Introduction to spin systems and phase transitions

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Phase transitions

- A thermodynamic (macroscopic) system can exist in different phases
  - Example 1: Water, ice, steam
  - Example 2: paramagnet, ferromagnet
- When external controls (temperature) are changed slightly, properties (density)
  - Most of the time change slightly
  - Sometimes abruptly, changing phase $\Longrightarrow$ phase transition
- Study of phase transitions has been a central theme of statistical mechanics.

Role of statistical mechanics

- Discussed in detail by Sitabhra
- Bridging scales from micro to macro
- Example: start with gas of particles and determine macroscopic properties like pressure, temperature
- Molecules to protein to DNA to cells to tissues to organs
- People to society to country

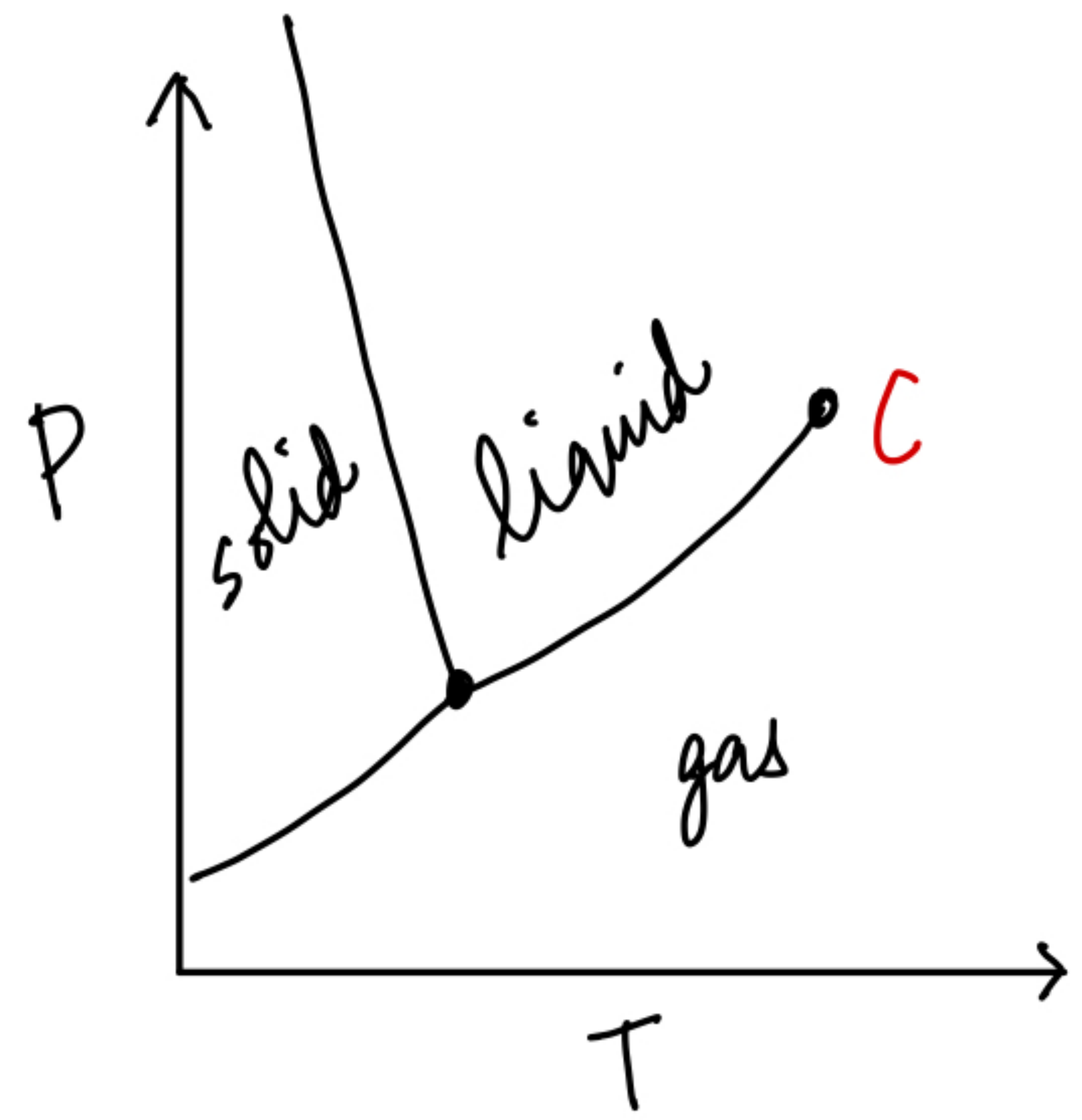
In these lectures …

- Introduce spin models as prototypical models for studying past transitions
- Later, they will have their own importance as minimal models for different phenomena
- Will discuss how to study them
  - Mean field theories
  - Phase transitions
  - Critical behaviour
  - Numerical methods (Markov models and detailed balance)
  - How to numerically characterise phase transitions

These might look intimidating to some, but

Fortunately, in my first year of graduate school, I had the good luck to fall into the hands of senior physicists who insisted, over my anxious objections, that I must start doing research, and pick up what I needed to know as I went along. It was sink or swim. To my surprise, I found that this works. I managed to get a quick PhD - though when I got it I knew almost nothing about physics. But I did learn one big thing: that no one knows everything, and you don't have to. [Weinberg, first golden rule of research]

Phase diagram of water



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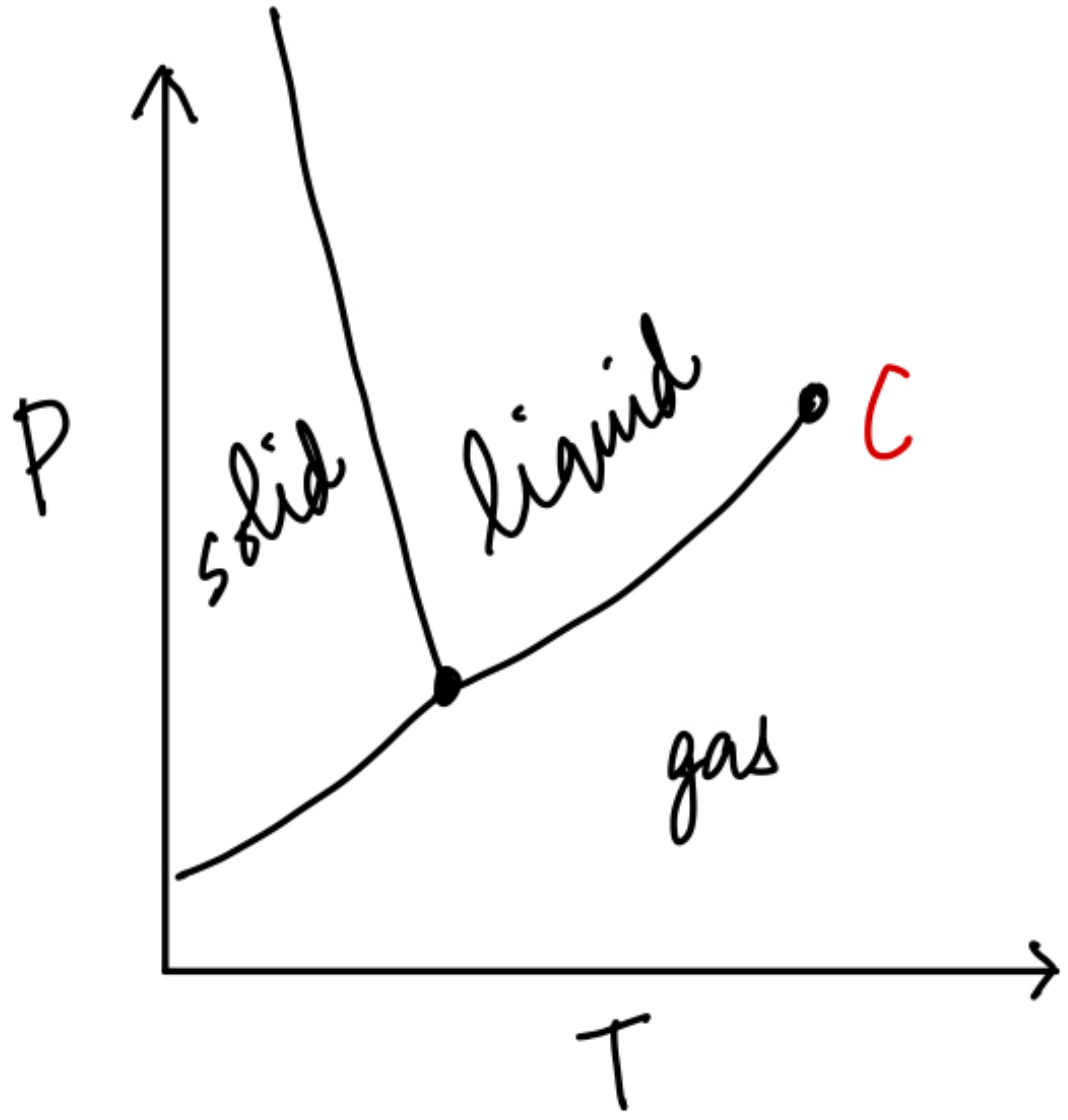

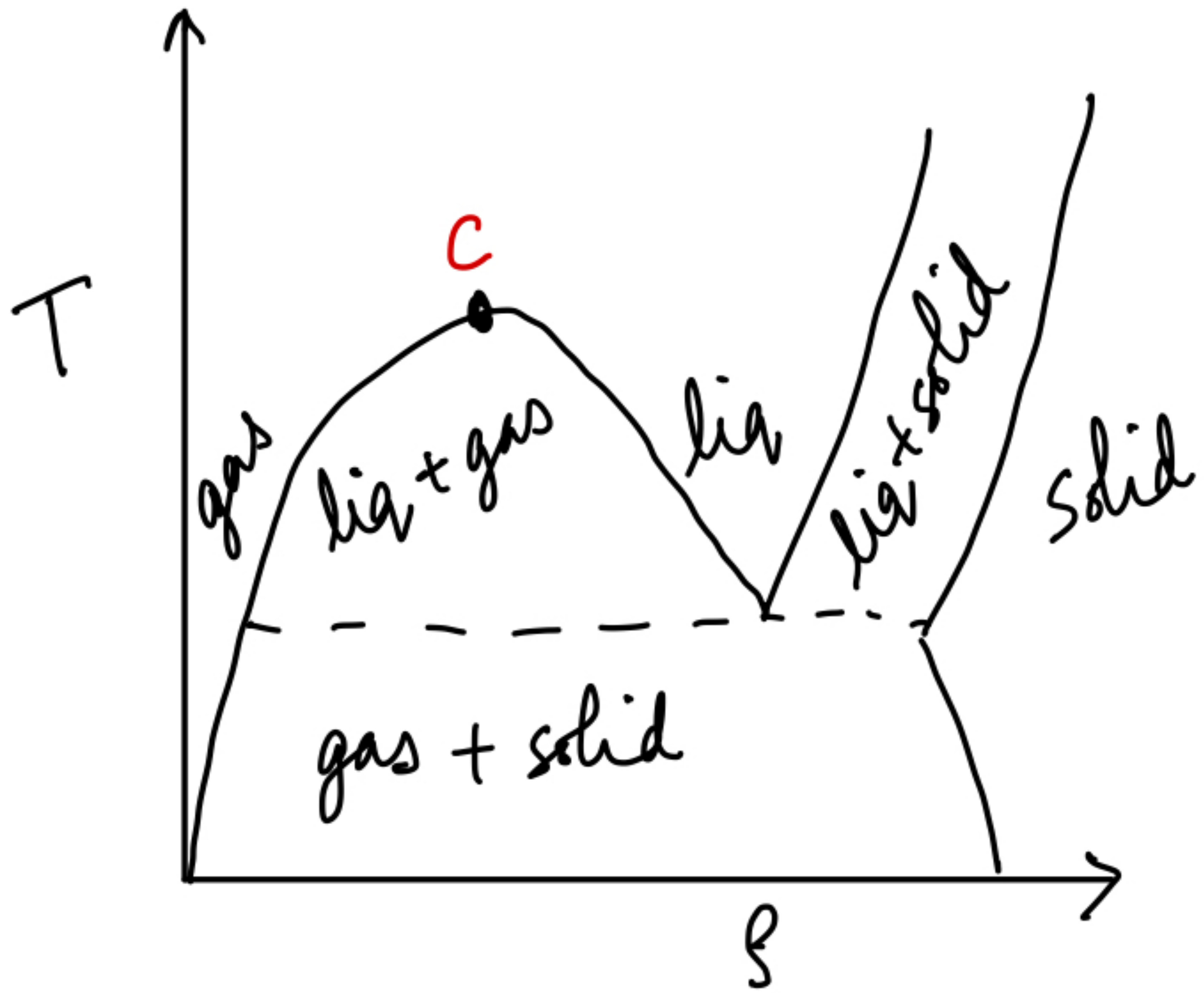

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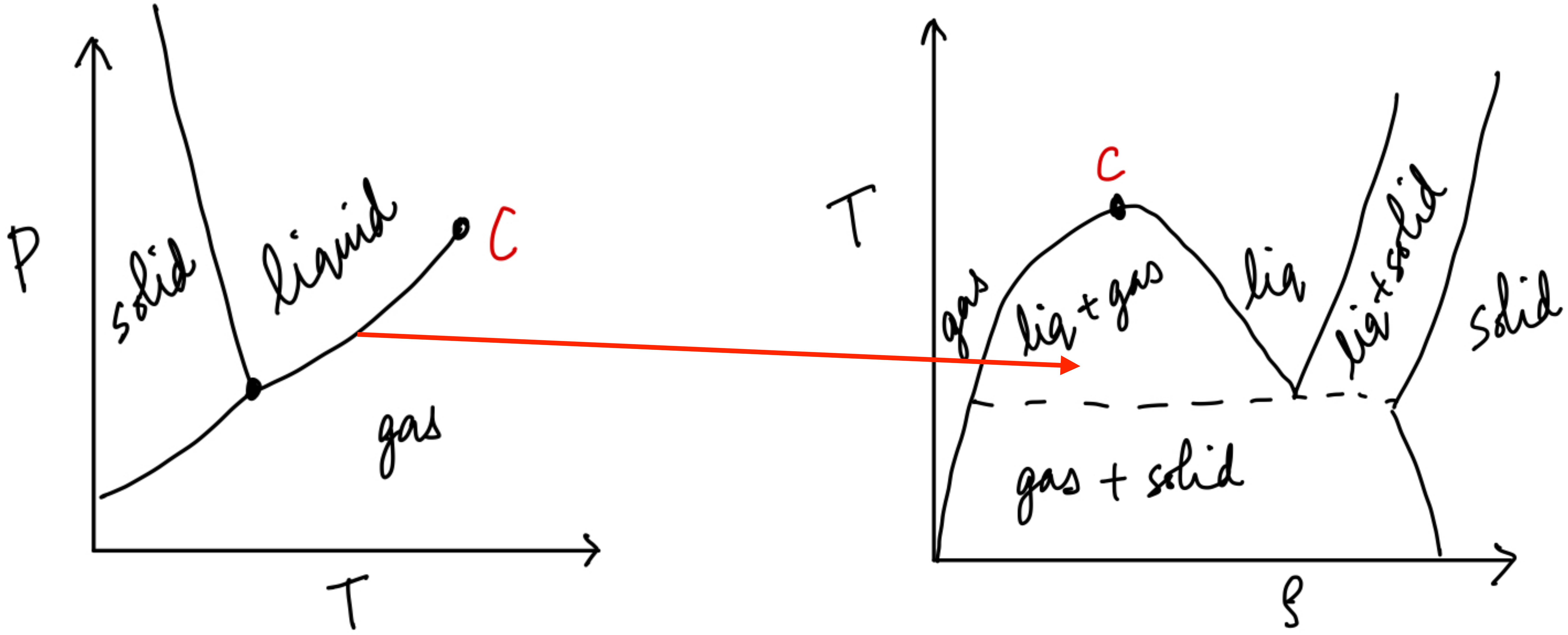

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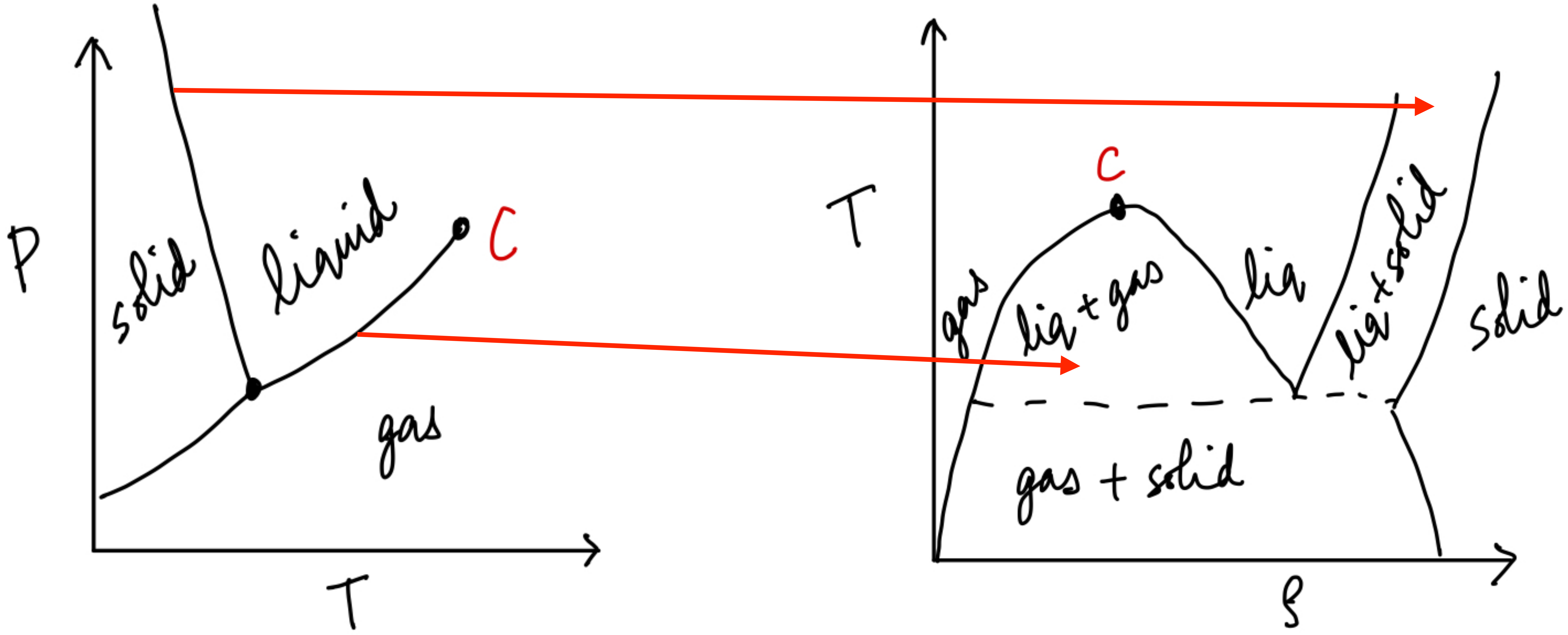

