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Existence of phase transitions only in TD limit

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Existence of phase transitions only in TD limit

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Phase transitions occur only in thermodynamical limit

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Phase transitions occur only in thermodynamical limitWant 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

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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

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• No problem in Thermodynamical limit

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How to find T_c

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- No problem in Thermodynamical limit
- Look at finite system

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- 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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• No problem in Thermodynamical limit

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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

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Problems:

• Cannot simulate infinite system



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- Cannot simulate infinite system
- Finding T_c

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Problems:

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

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Motivating the Scaling Function

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Consider the magnetic susceptibility:

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Motivating the Scaling Function

Consider the magnetic susceptibility:

• 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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Consider the magnetic susceptibility:

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

• Approaching T_c results in divergence of ξ

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Consider the magnetic susceptibility:

- Can be defined as $k_B T \chi_M = \sum_{\{i,j\}} \langle \sigma_i \sigma_j \rangle \langle \sigma_i \rangle \langle \sigma_j \rangle$
- Approaching T_c results in divergence of $\xi \to$ susceptibility saturates as $\xi \sim L$

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Consider the magnetic susceptibility:

- Can be defined as $k_B T \chi_M = \sum_{\{i,j\}} \langle \sigma_i \sigma_j \rangle \langle \sigma_i \rangle \langle \sigma_j \rangle$
- Approaching T_c results in divergence of $\xi \to$ 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 $t = (T - T_c)/T_c$

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

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

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

• $g(x) \rightarrow \text{const.}$ as $x \rightarrow \infty$

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

 $g(x)$ should also satisfy:

•
$$g(x) \rightarrow \text{const.}$$
 as $x \rightarrow \infty$
• $g(x) \propto x^{\gamma/\nu}$ as $x \rightarrow 0$

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Motivating the Scaling Function

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

•
$$g(x) \rightarrow \text{const.}$$
 as $x \rightarrow \infty$

•
$$g(x) \propto x^{\gamma/\nu}$$
 as $x \to 0$

 First constraint: Ensures correct powerlaw behaviour in TD limit.

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

g(x) should also satisfy:

•
$$g(x) \rightarrow \text{const.}$$
 as $x \rightarrow \infty$

•
$$g(x) \propto x^{\gamma/\nu}$$
 as $x \to 0$

- First constraint: Ensures correct powerlaw behaviour in TD limit.
- Second constraint: Ensures temperature independent Magnetic Susceptibility for $\xi \gg L$

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

•
$$g(x) \to \text{const.}$$
 as $x \to \infty$

•
$$g(x) \propto x^{\gamma/\nu}$$
 as $x \to 0$

- First constraint: Ensures correct powerlaw behaviour in TD limit.
- $\, \circ \,$ 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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$$\begin{split} M &= L^{-\beta/\nu} g_M(t L^{1/\nu})\\ \chi &= L^{\gamma/\nu} g_\chi(t L^{1/\nu}) \end{split}$$

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Note: Only valid for

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Note: Only valid for

• Temperatures close enought to T_c

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Note: Only valid for

- 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 $C = L^{\alpha/\nu}g_C(tL^{1/\nu})$

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



Figure: With correct exponents we see data collapse near T_c

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

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

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

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



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

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

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How to obtain T_c ? • Order Parameter $\neq 0$ $\forall T < \infty$

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How to obtain T_c ? • Order Parameter $\neq 0$ $\forall T < \infty$



Figure: The order parameter is never zero.

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How to obtain T_c ?

 No divergence of Correlation Length, Magnetic Susceptibility or HeatCapacity

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Figure: The quantities do not diverge.

