MATH327: StatMech and Thermo

Wednesday, 7 May 2025

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Something to consider

Suppose we want to *approximately* compute expectation values

$$\langle \mathcal{O} \rangle = \sum_{i=1}^{M} \mathcal{O}_i \, p_i = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{O}_i \, e^{-\beta E_i} = \frac{\sum_{i=1}^{M} \mathcal{O}_i \, e^{-\beta E_i}}{\sum_{i=1}^{M} e^{-\beta E_i}}.$$

How many of the system's micro-states do we really need to analyse?

Recap

Ising model magnetization as order param.

transition vs. crossover

Mean-field approx. $\to$ self-consistency condition

$\langle m \rangle = \tanh(\beta(2d \langle m \rangle + H))$

Plan

Wrap up mean-field approx. for Ising model

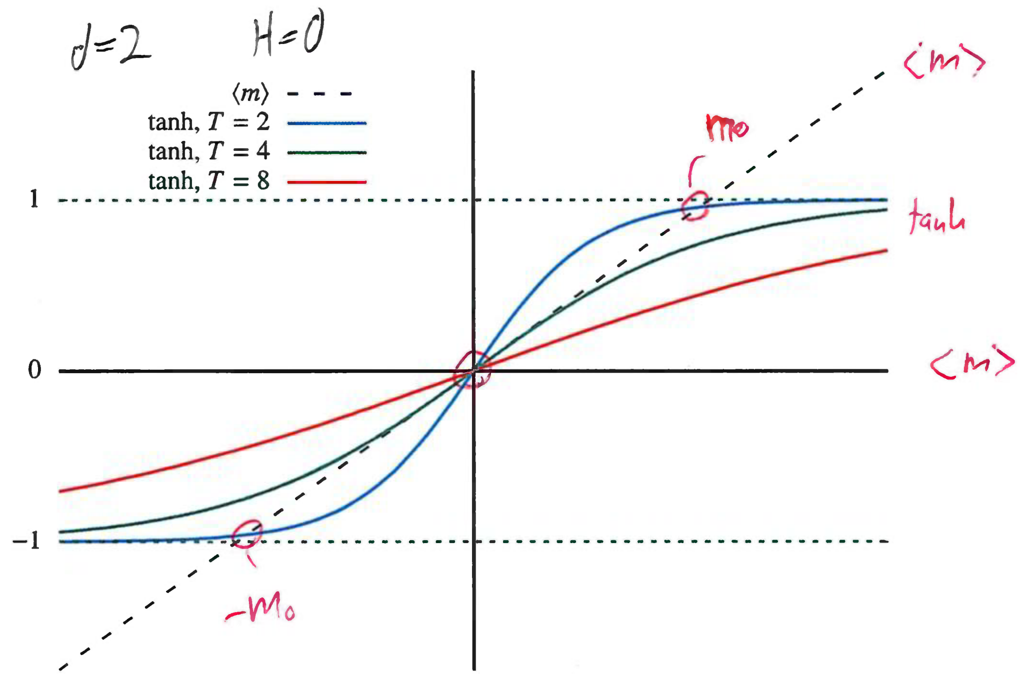
Numerical methods – more broadly applicable