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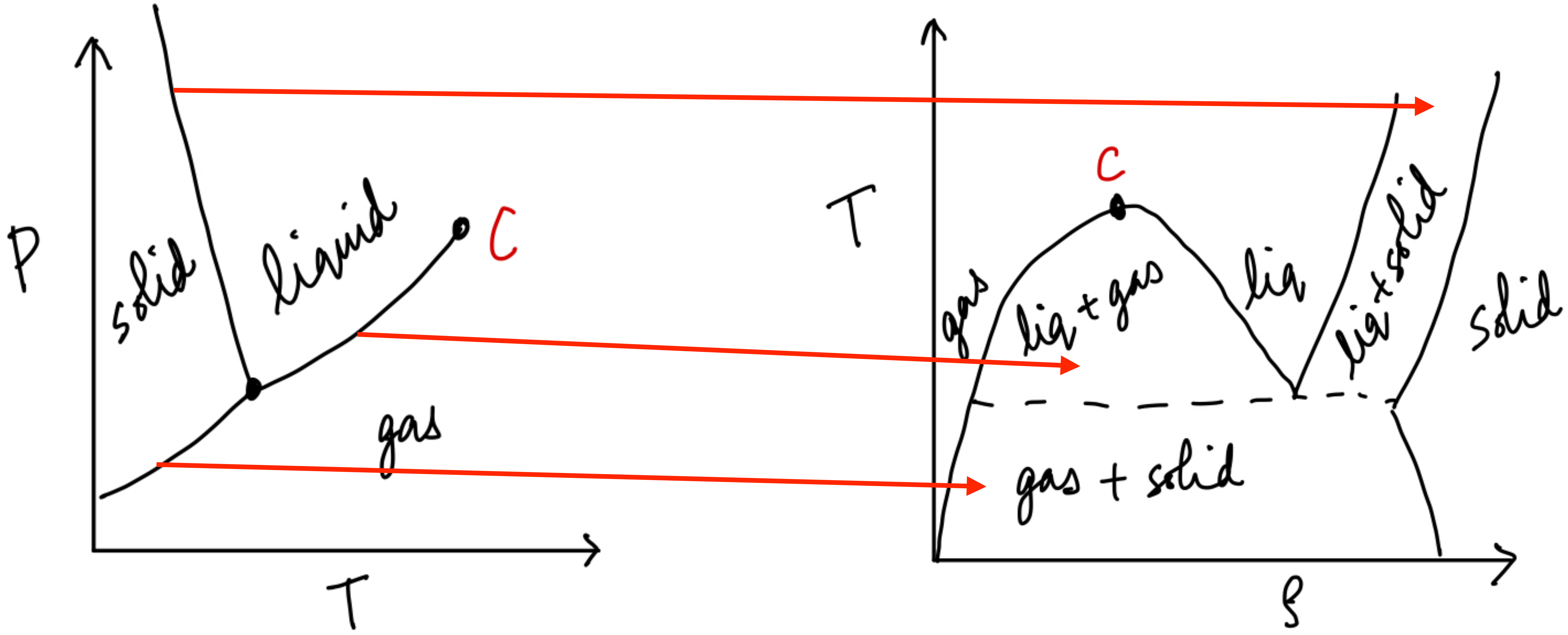
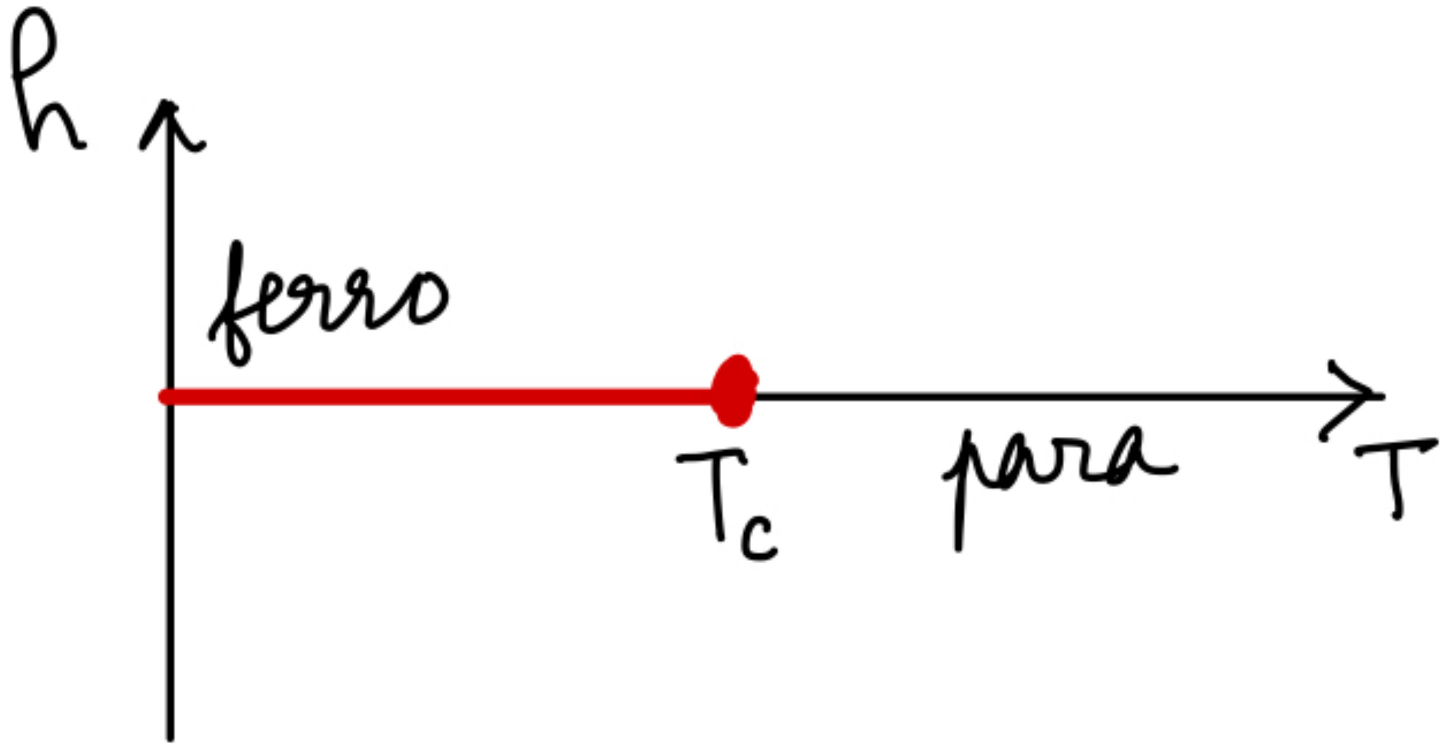
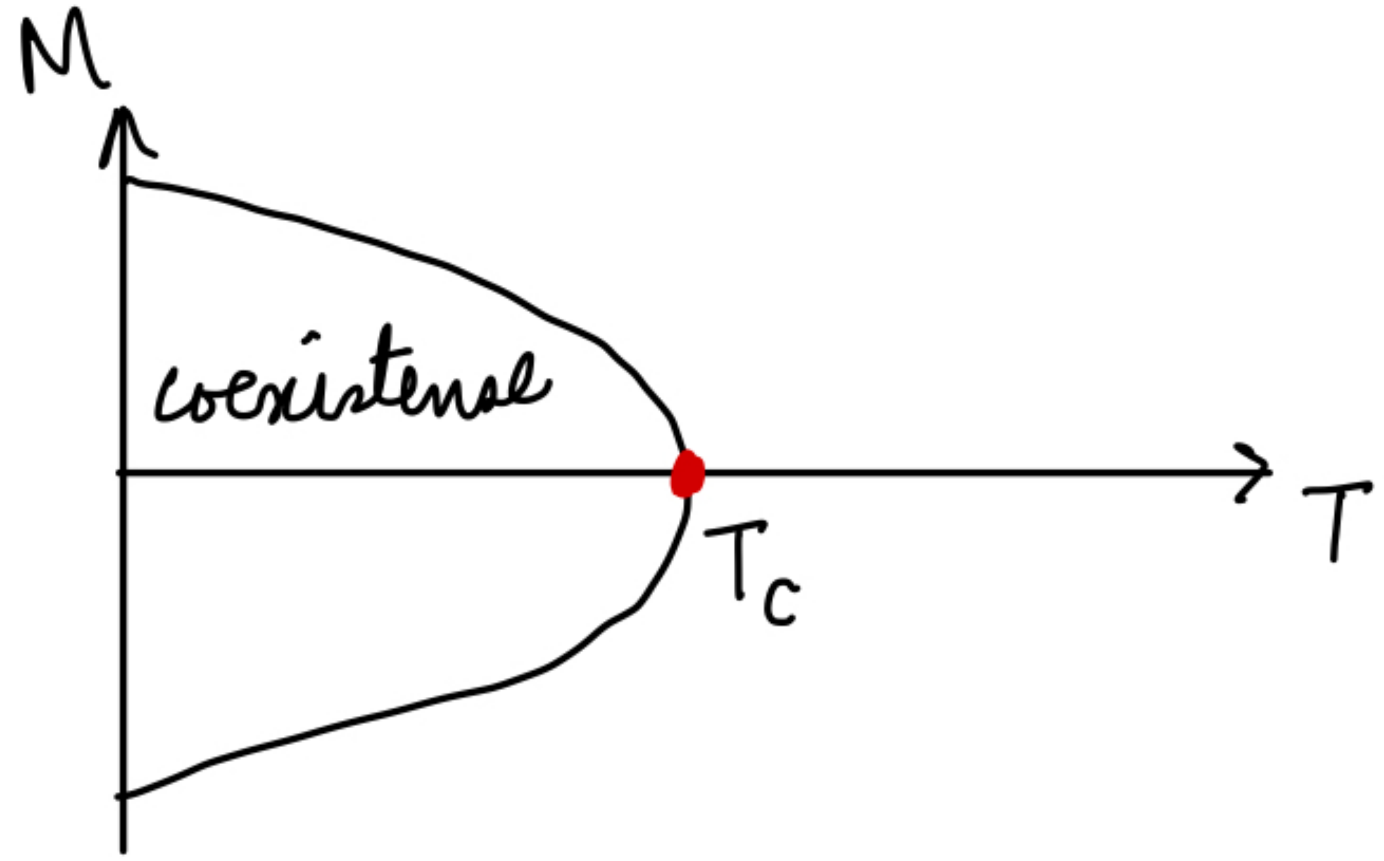
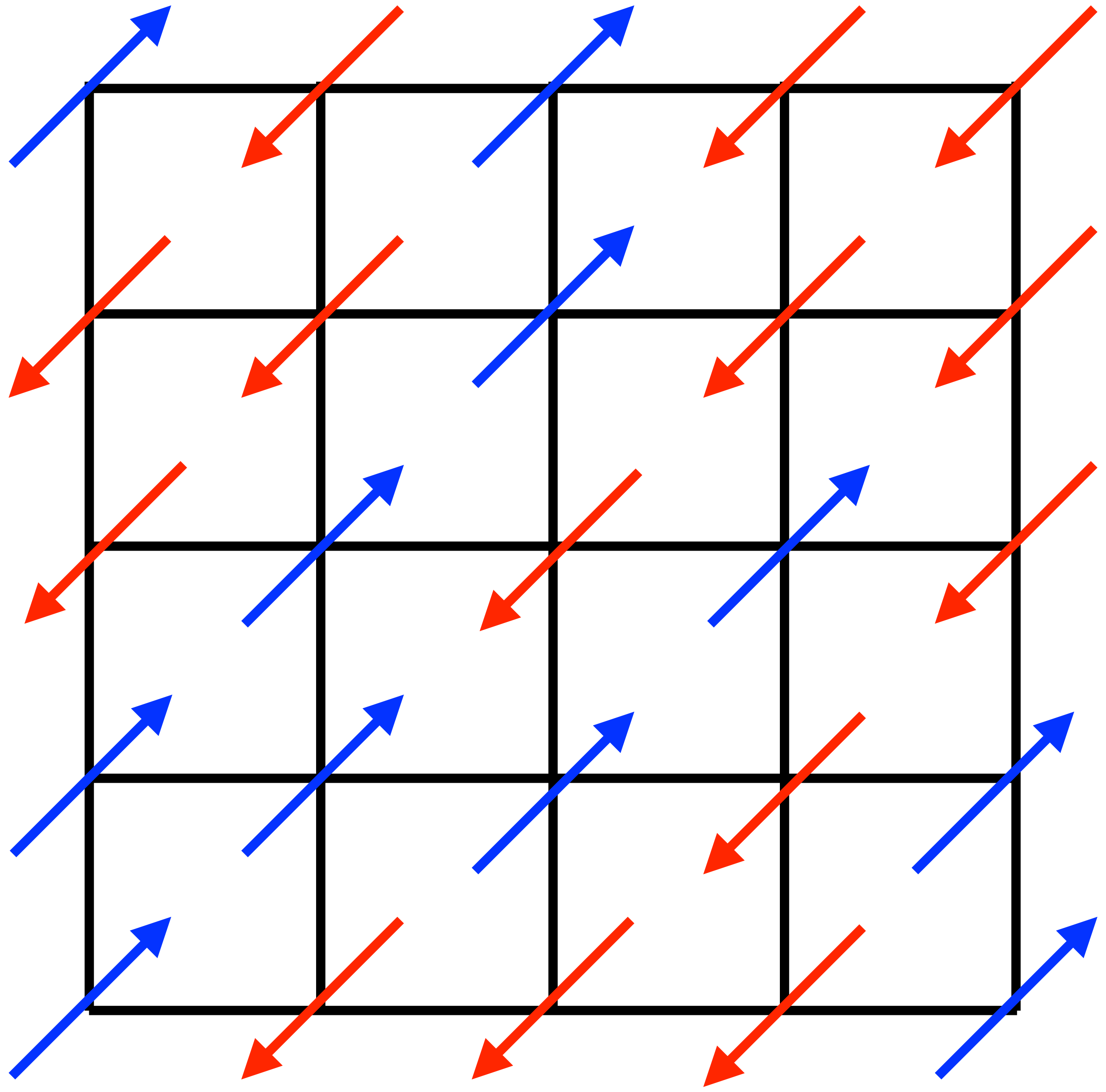


Phase diagram of a magnet





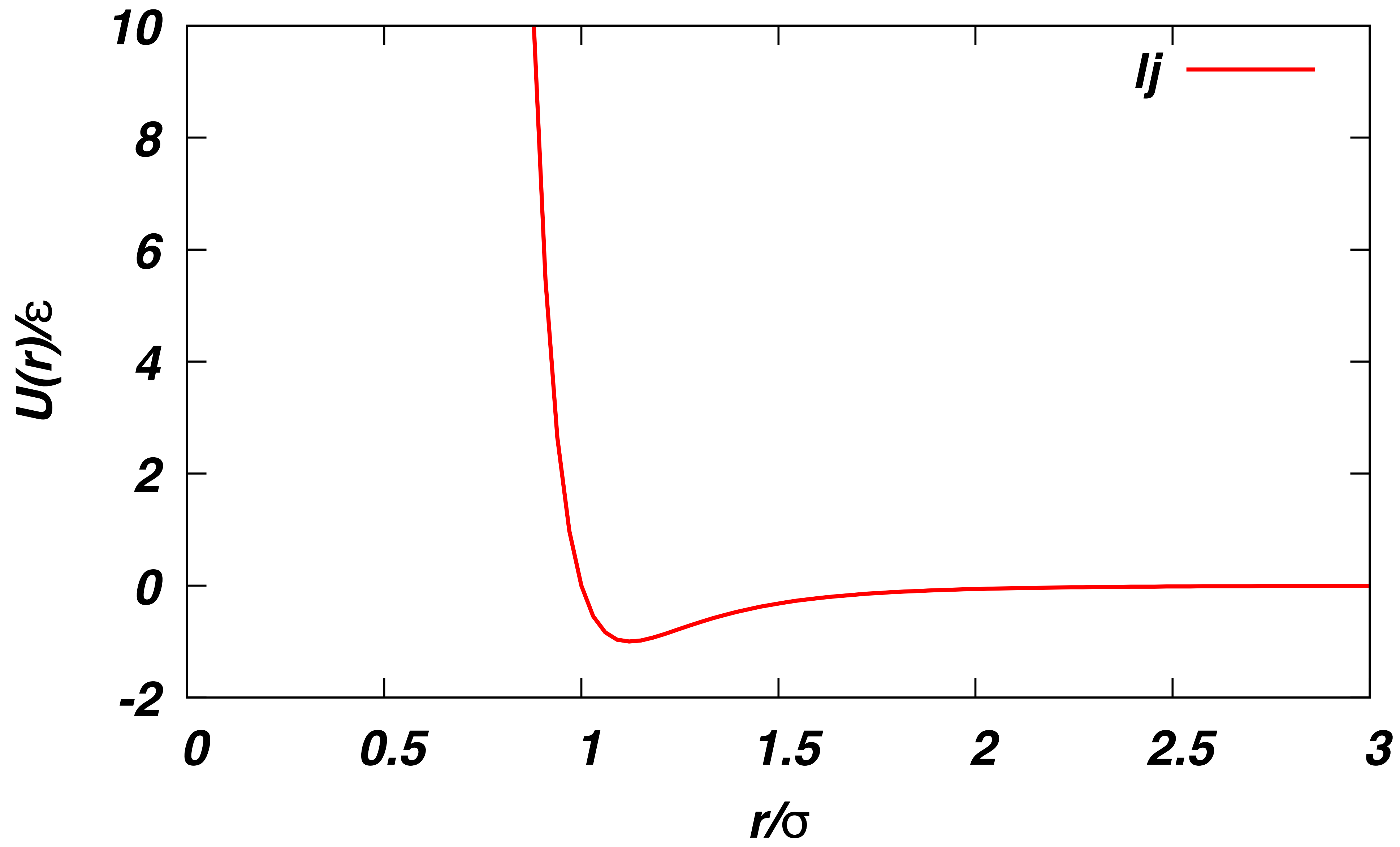
Ising Model



- At each site a spin
  - 2 orientations $S_i = \pm 1$
- Energy $\mathscr{H} = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$
- Neighbouring spins aligning decreases energy
- Magnetic field breaks plus/minus symmetry
- Boundary conditions
  - Periodic (not necessary)
  - Translational symmetry (no edge effects)

Lattice gas

- A generic inter-particle potential
  - Lennard Jones
  - $$U(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



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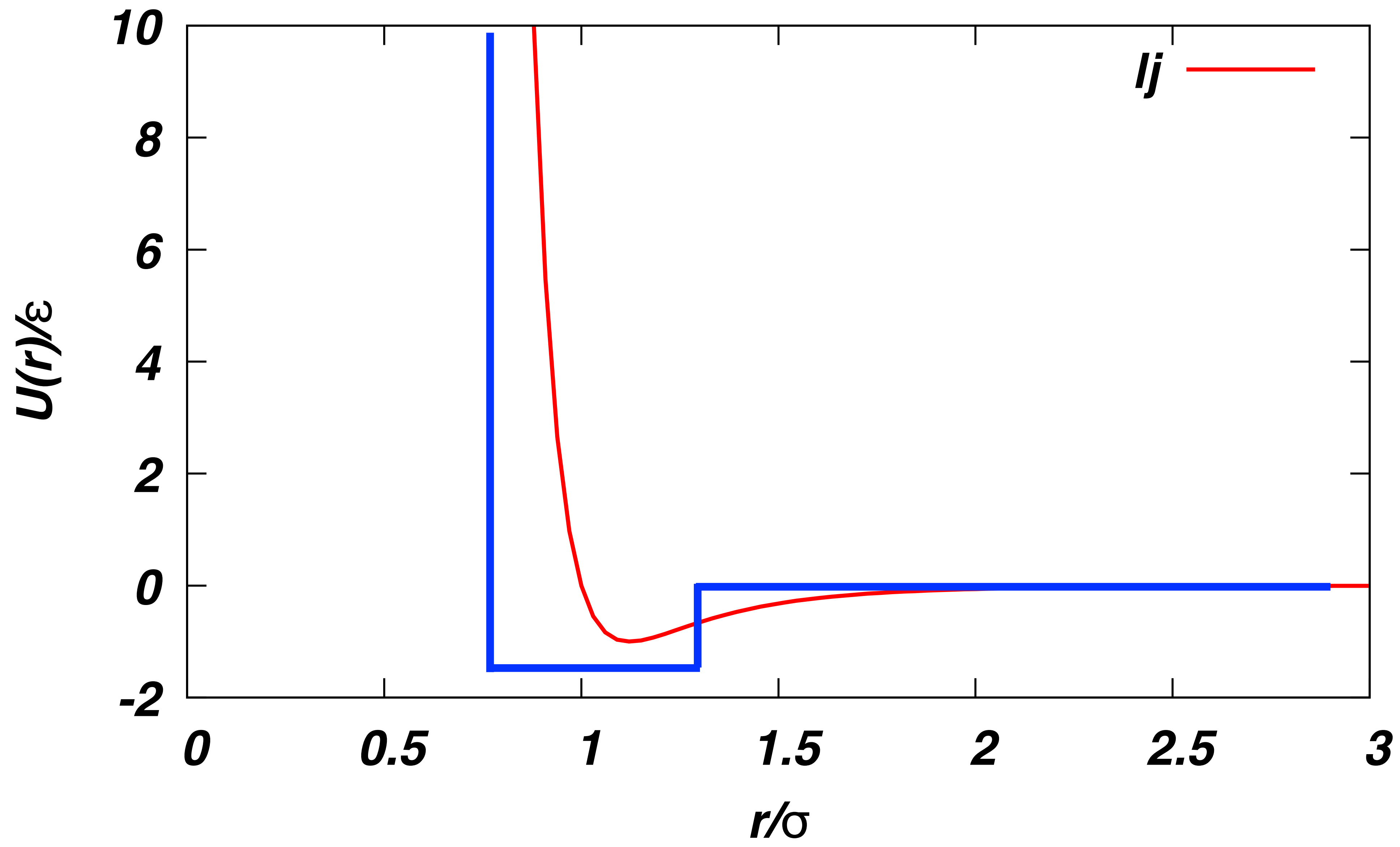

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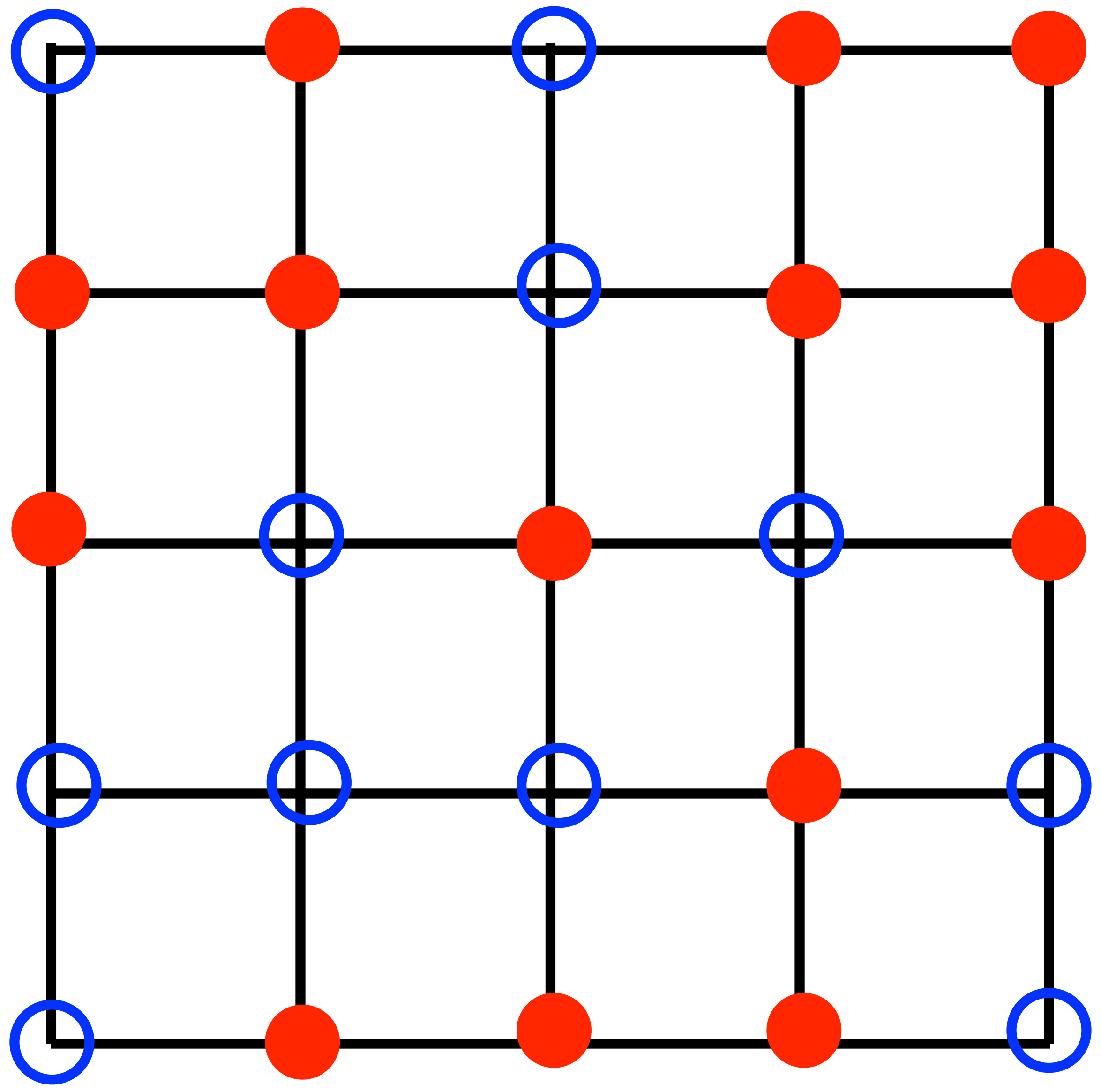

