MATH327: Statistical Physics

Friday, 10 May 2024

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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 analyze?

Plan

Mean-field approx. for Ising model

Numerical methods (more broadly applicable)

Recap

~~Ave~~ Assume on average small fluctuations around mean spin $\langle m \rangle$

$\rightarrow$ non-interacting system w/ effective magnetic field H_{eff}

$$E = -\sum_{(jk)} s_j s_k - H \sum_n s_n \rightarrow d \cdot N \langle m \rangle^2 - (2d\langle m \rangle + H) \sum_n s_n$$

Self-consistency condition $\langle m \rangle = \tanh(\beta(2d\langle m \rangle + H))$

$H = 0$ & low T $\rightarrow$ three solutions $\langle m \rangle = 0, \pm m_0$

which is true?

Imagine perturbing $\langle m_i \rangle = 0 \rightarrow \langle m_i \rangle = \varepsilon > 0$

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

$\rightarrow$ decrease to stable $\langle m_i \rangle = 0$

$T=2$: $\langle m_i \rangle$ too small compared to tanh

$\rightarrow$ increase to stable $\langle m_i \rangle = m_0 > 0$

Similarly go to $-m_0 \neq 0$ from $-\varepsilon < 0$

$\therefore$ $\langle m_i \rangle = 0$ unstable $\rightarrow$ $\langle m_i \rangle \neq 0$ ordered phase ✓

Another way to see (in)stability

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

└ Positive $\rightarrow$ $\langle m_i \rangle$ too small

Negative $\rightarrow$ $\langle m_i \rangle$ too large

So mean-field approx $\rightarrow$ ordered/disordered like Full Ising model ✓

When does $\langle m_i \rangle = 0$ becomes unstable?

Need $\tanh > \langle m_i \rangle$ for $\langle m_i \rangle = \varepsilon > 0 \rightarrow$ slope > 1 at $\langle m_i \rangle = 0$

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

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Is this a phase transition (w/discontinuity)?

