Statistical Physics 2019/20
MATH327
Kurt Langfeld & David Schaich

Interacting systems & Ising model

Tuesday 21 April

Plan

Today: Start Chapter 9 on phase transitions

This Friday: Final virtual computer lab
Review computer project part A, any questions on part B

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Monday, 11 May: Optional exam revision (rescheduled due to 8 May holiday)

Questions?

Recap: Phase transition overview (page 134)

Many systems exist in very different **phases**

depending on temperature, pressure, other conditions

Examples: Water transitions from liquid to solid (ice) as temperature decreases

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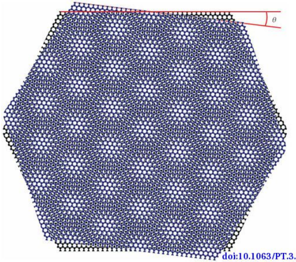
<u>Twisted bilayer graphene</u>

Transitions from electrical insulator to superconductor

at low temperature $T_c \approx 1.7$ K

(for 'magic' twist angle $\theta \approx 1.1^\circ$)



doi:10.1063/PT.3.4384

Phase transitions require interactions (page 134)

Many systems exist in very different **phases**

depending on temperature, pressure, other conditions

Questions: What causes such dramatic **phase transitions**?

What distinguishes the different phases of a system?

Phase transitions require interactions (page 134)

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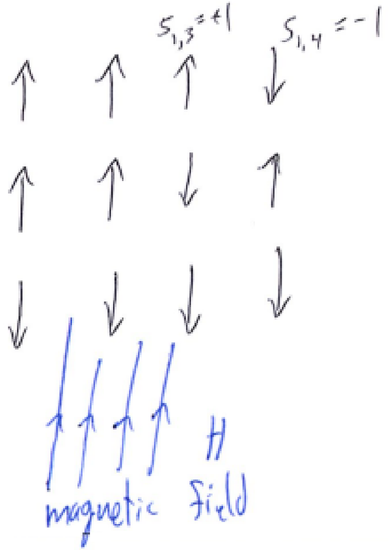
What distinguishes the different phases of a system?

Key ingredient: Interactions between degrees of freedom (DoF) in system

Review non-interacting spin system (pages 134–135)



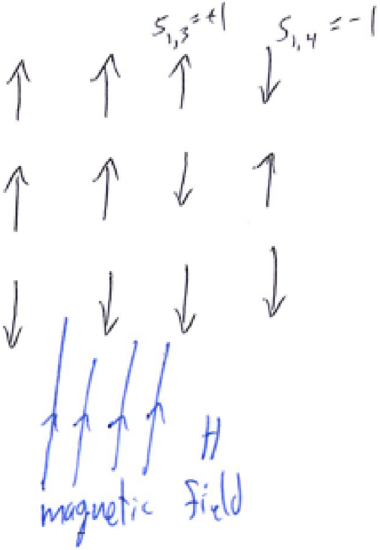
Spin DoF are $s_i \in \{-1, +1\}$ with $i = 1, \cdots, N$

Distinguishable by location in **lattice**

- Two-dimensional lattice drawn to left
- One-dimensional lattice (chain) considered in Section 3.3.1

Want to compute energy as starting point for statistical analyses

Review non-interacting spin system (pages 134–135)



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Distinguishable by location in **lattice**

Two-dimensional lattice drawn to left

One-dimensional lattice (chain) considered in Section 3.3.1

External magnetic field with strength H

Spin s_i has energy $-H \cdot s_i$

Total energy is simply sum $E = -H \sum_i s_i$

(sign from Eq. 91 on page 138)

Definition of non-interacting system (page 135)

ΔE_i is change in system's total energy E upon changing ith DoF

System is **non-interacting** if and only if ΔE_i is independent of **all** DoF $k \neq i$

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System is **non-interacting** if and only if ΔE_i is independent of **all** DoF $k \neq i$