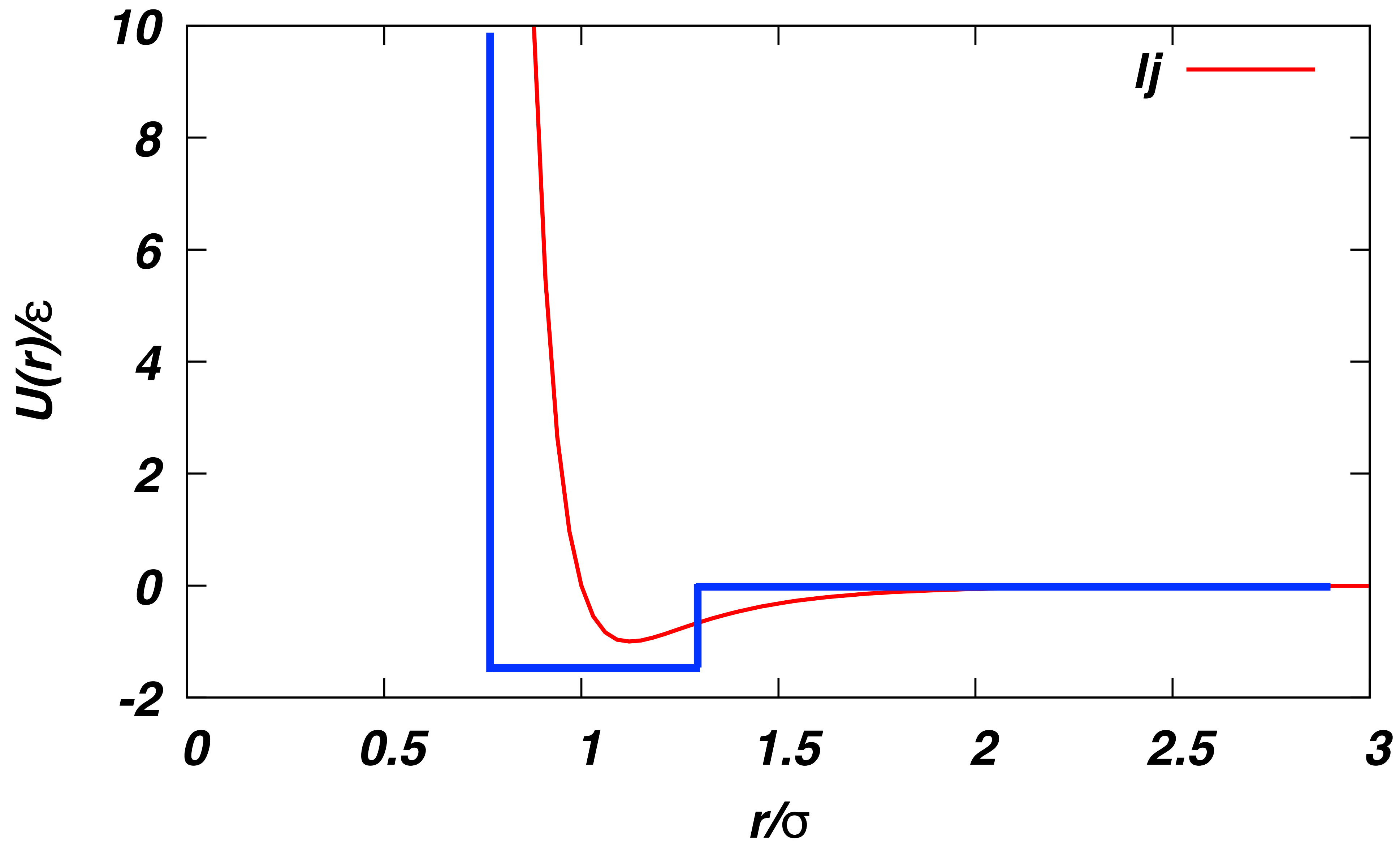

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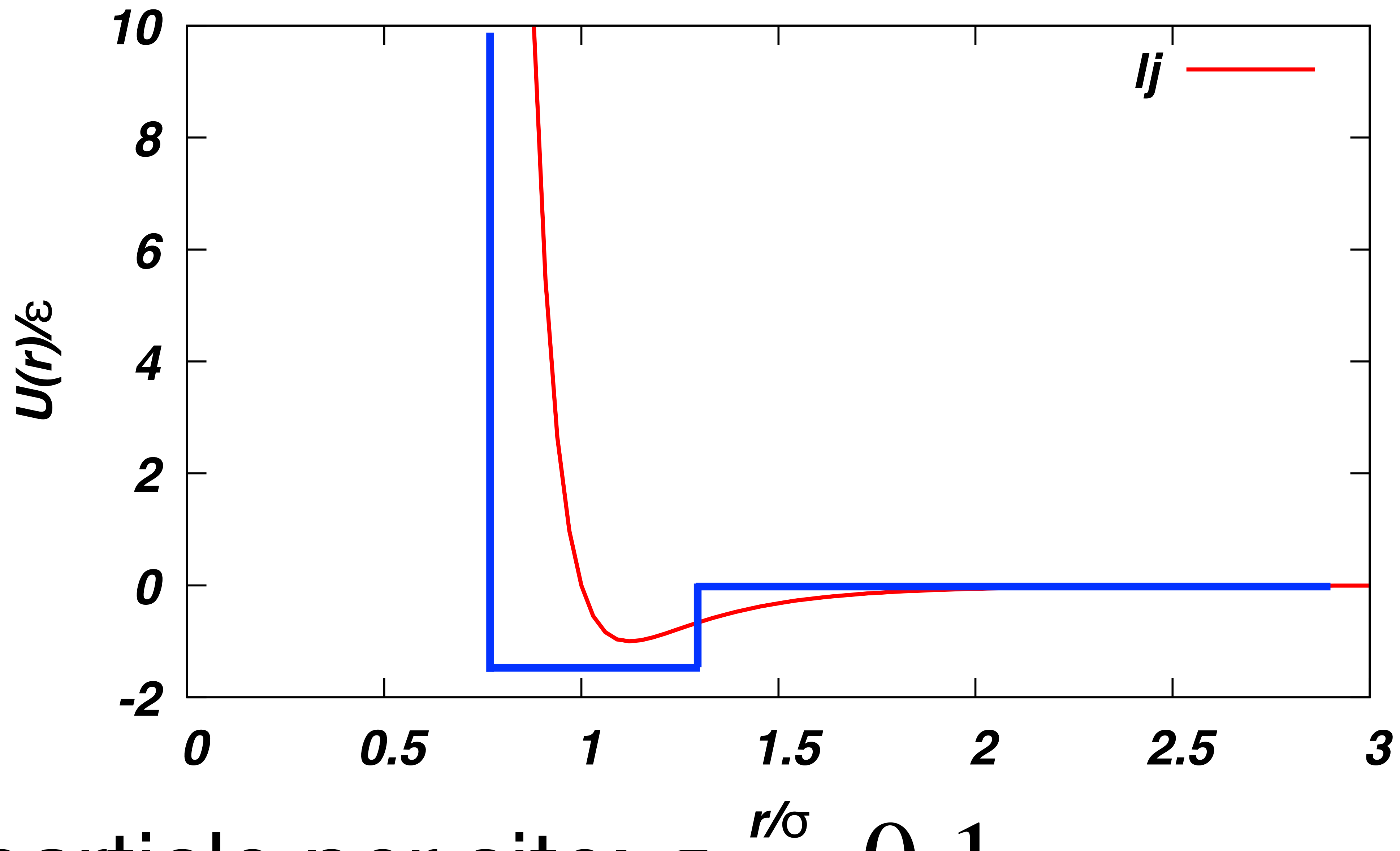
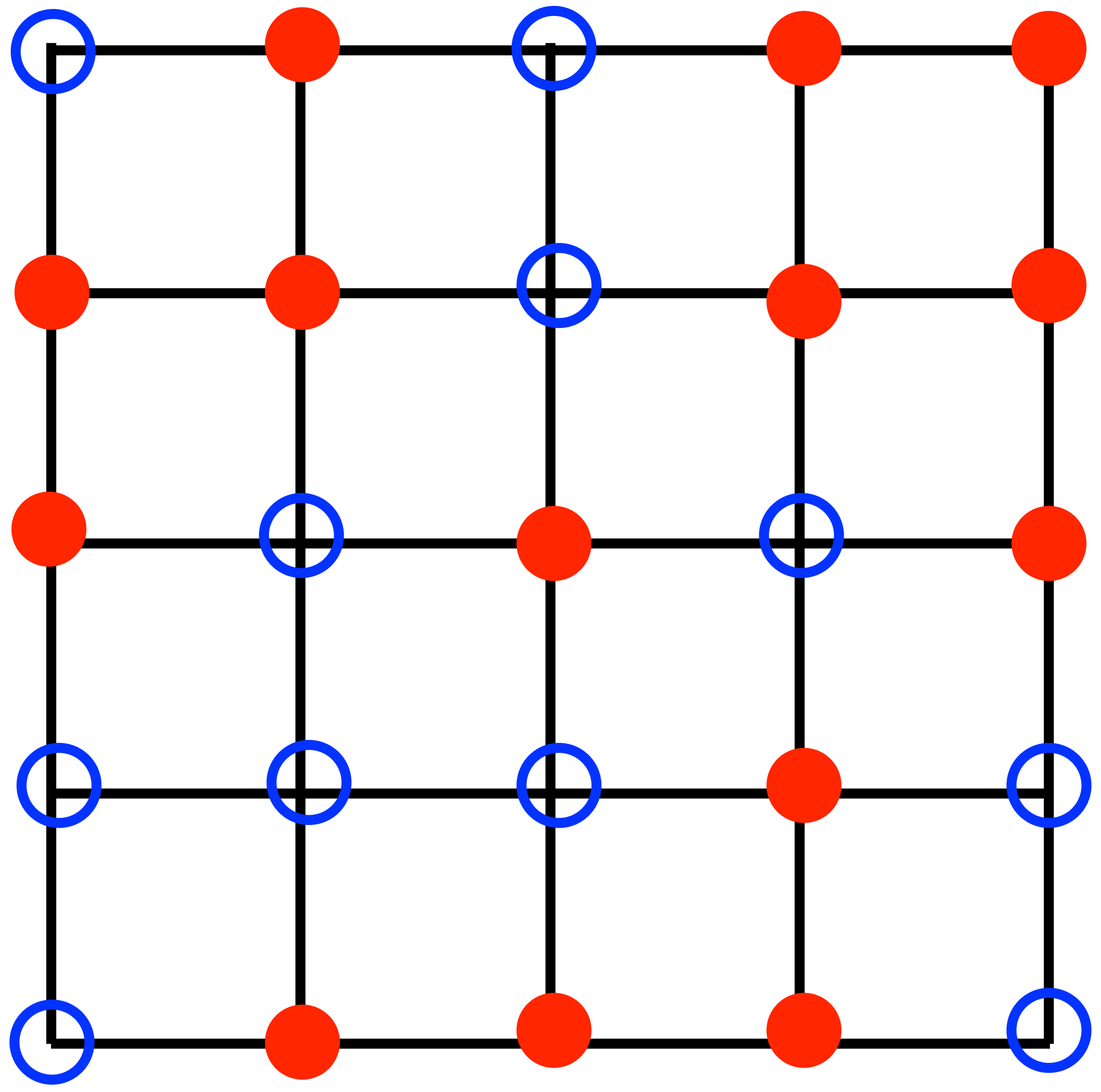




- Utmost one particle per site: $\tau_i = 0,1$
- Energy $\mathscr{H} = -\epsilon \sum_{\langle ij \rangle} \tau_i \tau_j - \mu \sum_i \tau_i$
- Change variables: $\sigma_i = 2\tau_i - 1$
- $\sigma_i = \pm 1$

Ising $\leftrightarrow$ Lattice gas

$$H = -\epsilon \sum_{\langle ij\rangle} \left(\frac{1+\sigma_i}{2}\right)\left(\frac{1+\sigma_j}{2}\right) - \mu \sum_j \frac{1+\sigma_j}{2}$$

$$= -\frac{\epsilon}{4} \sum_{\langle ij\rangle} \left(1 + \sigma_i + \sigma_j + \sigma_i \sigma_j\right) - \frac{\mu N}{2} - \mu \sum_j \sigma_j$$

$$= \underbrace{-\frac{\epsilon}{4} \sum_{\langle ij\rangle} \sigma_i \sigma_j - \left(\frac{\epsilon}{2} + \mu\right) \sum_j \sigma_j}_{\text{Ising model}} - \underbrace{\frac{\epsilon q}{8} - \frac{\mu N}{2}}_{\text{constant}}$$

$$J = -\frac{\epsilon}{4} \,;\quad h = \mu + \frac{\epsilon}{2} \,;\quad \sigma_i = S_i = \pm 1$$

How to analyse?

- Given $\mathscr{H} = -J\sum_{\langle ij \rangle} S_i S_j - h\sum_i S_i$, how to proceed?
- Recipe for calculation
  - A configuration C has energy $E(C)$
  - Then $\mathrm{Prob}(C) = \dfrac{\exp[-\beta E(C)]}{\sum_{C'} \exp[-\beta E(C')]}$
  - $\langle O \rangle = \sum_C O(C)\mathrm{Prob}(C)$

Different ways to analyse

- Solve exactly (unlikely)
- Low temperature expansion
- High temperature expansion
- Mean field theory
  - Curie-Weiss
  - Bethe lattice
  - Variational
- Simulations
- Etc

Symmetries

- $\mathscr{H} = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$
- When $h = 0$ then $\mathscr{H}(\{S\}) = \mathscr{H}(\{-S\})$
- Then, can we have a phase where $m = \langle S \rangle \neq 0$
- Such a phase would break the symmetry
- Similar example is a crystal
  - Hamiltonian has continuous translational symmetry
  - Crystal has discrete translational symmetry

Low and high temperature limits

Free Energy $F = E - TS$ $[F = -kT \ln Z]$

F is minimized

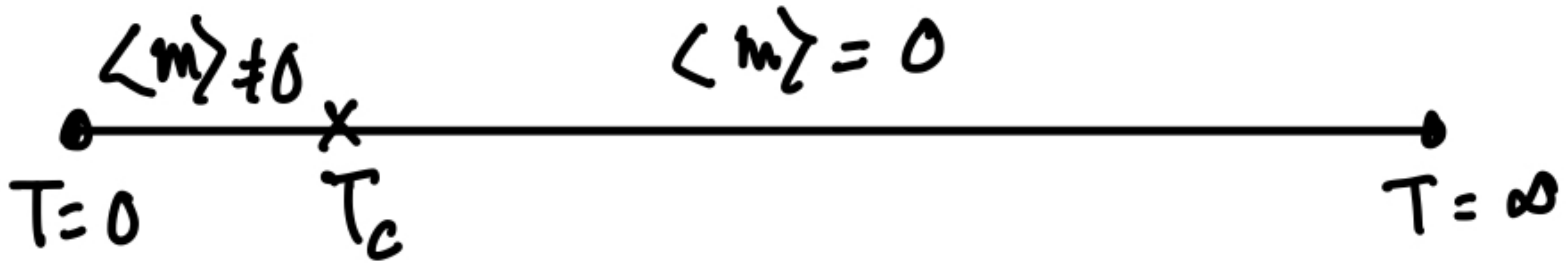
When $T = 0$, no entropic contribution

$\Rightarrow \uparrow\uparrow\uparrow\uparrow\ldots$ or $\downarrow\downarrow\downarrow\downarrow$ $\qquad \langle |m| \rangle = 1$

When $T = \infty$, entropy is maximised

$\Rightarrow \uparrow\downarrow\uparrow\uparrow\downarrow$ - each spin random

$\Rightarrow \langle m \rangle = 0$



Is $T_c > 0$?

Ans: only in $d \geq 2$ [Peierls argument]

Age old Curie-Weiss MFT

- Isolate a spin from its environment
- Spin sees an effective magnetic field
    - $h + J \sum_{j \in nn} S_j$: fluctuating
    - MFA: $\sum_j S_j \approx \sum_j \langle S_j \rangle = qm$
    - $H_{mf} = -(Jqm + h) \sum_i S_i = -h_{eff} S_i$

Curie-Weiss MFT

$$H_{mf} = -h_{eff} \sum_i S_i$$

Partition fn $Z = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} e^{\beta h_{eff}(S_1 + S_2 + \cdots + S_N)}$

$$= \left(e^{\beta h_{eff}} + e^{-\beta h_{eff}}\right)^N$$

$$= \left[2 \cosh(\beta h_{eff})\right]^N$$

$$M = \frac{1}{\beta} \frac{\partial}{\partial h_{eff}} (\ln Z)$$

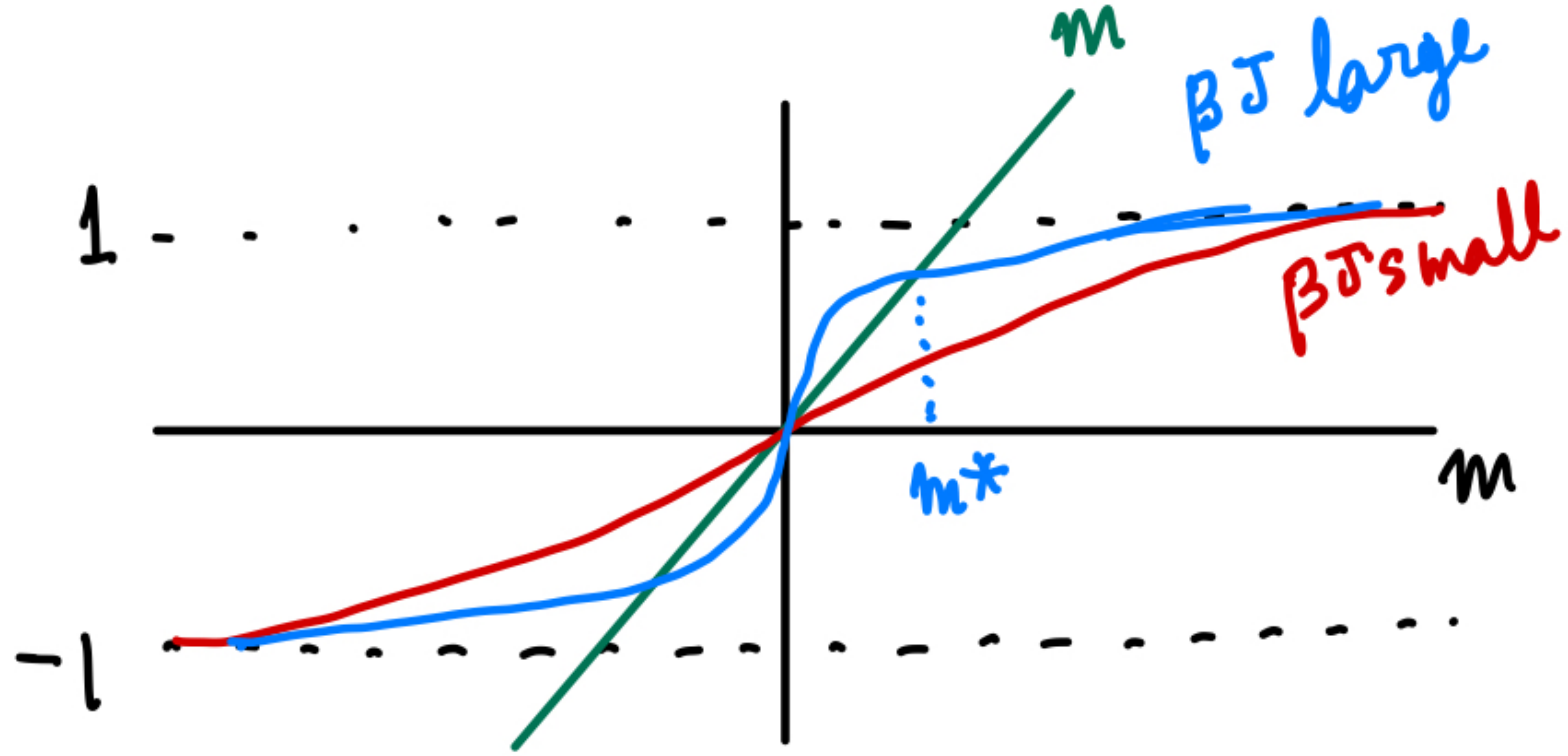
$$= kTN\beta \tanh(\beta h_{eff})$$

$$\Rightarrow m = \frac{M}{N} = \tanh(\beta h_{eff})$$

Solving self-consistent equation

$$m = \tanh \beta(h + Jqm)$$

Consider $h = 0$; $m = \tanh(\beta J q m)$



When does $m^* \neq 0$ exist?

MFT: solution

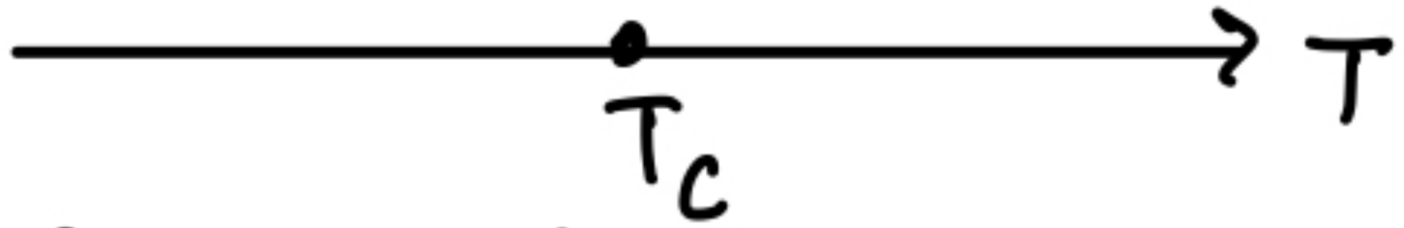
$m = \tanh(\beta J q m)$

When does $m^* \neq 0$ exist?