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

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

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

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

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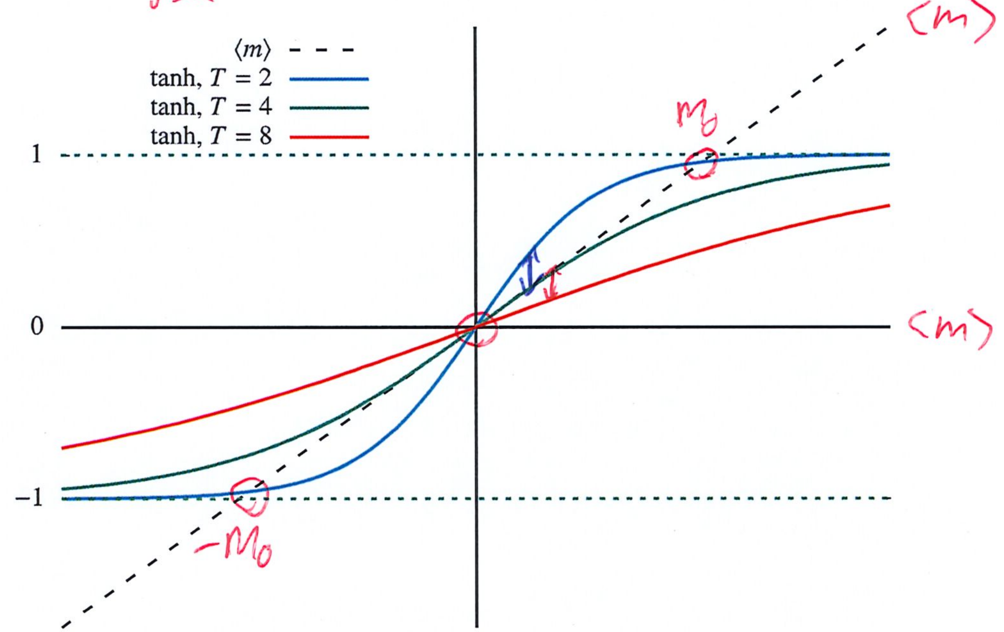
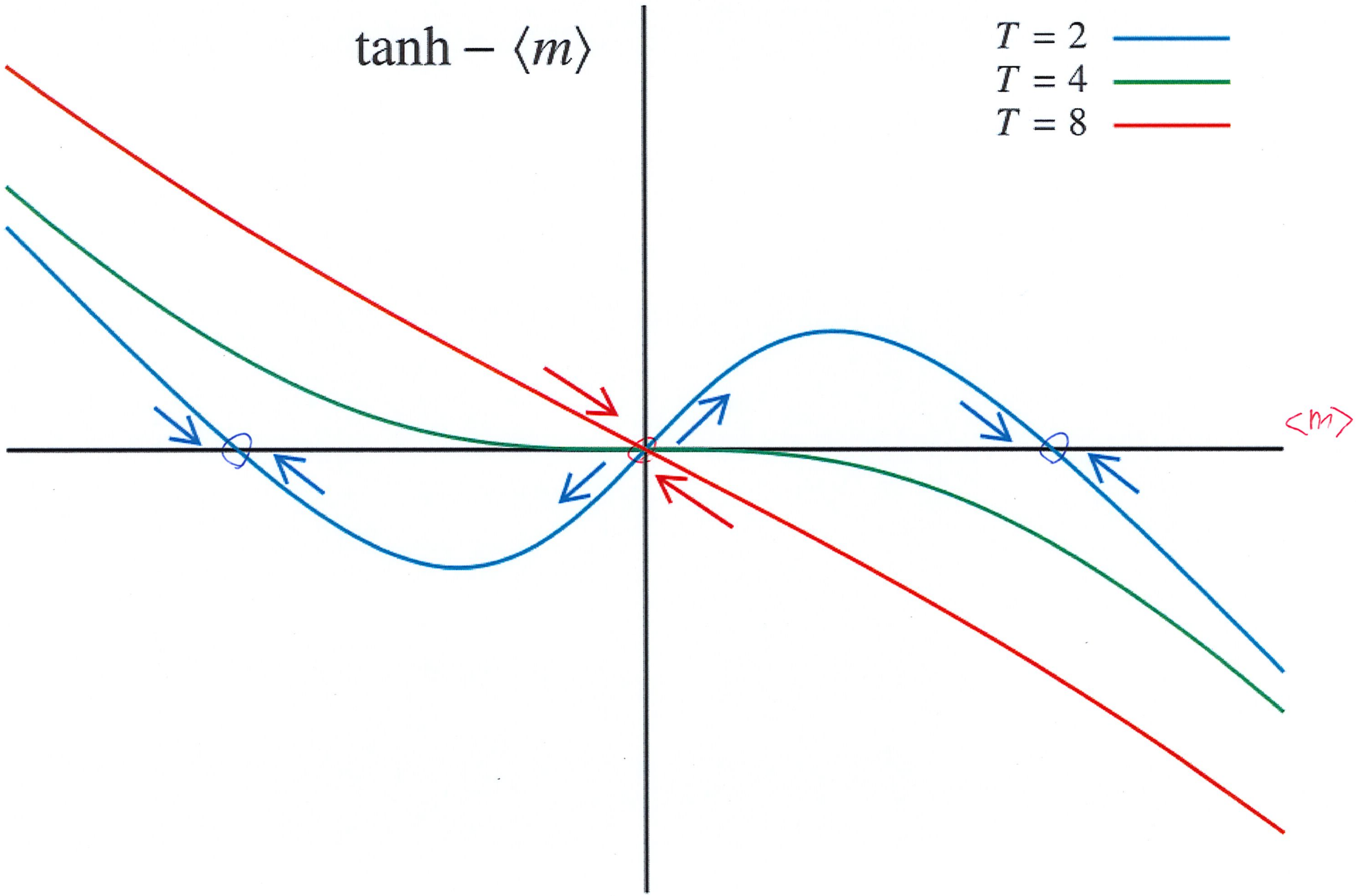
$J=2$



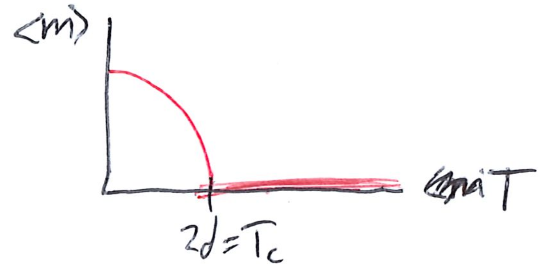
$\langle m \rangle$
tanh, $T = 2$
tanh, $T = 4$
tanh, $T = 8$
1
0
−1
m_0
$-m_0$
$\langle m \rangle$
$\langle m \rangle$


tanh − ⟨m⟩
T = 2
T = 4
T = 8
⟨m⟩

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

∴ magnetization is continuous at T_c

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



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

diverges as $T \rightarrow T_c$ from below

→ mean-field approx predicts 2nd-order PT for Ising model

General result when OP $\propto (T_c - T)^b$

with non-integer <u>critical exponent</u> $(b = 1/2)$

Many phase trans. have same sets of critical exponents

→ <u>universality</u> emergent large-scale behaviour near critical point independent of "microscopic" details

Are mean-field predictions correct? ($H=0$ 2nd-order PT $T_c = 2d$, $b = 1/2$)

