MATH327: Statistical Physics

Monday, 15 May 2023

604213

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

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

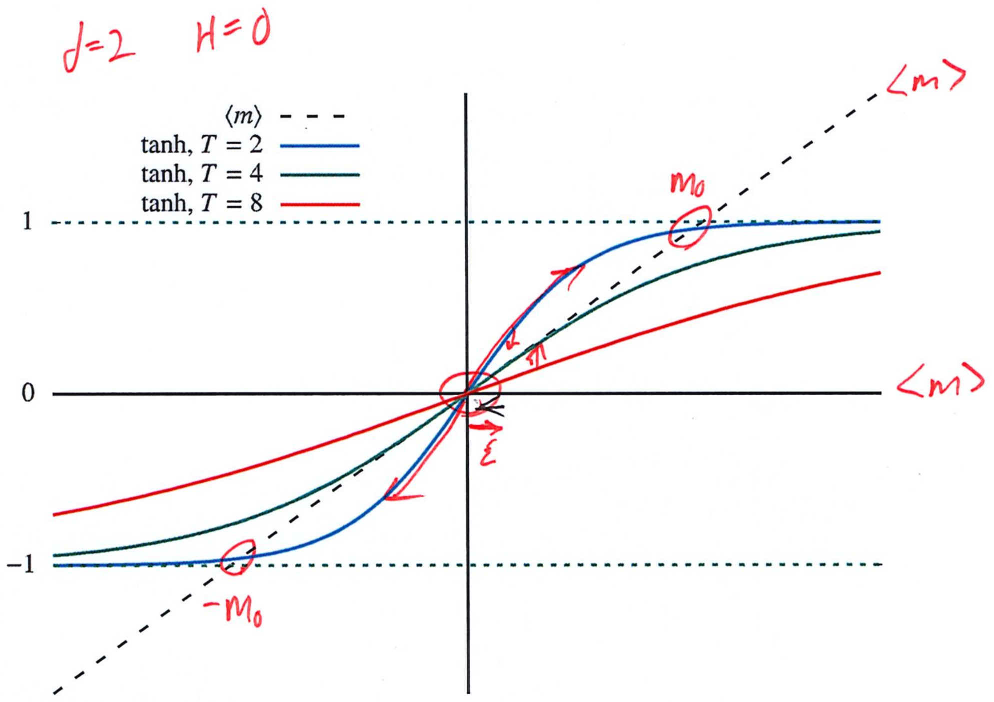
Assuming small average fluctuations

→ non-interacting w/ effective magnetic field involving mean spin & 2d n.n.'s

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

$H=0$ & low temperature → three solutions $\langle m \rangle = 0$ (unstable)

$\langle m \rangle = \pm m_0 \neq 0$



J=2 H=0
⟨m⟩
tanh, T = 2
tanh, T = 4
tanh, T = 8
1
0
−1
m₀
−m₀
⟨m⟩
⟨m⟩

Another way to see $\langle m \rangle = 0$ instability

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

Postive $\rightarrow$ $\langle m \rangle$ too small

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

Conclude $\langle m \rangle = 0$ unstable for low temperature $(H=0)$

Mean-field approx $\rightarrow$ ordered/disordered like full Ising model

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

(If phase trans., this will be T_c)

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

$$\left.\frac{d}{d\langle m \rangle} \tanh(2\beta d \langle m \rangle)\right|_{\langle m \rangle = 0} = \frac{d}{d\langle m \rangle}\left(2\beta d \langle m \rangle + \mathcal{O}(\langle m \rangle^3)\right)_{\langle m \rangle = 0}$$

$$= 2\beta d = 1$$

$$T_c = \frac{1}{\beta_c} = 2d$$

page 144

Is there a phase transition (w/discontinuity)?