Ans: when slope of $\tanh(\beta J q m) \geqslant 1$ at $m = 0$

$$\Rightarrow \operatorname{sech}^2(\beta J q m)\, \beta_c J q \Big|_{m=0} = 1$$

or $$\frac{kT_c}{J} = q$$



$T \geqslant T_c$ only one solution $m = 0$

$T < T_c$ three solutions $m = 0, m^*, -m^*$

Which one do we choose?

Choosing solution

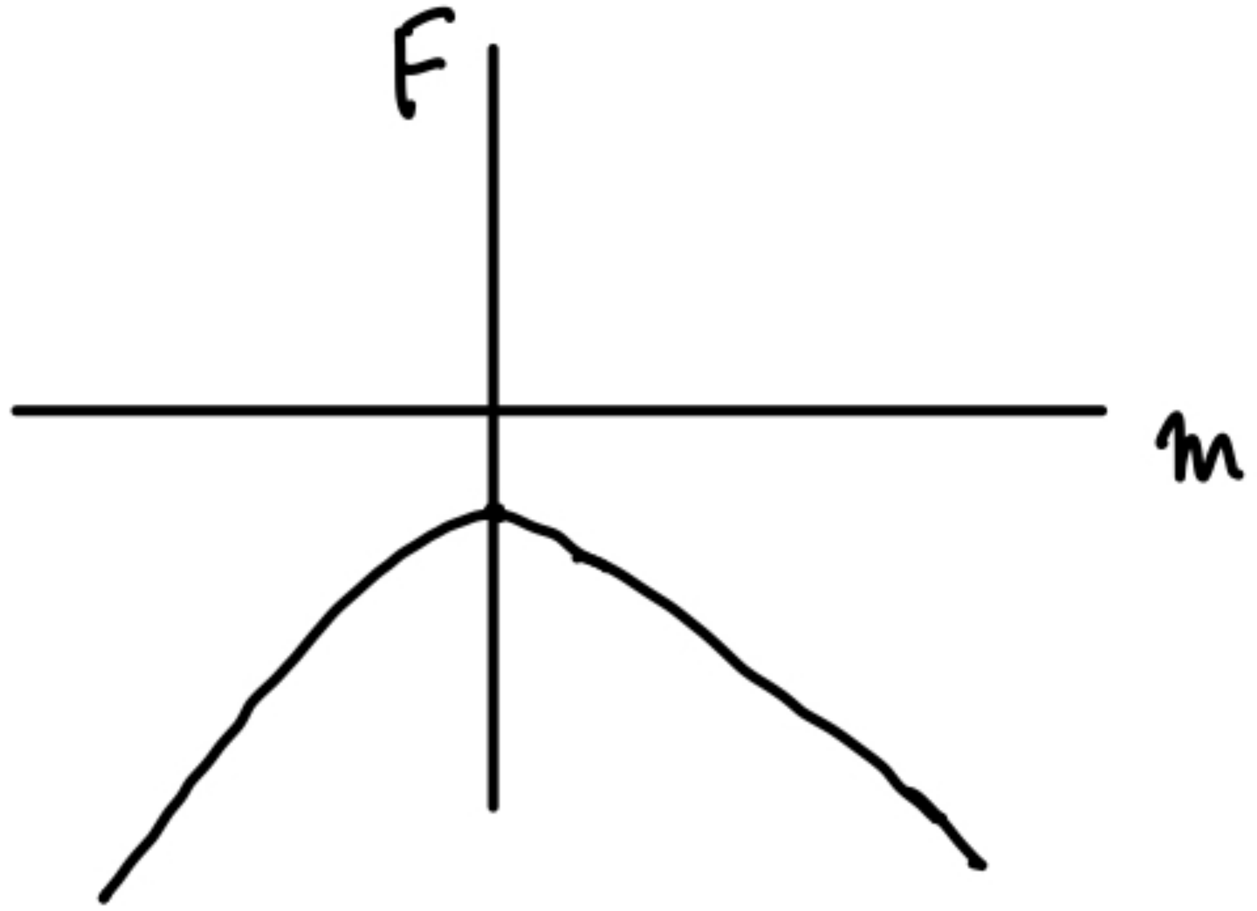
Remember $F = -kT \ln Z$

$= -kTN \ln(2 \cosh \beta J q m)$

$\frac{\partial F}{\partial m} = -kTN \tanh(\beta J m q)\, \beta J q$

$= -NJq \tanh(\beta J m q)$ > 0 for $m < 0$

< 0 for $m > 0$



$\Rightarrow m^* \neq 0$ has lower free energy

$\Rightarrow m^* \neq 0$ is correct solution

Sketching magnetisation

$$m = \tanh\left(\frac{Jq\,m}{T}\right)$$

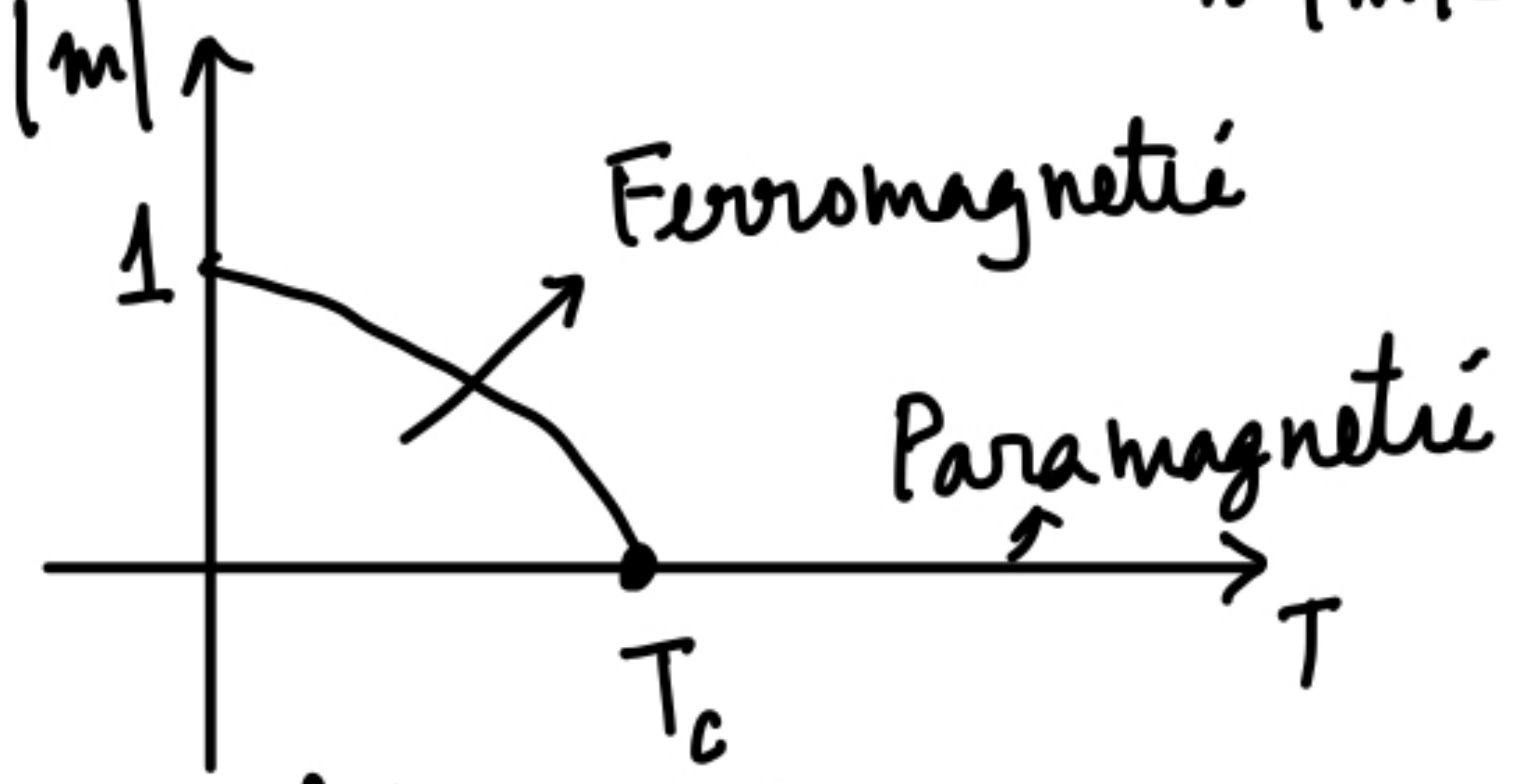
$T > T_c$: $m = 0$

$T = T_c$: $m = 0$

$T < T_c$: $m = m^* \neq 0$

$T = 0$: $RHS = \pm 1$ if $m \gtrless 0$ $\Rightarrow m = \pm 1$

or $|m| = 1$



$\Rightarrow$ non-analytic at T_c

Behaviour near T_c

Let $T = T_c(1-\epsilon)$

$$m^* = \tanh \frac{Jq\, m^*}{T_c(1-\epsilon)} \quad \text{but } T_c = Jq$$

$$m^* = \tanh\left(\frac{m^*}{1-\epsilon}\right) \quad ; \tanh x = x - \frac{x^3}{3} + \cdots$$

$$m^* = \frac{m^*}{1-\epsilon} - \frac{m^{*3}}{(1-\epsilon)^3 3}$$

$$\text{or } \frac{m^{*2}}{3(1-\epsilon)^3} = \frac{1}{1-\epsilon} - 1 = \frac{\epsilon}{1-\epsilon}$$

$$\Rightarrow \quad m^{*2} \approx 3\epsilon$$

$$m^* \propto \sqrt{\epsilon}$$

Critical Exponents

$$m^* \propto \sqrt{\epsilon}$$

Usual Taylor expansion : $m^* \propto \epsilon$

Non-analytic behaviour captured by critical exponent

$$m^* \propto \epsilon^{\beta}$$

$$\beta_{mf} = \frac{1}{2} \qquad [\text{This } \beta \text{ not } 1/kT!]$$

Other exponents (Susceptibility)

Susceptibility $\chi = \left.\frac{\partial m}{\partial h}\right|_{h\to 0}$

$$T = T_c(1+\epsilon)$$

$$m = \tanh \frac{h + Jmq}{Jq(1+\epsilon)}$$

$$\chi = \left.\operatorname{sech}^2 \frac{h+Jmq}{Jq(1+\epsilon)} \times \frac{1}{Jq(1+\epsilon)}\left[1 + Jq\chi\right]\right|_{m=0,\, h=0}$$

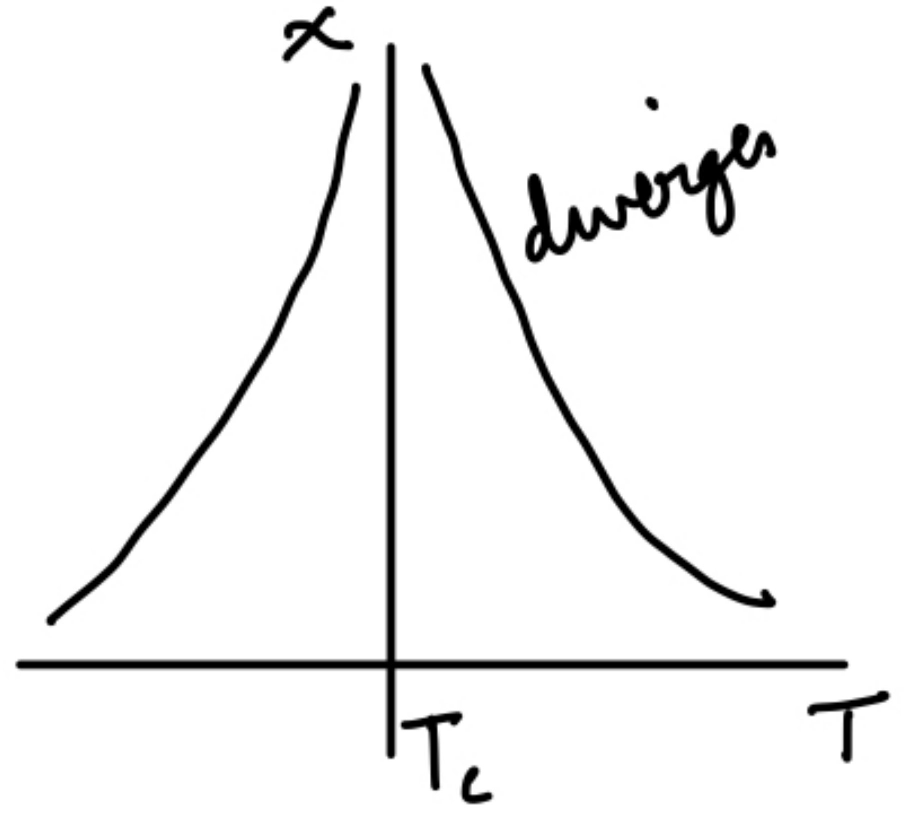
$$\chi\left[1 - \frac{1}{1+\epsilon}\right] = \frac{1}{Jq(1+\epsilon)}$$

$$\chi \frac{\epsilon}{1+\epsilon} = \frac{1}{Jq(1+\epsilon)}$$

$$\chi_{T>T_c} = \frac{1}{Jq\epsilon}$$

$$\chi_{T<T_c} = \frac{1}{2Jq\epsilon}$$

$$\chi \sim |\epsilon|^{-\gamma} \Rightarrow \gamma_{mf} = 1$$



At T_c?

At T_c $$m = \tanh\left[\frac{h + Jqm}{Jq}\right]$$

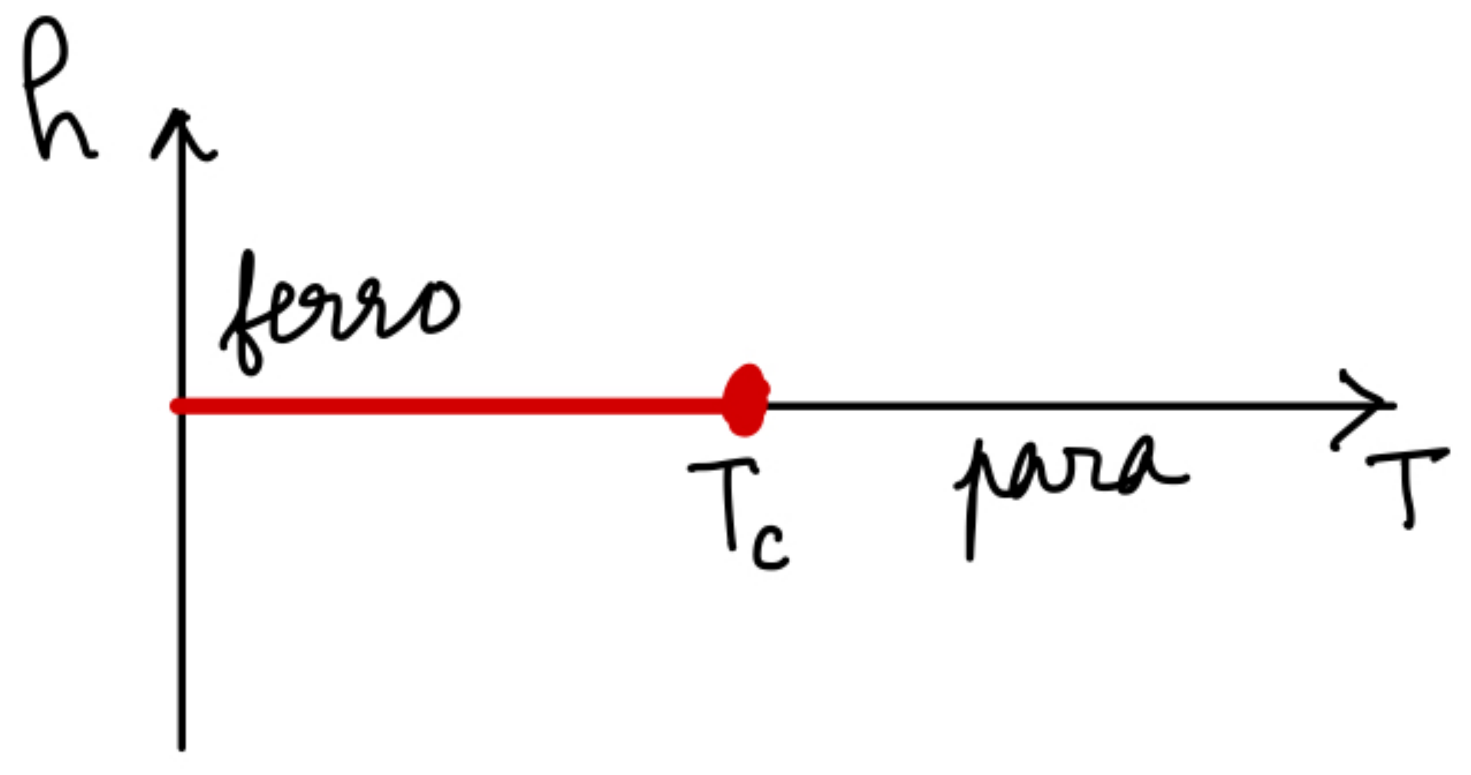
$$m = \frac{h + Jqm}{Jq} - \frac{m^3}{3} + \cdots$$

$$m^3 \approx h$$

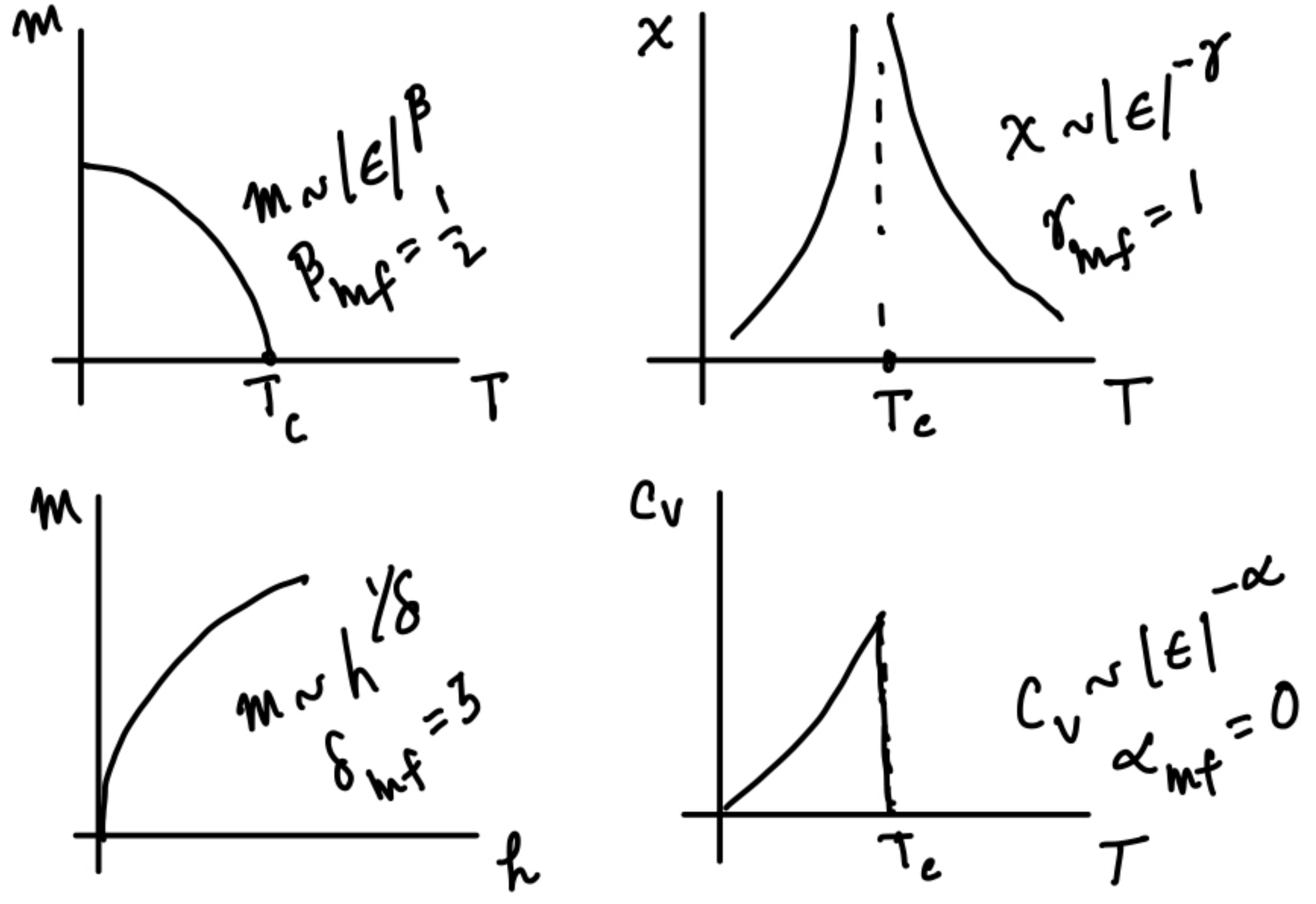
$$m^\delta \sim h$$

$$\delta_{mf} = 3$$

Summary of MFT



$$T_c = Jq$$



Minimal models and MFT

- Water and magnets complicated objects
- But a simple interacting spin model
  - Correct phases
  - Qualitative phase diagram
  - Not the correct T_c
  - What about critical exponents?
- MFT
  - Calculation simple
  - Value of critical exponents wrong ($\beta_{2d} = 1/8; \beta_{mf} = 1/2$)

