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Tutor: Munehisa Matsumoto

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Existence of phase transitions only in TD limit

Existence of phase transitions only in TD limit

Phase transitions occur only in thermodynamical limit

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- Want to simulate such systems

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Existence of phase transitions only in TD limit

Phase transitions occur only in thermodynamical limit

- Want to simulate such systems
  - Problem: finite memory and processing time
  - Idea: Analyse finite systems and deduce conclusions for TD limit

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How to find T_c

- No problem in Thermodynamical limit

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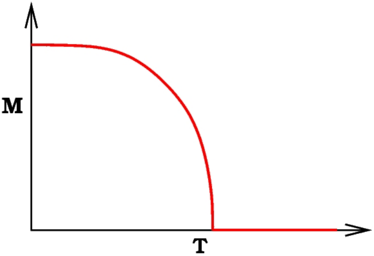

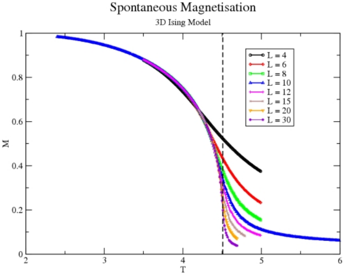

Figure: In TD limit the order parameter is 0 for $T > T_c$ but in FS the transition is smeared out.

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1st or 2nd order transition?

- No problem in Thermodynamical limit
- Look at finite system

Equilibrium TD behaviour of FS smooth for both 1st AND 2nd order transitions

Summary of Problems

Problems:

- Cannot simulate infinite system

Summary of Problems

Problems:

- Cannot simulate infinite system
- Finding T_c

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- Cannot simulate infinite system
- Finding T_c
- Distinguishing between 1st and 2nd order transitions

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Consider the magnetic susceptibility:

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- Can be defined as $k_B T \chi_M = \sum_{\{i,j\}} \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$

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- Can be defined as $k_B T \chi_M = \sum_{\{i,j\}} \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$
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Motivating the Scaling Function

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Motivating the Scaling Function

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- Approaching T_c results in divergence of ξ $\rightarrow$ susceptibility saturates as $\xi \sim L$
- Including this into scaling theorie gives $\chi(L,T) = |t|^{-\gamma} g\left(\frac{L}{\xi(t)}\right)$, where $t = (T - T_c)/T_c$

Motivating the Scaling Function

$$\chi(L,T) = |t|^{-\gamma} g\left(\frac{L}{\xi(t)}\right)$$

Motivating the Scaling Function

$\chi(L,T) = |t|^{-\gamma} g\left(\frac{L}{\xi(t)}\right)$
$g(x)$ should also satisfy:

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$\chi(L,T) = |t|^{-\gamma} g\left(\frac{L}{\xi(t)}\right)$

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- $g(x) \to$ const. as $x \to \infty$

Motivating the Scaling Function

$\chi(L,T) = |t|^{-\gamma} g\left(\frac{L}{\xi(t)}\right)$

$g(x)$ should also satisfy:

- $g(x) \to$ const. as $x \to \infty$
- $g(x) \propto x^{\gamma/\nu}$ as $x \to 0$

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  - Second constraint: Ensures temperature independent Magnetic Susceptibility for $\xi \gg L$

Motivating the Scaling Function

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- $g(x) \rightarrow$ const. as $x \rightarrow \infty$
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  - First constraint: Ensures correct powerlaw behaviour in TD limit.
  - Second constraint: Ensures temperature independent Magnetic Susceptibility for $\xi \gg L$
- Sideproduct: Maximum of TD quantity grows like $L^{\gamma/\nu}$

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TD limit	FS system

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Scaling Functions

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$M \propto \|t\|^{-\beta}$	$M = L^{-\beta/\nu} g_M(tL^{1/\nu})$

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Scaling Functions

TD limit	FS system
$M \propto \lvert t\rvert^{-\beta}$	$M = L^{-\beta/\nu} g_M(tL^{1/\nu})$
$\chi \propto \lvert t\rvert^{\gamma}$	$\chi = L^{\gamma/\nu} g_\chi(tL^{1/\nu})$

