Statistical Physics 2019/20
MATH327
Kurt Langfeld & David Schaich

Ising model analyses: Mean-field & maybe more

Tuesday 28 April

Plan

Today: Complete Chapter 9, with some additions

This Friday, 1 May: Lecture loose ends, tutorial on sample exam

Next Tuesday, 5 May: Course review for exam revision

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Monday, 11 May: Optional exam revision (if no conflicting exams...)

Friday, 29 May: Exam available 9AM, due in 24 hours

Questions?

Recap

Interacting theories can exhibit **phase transitions**

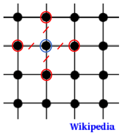
Interacting means ΔE_i from change in ith DoF depends on other DoF $k \neq i$

$\longrightarrow$ **much** more complicated than non-interacting systems we've studied so far

Famous (simple) example: **Ising model** in d dimensions

System of N **spins** arranged in a **lattice** with nearest-neighbour interaction

$$E = -\sum_{(ij)} s_i s_j - H \sum_i s_i$$



Recap

Magnetization $|m| = \frac{|M|}{N} = \frac{|n_+ - n_-|}{n_+ + n_-}$ characterizes Ising model's phases

High-temperature **disordered phase** with magnetization $|m| = 0$

Low-temperature **ordered phase** with magnetization $|m| = 1$

$d = 1$: Smooth **crossover** (not transition) between phases

$d \geq 2$: Rapid **second-order transition** between phases (in limit $N \to \infty$)

Magnetization continuous but first derivative $\frac{dM}{dT}$ discontinuous

Questions?

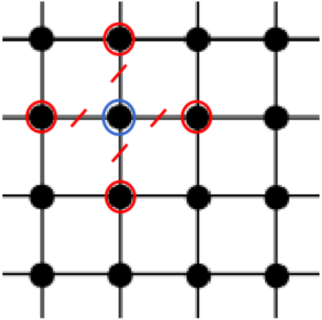
Preparation for mean-field approximation (page 142)

Mea culpa: Last week's preview was more ambitious than it had to be

Only need to consider 'local magnetic field' at single site i

$$E = -\sum_{(jk)\not\ni i} s_j s_k - H\sum_{k\neq i} s_k - s_i \sum_{k\in(ik)} s_k - H\cdot s_i$$

$$= -\sum_{(jk)\not\ni i} s_j s_k - H\sum_{k\neq i} s_k - (h_i + H)s_i$$



Wikipedia

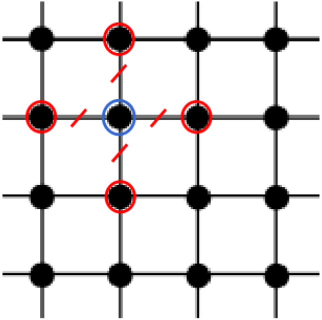
Preparation for mean-field approximation (page 142)

Only need to consider 'local magnetic field' at single site i

$$E = -\sum_{(jk)\not\ni i} s_j s_k - H \sum_{k \neq i} s_k - (h_i + H) s_i$$

$$Z(\beta, N, H) = \sum_{\{s_i\}} \exp\left[-\beta E\right]$$

$$= \sum_{\{s_k, k \neq i\}} \left(F(s_k) \sum_{s_i = \pm 1} \exp\left[\beta (h_i + H) s_i\right] \right)$$



Wikipedia

$$\sum_{\{s_k, k \neq i\}} F(s_k) \equiv c(\beta, N, H) \sim$$ modified partition function for portion of system that doesn't interact with ith DoF

Preparation for mean-field approximation (page 142)

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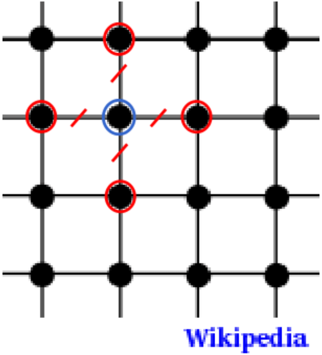

Still complicated since h_i depends on $2d$ s_k nearest neighbours of s_i

Mean-field approximation (pages 142–143)

$$Z(\beta, N, H) = \sum_{\{s_k, k \neq i\}} \left(F(s_k) \sum_{s_i = \pm 1} \exp\left[\beta(h_i + H)s_i\right] \right)$$

Assume $h_i = \sum_{k \in (ik)} s_k$ doesn't fluctuate much on average

$\longrightarrow$ **approximate** $h_i \approx \langle h_i \rangle = \sum_{k \in (ik)} \langle s_k \rangle = 2d \langle m \rangle$

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Depends on **constant expectation value** of magnetization

$$m = \frac{M}{N} = \frac{n_+ - n_-}{N} = \frac{1}{N}\sum_{i=1}^{N} s_i \qquad \langle m \rangle = \frac{1}{Z}\sum_{\{s_i\}} m \exp\left[-\beta E\right]$$

$\longrightarrow$ independent of spin configuration!