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

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

$$2\beta d = \frac{T_c}{T}$$

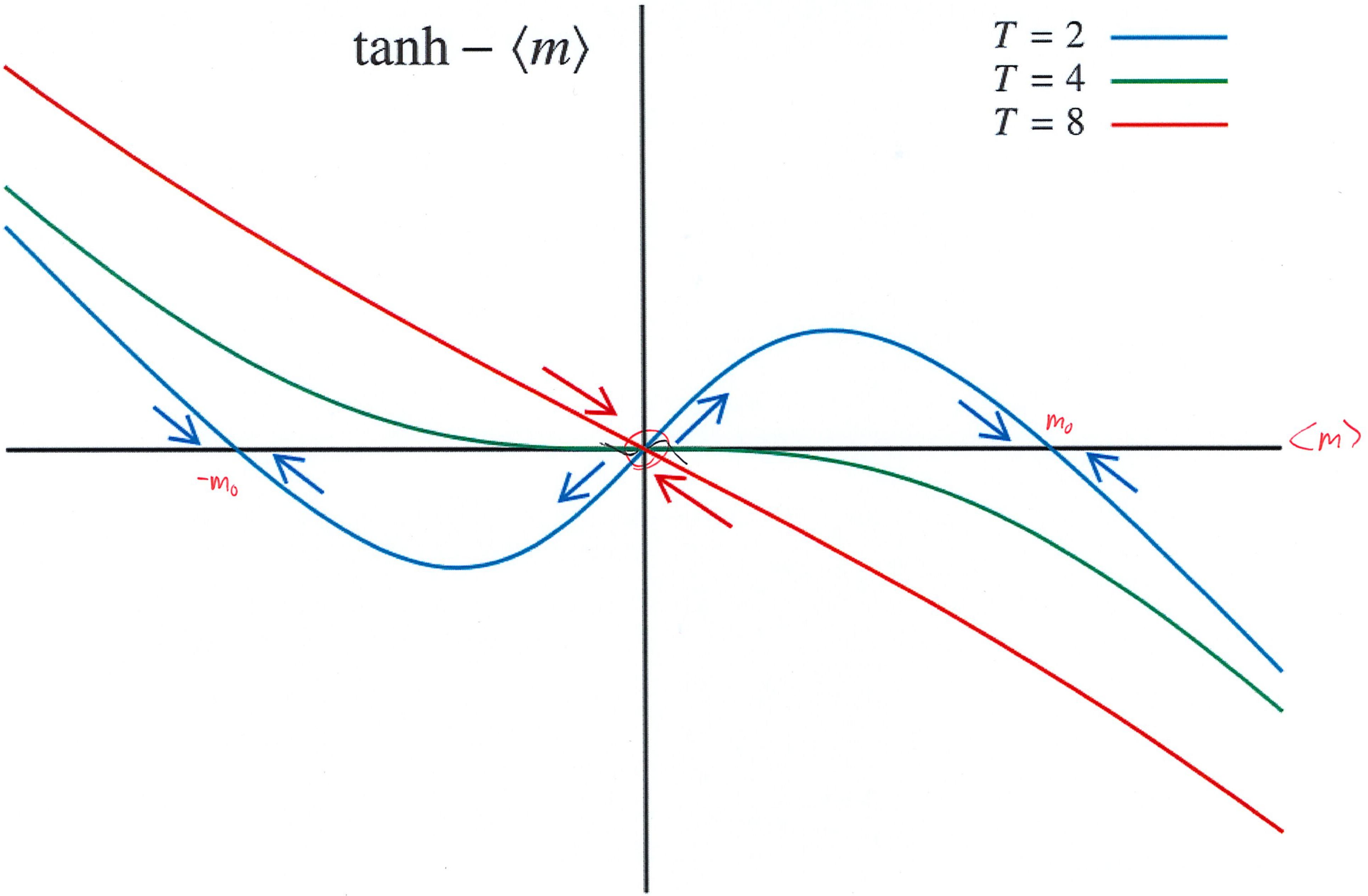
$$\frac{1}{3}\left(\frac{T_c}{T}\right)^3 \langle m \rangle^2 = \frac{T_c}{T} - 1$$

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

Approximating $\left(\frac{T}{T_c}\right)^2 \simeq 1$

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

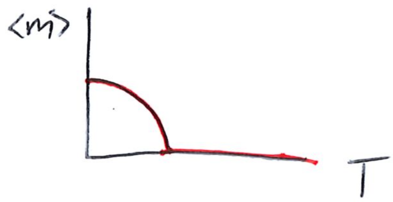
page 145



$\tanh - \langle m \rangle$
$T = 2$
$T = 4$
$T = 8$
$-m_0$
m_0
$\langle m \rangle$

So magnetization is continuous at $T=T_c$

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



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

diverges as $T \to T_c$ from below

→ 2nd-order phase trans. predicted by mean-field approx.

General result when $\langle m \rangle \propto (T_c - T)^b$

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 crit. pt. indendent of microscopic details

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Mean-field predictions $(H=0)$ 2nd-order PT

$T_c = 2d$ $b = 1/2$

Are these predictions correct?