Check that spin system is non-interacting

$$E_{\text{before}} = -H \sum_j s_j = -H \left(\sum_{k \neq i} s_k + s_i \right)$$

$$E_{\text{after}} = -H \left(\sum_{k \neq i} s_k - s_i \right)$$

$\Delta E_i = E_{\text{after}} - E_{\text{before}} = 2H \cdot s_i$ independent of all $k \neq i$ ✓

Simplifications for non-interacting systems (page 136)

Enormous simplifications possible when systems are non-interacting

(That's why we have only considered non-interacting systems so far)

Example: Canonical partition function for N distinguishable spins

$$
\begin{aligned}
Z_{\text{dist}} &= \sum_{\{s_i\}} \exp\left[-\beta E(s_i)\right] = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left[\beta H \sum_i s_i\right] \\
&= \left(\sum_{s_1=\pm 1} \exp\left[\beta H s_1\right]\right) \times \cdots \times \left(\sum_{s_N=\pm 1} \exp\left[\beta H s_N\right]\right) \\
&= \left(e^{-\beta H} + e^{\beta H}\right) \times \cdots \times \left(e^{-\beta H} + e^{\beta H}\right) = \left(e^{-\beta H} + e^{\beta H}\right)^N = Z_1^N
\end{aligned}
$$

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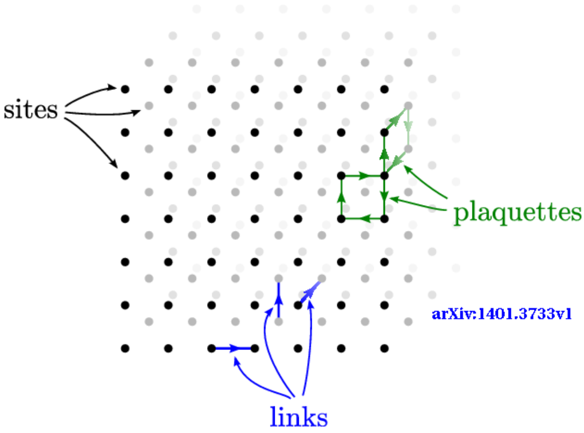
$$= \left(e^{-\beta H} + e^{\beta H}\right) \times \cdots \times \left(e^{-\beta H} + e^{\beta H}\right) = \left(e^{-\beta H} + e^{\beta H}\right)^N = Z_1^N$$

Non-interacting form of E lets us rearrange & simplify 2^N terms

Even $2^{100\times 100} = 2^{10,000} \sim 10^{3000}$ terms hard to handle, let alone realistic $2^{10^{23}}$

Fix lattice structure (pages 136–137)

For simplicity, define spin system on (hyper-)cubic lattice in d dimensions



In nature, only have $d = 1, 2,$ or 3
($d = 3$ lattice drawn to left)

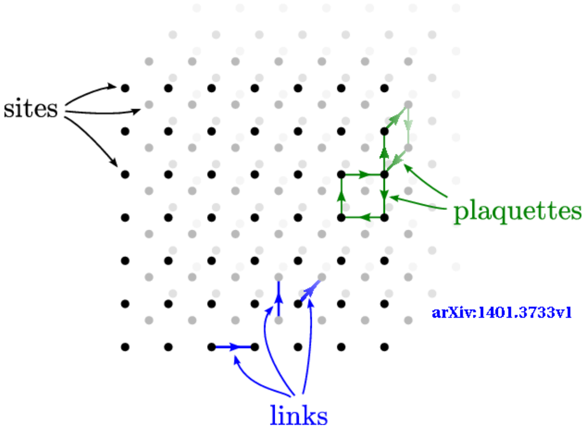
Can mathematically define
d-dim'l lattice for any integer $d \geq 1$

All spins at **sites** in regular grid,
separated by constant distance

Links connect nearest-neighbour sites
in all d dimensions

Fix lattice structure (pages 136–137)