Mean-field approximation (pages 142–143)

$$Z(\beta, N, H) = \sum_{\{s_k, k \neq i\}} \left(F(s_k) \sum_{s_i = \pm 1} \exp\left[\beta(h_i + H)s_i\right] \right)$$

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$\longrightarrow$ **approximate** $h_i \approx \langle h_i \rangle = \sum_{k \in (ik)} \langle s_k \rangle = 2d \langle m \rangle$

Now s_i is decoupled from all other DoF $k \neq i$:

$$Z(\beta, N, H) \approx Z_{\text{MF}}(\beta, N, H) = \left(\sum_{\{s_k, k \neq i\}} F(s_k) \right) \sum_{s_i = \pm 1} \exp\left[\beta(2d \langle m \rangle + H)s_i\right]$$

$$= c(\beta, N, H) \cdot 2 \cosh\left[\beta(2d \langle m \rangle + H)\right]$$

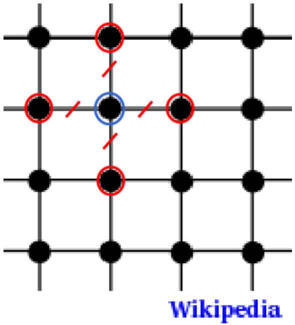
Mean-field partition function (page 143)

We have the N-spin partition function Z_{MF}
expressed in terms of the $(N-1)$-spin modified partition function c

$$Z_{\text{MF}}(\beta, N, H) = 2c(\beta, N, H) \cosh\left[\beta(2d\langle m\rangle + H)\right]$$

Conjecture that iterating will produce

$$Z_{\text{MF}}(\beta, N, H) \propto \left(2\cosh\left[\beta(2d\langle m\rangle + H)\right]\right)^N$$



Let's derive this explicitly...

Mean-field approximation alternate derivation (D. Tong section 5.2)

Rewrite interaction $s_i s_j$ in terms of fluctuations about average $\langle m \rangle$

$$s_i s_j = \left[(s_i - \langle m \rangle) + \langle m \rangle \right] \times \left[(s_i - \langle m \rangle) + \langle m \rangle \right]$$
$$= (s_i - \langle m \rangle)(s_j - \langle m \rangle) + (s_i - \langle m \rangle) \langle m \rangle + (s_j - \langle m \rangle) \langle m \rangle + \langle m \rangle^2$$

Assume small fluctuations $|s_i - \langle m \rangle| \ll 1$ on average

$\longrightarrow$ **approximate** by neglecting quadratic term

$$E = -\sum_{(ij)} s_i s_j - H \sum_i s_i$$

$$\longrightarrow \ E_{\text{MF}} = -\sum_{(ij)} \left[(s_i + s_j) \langle m \rangle - \langle m \rangle^2 \right] - H \sum_i s_i$$

Mean-field approximation alternate derivation (D. Tong section 5.2)

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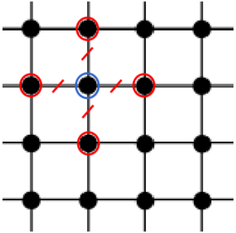

Nearest-neighbour sum runs over $d \cdot N$ links

Includes both $(s_i + s_j) \longrightarrow$ each spin appears $2d$ times in sum:

$$E_{\mathrm{MF}} = d \cdot N \langle m \rangle^2 - (2d \langle m \rangle + H) \sum_{i=1}^{N} s_i$$

You can check E_{MF} is non-interacting $\longrightarrow$ significant simplifications

Mean-field approximation alternate derivation (D. Tong section 5.2)

$$E_{\text{MF}} = d \cdot N \langle m \rangle^2 - (2d \langle m \rangle + H) \sum_i s_i$$

