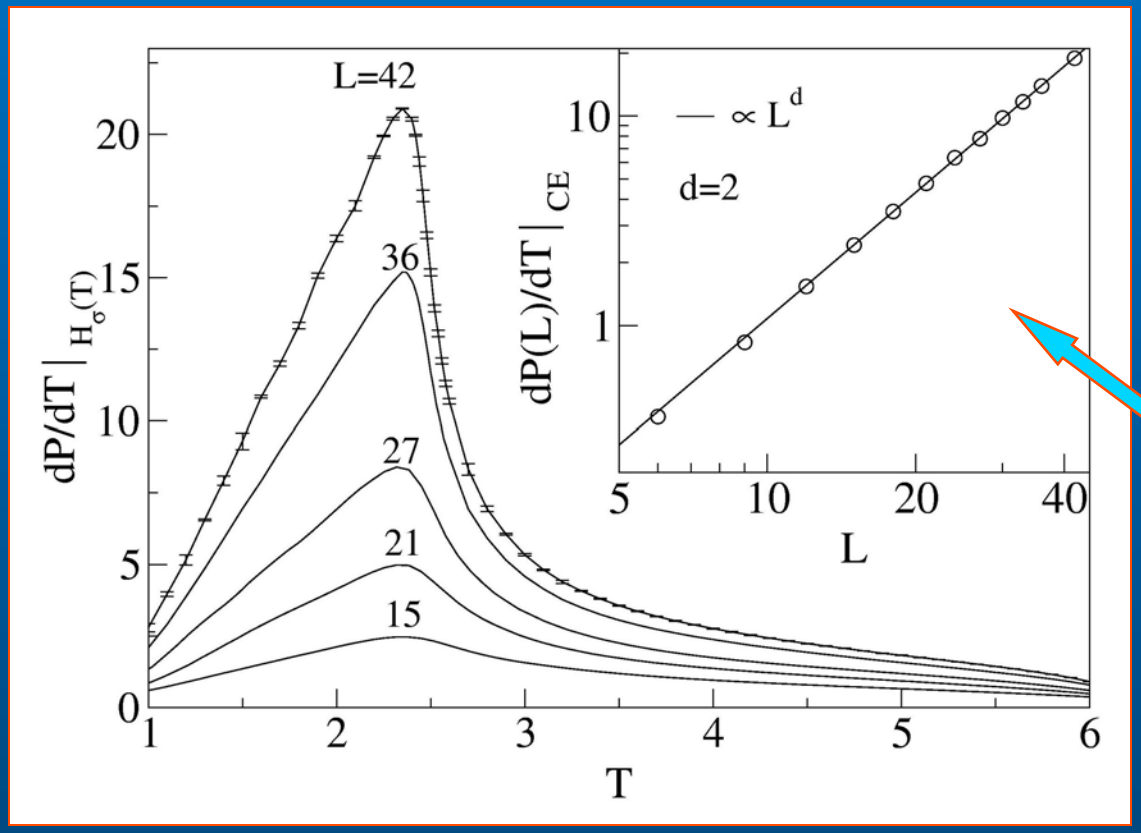
Triangular Ising Model with Two-Body and Three-Body Interactions