Minimal models and exponents

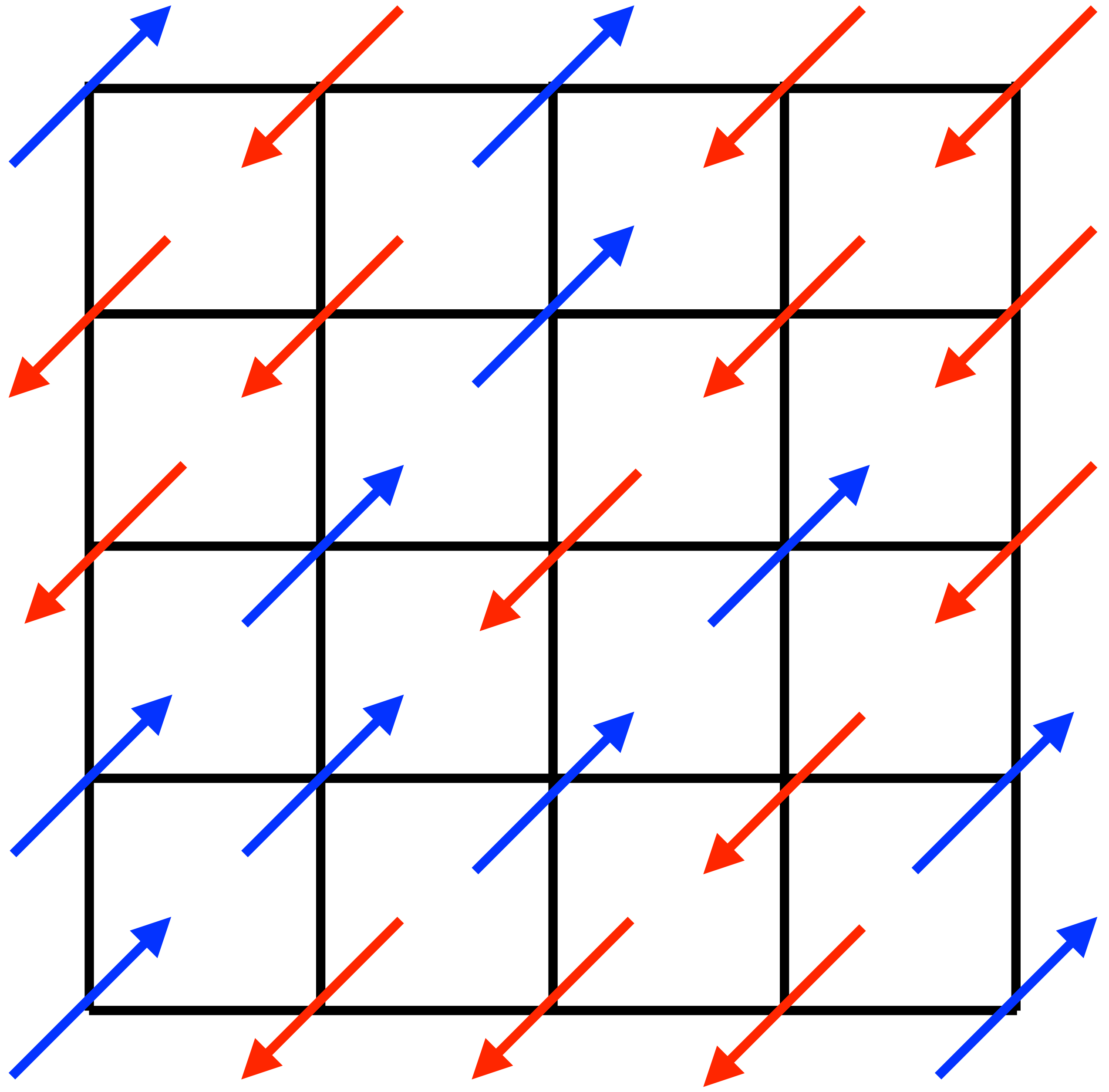
- If we could calculate the critical exponents, then it would be the value observed in experiments
- Different from usual modelling
  - More complicated models for better results
  - Here, simple enough but not too simple
  - Results will not improve with more complicated models (next nearest neigbour? Full LJ?)
- Why? Ans: universality
- Depends only on certain symmetries

Drawbacks of Curie-Weiss MFT

- Ad hoc approximation: Hamiltonian itself changed, now depends on observable itself!
- No way to do systematically
- Predicts phase transition for one dimension [not true]
- Specific heat is zero for $T > T_c$
- Better way of doing MFT?
- Simulations for better quantitative answers?
- Other well-studied spin systems?

Recap

Ising Model



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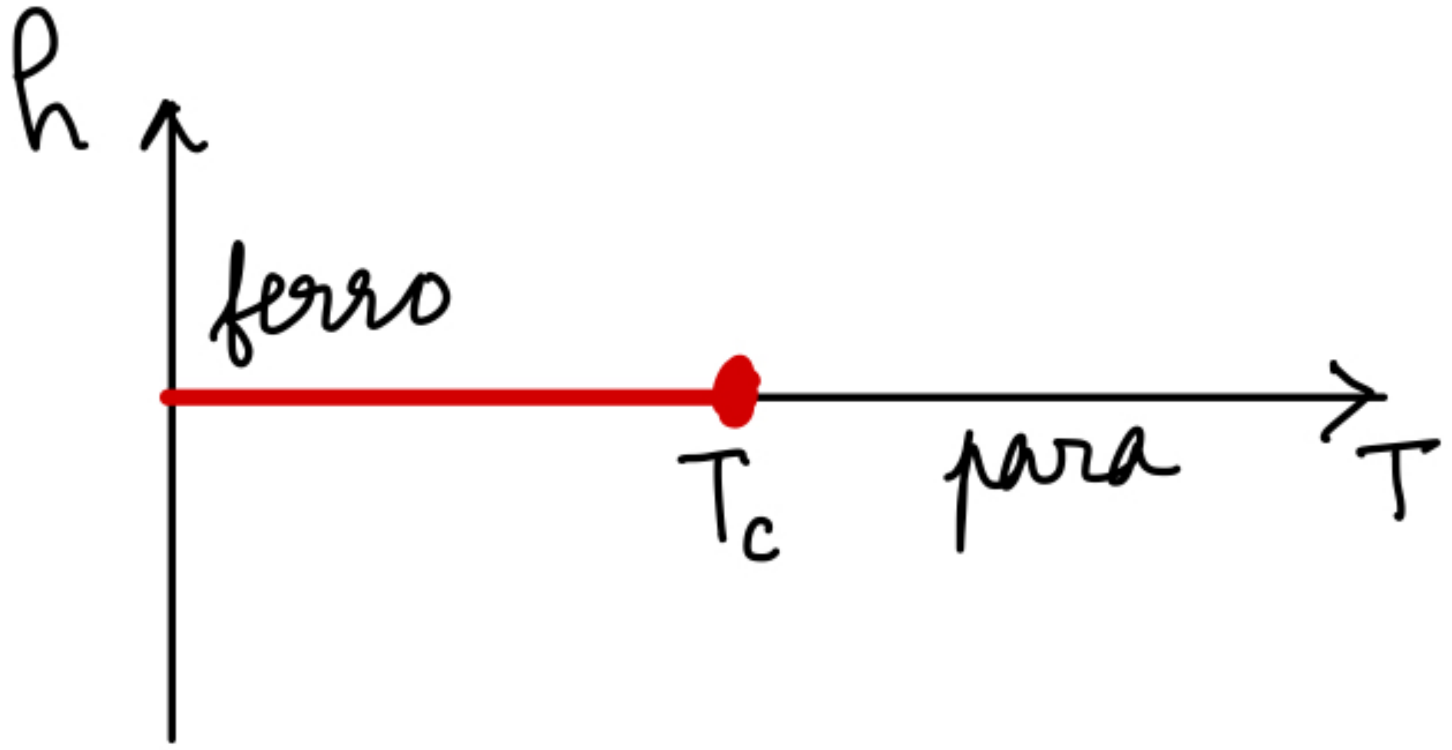
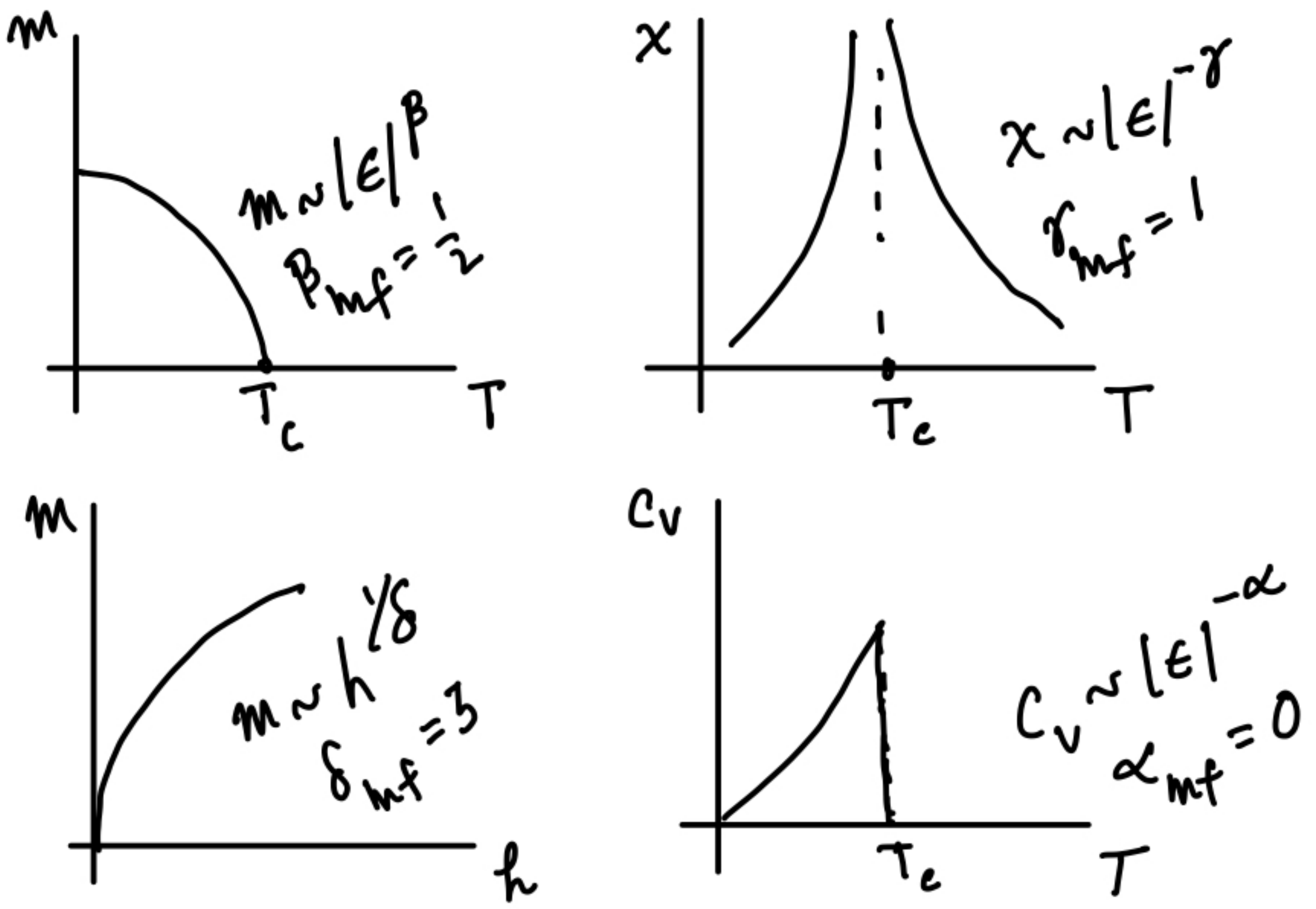
Summary of MFT



$$T_c = Jq$$



Lecture 2
Monte Carlo simulations

Motivation

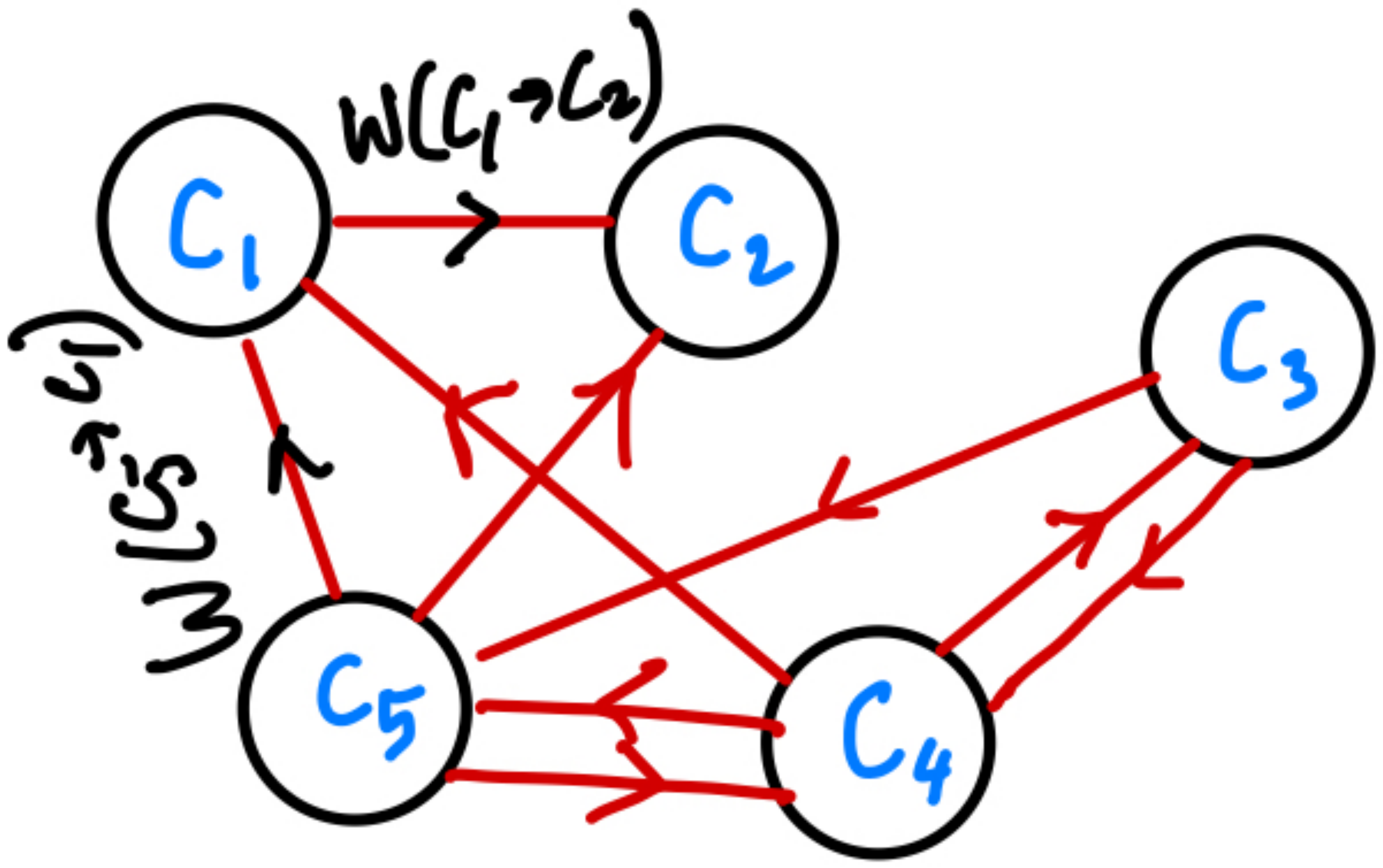
- Equilibrium statistical mechanics (no dynamics, only Hamiltonian)
- Recipe for calculation
  - A configuration C has energy $E(C)$
  - Then $\mathrm{Prob}(C) = \dfrac{\exp[-\beta E(C)]}{\sum_{C'} \exp[-\beta E(C')]}$
  - Aim: generate configurations $C_1, C_2, \ldots \propto$ to their equilibrium weights
  - Then $\langle O \rangle = \dfrac{1}{T} \sum_{t=1}^{T} O(C_t)$

Motivation

- Model defined through dynamics
  - Example: random walkers that repel each other
- Simplest and most common dynamics: Markovian
  - Dynamical rules depend only on the current state
- For generating equilibrium configurations also, we will choose Markovian dynamics
- Questions
  - How to define the dynamics?
  - How to simulate on a computer?
  - What dynamics will generate equilibrium weights?

Defining a model

- What should be given to define a model?
  - The configurations a system can be in $(C_1, C_2, C_3 \ldots)$
  - The transition rates to go from C_i to C_j: $W(C_i \to C_j)$



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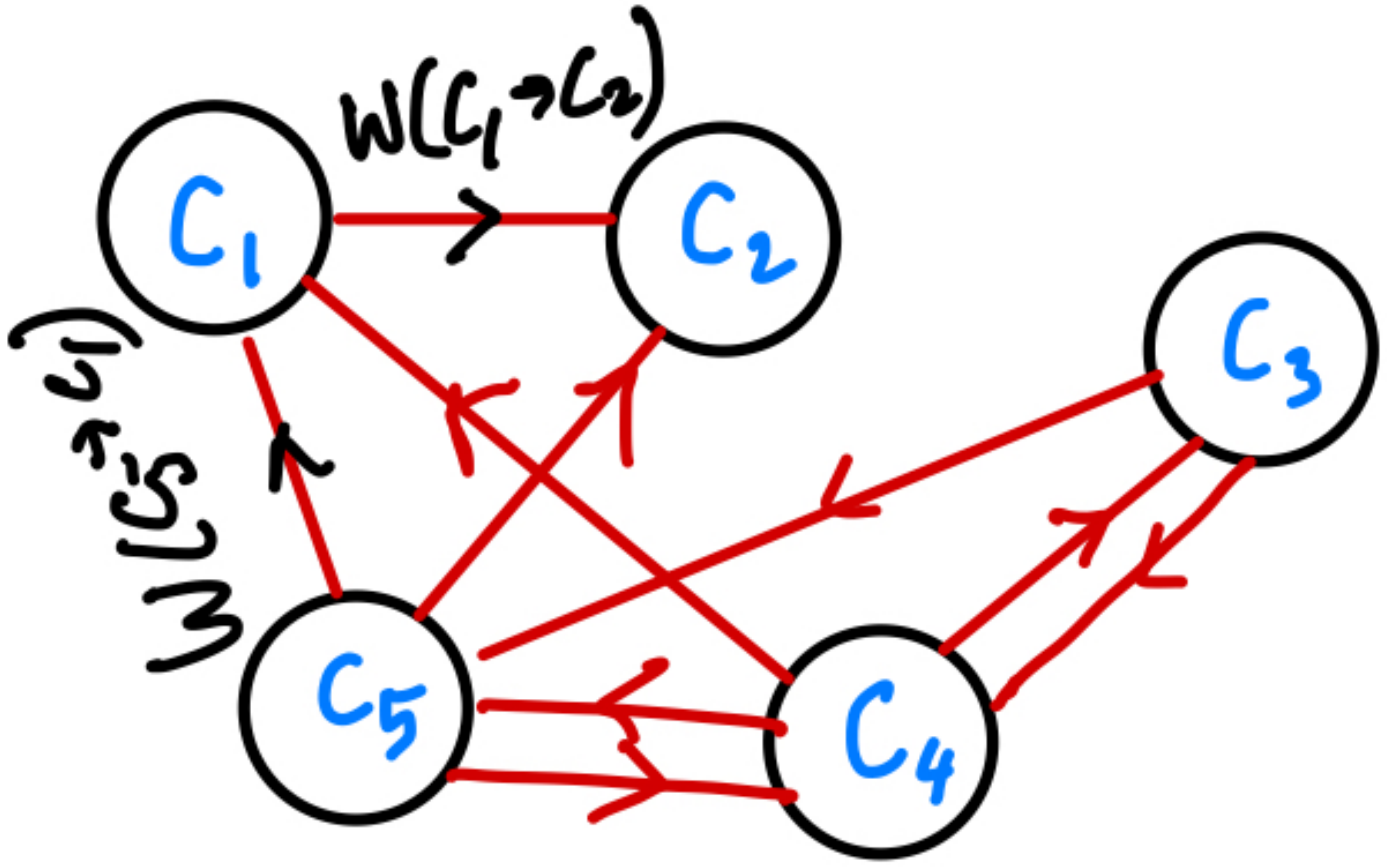

Rates?

What does rate mean?

- Suppose an event occurs at rate λ
- Probability of the event occurring in time $dt \equiv \lambda dt$
- What is the probability of it occurring for the first time at time t?