Repeating the derivation of Eq. 32 on pages 54–55 confirms our conjecture:

$$\begin{aligned} Z_{\text{MF}}(\beta, N, H) &= \sum_{\{s_i\}} \exp\left[-\beta E\right] \\ &= \exp\left[-\beta d \cdot N \langle m \rangle^2\right] \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \exp\left[\beta(2d \langle m \rangle + H)(s_1 + \cdots + s_N)\right] \end{aligned}$$

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$$= \left(\sum_{s_1=\pm 1} \exp\left[\beta(2d \langle m \rangle + H)s_1\right] \right) \times \cdots \times \left(\sum_{s_N=\pm 1} \exp\left[\beta(2d \langle m \rangle + H)s_N\right] \right)$$

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$$Z_{\text{MF}}(\beta, N, H) = \exp\left[-\beta d \cdot N \langle m \rangle^2\right] \left(\sum_{s=\pm 1} \exp\left[\beta(2d \langle m \rangle + H)s\right] \right)^N$$

$$= \exp\left[-\beta d \cdot N \langle m \rangle^2\right] \left(2 \cosh\left[\beta(2d \langle m \rangle + H)\right]\right)^N \qquad \checkmark$$

Magnetization in mean-field approximation (pages 143–144)

The mean-field partition function depends on the magnetization:

$$Z_{\mathrm{MF}}(\beta) = \exp\left[-\beta d \cdot N \langle m \rangle^2\right] \left(2\cosh\left[\beta(2d\langle m \rangle + H)\right]\right)^N$$

What can we say about $\langle m \rangle$?

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What can we say about $\langle m \rangle$?

1) Observe $M = n_+ - n_- = \sum_{i=1}^{N} s_i$ appears in full Ising model energy

$$E = -\sum_{(ij)} s_i s_j - H \sum_i s_i = -\sum_{(ij)} s_i s_j - H \cdot M$$

Magnetization in mean-field approximation (pages 143–144)

1)

$$E = -\sum_{(ij)} s_i s_j - H \cdot M$$

2) Expectation value $\langle M \rangle = \frac{1}{Z} \sum_{\{s_i\}} M \exp\left[-\beta E\right]$

related to derivative $\frac{\partial}{\partial H} \exp\left[\beta \sum_{(ij)} s_i s_j + \beta H \cdot M\right] = \beta M \exp\left[\beta \sum_{(ij)} s_i s_j + \beta H \cdot M\right]$

Magnetization in mean-field approximation (pages 143–144)

2)

$$\frac{\partial}{\partial H}\exp\left[\beta\sum_{(ij)} s_i s_j + \beta H\cdot M\right] = \beta M \exp\left[\beta\sum_{(ij)} s_i s_j + \beta H\cdot M\right]$$

3) Pull derivative outside sum over configurations:

$$\langle M\rangle = \frac{1}{Z}\sum_{\{s_i\}} M \exp\left[\beta\sum_{(ij)} s_i s_j + \beta H\cdot M\right] = \frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial H}\sum_{\{s_i\}}\exp\left[\beta\sum_{(ij)} s_i s_j + \beta H\cdot M\right]$$

$$= \frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial H}Z = \frac{1}{\beta}\frac{\partial \ln Z}{\partial H} = -\frac{\partial}{\partial H}F$$

in terms of Helmholtz free energy $F = -\frac{\ln Z}{\beta}$

Magnetization in mean-field approximation (pages 143–144)

We have
$$\langle m \rangle = \frac{\langle M \rangle}{N} = \frac{1}{N\beta}\frac{\partial \ln Z}{\partial H}$$

Apply the mean-field approximation

$$\ln Z \;\longrightarrow\; \ln Z_{\mathrm{MF}} = N \ln\cosh\left[\beta(2d\,\langle m \rangle + H)\right] + \{H\text{-independent terms}\}$$

Magnetization in mean-field approximation (pages 143–144)

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$$\ln Z \longrightarrow \ln Z_{\text{MF}} = N \ln\cosh\left[\beta(2d\langle m \rangle + H)\right] + \{H\text{-independent terms}\}$$

Result: $$\langle m \rangle = \frac{1}{\beta}\frac{1}{\cosh\left[\beta(2d\langle m \rangle + H)\right]}\frac{\partial}{\partial H}\cosh\left[\beta(2d\langle m \rangle + H)\right]$$