Recall mean-field solutions for $d=2$ $T=4$

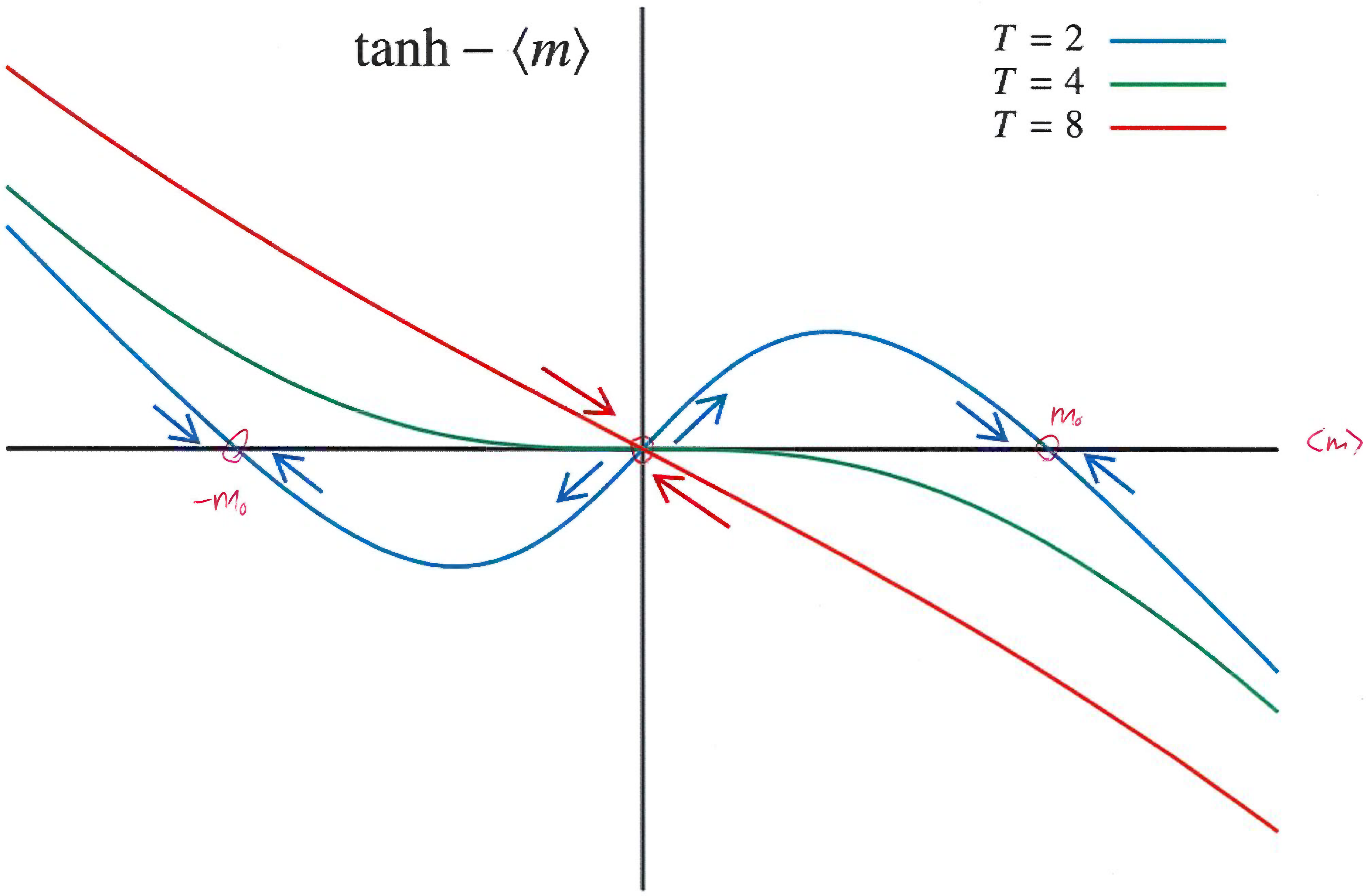
$H=0 \to \langle m \rangle = 0$ (disordered)

$H \neq 0 \to \langle m \rangle = \pm m_0 \neq 0$ (ordered)

$\hookrightarrow m_0 \to 1$ as $T \to 0$



$d=2$ $H=0$
$\langle m \rangle$
tanh, $T = 2$
tanh, $T = 4$
tanh, $T = 8$
1
0
−1
$\langle m \rangle$
m_0
tanh
$\langle m \rangle$
$-m_0$



tanh − ⟨m⟩
T = 2
T = 4
T = 8
−m0
m0
⟨m⟩

Expect low-T ordered phase even with $H=0$

Compare $T = 2, 4, 8$

$\langle m \rangle = 0$ always possible

Lower T → additional solutions $\langle m \rangle = \pm m_0 \neq 0$

$m_0 \to 1$ as $T \to 0$

Which intersection is true solution adopted by the system?

Consider perturbing $\langle m \rangle = 0 \to \langle m \rangle = \varepsilon > 0$

$T=8$: $\langle m \rangle$ too large compared to tanh

→ decrease to stable $\langle m \rangle = 0$

$T=2$: $\langle m \rangle$ too small

→ increase to stable $\langle m \rangle = m_0 \neq 0$

Similarly $-\varepsilon \to -m_0$

Conclude $\langle m \rangle = 0$ unstable → ordered phase for low T

Another way to see (in)stability

Plot $\tanh(2\beta d \langle m \rangle) - \langle m \rangle$ to find zeros

Positive → $\langle m \rangle$ too small

Negative → $\langle m \rangle$ too large

So $H=0$ mean-field approx. give expected phases

When does $\langle m \rangle = 0$ become unstable?