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Different Solutions for this problem

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

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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 $T_c(L)$

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• Denote temperature where χ has maximum by $T_c(L)$

• Assumption: $\xi(T_c(L) - T_c) = aL$

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• 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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• Denote temperature where χ has maximum by $T_c(L)$

• Assumption:
$$\xi(T_c(L) - T_c) = aL$$

Since $\xi(x) \propto |x|^{-\nu}$
 $T_c(L) = T_c + bL^{-1/\nu}$

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

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$T_c(L) = T_c + bL^{-1/\nu}$ Problem: 3 tunable Parameters (T_c, b, ν)
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$T_c(L) = T_c + bL^{-1/\nu}$ Problem: 3 tunable Parameters (T_c, b, ν)

Need data with good statistical accuracy

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$T_c(L) = T_c + bL^{-1/\nu}$ 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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Figure: Prof. Dr. Kurt Binder

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

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

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

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

• For $T < T_c \langle M^4 \rangle_L = \langle M^2 \rangle_L^2$

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Figure: Binder Parameter for the 3D Ising Model

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Figure: Obtaining of ν with FSS of U_L

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Figure: Obtaining of ν with FSS of U_L

• β canceled out

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Figure: Obtaining of ν with FSS of U_L

- β canceled out
- T_c obtained via point of intersection

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Figure: Obtaining of ν with FSS of U_L

- $\bullet \ \beta$ canceled out
- T_c obtained via point of intersection
- \Longrightarrow Have to tune only ν

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Similarly to the Binder Cumulant method we can derive T_c with $\boldsymbol{\xi}$

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Similarly to the Binder Cumulant method we can derive T_c with $\boldsymbol{\xi}$

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

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Similarly to the Binder Cumulant method we can derive T_c with $\boldsymbol{\xi}$

since
$$\xi_L = Lg_{\xi}(tL^{1/\nu}) \qquad \stackrel{T \to T_c}{\longrightarrow} \qquad \xi_L/L = g_{\xi}(0)$$

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Similarly to the Binder Cumulant method we can derive T_c with $\boldsymbol{\xi}$

since
$$\xi_L = Lg_{\xi}(tL^{1/\nu}) \qquad \stackrel{T \to T_c}{\longrightarrow} \qquad \xi_L/L = g_{\xi}(0)$$

Therefore ξ_L for different L intersect at T_c

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Similarly to the Binder Cumulant method we can derive T_c with ${\ensuremath{\mathcal E}}$

since $\xi_L = Lg_{\xi}(tL^{1/\nu}) \xrightarrow{T \to T_c} \xi_L/L = g_{\xi}(0)$ Therefore ξ_L for different L intersect at T_c



Figure: Obtaining T_c with ξ

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 $\bullet~T_c$ obtained via point of intersection

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• T_c obtained via point of intersection

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• Finite Size Scaling will not work

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

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Big Problem!

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

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Example: Ising Model

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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

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• Plot Histogram of ${\cal M}$ - increase system size

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Plot Histogram of M - increase system size If Peaks merge ⇒ 2nd order transition

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${\ensuremath{\, \bullet }}$ 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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• Can not obtain good values for critical exponents

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Or Can not obtain good values for critical exponents
 ⇒ No data collapse

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

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• Look at Maxima of TD quantities at T_c



Figure: 1st Order Phase Transition

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

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= 900

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

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- Behaviour of Histogram Peaks
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= 900

If we have weak 1st order phase transition

Scaling might work quite well (with completely wrong exponents)

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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

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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

 \implies Active area of research

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• Finite Size Effects

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$$\begin{split} \tau_A &\equiv \int_0^\infty \phi_A dt \\ \langle (\delta A)^2 \rangle &\equiv \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left(1 + 2 \frac{\tau_A}{\delta t} \right) \end{split}$$

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Summary

$$\tau_A \equiv \int_0^\infty \phi_A dt$$
$$\langle (\delta A)^2 \rangle \equiv \frac{1}{\mathcal{N}} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \left(1 + 2 \frac{\tau_A}{\delta t} \right)$$

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

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

Near 2nd order phase transitions \(\tau_A\) diverges (critical slowing down)

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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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- - Binder Cumulant

- Problem of the Weak 1st Order Transition



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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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- Have seen different possibilities to obtain T_c
- Problem: Distinguishing between 1st and 2nd order transitions

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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
- Have seen one of the important error contributions

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• I would like to thank Dr. Munehisa Matsumoto