Maximum of the derivative of the magnetization coexistence diameter

Triangular Ising Model with Two-Body and Three-Body Interactions

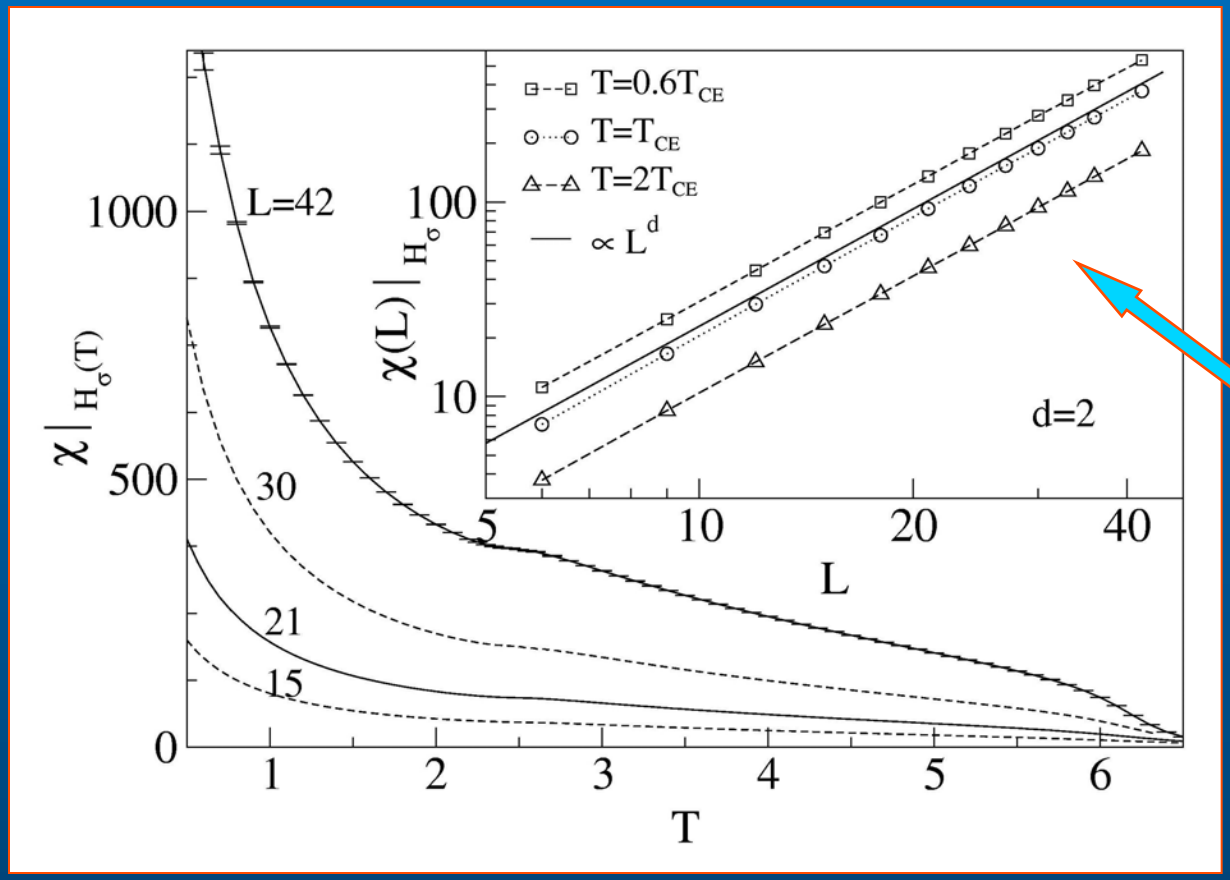
Singularity along the spectator phase boundary