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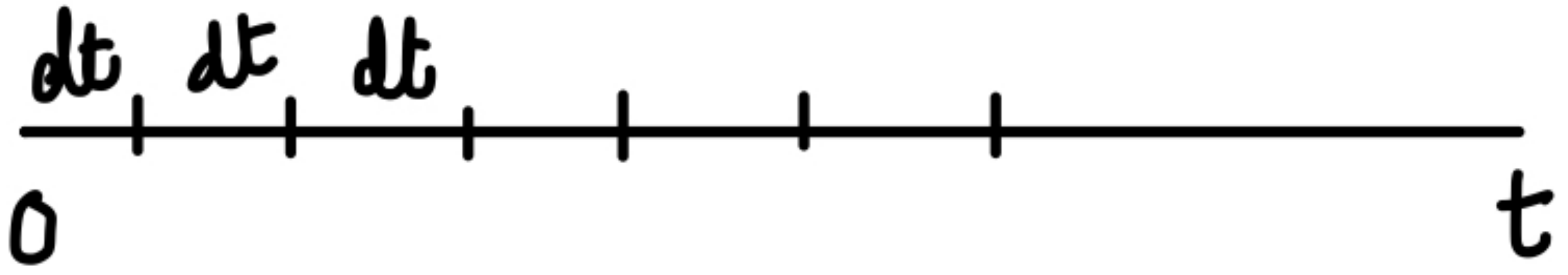

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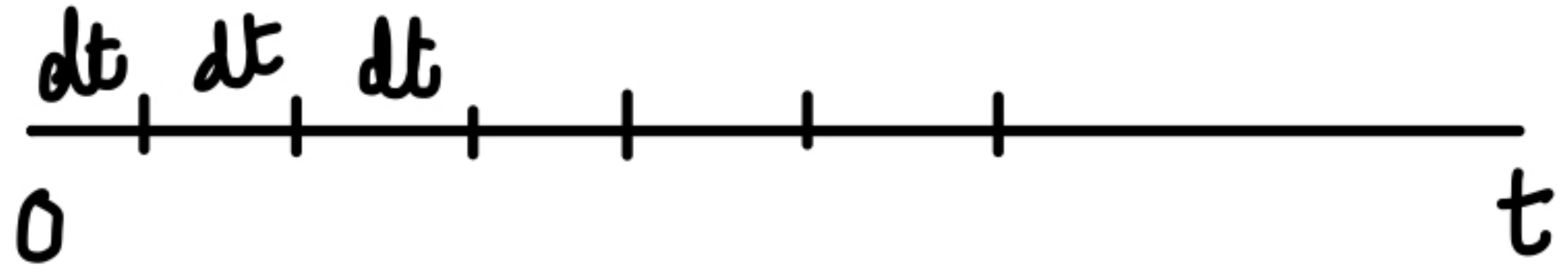

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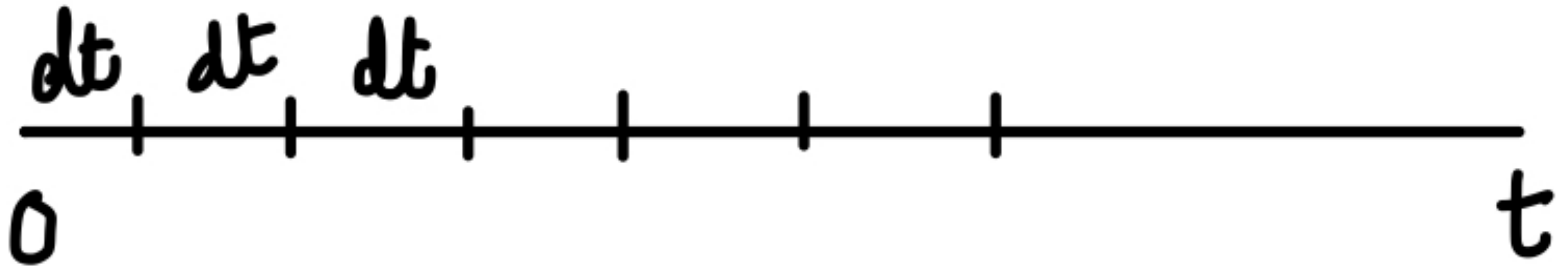

- Probability = $(1 - \lambda dt)^{t/dt} \times \lambda dt$
- Probability = $e^{-\lambda dt \times t/dt} \times \lambda dt$

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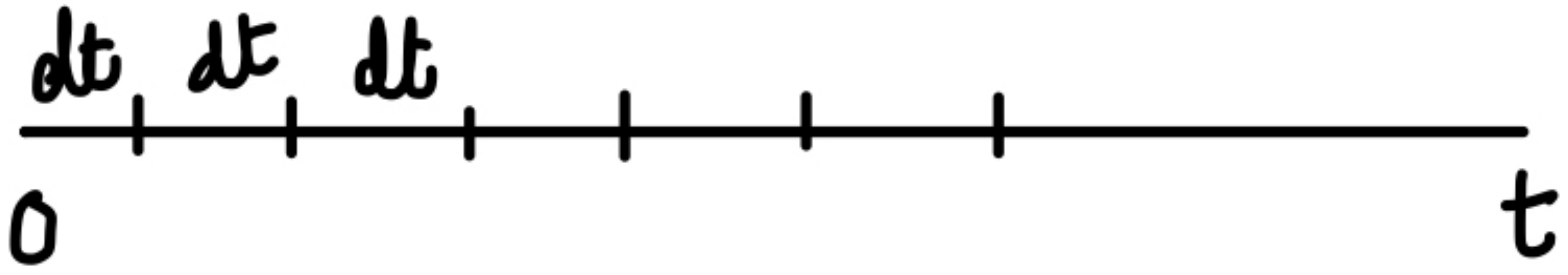

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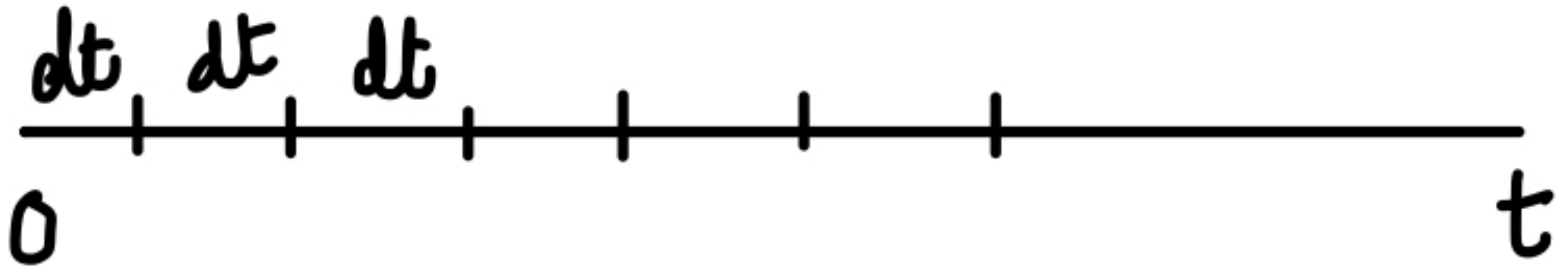

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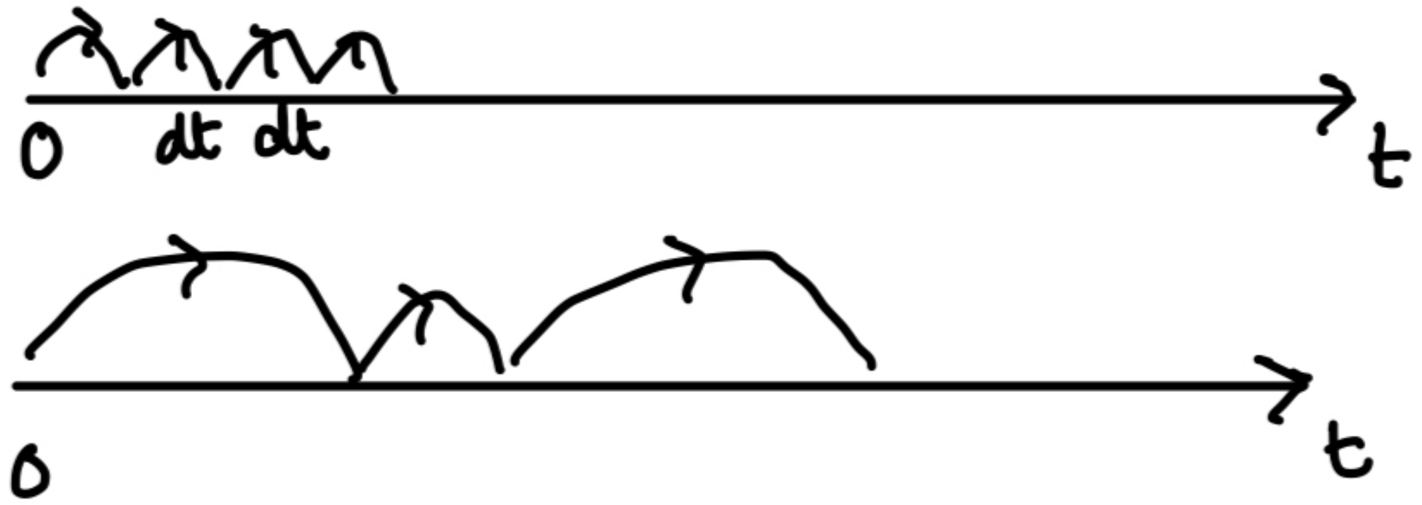
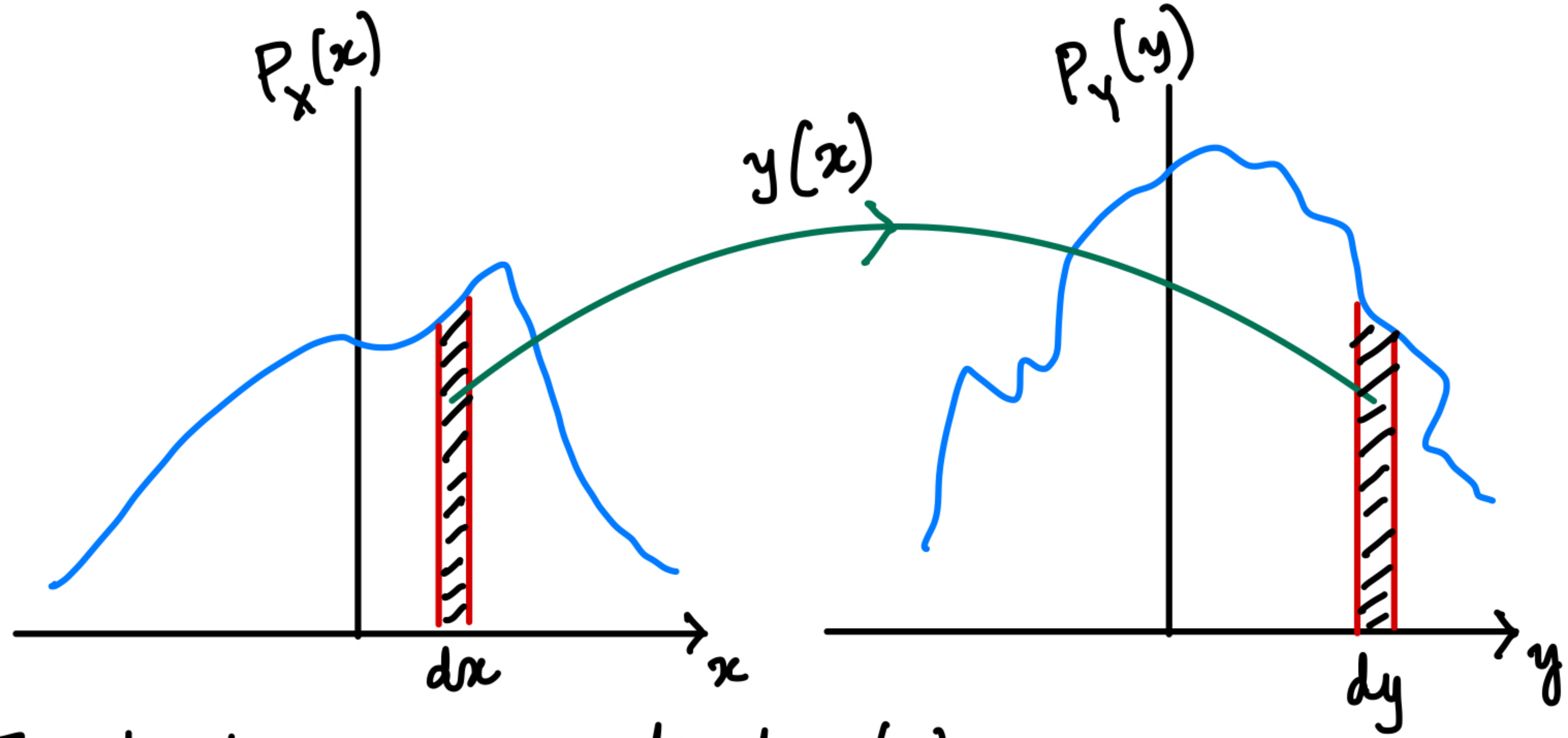
- Summary
  - Infinitesimal time: λdt
  - Waiting time: $P(t) = e^{-\lambda t} \times \lambda$



Generating probabilities

- Usually a random number generator in (0,1) is available
- Event occurs with probability λdt
  - draw a random number r in (0,1)
  - If $r < \lambda dt$ then event occurs, else not
- What about distributions like $P(t) = e^{-\lambda t} \times \lambda$? (You are only given a random number generator in (0,1))
- Given $P_X(x)$ for x, and $y(x)$ what is $P_Y(y)$ for y?

Changing variables



Event at x $\Rightarrow$ event at $y(x)$

$$\Rightarrow P_x(x)\,dx = P_y(y)\,dy$$

Generating exponential distribution

- Let $P_x(x)$ be uniform distribution in (0,1)
- Let $P_Y(y) = \lambda e^{-\lambda y}$
- What should $y(x)$ be?

Generating exponential distribution

- Let $P_x(x)$ be uniform distribution in (0,1)
- Let $P_Y(y) = \lambda e^{-\lambda y}$
- What should $y(x)$ be?

$$dx = \lambda e^{-\lambda y} dy$$

$$\int_0^x dx = \int_0^y \lambda e^{-\lambda y} dy$$

$$x = -e^{-\lambda y}\Big|_0^y = 1 - e^{-\lambda y}$$

$$\Rightarrow \quad y = \frac{1}{\lambda} \ln(1-x)$$

$x = 0, y = 0$; $x = 1, y = \infty$.

Coming back to Markov process

- What is a complete description of the stochastic process?
- Configurations keep changing probabilistically, so trajectory cannot be predicted
- Interested in $P(C, t)$: the probability of being in configuration C at time t

Master equation

$$\frac{dP(C_i, t)}{dt} = \sum_j W(C_j \to C_i)P(C_j, t) - \sum_j W(C_i \to C_j)P(C_i, t)$$

Ways of generating C_i

Ways of going out of C_i

Matrix form

$$\frac{d}{dt}\begin{bmatrix} P(C_1) \\ P(C_2) \\ P(C_3) \\ P(C_4) \end{bmatrix} = \begin{bmatrix} -W_{12}-W_{13}-W_{14} & W_{21} & W_{31} & W_{41} \\ W_{12} & -W_{21}-W_{23}-W_{24} & W_{32} & W_{42} \\ W_{13} & W_{23} & -W_{31}-W_{32}-W_{34} & W_{43} \\ W_{14} & W_{24} & W_{34} & -W_{41}-W_{42}-W_{43} \end{bmatrix} \begin{bmatrix} P(C_1) \\ P(C_2) \\ P(C_3) \\ P(C_4) \end{bmatrix}$$

$$\frac{dP}{dt} = W P$$

Properties of W?

(1) $W_{ij} \geq 0 \,, i \neq j$

(2) $W_{ii} < 0$

(3) $\sum_i W_{ij} = 0$ [column sum = 0]

Conservation of probability

$$\frac{dP_i}{dt} = \sum_j W_{ij} P_j$$

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$$\frac{d \sum_i P_i}{dt} = 0$$

$$\sum_i P_i = 1$$

Properties of W matrix

- $\dfrac{dP}{dt} = WP$ looks like Schrödinger equation
- But W need not be Hermitian ($W_{ij} \neq W_{ji}$ in general)
- Interested in eigenvectors and eigenvalues
- Important: left and right eigenvectors need not be same!
- (1, 1, 1, …) is a left eigenvector. Why?

Properties of W matrix

- $\frac{dP}{dt} = WP$ looks like Schrödinger equation
- But W need not be Hermitian ($W_{ij} \neq W_{ji}$ in general)
- Interested in eigenvectors and eigenvalues
- Important: left and right eigenvectors need not be same!
- (1, 1, 1, …) is a left eigenvector. Why?

- (1, 1, 1, …) times any column = 0 (because column sum=0)
- Therefore, 0 is an eigenvalue
- Denote right eigenvector as $P_s(C)$

Other Properties of W matrix

- $\lambda_1 = 0$ is non-degenerate
- All entries of $P_s(C) \geq 0$
- $Re(\lambda_j) < 0 \text{ for } j > 1$
- Eigenvectors are orthogonal as usual

Analysing the master equation

Now expand $P(C,t)$ in terms of e.vectors of W

$$P(C,t) = a_1(t)\,|\psi_1\rangle + a_2(t)\,|\psi_2(t)\rangle + \cdots$$

$$\langle 1111|P(C,t)\rangle = a_1(t)$$

but $LHS = 1$! $\Rightarrow a_1(t) = 1 \quad \forall t$

From master eq

$$\frac{da_1}{dt}|\psi_1\rangle + \frac{da_2}{dt}|\psi_2\rangle + \cdots = a_1(t)\,W|\psi_1\rangle + a_2(t)\,W|\psi_2\rangle + \cdots$$

$$= |\psi_1\rangle + \lambda_2 a_2(t)\,|\psi_2\rangle + \cdots$$

Take inner product with $\langle\psi_2^L|$

$$\frac{da_2}{dt} = \lambda_2 a_2(t) \Rightarrow a_2(t) = a_2(0)\,e^{\lambda_2 t}$$

and so on

Long time behaviour

Thus $P(c,t) = |\psi_1\rangle + a_2(0)\, e^{\lambda_2 t} |\psi_2\rangle + a_3(0)\, e^{\lambda_3 t} |\psi_3\rangle + \cdots$

but $\mathrm{Re}(\lambda_j) < 0$

When $t \to \infty$ $\quad P(c,t) = P_s(c)$

and $\quad P(c,t) - P_s(c) \propto e^{\lambda_2 t}$

- Long time behaviour unique: steady state
- Eigenvector of eigenvalue 0
- Independent of initial condition
- True if system is ergodic

Determining steady state

- Apriori not known
- Given relevant model, determining steady state becomes the key
- Can give unexpected results
- Approach to steady state: controlled by second eigenvalue λ_2

Simulating a Markov process

- Multiple events possible
  - Do in infinitesimal time
  - Do in finite time
- No generic speed up routines (I do not know)
- Problem specific

Infinitesimal time updates

Suppose N possibilities with rate $\lambda_1, \ldots, \lambda_N$

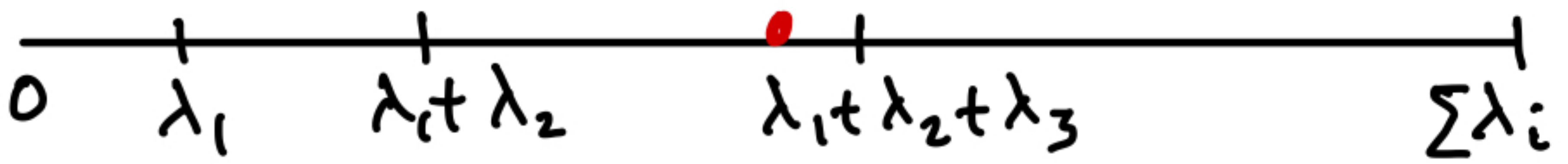
Probability of $i = \lambda_i dt$

Total probability $= (\lambda_1 + \lambda_2 + \cdots + \lambda_N) dt$

Rejection free $\Rightarrow (\lambda_1 + \lambda_2 + \cdots + \lambda_N) dt = 1$

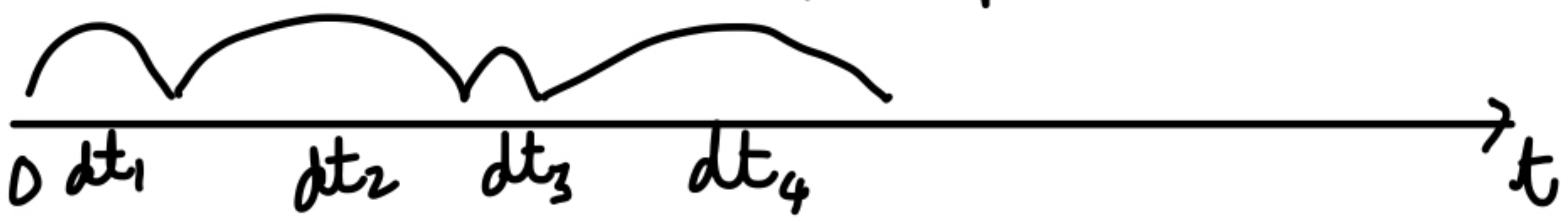
or $dt = \dfrac{1}{\lambda_1 + \lambda_2 + \cdots + \lambda_N}$

Then $\text{Prob}(i) = \dfrac{\lambda_i}{\lambda_1 + \lambda_2 + \cdots + \lambda_N}$



Pick random # in $(0, \Sigma \lambda_i)$:

In example, pick up 3.



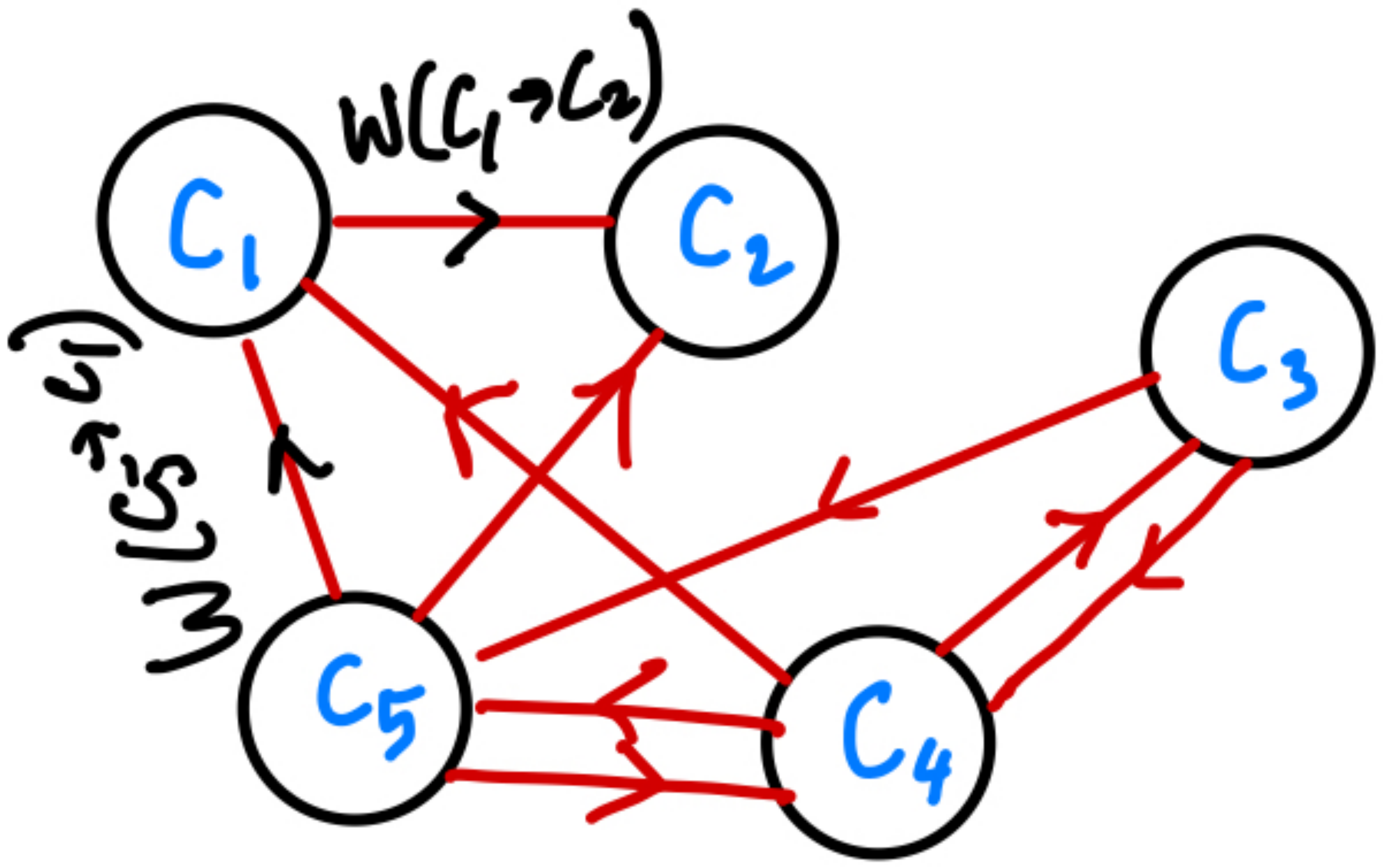
Finite waiting time updates

- Multiple waiting times
- Reduces to sorting them
- And keeping them sorted!
- Efficiency can be gained
  - by tricks
  - Parallelisation

Recap

Markov processes

- What should be given to define a model?
  - The configurations $(C_1, C_2, C_3 \ldots)$
  - The transition rates to go from C_i to C_j: $W(C_i \to C_j)$



Master equation

- $\dfrac{dP}{dt} = WP$
- $P = [P(C_1), P(C_2), \ldots]^T$
- $W_{ij} = W(C_j \to C_i)$
- Column sums of W=0

Long time behaviour

Thus $P(c,t) = |\psi_1\rangle + a_2(0)e^{\lambda_2 t}|\psi_2\rangle + a_3(0)e^{\lambda_3 t}|\psi_3\rangle + \cdots$

but $\mathrm{Re}(\lambda_j) < 0$

When $t \to \infty$ $P(c,t) = P_s(c)$

and $P(c,t) - P_s(c) \propto e^{\lambda_2 t}$

- Long time behaviour unique: steady state
- Eigenvector of eigenvalue 0
- Independent of initial condition
- True if system is ergodic

Simulating on a computer

- What are rates
- How to implement them on a computer
  - Small time increments
  - Waiting time calculations
- Two events do not occur at same time
- Because continuous time Markov process
- Equivalently one could have discrete time Markov processes
- Examples: all agents change their decision for second round
- $P(t+1) = TP(t)$
- Similar properties (steady state, $\lambda_{max} = 1$, etc)

Lecture 3
Simulating Equilibrium Systems

Equilibrium systems

- All this talk about Markov process
- But equilibrium models defined by $E(C)$
- No dynamics specified

Equilibrium systems

- All this talk about Markov process
- But equilibrium models defined by $E(C)$
- No dynamics specified
- Question now reversed
- $P_s(C) \propto e^{-\beta E(C)}$ is given
- What is the dynamics that gives above?