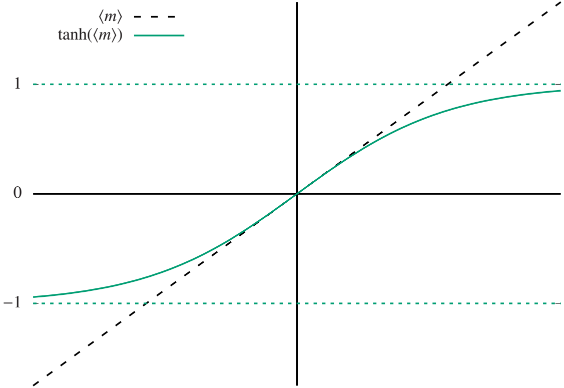
$$= \tanh\left[\beta(2d\langle m \rangle + H)\right]$$

Self-consistency condition for mean-field $\langle m \rangle$ (pages 144–145)

Find solutions of $\langle m \rangle = \tanh\left[\beta(2d\,\langle m \rangle + H)\right]$

by plotting intersections of $f(x) = x$ and $g(x) = \tanh\left[\beta(2d\cdot x + H)\right]$

First recall how $\tanh\left[\langle m \rangle\right]$ looks:



Corresponds to

$$d = 2$$

$$\beta = \frac{1}{2d} = \frac{1}{4}$$

$$H = 0 \qquad \longrightarrow \langle m \rangle = 0$$

Self-consistency condition for mean-field $\langle m \rangle$ (pages 144–145)

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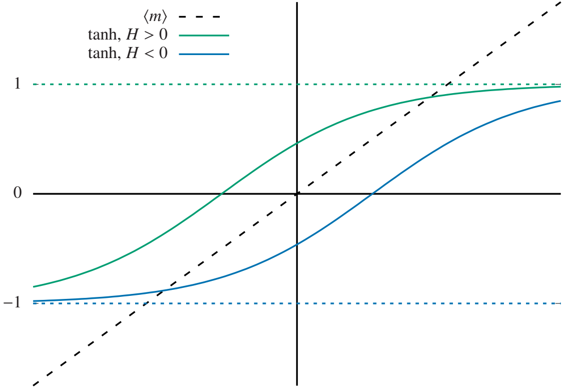
Positive $H > 0$ shifts $\texttt{tanh}$ to left:

Corresponds to

$d = 2$

$\beta = \frac{1}{2d} = \frac{1}{4}$

$H = \pm 2 \quad \longrightarrow \langle m \rangle = \pm 0.88$



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Increasing β makes tanh steeper:

Corresponds to

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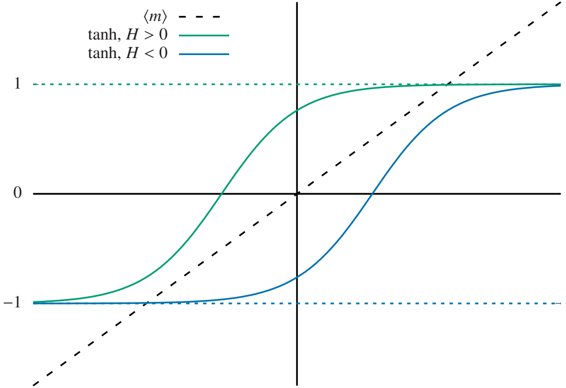
$H = \pm 2 \qquad \longrightarrow \langle m \rangle \approx \pm 1$



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Increasing β makes `tanh` steeper:

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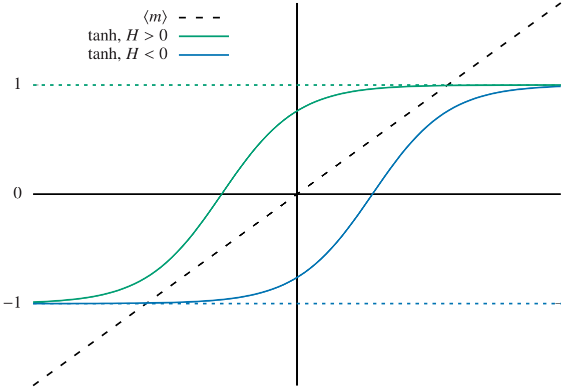