$d=1$: No phase transition (Ising 1924) ✗

$d=2$: 2nd-order phase transition (Onsager 1944) ✓

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

$b = 1/8$, MF off by 4x

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

$b \approx 0.32$

$d \geq 4$: $b = 1/2$, $T_c \rightarrow 2d$ as $d \rightarrow \infty$

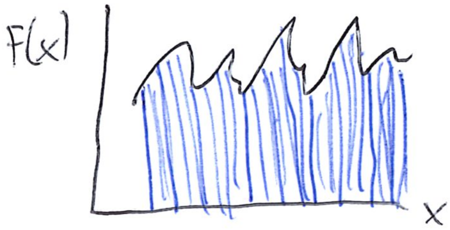
↳ Mean-field becomes exact

How do we carry out numerical analyses in less than $\sim 500{,}000\times$ age of universe?
(2d 10×10 part. func.)

Needed for $d \geq 3$ Ising model
and most interacted systems

Sample <u>small</u> subset of micro-states to approximate $\langle O \rangle$
Pseudo-random $\rightarrow$ "Monte Carlo" methods

<u>Example</u>: Compute integral by evaluating integrand at random points



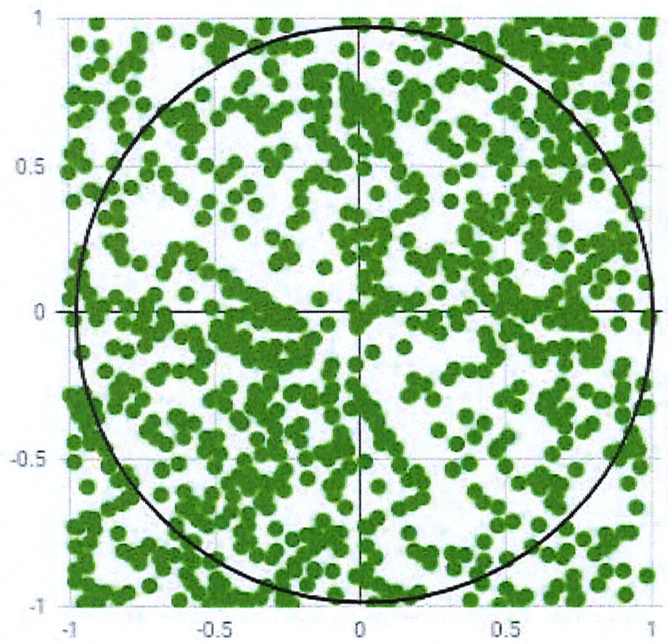
$$\int_{-1}^{1} dx \int_{-1}^{1} dy \; H\left(1 - \{x^2 + y^2\}\right) = \text{area of disk w/ radius } 1 = \pi$$

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

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

$$\frac{\text{length of computation}}{\text{age of universe}} \lll 1 \rightarrow$$ <u>very</u> small fraction of micro-states
How can this give reliable approx.

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



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

Low T: $\langle O \rangle$ dominated ground state

Other contribution suppressed $\sim e^{-E/T}$

Solution: Sample w_i with prob. $p_i \propto e^{-\beta E_i}$

without knowing p_i distribution

Importance sampling algorithms use pseudo-randomness to find large p_i w/out bias

Example: MRRTT algorithm (1953)

Start from any micro-state

Make a pseudo-random change $\to \Delta E$

$P_{accept} = \min\{1, \exp(-\beta \Delta E)\}$ otherwise rejected

$\to$ New micro-state (possibly unchanged)

Repeat!

Sequence of micro-states is "Markov chain"

(each w_i based on previous one, no memory)

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

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

Ergodicity depending on specific system & pseudo-random update

May take many updates to produce statistically independent w_i

$\to$ auto-correlations increase costs, increasing uncertainties $\propto 1/\sqrt{S}$

indep. samples

For Ising-~~mod~~like systems, huge benefits ~~&~~
from flipping "cluster" of spins, not just one
(avoid "critical slowing down" near 2nd-order phase trans.
with fluctuation on all length scales)

<u>Example</u>: Lattice quantum field theory

Relativity + QM → Fields $\Phi(\vec{x}, t)$ fill all space & time

Interactions governed by lagrangian $\mathcal{L}[\Phi(\vec{x}, t)]$

→ Feynman path integral

$$Z[\Phi(\vec{x},t)] = \int D\Phi \, \exp\left[\frac{i}{\hbar} \int d^3x \, dt \, \mathcal{L}[\Phi(\vec{x},t)]\right]$$

~ part. func. $T \leftrightarrow \hbar$

$t \to i\tau$

We have reached open research questions
just a few months after starting
w/probability foundations!