Need $\tanh > \langle m \rangle$ for $\langle m \rangle = \varepsilon > 0$ → slope > 1 at $\langle m \rangle = 0$

$$\boxed{\left.\frac{d}{d\langle m \rangle} \tanh(2d\beta\langle m \rangle)\right|_{\langle m \rangle = 0} = \frac{d}{d\langle m \rangle}\left[2d\beta\langle m \rangle + \mathcal{O}(\langle m \rangle^3)\right]_{\langle m \rangle = 0} = 2d\beta = 1 \to T_c = \frac{1}{\beta_c} = 2d}$$

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Is this a phase trans. w/ discontinuity?

Consider $T \lesssim T_c \rightarrow 0 < |\langle m \rangle| \ll 1$

$$\cancel{\langle m \rangle} = \tanh(2d\beta\langle m \rangle) = 2d\beta \cancel{\langle m \rangle} - \frac{1}{3}(2d\beta\langle m \rangle)^3 + \mathcal{O}(\langle m \rangle^5)$$

$$\frac{1}{3}\left(\frac{T_c}{T}\right)^3 \langle m \rangle^2 = \frac{T_c}{T} - 1$$

$$\langle m \rangle^2 = 3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T} - 1\right) = 3\left(\frac{T}{T_c}\right)^2\left(1 - \frac{T}{T_c}\right)$$

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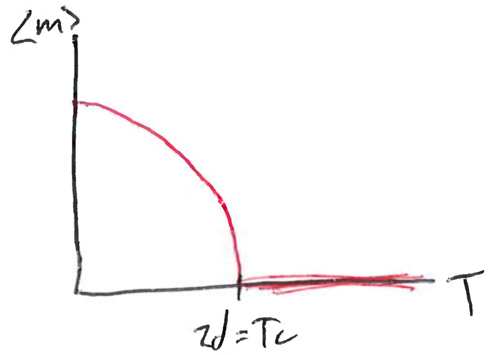
For $\frac{T}{T_c} \approx 1 \rightarrow \langle m \rangle \approx \pm\sqrt{3}\left(1 - \frac{T}{T_c}\right)^{1/2} = \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2}$

So OP continuous:

$$\langle m \rangle \propto \begin{cases} (T_c - T)^{1/2} & \text{for } T \lesssim T \\ 0 & \text{for } T \gtrsim T_c \end{cases}$$



But $\frac{d\langle m \rangle}{dT} \propto \frac{1}{(T_c - T)^{1/2}}$ for $T \lesssim T_c$

diverges as $T \rightarrow T_c$ from below

Mean-field approx. predicts second-order PT for Ising model

occurs whenever $OP \propto (T_c - T)^b$

with critical exponent $0 < b < 1$

Many phase trans. have same sets of critical exponents

$\rightarrow$ universality: emergent behaviour near critical point independent of microscopic details

$H = 0$ mean-field predicts second-order PT at $T_c = 2d$, $b = 1/2$

Is this correct?

$d = 1$: No phase trans. (Ising 1924) X

$d = 2$: Second-order PT (Onsager 1944) ✓

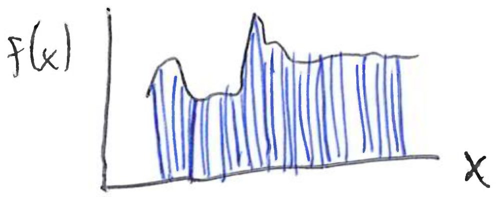
$$T_c = \frac{2}{\log(1+\sqrt{2})} \approx 2.27 \rightarrow \text{MF } T_c = 4 \text{ off by } \sim 2\times$$

$$b = \frac{1}{8} \rightarrow \text{MF off by } 4\times$$

$d=3$: <u>Numerical analyses</u> → 2nd-order PT $T_c \approx 4.5$ (vs. 6)
$b \approx 0.32$