Sufficiently large $|H| \longrightarrow$ single solution to self-consistency condition:
ordered $\langle m \rangle \approx \text{sign}(H)$ in alignment with external field

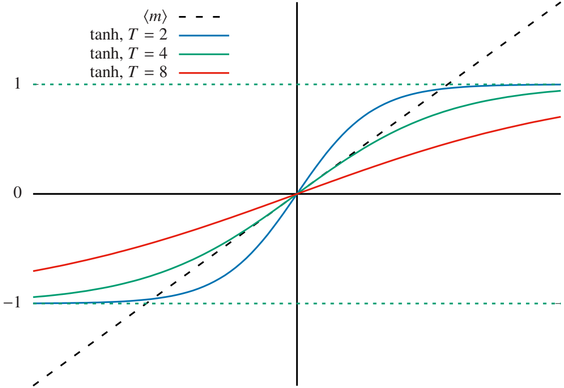
Mean-field $\langle m \rangle$ temperature dependence (pages 145–146)

Consider $H = 0$ for various temperatures

Disordered $\langle m \rangle = 0$
is always possible solution

Steeper `tanh` at lower temperature
$\longrightarrow$ additional solutions $\langle m \rangle = \pm m_0$

Approach **ordered** $m_0 \to 1$ as $T \to 0$



Not hard to see $\langle m \rangle = 0$ solution **unstable** at low temperatures

Mean-field $\langle m \rangle$ solution stability (page 146)

Not hard to see $\langle m \rangle = 0$ solution **unstable** at low temperatures

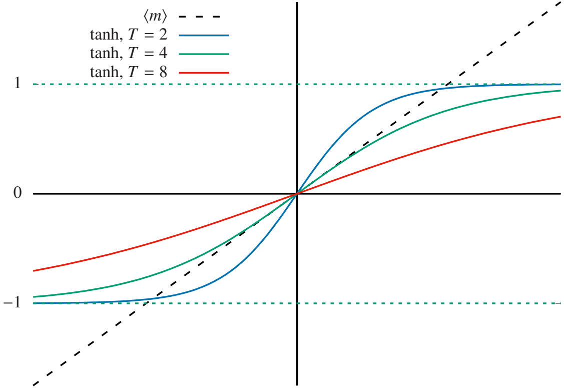
Start with $\langle m \rangle = 0$

Small positive fluctuation

produces $\langle m \rangle < \tanh$

$\Longrightarrow$ $\langle m \rangle$ must increase further

until it reaches $\langle m \rangle = m_0$



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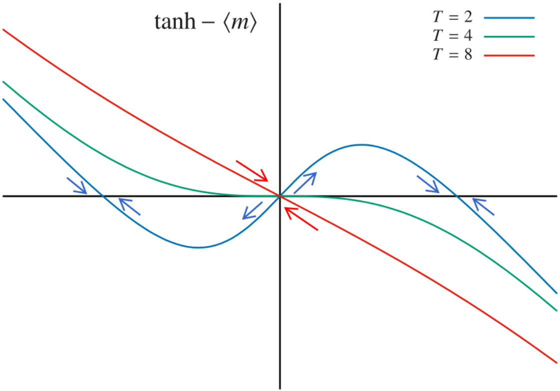


Equivalent to $\tanh - \langle m \rangle > 0$ for small $\langle m \rangle > 0$

Mean-field critical temperature (page 146)

Conclusion: Rapid change from disordered $\langle m \rangle = 0$ to ordered $|\langle m \rangle| = m_0 > 0$

when tanh steeper than $\langle m \rangle$ around $\langle m \rangle = 0$

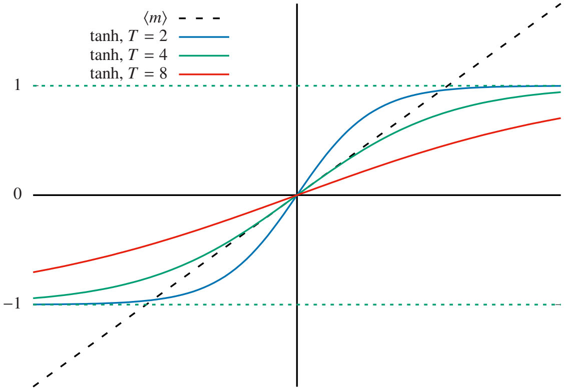
Around $\langle m \rangle = 0$,

$$\tanh(u) = u + \mathcal{O}\left(u^3\right)$$

$$\implies \frac{d}{d\langle m \rangle} \tanh\left[2d \cdot \beta \langle m \rangle\right]\Big|_{\langle m \rangle = 0} = 2d \cdot \beta$$

tanh slope $2d \cdot \beta = 1$

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



Mean-field phase transition (pages 146–147)

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around $\beta_c = \dfrac{1}{2d}$

Question: Is this rapid change a true phase transition?