For simplicity, define spin system on (hyper-)cubic lattice in d dimensions



All spins at **sites** in regular grid, separated by constant distance

Links connect nearest-neighbour sites in all d dimensions

For $d \geq 2$ **plaquettes** are elementary units of surface area

For $d \geq 3$ cubes are elementary units of volume

Add short-range interaction to spin system (page 137)

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

Definition: (ij) is set of all nearest-neighbour (n.n.) pairs in lattice,
equivalent to set of all links $\ell = (ij)$ in lattice

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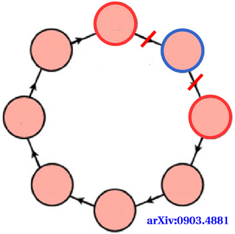
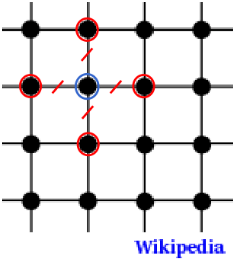


$d = 1$:
2 n.n. per site
N sites
$\longrightarrow$ N links



$d = 2$:
4 n.n. per site
N sites
$\longrightarrow$ $2N$ links

Aside: Assume lattices are periodic hyper-tori (negligible for large N)

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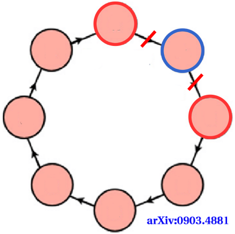

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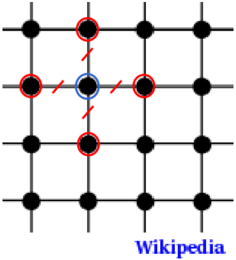

$d = 2$:
4 n.n. per site
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General d: $2d$ n.n. per site, N sites $\longrightarrow$ $d \cdot N$ links

Confirm this is interacting system (pages 137–138)

Compute ΔE_i for $E = -\sum_{(jk)} s_j s_k - H \sum_j s_j$

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

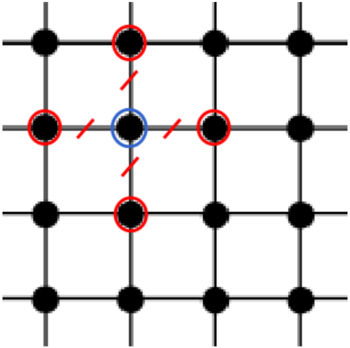
$$E_{\text{after}} = -\sum_{(jk)\not\ni i} s_j s_k - H \sum_{k\neq i} s_k + s_i \sum_{k\in(ik)} s_k + H s_i$$

$$\Delta E_i = E_{\text{after}} - E_{\text{before}} = 2\left(\sum_{k\in(ik)} s_k + H\right) s_i \quad \text{depends on } k \neq i \quad \checkmark$$

Confirm this is interacting system (pages 137–138)

$$\Delta E_i = 2 \left(\sum_{k \in (ik)} s_k + H \right) s_i \equiv 2(h_i + H) s_i$$

Sites $k \in (ik)$ are nearest neighbours of site i



Wikipedia

Interpretation

Nearest-neighbour sites generate

local magnetic field $h_i \equiv \sum_{k \in (ik)} s_k$ at site i

On page 142, will rewrite system in terms of h_i

Canonical partition function for Ising model (page 138)

Definition: Ising model is spin system on d-dim'l (hyper-)cubic lattice with energy $E = -\sum_{(ij)} s_i s_j - H \sum_i s_i$

Invented by Lenz (1920)

$d = 1$ case solved by Ising (1925)

$d = 2$ case solved by Onsager (1944)

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"Solving" means evaluating the partition function

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

Extremely difficult for interacting systems

Qualitative behaviour of Ising model (page 139)

Recall initial **question:** What distinguishes the different phases of a system?