Detailed Balance

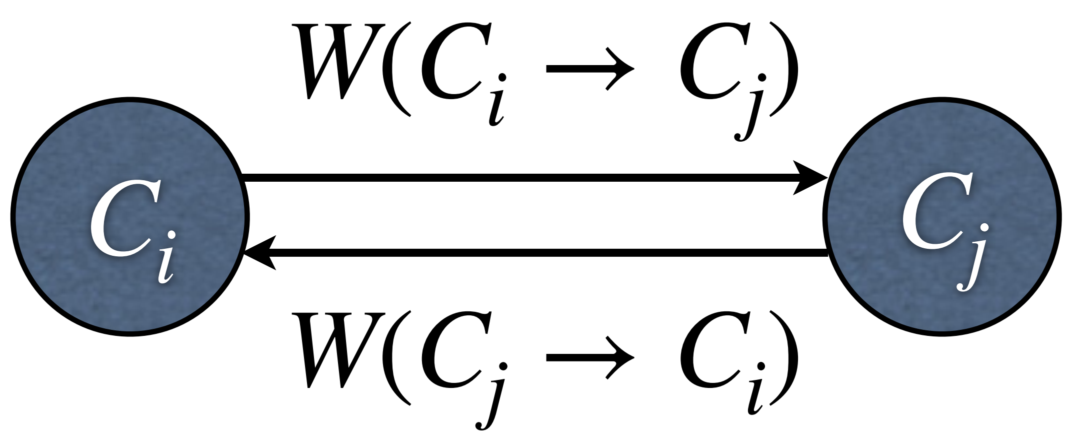
- Steady state of Markov process is unique
- If we find one solution to the master equation, that is the unique solution

$$\frac{dP(C_i,t)}{dt} = \sum_j W(C_j \to C_i)P(C_j,t) - \sum_j W(C_i \to C_j)P(C_i,t)$$

$$\frac{dP(C_i,t)}{dt} = \sum_j \left[W(C_j \to C_i)P(C_j,t) - W(C_i \to C_j)P(C_i,t) \right]$$

choose dynamics such that $W(C_j \to C_i)P(C_j,t) = W(C_i \to C_j)P(C_i,t)$

Detailed balance condition



Detailed Balance

$$W(C_j \to C_i)P(C_j, t) = W(C_i \to C_j)P(C_i, t)$$

$$P(C_j, t) = \frac{e^{-E(C_j)}}{Z}$$

How to implement on a computer?

Comment about equilibrium vs nonequilibrium

A Convenient Rule: Metropolis

- At some time step let energy=E_{old}
- Make a dynamical move that changes configuration
- Let new energy=E_{new} and $\Delta E = E_{new} - E_{old}$
- Accept new configuration with probability

$$\min[1,\frac{Prob(new)}{Prob(old)}] = \min[1, \exp(-\beta \Delta E)]$$

- Acceptance rule obeys detailed balance (Why?)
- If we run with this rule, we will generate configurations with equilibrium weight

A Convenient Rule: Metropolis

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$$\min[1, \frac{Prob(new)}{Prob(old)}] = \min[1, \exp(-\beta \Delta E)]$$

- Acceptance rule obeys detailed balance (Why?)
- If we run with this rule, we will generate configurations with equilibrium weight

Let $E_{old} \leq E_{new}$

Acceptance probability $= e^{-\beta(E_{new} - E_{old})}$

$$Prob(E_{old})\, W(E_{old} \to E_{new}) = \frac{e^{-\beta E_{old}}}{Z} e^{-\beta(E_{new} - E_{old})}$$

$$= \frac{e^{-\beta E_{new}}}{Z}$$

$$Prob(E_{new})\, W(E_{new} \to E_{old}) = \frac{e^{-\beta E_{new}}}{Z} \times 1$$

$\parallel^{ly}$ for $E_{old} > E_{new}$

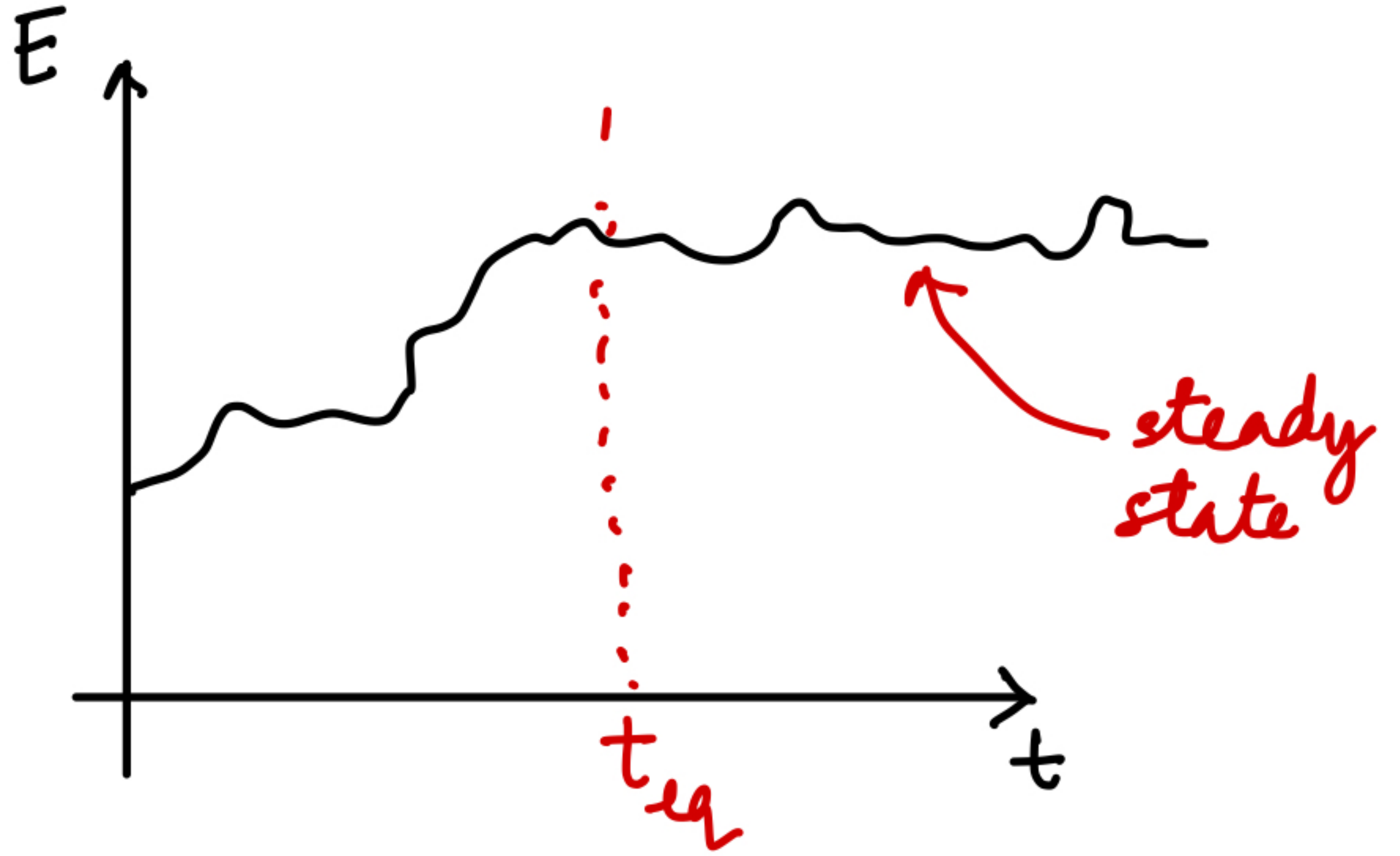
Coming back to Ising model

- Local moves
  - Glauber dynamics
    - Pick a spin at random and flip it (old and new)
    - Does not conserve magnetisation
  - Kawasaki dynamics
    - Pick a pair of neighbouring spins and exchange them
    - Conserves magnetisation

What happened to rates, time?

- Say, each spin flips with rate λ
- In a time dt the total rate of all events $= N\lambda dt$
- We are going to choose dt such that $N\lambda dt = 1$
- $\implies \lambda dt = \dfrac{1}{N}$
- In metropolis, probability that a spin is attempted to flip $= \dfrac{1}{N}$
- $\implies$ consistent
- All time defined in terms of λ^{-1}
- Convenient to choose $\lambda = 1 \implies N$ flips = 1 Monte Carlo step

Equilibration



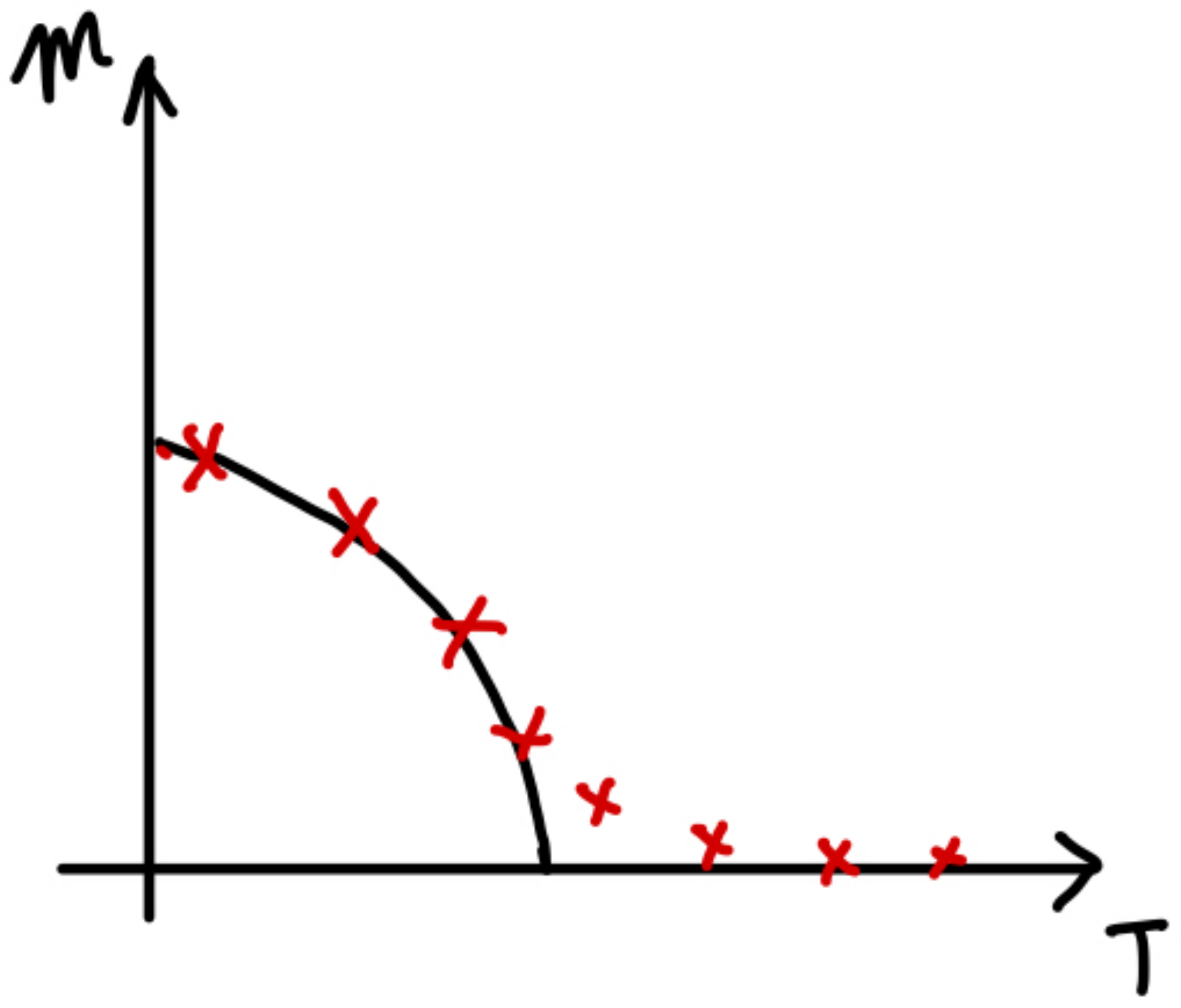
How to check whether equilibrated?

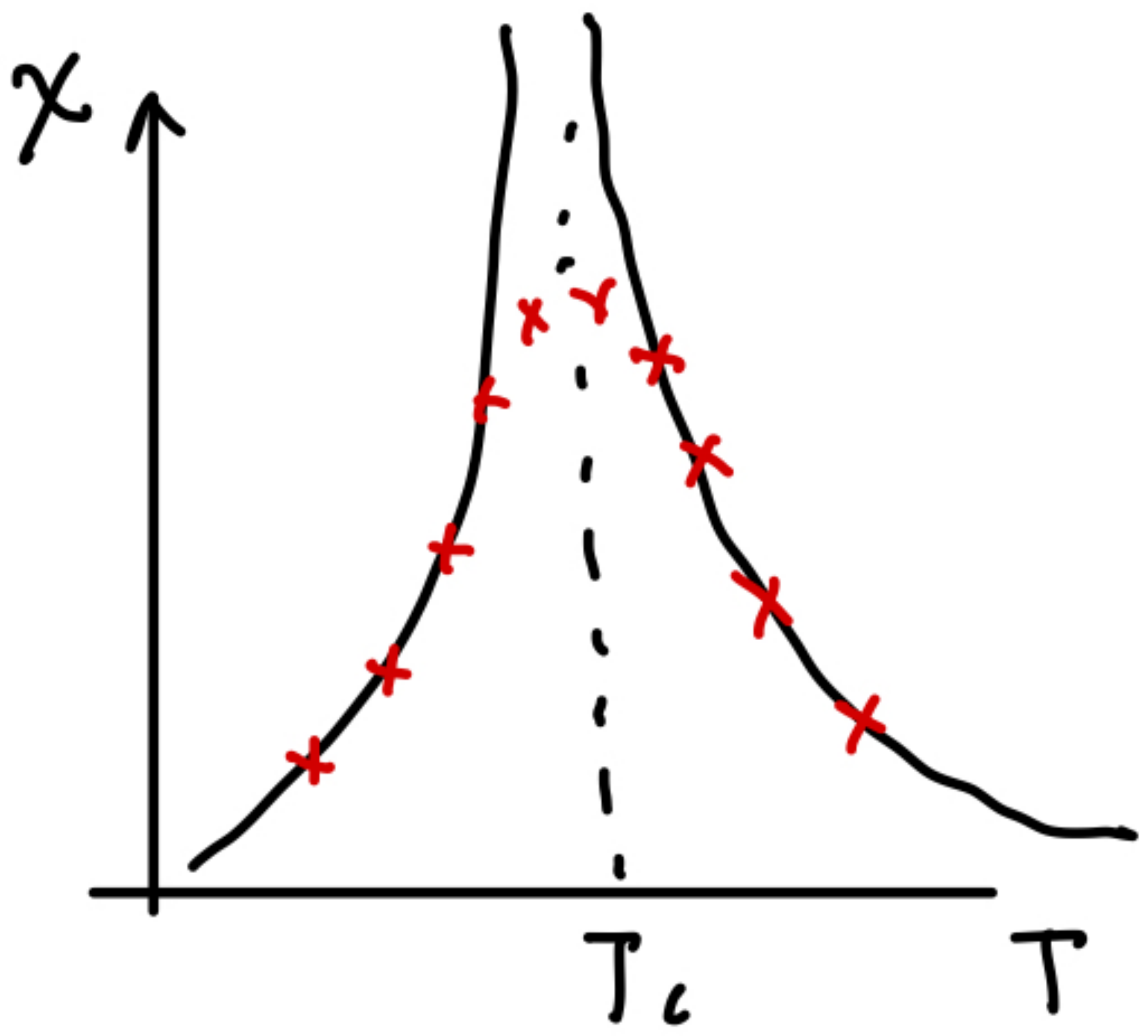
- Run with few extreme initial conditions
- Stationarity

$$\langle E(t_1)\, E(t_2) \rangle = f(t_1 - t_2)$$

- Equilibration time will depend on L

Simulations on finite lattices





- Simulations are on finite lattices
- How does one extrapolate to infinite lattices: finite size scaling
- Tells about nature of transition, exponents, etc

Going back to Metropolis

- At some time step let energy=E_{old}
- Make a dynamical move that changes configuration
- Let new energy=E_{new} and $\Delta E = E_{new} - E_{old}$
- Accept new configuration with probability
$$\min[1, \frac{Wt(new)}{Wt(old)}] = \min[1, \exp(-\beta \Delta E)]$$
- Acceptance rule obeys detailed balance
- Note that each simulation is done at a fixed value of temperature (and/or other parameters)

Can we determine density of states g(E)?

density of states

- $$Z = \sum_E g(E)\exp(-\beta E)$$
- $$\langle E^n \rangle = Z^{-1} \sum_E E^n g(E)\exp(-\beta E)$$
- If g(E) is known, then data for whole temperature range can be found in one go.
- In regular Monte Carlo, each temperature has to be simulated separately
- How to determine g(E) in a Monte Carlo simulation?