$d \geq 4$: $b = \frac{1}{2}$ ✓
$T_c \to 2d$ as $d \to \infty$
Mean-field becomes exact
(more n.n. → more reliable)

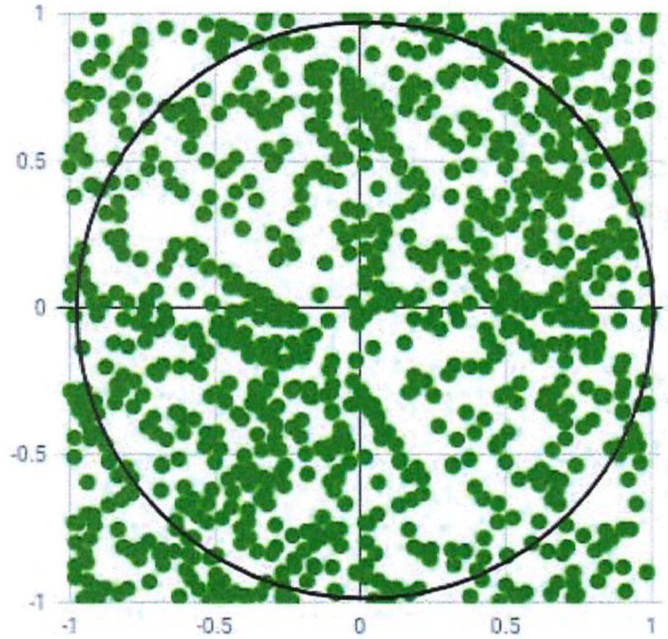
How to do numerical calcs in less than ~500,000× age of universe?
Needed for most interacting statistical system
including $d \gtrsim 3$ Ising model
Sample small subset of micro-states to approximate $\langle O \rangle$
Pseudo-random → ~~Math~~ "Monte Carlo" methods
Example: Estimate integral by evaluating integrand at random points



$$\int_{-1}^{1} dx \int_{-1}^{1} dy \; H(1 - \{x^2 + y^2\}) = \text{area of disk w/radius } 1 = \pi$$

$$H(r) = \begin{cases} 1 & \text{for } r \geq 0 \\ 0 & \text{for } r < 0 \end{cases}$$

Monte Carlo integration most useful for high-dim'l integrals like $\langle O \rangle$ for $N \gg 1$ ~~integ~~interacting statistical systems!



Fraction = $\frac{\pi}{4}$

$\dfrac{\text{length of calc}}{\text{age of universe}} \ll 1$ → <u>very</u> small fraction of micro-states
How can this give reliable approx?

High-T Ising model: All p_i roughly equal
$\langle O \rangle$ determined by degeneracies
Large degeneracy → more likely to sample...
could be okay

Low T: $\langle O \rangle$ dominated by ground states
Other contributions suppressed $\sim e^{-E/T}$

Solution: Sample w_i with prob. $p_i \propto e^{-\beta E_i}$
without knowing p_i distribution

<u>Importance sampling</u> algorithms use pseudo-randomness
to find large p_i without bias

Example: MRRTT algorithm (1953)
Start from any micro-state
Pseudo-randomly change → ΔE
$P_{accept} = \min\{1, \exp(-\beta \Delta E)\}$, otherwise reject
→ New micro-state (possibly unchanged)

Repeat

Sequence of micro-states is Markov chain
→ each w_i based on previous one, no memory

$$w_1 \to w_2 \to w_3 \to \cdots$$

$$\frac{P(A \to B)}{P(B \to A)} = \frac{\min\{1, e^{-\beta(E_B - E_A)}\}}{\min\{1, e^{-\beta(E_A - E_B)}\}} = e^{-\beta(E_B - E_A)} = \frac{e^{-\beta E_B}}{e^{-\beta E_A}} = \frac{P_B}{P_A} \checkmark$$

To avoid bias, must (in principle) be able to reach any w_i
from any other w_j

<u>Ergodicity</u> of random update depending on system

May take many updates to produce statistically independent w_i
→ <u>auto-correlation</u> increase costs and uncertainties
$\propto 1/\sqrt{S}$
indep. samples

For spin systems, huge benefits
from flipping "cluster" of spins, not just one

Reduce "critical slowing down" near 2nd-order phase trans.
with fluctuations on all length scales

We have reached areas of ongoing research
just a few months after starting
w/probability foundations!