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Note: Only valid for

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- Temperatures close enought to T_c
- Sufficently large system sizes L

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Let's look at heat capacity $C = L^{\alpha/\nu} g_C(tL^{1/\nu})$

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Let's look at heat capacity $C = L^{\alpha/\nu} g_C(tL^{1/\nu})$

Plot $C/L^{\alpha/\nu}$ with respect to $tL^{1/\nu}$

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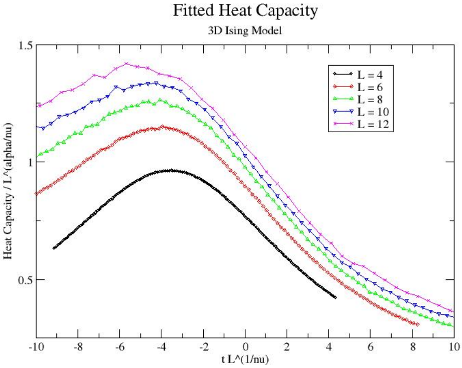

Figure: With correct exponents we see data collapse near T_c

Interpretation

Another example $\chi = L^{\gamma/\nu} g_C(tL^{1/\nu})$

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Plot $\chi/L^{\gamma/\nu}$ with respect to $tL^{1/\nu}$

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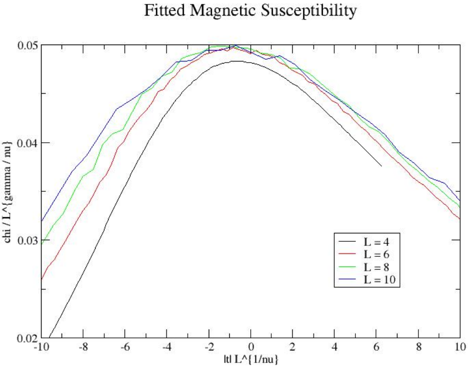

Figure: With correct exponents we see data collapse near T_c

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- Numerical algorithms for data fitting exist

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Remarks

- Numerical algorithms for data fitting exist
- One obtains all parameters at once

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- Order Parameter $\neq 0 \qquad \forall T < \infty$

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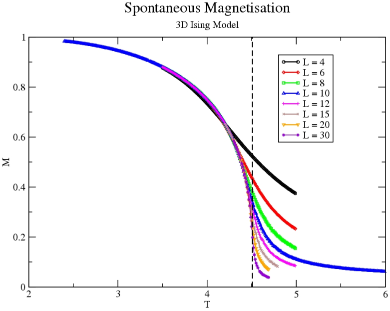

Figure: The order parameter is never zero.

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- No divergence of Correlation Length, Magnetic Susceptibility or HeatCapacity

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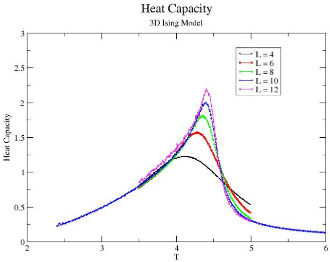

Figure: The quantities do not diverge.

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- Behaviour of Maximum of χ or C

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Different Solutions for this problem

- Behaviour of Maximum of χ or C
- Binder Cumulant $U_L := 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L^2}$

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Different Solutions for this problem

- Behaviour of Maximum of χ or C
- Binder Cumulant $U_L := 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L^2}$
- Behaviour of Correlation Length ξ

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Maximum of χ

Behaviour of Maximum of TD quantities (e.g. χ or C)

Maximum of χ

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Temperature where χ or C experiences maximum is not exactly T_c

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Behaviour of Maximum of TD quantities (e.g. χ or C)
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- Denote temperature where χ has maximum by $T_c(L)$

Maximum of χ

Behaviour of Maximum of TD quantities (e.g. χ or C)
Temperature where χ or C experiences maximum is not exactly T_c

- Denote temperature where χ has maximum by $T_c(L)$
- Assumption: $\xi(T_c(L) - T_c) = aL$