Is there a discontinuity in the order parameter $\langle m \rangle$ or its derivative(s)?

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For β above but close to β_c we have $0 < |\langle m \rangle| \ll 1$

and can expand the self-conistency equation,

$$\langle m \rangle = \tanh\left[2d \cdot \beta \langle m \rangle\right] \approx 2d \cdot \beta \langle m \rangle - \frac{1}{3}\left(2d \cdot \beta \langle m \rangle\right)^3$$

Mean-field phase transition (pages 146–147)

Self-consistency equation: $2d\cdot\beta - 1 = \frac{1}{3}(2d\cdot\beta)^3 \langle m\rangle^2$

In terms of $T = \frac{1}{\beta}$ close to but lower than $T_c = 2d$,

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

Mean-field phase transition (pages 146–147)

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

Mean-field phase transition (pages 146–147)

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With $\left(\dfrac{T}{T_c}\right)^2 \approx 1$ we have $$\langle m\rangle = \pm\sqrt{\frac{3}{2d}}\,(T_c - T)^{1/2} \text{ for } T < T_c$$

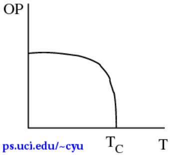
Mean-field phase transition (pages 146–147)

Conclusion: $\langle m \rangle = \pm\sqrt{\frac{3}{2d}}\,(T_c - T)^{1/2}$ for $T < T_c$

The coefficient on page 147 is correct in $d = 6$ dimensions ;)

What matters is the **critical exponent** $1/2$:

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



Mean-field phase transition (pages 146–147)

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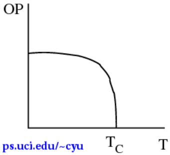


The order parameter $\langle m \rangle$ is continuous at $T = T_c$

while $\frac{d\langle m \rangle}{dT} \propto \frac{1}{(T_c - T)^{1/2}}$ diverges $\longrightarrow$ predict **second-order transition**

Accuracy of mean-field approximation (page 147)

Recap: Mean-field approximation predicts

* Second-order transition at critical $\beta_c = \dfrac{1}{2d}$

* Order parameter $\langle m \rangle \propto (T_c - T)^{1/2}$ just below transition

Question: How accurate are these results?

Accuracy of mean-field approximation (page 147)

Question: How accurate are these results?

For $d = 2$ we have Onsager's 1944 exact solution:

Second-order transition ✓

Critical $\beta_c = \dfrac{\ln(1+\sqrt{2})}{2} \approx 0.44$ almost twice mean-field $\beta_c = \frac{1}{2d} = \frac{1}{4}$

$\langle m \rangle \propto (T_c - T)^{1/8} \longrightarrow$ critical exponent $1/8$

four times smaller than mean-field $1/2$

So mean-field approximation predicts right qualitative behaviour

with significant quantitative shortcomings

Accuracy of mean-field approximation (page 147)

Question: How accurate are these results?

For $d = 1$ we have Ising's 1925 exact solution:

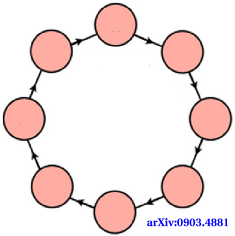
No phase transition $\longrightarrow$ mean-field approximation fails badly

If time permits, let's solve the one-dimensional Ising model ourselves...