Flat Histogram Methods

- Suppose $Wt(E) \neq \exp(-\beta E)$
- Run a simulation satisfying detailed balance: prob= $\min[1, \frac{Wt(new)}{Wt(old)}]$
- Measure histogram $H(E)$, the number of times E is visited
- Then $H(E) \propto g(E)Wt(E)$
- If $Wt(E) = 1/g(E)$, then histogram would be flat
- Of course, one does not know $g(E)$, but one could use the fact that if the correct $Wt(E)$ is chosen, then histogram would be flat

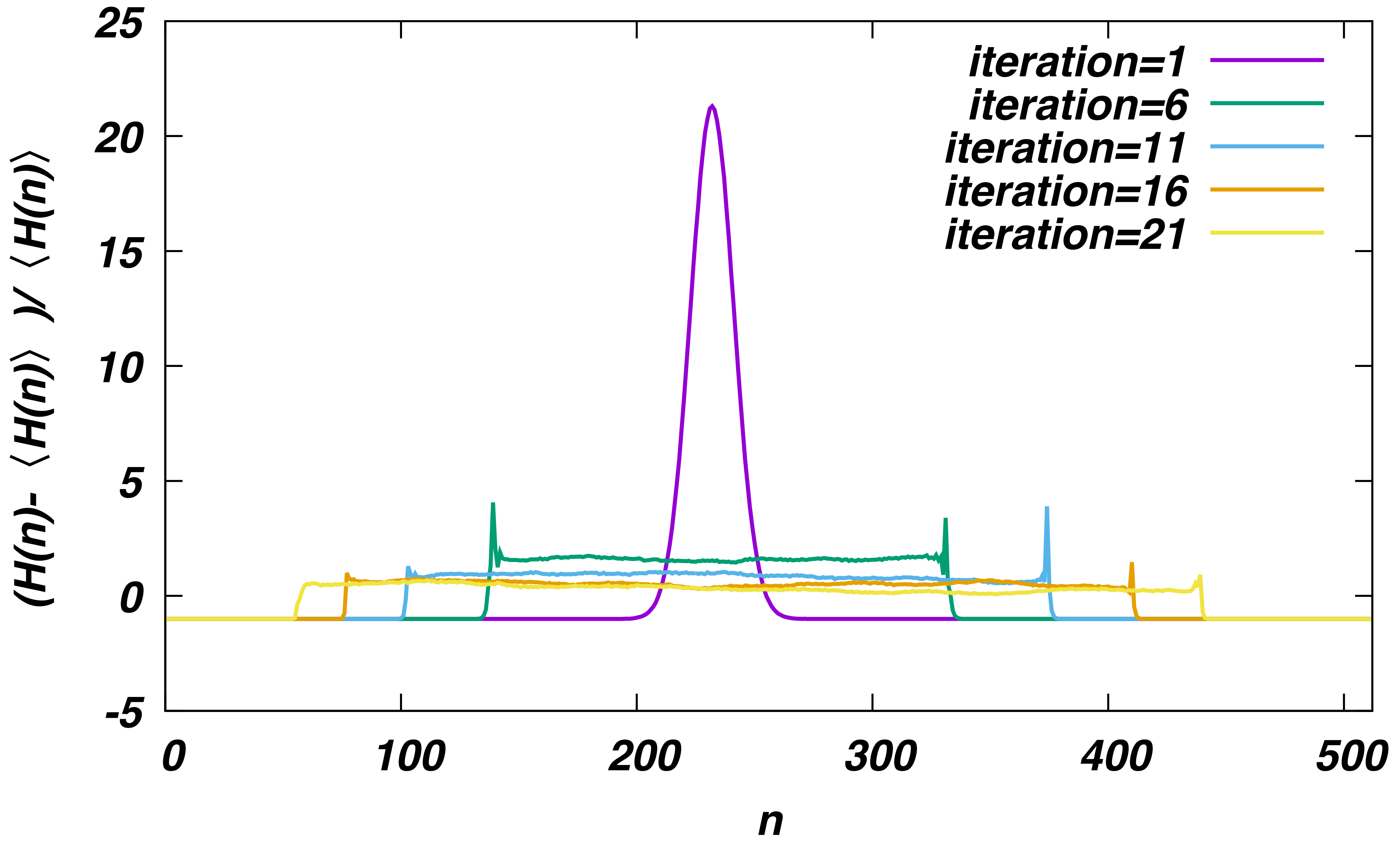
A Direct Implementation

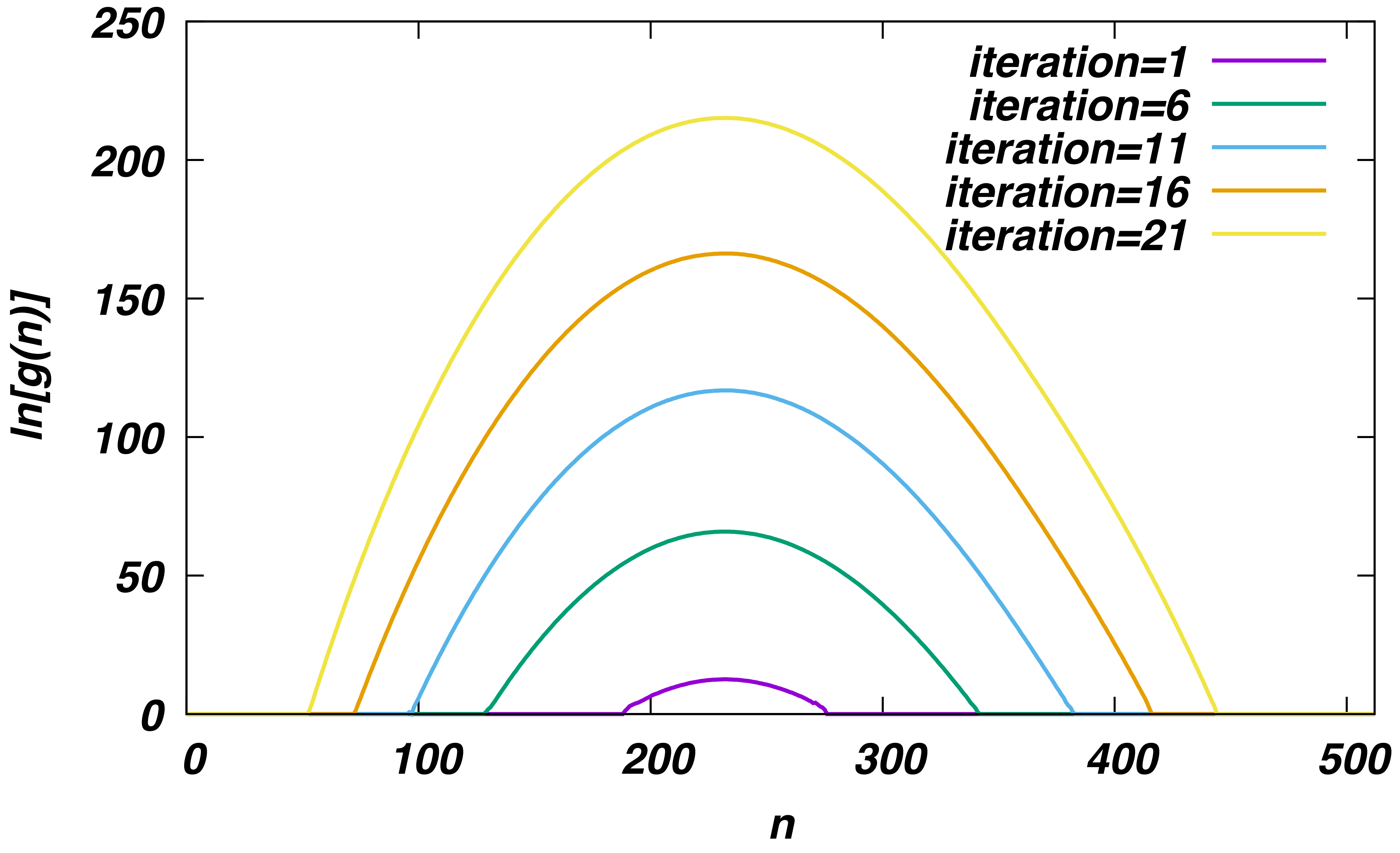
- Make a guess for $g(E) = g_1(E) \implies Wt(E) = 1/g_1(E)$
- Then $H(E) \propto g(E)Wt(E) = g(E)/g_1(E)$
- $g_2(E) = g(E) = H(E)g_1(E)$
- Conceptually, one could stop now, but in practice $g_2(E)$ is a poor estimate
- Iterate above a few times to get $g_1, g_2, \ldots \to g(E)$

An example

- Issues: convergence is very slow. For larger system sizes, it depends crucially on initial guess $g_1(E)$

Data for NN exclusion model (L=32)





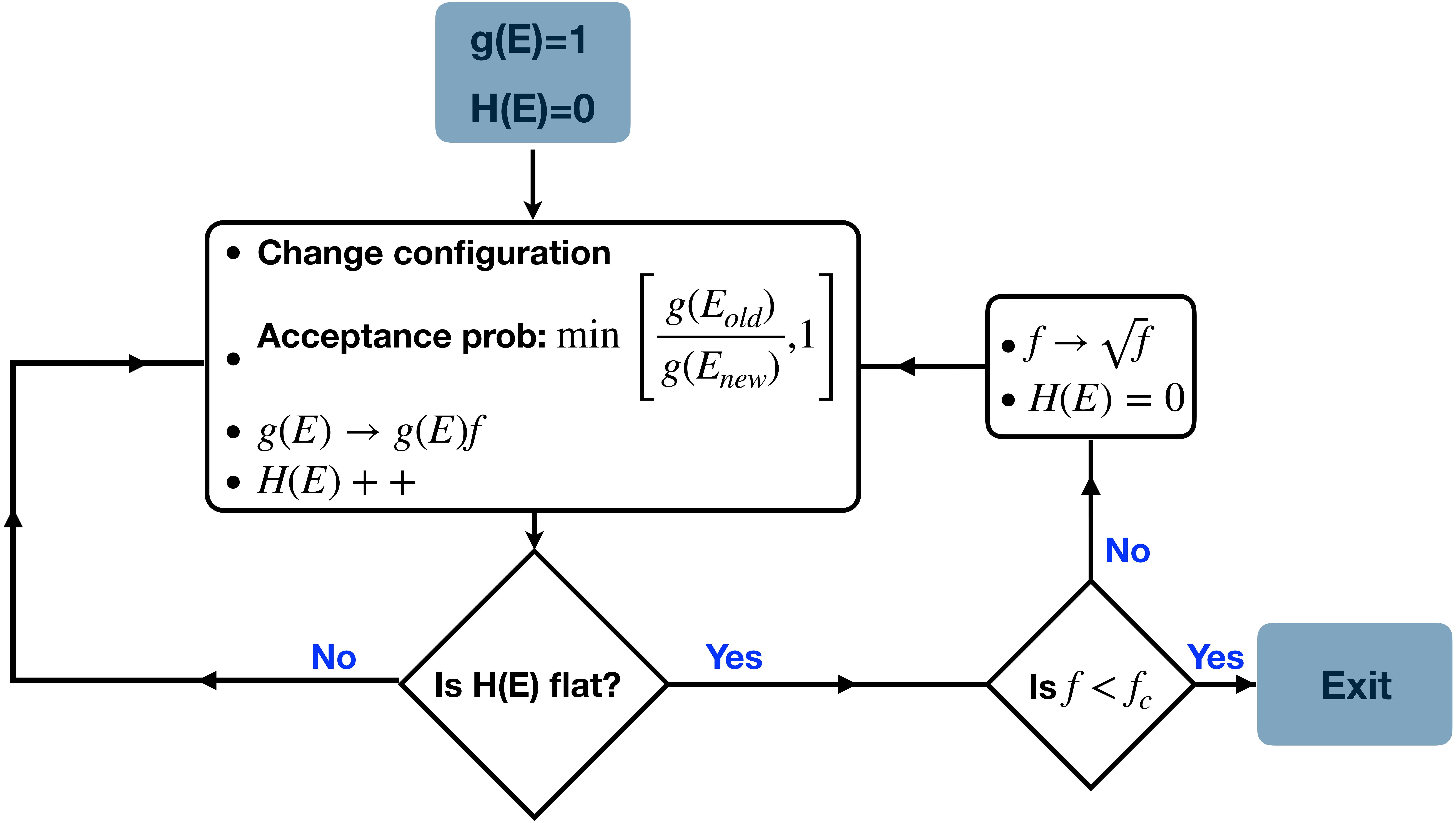
- How can one improve the convergence?

Wang Landau algorithm

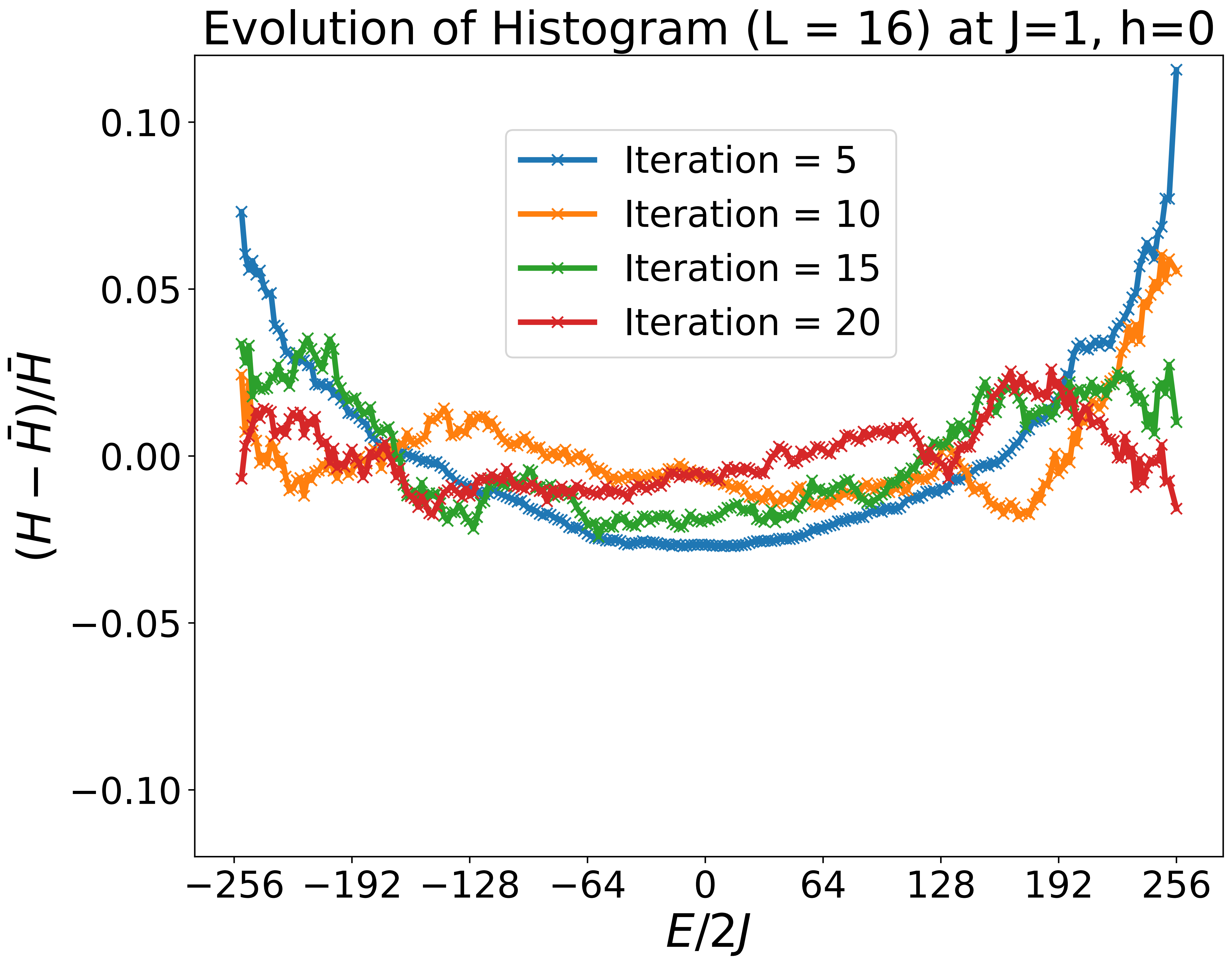
- $g(E)$ continuously evolves during the simulation (next slide)
- Simulation does not satisfy detailed balance because g(E) is changing
- But convergence is very fast
- A very popular and efficient algorithm

Wang et al, PRL, 2001

Wang Landau protocol



Flattening of Histograms



- Ising Model (2D): 16x16

Benchmarking

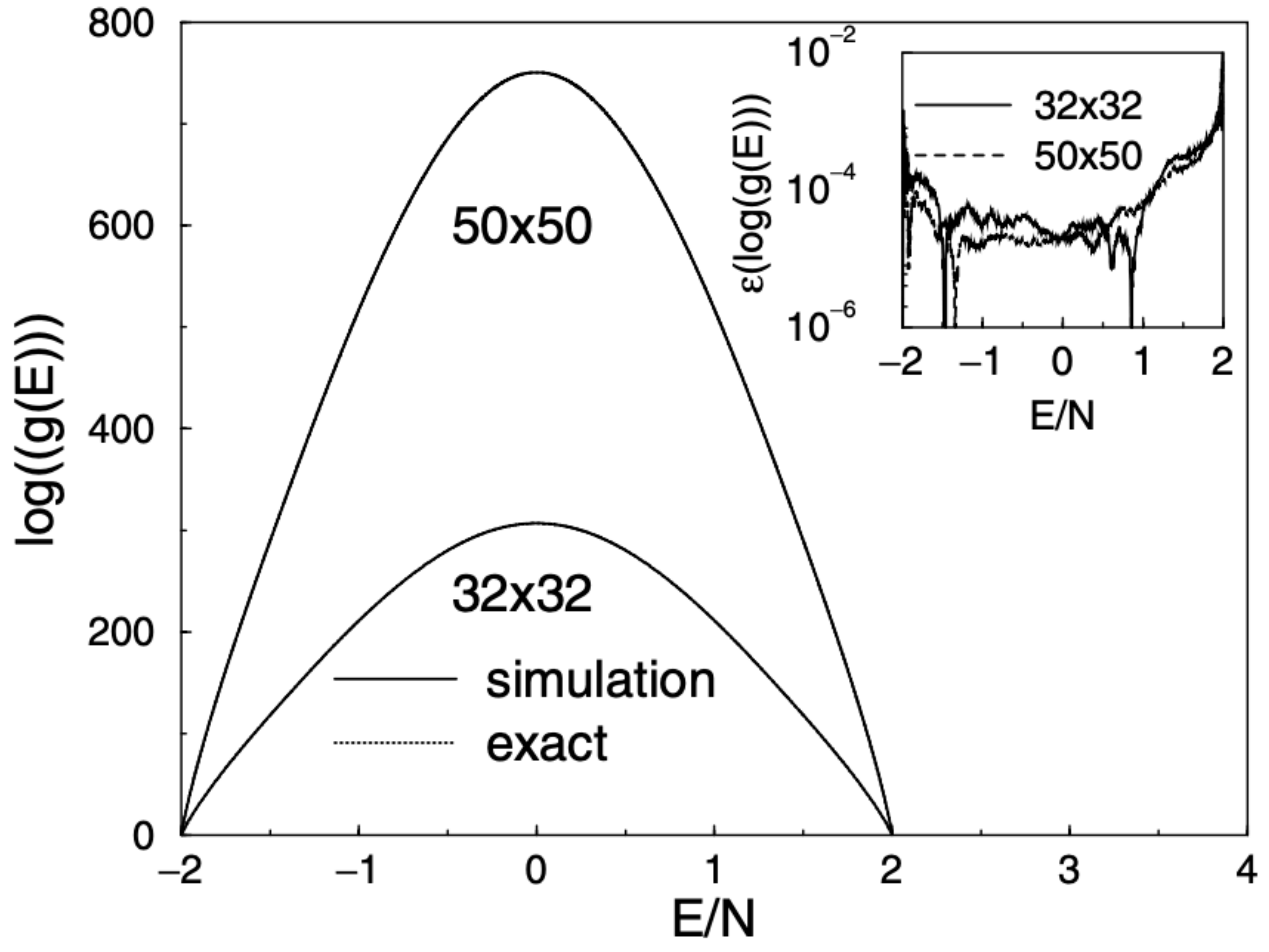


FIG. 1. Comparison of the density of states obtained by our algorithm for 2D Ising model and the exact results calculated by the method in Ref. [13]. Relative errors $\varepsilon(\log(g(E)))$ are shown in the inset.

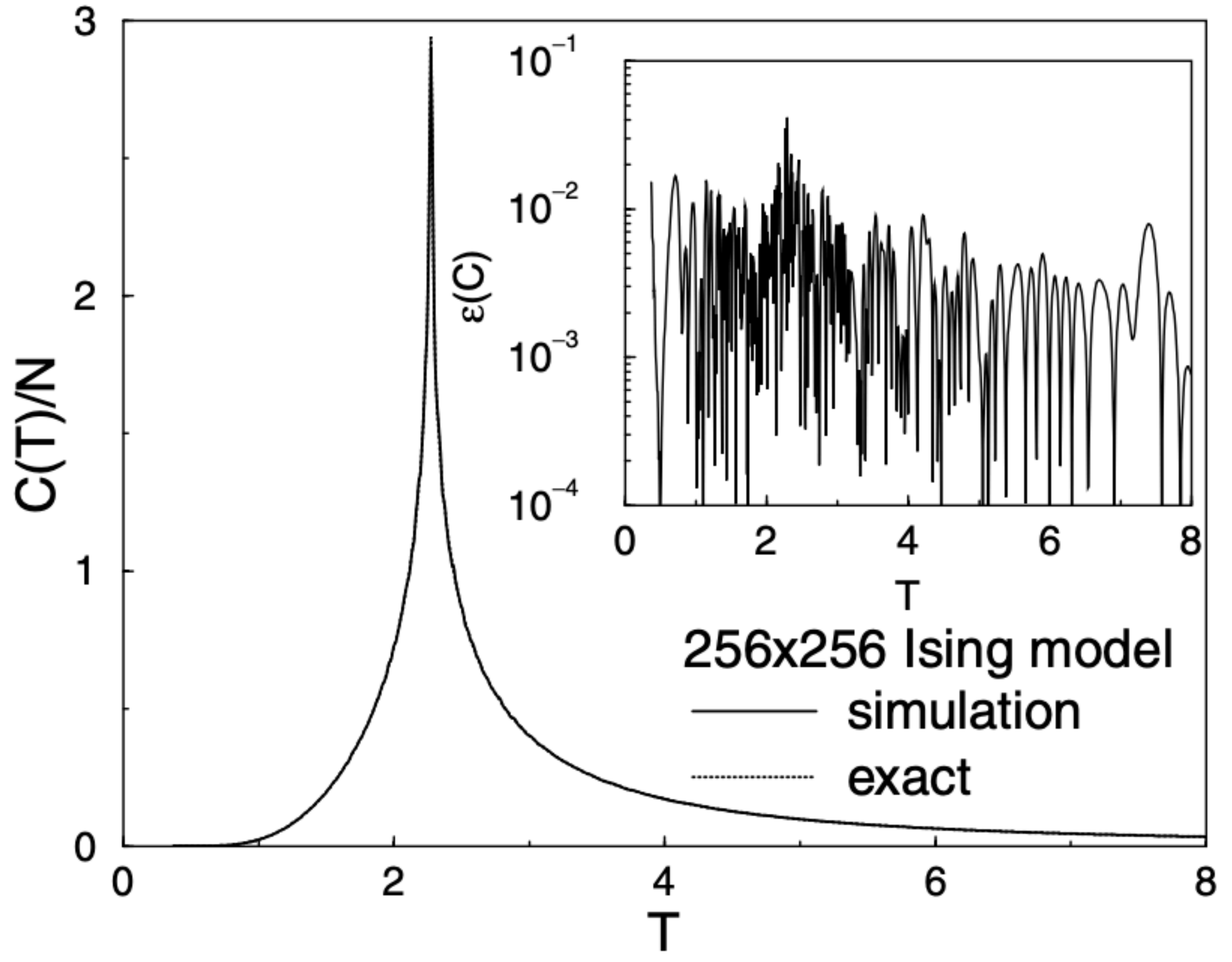


FIG. 3. Specific heat for the 2D Ising model on a 256×256 lattice in a wide temperature region. The relative error $\epsilon(C)$ is shown in the inset in the figure.

Wang et al, PRL, 2001

Many spin models

- Potts model: $S_i = 1,2,3,\ldots,q$
  - $\mathscr{H} = -J\sum_{\langle ij \rangle}\delta_{S_i,S_j}$
- Clock model: $S = \frac{2\pi ij}{q}, j = 0,1,\ldots,q-1$
  - $\mathscr{H} = -J\sum_{\langle ij \rangle}\cos(\theta_i - \theta_j)$
- XY model: $q \to \infty$ limit of clock model