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Maximum of χ

Behaviour of Maximum of TD quantities (e.g. χ or C)
Temperature where χ or C experiences maximum is not exactly T_c

- Denote temperature where χ has maximum by $T_c(L)$
- Assumption: $\xi(T_c(L) - T_c) = aL$
  Since $\xi(x) \propto |x|^{-\nu}$

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Maximum of χ

Behaviour of Maximum of TD quantities (e.g. χ or C)
Temperature where χ or C experiences maximum is not exactly T_c

- Denote temperature where χ has maximum by $T_c(L)$
- Assumption: $\xi(T_c(L) - T_c) = aL$
  Since $\xi(x) \propto |x|^{-\nu}$
  $T_c(L) = T_c + bL^{-1/\nu}$

Maximum of χ

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Maximum of χ

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Problem: 3 tunable Parameters (T_c, b, ν)

Maximum of χ

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Problem: 3 tunable Parameters (T_c, b, ν)

- Need data with good statistical accuracy

Maximum of χ

$T_c(L) = T_c + bL^{-1/\nu}$

Problem: 3 tunable Parameters (T_c, b, ν)

- Need data with good statistical accuracy
- Measure different quantities (since all have same T_c, b, ν)

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Binder Cumulant

Figure: Prof. Dr. Kurt Binder

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Binder Cumulant

Binder Cumulant $U_L := 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L^2}$

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Binder Cumulant not depending on L at T_c

$$\frac{\langle M^4 \rangle_L}{\langle M^2 \rangle_L^2} = \frac{L^{-4\beta/\nu} g_{M^4}(tL^{1/\nu})}{\left(L^{-2\beta/\nu} g_{M^2}(tL^{1/\nu})\right)^2} = g_c(tL^{(1/\nu)})$$

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- For $T > T_c$ $\langle M^4 \rangle_L = 3\langle M^2 \rangle_L^2$
- For $T < T_c$ $\langle M^4 \rangle_L = \langle M^2 \rangle_L^2$

Binder Cumulant

$$U_L = 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L} \xrightarrow{L\to\infty} \begin{cases} 0 & \text{for } T > T_c \\ \frac{2}{3} & \text{for } T < T_c \end{cases}$$

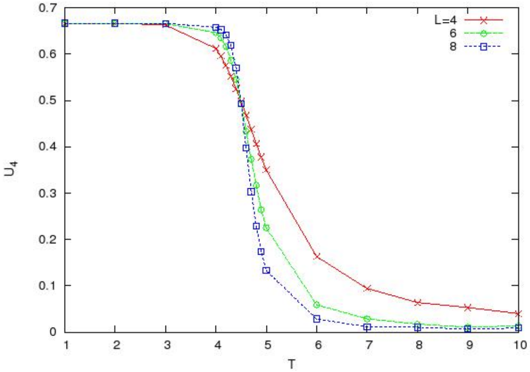

Figure: Binder Parameter for the 3D Ising Model

Binder Cumulant

Possible to apply FSS on Binder Cumulant

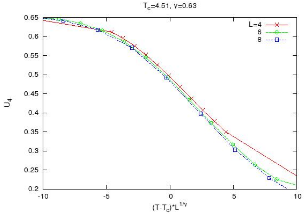

Figure: Obtaining of ν with FSS of U_L

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Possible to apply FSS on Binder Cumulant

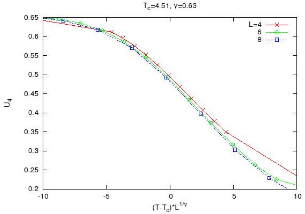

Figure: Obtaining of ν with FSS of U_L

- β canceled out

Binder Cumulant

Possible to apply FSS on Binder Cumulant

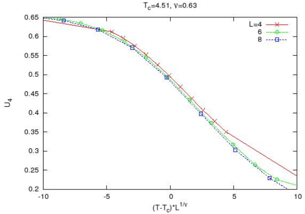

Figure: Obtaining of ν with FSS of U_L

- β canceled out
- T_c obtained via point of intersection

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Possible to apply FSS on Binder Cumulant