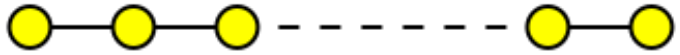
$d = 1$ Ising model exact solution (D. V. Schroeder section 8.2)

As before $H = 0$ is most interesting case, $Z(\beta, N, H) = \sum_{\{s_i\}} \exp\left[\beta \sum_{(ij)} s_i s_j\right]$

Simplify by 'unrolling' spin chain:

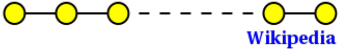


$\rightsquigarrow$



Miss 1 of N links $\longrightarrow$ accurate for large N

$d = 1$ Ising model exact solution (D. V. Schroeder section 8.2)



$$E = -(s_1 s_2 + s_2 s_3 + \cdots + s_{N-1} s_N)$$

$$\longrightarrow Z = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta s_1 s_2} e^{\beta s_2 s_3} \ldots e^{\beta s_{N-1} s_N}$$

Only last factor depends on s_N:

$$\left.\begin{array}{ll} \text{If } s_{N-1} = +1 & \sum_{s_N=\pm 1} e^{\beta s_{N-1} s_N} = e^{\beta} + e^{-\beta} \\ \text{If } s_{N-1} = -1 & \sum_{s_N=\pm 1} e^{\beta s_{N-1} s_N} = e^{-\beta} + e^{\beta} \end{array}\right\} = 2\cosh\beta$$

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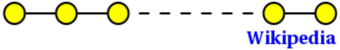

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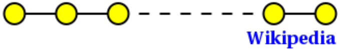
Now $Z = (2\cosh\beta) \sum_{s_1=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} e^{\beta s_1 s_2} e^{\beta s_2 s_3} \ldots e^{\beta s_{N-2} s_{N-1}}$

and we can repeat for s_{N-1}

$d = 1$ Ising model exact solution (D. V. Schroeder section 8.2)

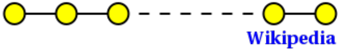


Result:

$$Z = \sum_{s_1=\pm 1} (2\cosh\beta)^{N-1} = 2^N (\cosh\beta)^{N-1}$$

Restoring omitted link adds Nth $\cosh$ factor $\longrightarrow$ $Z = (2\cosh\beta)^N$

$d = 1$ Ising model exact solution (D. V. Schroeder section 8.2)



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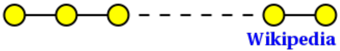
Internal energy: $$\langle E\rangle = -\frac{\partial}{\partial\beta}\ln Z = -N\tanh\beta$$

- Low temperatures $\beta \to \infty$ give $\langle E\rangle \to -N$ in ordered ground state ✓
- High temperatures $\beta \to 0$ give $\langle E\rangle \to 0$ in disordered phase ✓

$d = 1$ Ising model exact solution (D. V. Schroeder section 8.2)



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Low temperatures $\beta\to\infty$ give $\langle E\rangle\to -N$ in ordered ground state ✓

High temperatures $\beta\to 0$ give $\langle E\rangle\to 0$ in disordered phase ✓

No discontinuity in $\langle E\rangle$ or its derivatives for $T > 0$ $\longrightarrow$ smooth crossover

Revisit accuracy of mean-field approximation

For $d = 1$ mean-field approximation fails badly

For $d = 2$ it predicts right qualitative behaviour
with significant quantitative shortcomings

Conjecture mean-field approximation more accurate as d increases

Justification: $2d$ neighbours $\longrightarrow$ better averaging for larger d

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Mean-field predicts correct critical exponents for $d \geq 4$

Mean-field exact reproduces Ising model in formal limit $d \to \infty$

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Mean-field predicts correct critical exponents for $d \geq 4$

Mean-field reproduces exact theory in formal limit $d \to \infty$

Numerical methods required to analyze $d \geq 3$...

Wrap up

Mean-field approximation assumes small fluctuations on average

$\longrightarrow$ omit interactions in Ising model

Produces **self-consistency condition** for magnetization order parameter

Predicts second-order transition at critical $\beta_c = \dfrac{1}{2d}$

where $\langle m \rangle \propto (T_c - T)^{1/2}$ with critical exponent $1/2$

Accuracy of approximation improves as dimension d increases

Wrap up

Mean-field approximation assumes small fluctuations on average

$\longrightarrow$ omit interactions in Ising model

Predicts second-order transition at critical $\beta_c = \dfrac{1}{2d}$

where $\langle m \rangle \propto (T_c - T)^{1/2}$ with critical exponent $1/2$

Accuracy of approximation improves as dimension d increases

Fails badly compared to exact $d = 1$ solution

Qualitatively but not quantitatively correct compared to exact $d = 2$ solution

Exactly reproduces Ising model in formal limit $d \to \infty$

Numerical methods required to analyze $d \geq 3$ Ising model