Will show Ising model exists in different **phases** at high and low temperatures

This is necessary but not sufficient for there to be a phase transition

Qualitative behaviour of Ising model (page 139)

Recall initial **question:** What distinguishes the different phases of a system?

Will show Ising model exists in different **phases** at high and low temperatures

This is necessary but not sufficient for there to be a phase transition
Could instead be slow, smooth **crossover** rather than rapid **transition**

Will need more careful definition of “transition”
which will be motivated by phases of Ising model

Questions?

High-temperature limit of Ising model (page 139)

As $T \to \infty$ we have $\beta = \frac{1}{T} \to 0$ and

$$Z(\beta \to 0) = \sum_{\{s_i\}} \exp\left[\beta \sum_{(ij)} s_i s_j + \beta H \sum_i s_i\right] \longrightarrow \sum_{\{s_i\}} \exp[0] = 2^N$$

Identical to trivial system with $E = 0$!

(Obviously non-interacting since $\Delta E_i = 0$ independent of all DoF)

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Identical to trivial system with $E = 0$!

(Obviously non-interacting since $\Delta E_i = 0$ independent of all DoF)

All micro-states have same probability:

$$p_i = \frac{1}{Z} \exp[-\beta E_i] = \frac{1}{2^N}$$

(Eq. 18 on page 46)

Magnetization for $T \to \infty$ (page 139)

$Z(\beta \to 0) = 2^N \longrightarrow$ energy no longer distinguishes micro-states

Instead consider **magnetization** $M = n_+ - n_-$

$n_\pm$ is number of spins with value ± 1, so $n_+ + n_- = N$

Convenient to normalize: $|m| \equiv \dfrac{|M|}{N} = \dfrac{|n_+ - n_-|}{n_+ + n_-}$ so $0 \le |m| \le 1$

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Only 2 ways to have $|m| = 1$: $(n_+, n_-) = (N, 0)$ or $(0, N)$

In general, $\begin{pmatrix} N \\ n_+ \end{pmatrix} = \begin{pmatrix} N \\ n_- \end{pmatrix}$ micro-states with certain n_+

High-T phase is disordered (page 139)

Magnetization $|m| \equiv \dfrac{|M|}{N} = \dfrac{|n_+ - n_-|}{n_+ + n_-}$ with $0 \leq |m| \leq 1$

$\begin{pmatrix} N \\ n_+ \end{pmatrix} = \begin{pmatrix} N \\ n_- \end{pmatrix}$ micro-states with certain n_+, all equally likely with $p_i = \dfrac{1}{2^N}$

For large N, binomial coeff. factorially peaked around $n_+ = n_- = \frac{1}{2}N \longrightarrow |m| \approx 0$

$n_+ \approx n_-$ defines **disordered phase**

In "thermodynamical limit" $N \to \infty$

disordered-phase magnetization vanishes exactly, $|m| = 0$

Low-temperature limit of Ising model (pages 139)

With $H = 0$ for simplicity, we have $T \to 0$ and $\beta = \frac{1}{T} \to \infty$, with

$$Z(\beta) = \sum_{\{s_i\}} \exp\left[-\beta E(s_i)\right] \qquad \text{with} \qquad E = -\sum_{(ij)} s_i s_j$$

What is probability that spin system has energy E?

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What is probability that spin system has energy E?

Two factors:

Probability $p_i = \dfrac{1}{Z} \exp\left[-\beta E_i\right]$ for micro-state i with energy E_i

Number of micro-states with energy E — **density of states** $\rho(E)$

Put them together: $$p(E) = \frac{1}{Z}\, \rho(E)\, \exp\left[-\beta E\right]$$

Ground state $T \to 0$ (pages 139–140)

$$p(E) = \frac{1}{Z}\,\rho(E)\,\exp\left[-\beta E\right]$$ exponentially favours low energy $$E = -\sum_{(ij)} s_i s_j$$