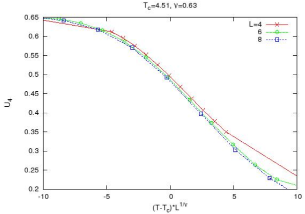

Figure: Obtaining of ν with FSS of U_L

- β canceled out
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$\Longrightarrow$ Have to tune only ν

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Obtaining T_c by observing ξ

Similarly to the Binder Cumulant method we can derive T_c with ξ

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since $\xi_L = Lg_\xi(tL^{1/\nu})$

Obtaining T_c by observing ξ

Similarly to the Binder Cumulant method we can derive T_c with ξ

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Similarly to the Binder Cumulant method we can derive T_c with ξ

since $\xi_L = L g_\xi(tL^{1/\nu}) \quad \xrightarrow{T \to T_c} \quad \xi_L / L = g_\xi(0)$

Therefore ξ_L for different L intersect at T_c

Obtaining T_c by observing ξ

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since $\xi_L = L g_\xi(tL^{1/\nu}) \quad \xrightarrow{T \to T_c} \quad \xi_L / L = g_\xi(0)$

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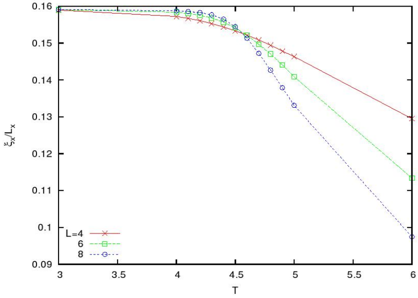

Figure: Obtaining T_c with ξ

Obtaining T_c by observing ξ

Possible to apply FSS to ξ_L/L

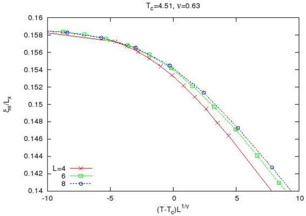

Figure: Obtaining ν with FSS of ξ/L

- T_c obtained via point of intersection

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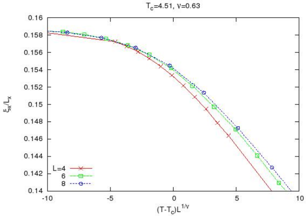

Figure: Obtaining ν with FSS of ξ/L

- T_c obtained via point of intersection

$\Longrightarrow$ Have to tune only ν

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1st or 2nd Order?

Big Problem!

1st or 2nd Order?

Big Problem!

- Finite Size Scaling will not work

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Big Problem!

- Finite Size Scaling will not work
- Histogram peaks will not merge

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1st or 2nd Order?

Big Problem!

- Finite Size Scaling will not work
- Histogram peaks will not merge
- No critical exponents

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Example: Ising Model

Phase diagram of the Ising Model

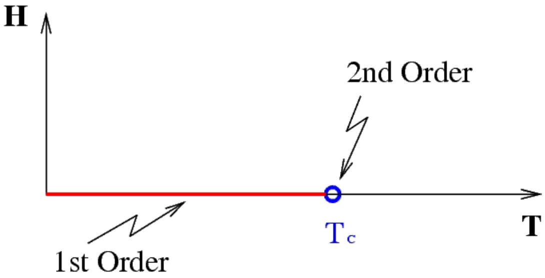

Figure: Phase Diagram of the Ising Model

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Histogram peaks

- Look at behaviour of M at $T < T_c$ and $H \approx 0$

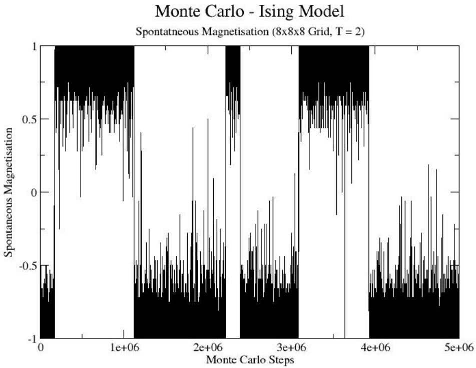

Figure: Spontaneous Magnetisation fluctuates from one ordered state to the other

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Histogram Peaks

- Plot Histogram of M - increase system size

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Histogram Peaks

- Plot Histogram of M - increase system size
  - If Peaks merge $\Rightarrow$ 2nd order transition