Finite size behavior at the critical endpoint

Triangular Ising Model with Two-Body and Three-Body Interactions

Susceptibility along the spectator phase boundary

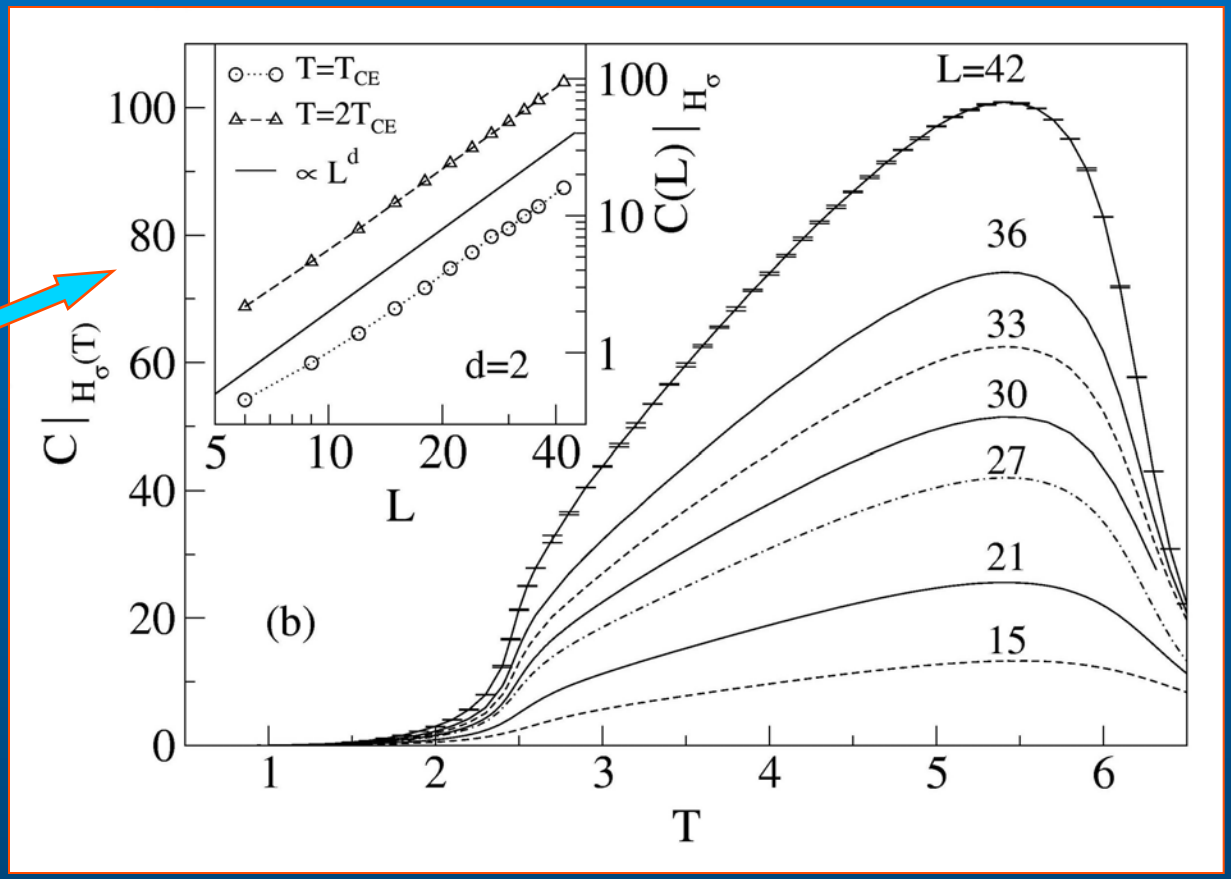


Finite size behavior

Triangular Ising Model with Two-Body and Three-Body Interactions

Specific heat along the spectator phase boundary

Finite size behavior



Can Wang-Landau Sampling be Applied to Quantum Models?

$$Z = \sum_{all\ states} e^{-\beta \mathcal{H}}$$

$$= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} Tr\left(-\mathcal{H}\right)^n \equiv \sum_{n=0}^{\infty} g(n)\beta^n$$

Can Wang-Landau Sampling be Applied to Quantum Models?

$$Z = \sum_{\text{all states}} e^{-\beta \mathcal{H}} \qquad 1/k_B T$$

$$= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} Tr\left(-\mathcal{H}\right)^n \equiv \sum_{n=0}^{\infty} g(n)\beta^n$$