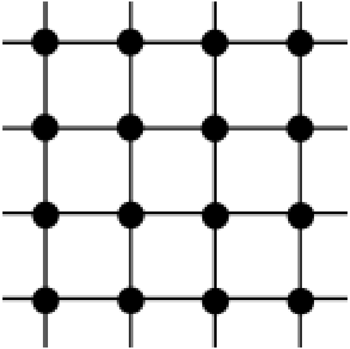
Lowest-energy (ground) states have all spins aligned:

$$(n_+, n_-) = (N, 0) \text{ or } (0, N) \longrightarrow \rho(E_{\text{min}}) = 2$$

Both have $E_{\text{min}} = -\sum_{(ij)} (\pm 1)^2 = -d \cdot N$

(count number of links)

Both have magnetization $|m| = 1$

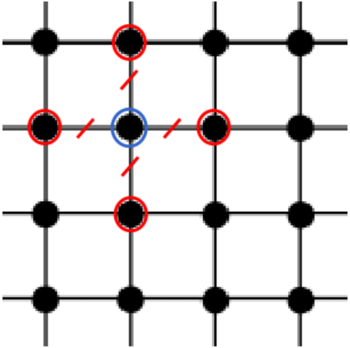


Wikipedia

First excited state for $T \to 0$ (pages 140–141)

$$p(E) = \frac{1}{Z}\,\rho(E)\,\exp\left[-\beta E\right] \text{ exponentially favours low energy } E = -\sum_{(ij)} s_i s_j$$

Next-lowest-energy comes from changing single spin ('first excited state')



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$2d$ links change from $(\pm 1)^2$ to $(+1)(-1)$ $(\delta E = 2)$

$$\longrightarrow E_1 = E_{\text{min}} + 4d = -(d \cdot N - 4d)$$

Magnetization is $|m| = \frac{N-1}{N} = 1 - \frac{1}{N}$

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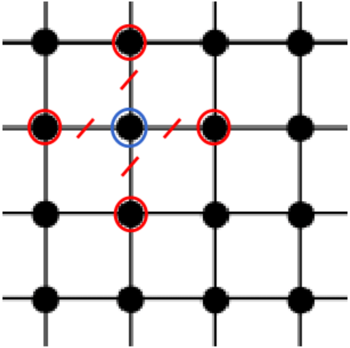
$$\longrightarrow E_1 = E_{\min} + 4d = -(d \cdot N - 4d)$$

Density $\rho(E_1) = \begin{pmatrix} N \\ 1 \end{pmatrix} + \begin{pmatrix} N \\ N-1 \end{pmatrix} = 2N$



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Low-T phase is ordered (page 141)

$$\text{Ground state probability:} \quad p(E_{\text{min}}) = \frac{1}{Z} 2 \, \exp\left[\beta d \cdot N\right]$$

$$\text{First excited state probability:} \quad p(E_1) = \frac{1}{Z} 2N \, \exp\left[\beta(d \cdot N - 4d)\right]$$

$$\text{Ratio:} \quad \frac{p(E_{\text{min}})}{p(E_1)} = \frac{\exp\left[4d \cdot \beta\right]}{N}$$

As $T \to 0$ and $\beta = \frac{1}{T} \to \infty$, ground state with $|m| = 1$ infinitely more likely!

$\longrightarrow$ **Ordered phase** with all spins aligned

Ising model phases (page 141)

Question: What distinguishes the different phases of the Ising model?