$d=1$: No phase transition (supplement) ✗

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

$$T_c = \frac{2}{\log(1+\sqrt{2})} \approx 2.27 \quad \text{(supplement)}$$

MF $T_c = 4$ off by $\sim 2\times$

$b = 1/8$. MF off by $4\times$

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

$b \simeq 0.32$

$d \geq 4$: $b = 1/2$ ✓

$T_c \to 2d$ as $d \to \infty$

MF becomes exact sol'n when $2d \to \infty$ ($2d$ n.n.'s to average over)

Numerical analyses

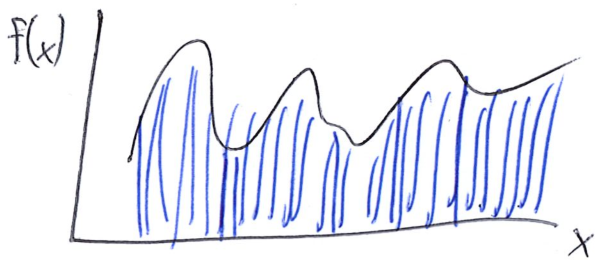
Needed for Ising model with $d>2$
and most interacting systems

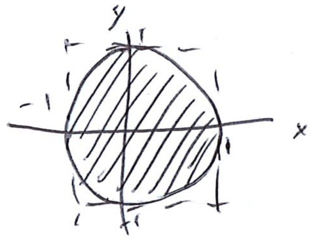
How? Recall $\sim 500{,}000 \times$ age of universe
to evaluate all $\sim 10^{32}$ terms in 10×10 Ising model part. func.

Sample small subset of micro-states
to approximate $\langle \mathcal{O} \rangle$

(Pseudo-) randomly $\to$ "Monte Carlo" methods

Example: Compute integral by evaluating integrand
at random points





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

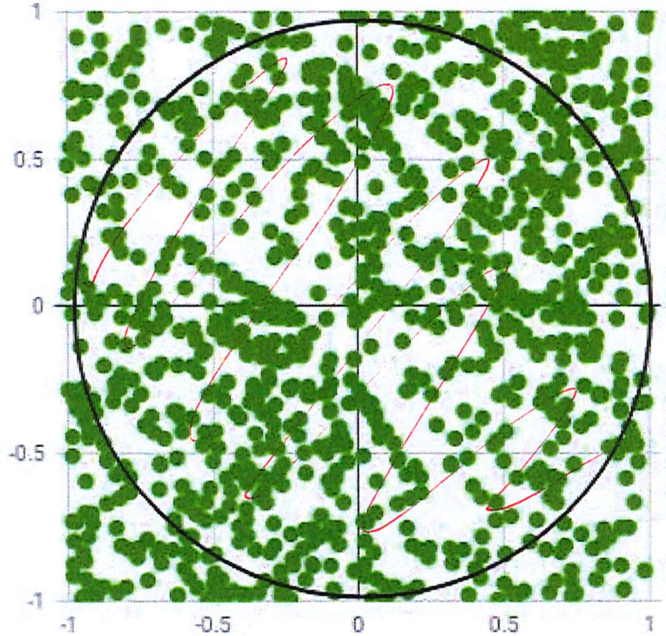
$$H(r) = \begin{cases} 1 & \text{for } r \geq 0 \\ 0 & \text{for } r < 0 \end{cases}$$

Monte Carlo integration most useful for high-dimensional integrals
... like part. func. for interacting statistical systems w/ $N \gg 1$

Can only consider very small fraction of micro-state

$$\cancel{\text{Ratio}}\ \text{fraction} \sim \frac{\text{length of computation}}{\text{many times age of universe}} \ll 1$$

How can this give reliable approximations?



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

Return ~~III~~ to Ising model

High-T limit → all micro-states equally probable

$\langle O \rangle$ determined by degeneracies

Large degeneracy more likely to be sample

... could be okay

Low-T limit → $\langle O \rangle$ determined by ground state

other micro-states' contributions suppressed $\sim e^{-\beta E_i}$

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

without knowing p_i distribution

→ Importance sampling algorithms use pseudo-randomness

Find important w_i w/ large p_i without bias

Example: MRRTT algorithm (1953)

Ising

spin config.

select s_j & flip it

Start from any micro-state

Make a pseudo-random 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)

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

To avoid bias, Markov chain must (in principle) be able to reach any micro-state from any other micro-state

→ <u>Ergodicity</u> depending on specific system and how state is updated

Statistical uncertainty $\propto \frac{1}{\sqrt{S}}$

number of samples

These are ongoing research question ~~we~~ which we've reached ~~at~~ just a few months after starting w/probability foundations!