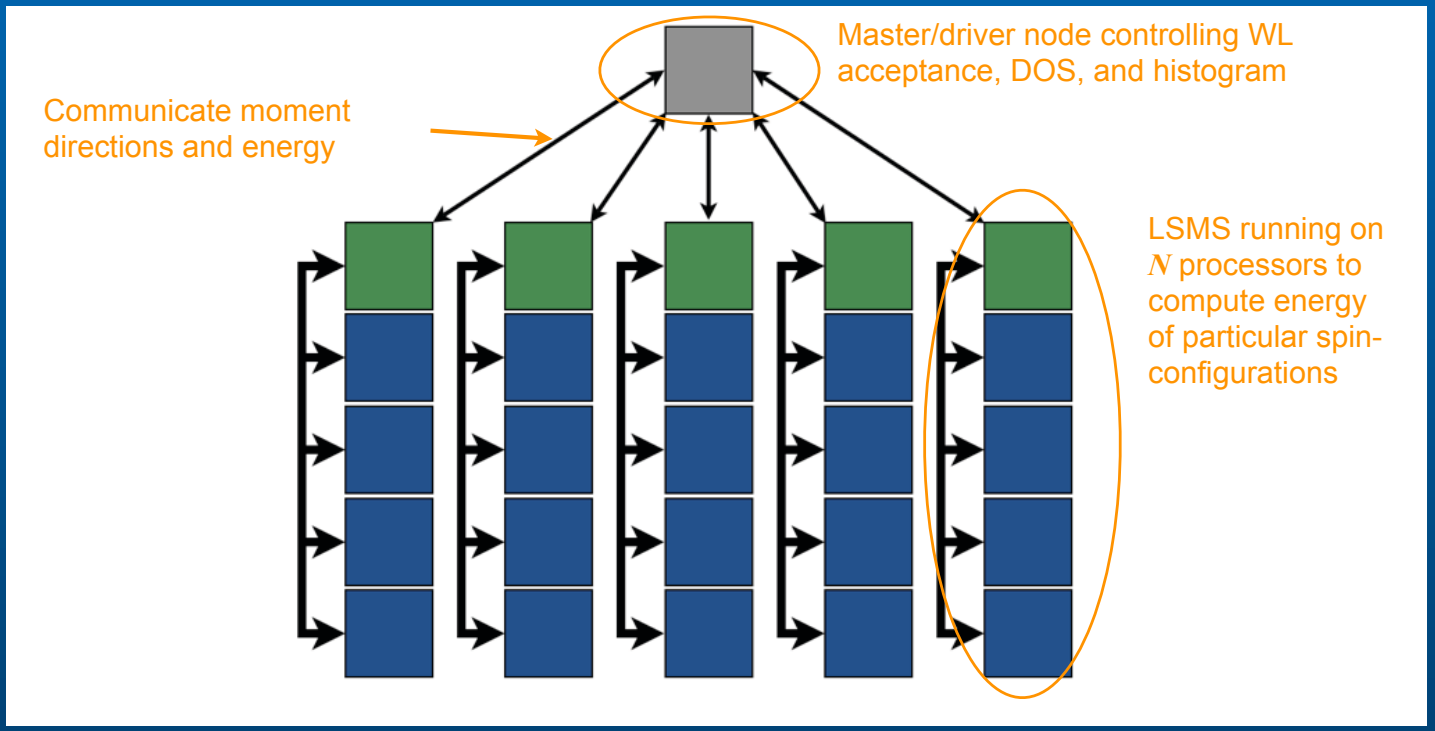
- Perform a random walk in the space of series expansion coefficients n
- Then, calculate properties from the partition function

(Troyer et al., 2003)

WL-LSMS Method and the Gordon Bell Award

Calculate the free energy of a magnetic nanoparticle by combining an LSMS *(locally self-consistent multiple scattering)* method with Wang-Landau sampling.

$$F(T,\vec{M}) = E(T,\vec{M}) - k_{\mathrm{B}}T \ln W(E,\vec{M})$$



Peak performance =1.8 Pflop on Jaguar at ORNL

(Eisenbach et al., 2009)

Can Wang-Landau Sampling be implemented differently?

Different functions cn be used to let the modification factor approach $f => 1$.

Suppose we don't use a modification factor at all but let $f => 1$ as $1/t$? (t is Monte Carlo time). *(Belardinelli, Manzi, and Peyrera, 2008)*

Can Wang-Landau Sampling be implemented differently?

After the density of states has converged, use the result to perform a multicanonical simulation

But updates do not have to be single spin-flips, *e.g.* perform a multibondic cluster flip trial.

(Berg and Janke, 2007)

Use an N-fold way algorithm to study interface unbinding in an Ising model with antisymmetric walls

(Schulz, Binder, and Mueller, 2005)

Overview and Conclusion

Wang-Landau sampling is powerful and flexible

- It provides direct access to the density of states
- It is easily parallelizable
- It is effective for the study of *critical phenomena*
- It eliminates the problem with energy barriers at *1st order* phase transitions
- It can be used to study subtle problems like critical endpoints
- It can be easily extended