Histogram Peaks

- Plot Histogram of M - increase system size
  - If Peaks merge $\Rightarrow$ 2nd order transition
  - If Peaks don't move $\Rightarrow$ 1st order transition

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Finite Size Scaling on 1st Order Transitions

- Can not obtain good values for critical exponents

Finite Size Scaling on 1st Order Transitions

- Can not obtain good values for critical exponents $\Longrightarrow$ No data collapse

Finite Size Scaling
Darko Pilav
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Finite Size Scaling on 1st Order Transitions

- Can not obtain good values for critical exponents $\Longrightarrow$ No data collapse
- No single intersection point of Binder cumulant or ξ/L

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Maxima of TD quantities at T_c

- Look at Maxima of TD quantities at T_c

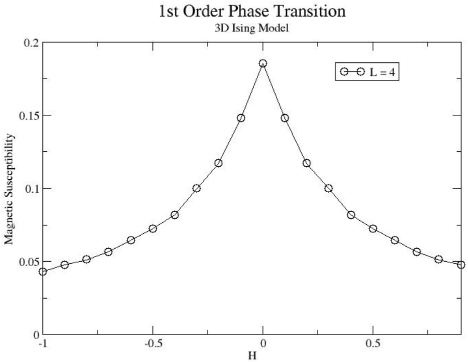

Figure: 1st Order Phase Transition

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Maxima of TD quantities at T_c

- Peaks scale like $L^{\alpha/\nu} \Rightarrow$ 2nd order transition

Maxima of TD quantities at T_c

- Peaks scale like $L^{\alpha/\nu} \Rightarrow$ 2nd order transition
- Peaks scale like $L^{d} \Rightarrow$ 1st order transition

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Weak 1st Order Transition

If we have weak 1st order phase transition

- Scaling might work quite well (with completely wrong exponents)

Weak 1st Order Transition

If we have weak 1st order phase transition

- Scaling might work quite well (with completely wrong exponents)
- Peaks in histogram might emerge only at large L

Weak 1st Order Transition

If we have weak 1st order phase transition

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$\Longrightarrow$ Active area of research

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- Finite Size Effects

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- Finite Size Effects
- Statistical Errors
- Relaxation Effects

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$$\tau_A \equiv \int_0^\infty \phi_A dt$$

$$\langle(\delta A)^2\rangle \equiv \frac{1}{\mathcal{N}}\left(\langle A^2\rangle - \langle A\rangle^2\right)\left(1 + 2\frac{\tau_A}{\delta t}\right)$$

Statistical Error

Summary

$$\tau_A \equiv \int_0^\infty \phi_A dt$$

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- $1 + 2\tau_A/\delta t$ is so called "Statistical Inefficiency"

Statistical Error

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$$\tau_A \equiv \int_0^\infty \phi_A dt$$
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- Near 2nd order phase transitions τ_A diverges (critical slowing down)

Statistical Error

Summary

$$\tau_A \equiv \int_0^\infty \phi_A dt$$

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- $1 + 2\tau_A/\delta t$ is so called “Statistical Inefficiency”
- Near 2nd order phase transitions τ_A diverges (critical slowing down)
- Algorithms that reduce critical slowing down very important

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- Can nummerically collect information of TD systems due to FSS

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- Can nummerically collect information of TD systems due to FSS
- Have seen different possibilities to obtain T_c

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- Can nummerically collect information of TD systems due to FSS
- Have seen different possibilities to obtain T_c
- Problem: Distinguishing between 1st and 2nd order transitions

Summary

- Can nummerically collect information of TD systems due to FSS
- Have seen different possibilities to obtain T_c
- Problem: Distinguishing between 1st and 2nd order transitions
- Have seen one of the important error contributions

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Questions?

- I would like to thank Dr. Munehisa Matsumoto