Answer: Magnetization $|m| = \frac{|M|}{N} = \frac{|n_+ - n_-|}{n_+ + n_-}$

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

Low-T phase is **ordered** with magnetization $|m| > 0 \quad (\to 1 \text{ as } T \to 0)$

(generic behaviour for interacting thermodynamical systems)

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(generic behaviour for interacting thermodynamical systems)

Magnetization is example of "**order parameter**",

vanishes in one phase, non-zero in other phase

Easy to check in numerical simulations of Ising model

Phase transitions (page 142)

Magnetization is **order parameter** for Ising model,

changing from $|m| = 0$ at high temperatures to $|m| > 0$ at low temperatures

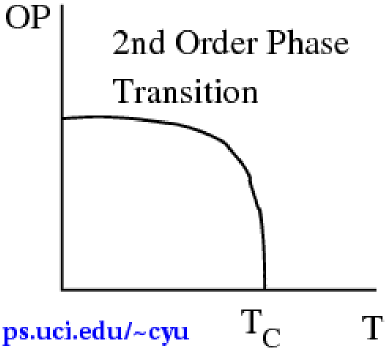
Change could be either slow, smooth **crossover** or rapid **transition**

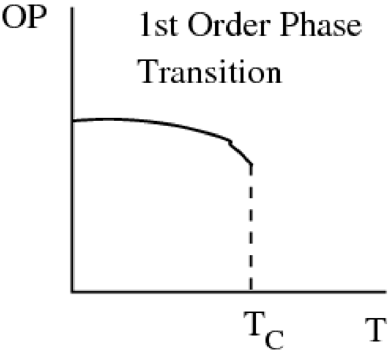
How to distinguish?

Phase transitions (page 142)

How to distinguish crossover vs. transition?

Transition typically involves discontinuity
in order parameter (OP) or its derivative(s) at 'critical temperature' T_c





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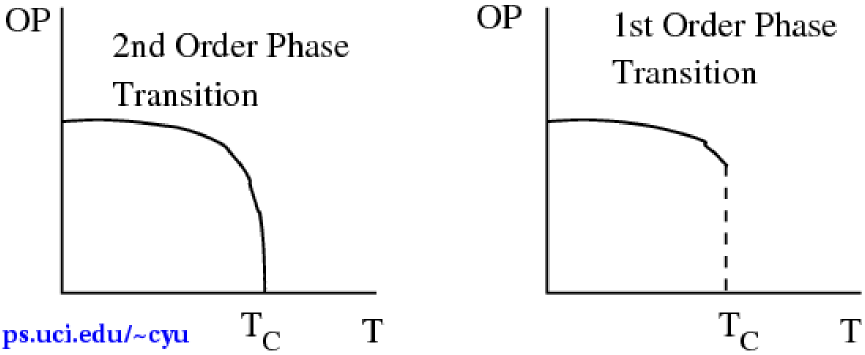


“Thermodynamical limit” $N \to \infty$ required to have true discontinuities
Approach to limit can reveal crossover vs. transition

Ising model phase transitions (page 142)

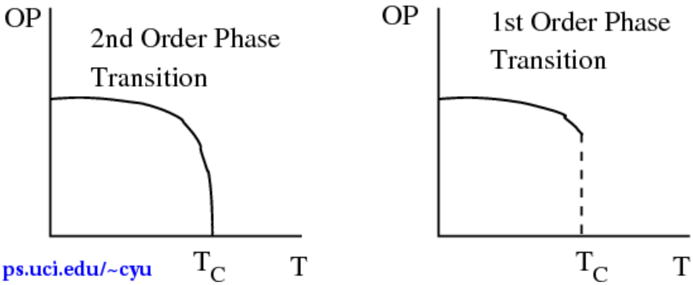
Transition would involve discontinuity in magnetization or its derivative(s)

Ising model invented by Lenz (1920)

$d = 1$ case solved by Ising (1925) $\longrightarrow$ smooth crossover rather than transition

$d \geq 2$ found to have second-order transition by Peierls (1936)

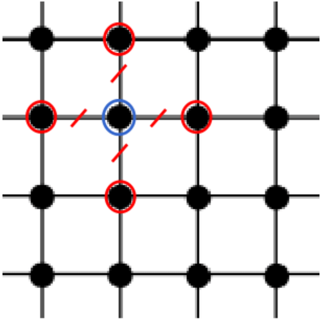
prior to full $2d$ solution by Onsager (1944)



Next time: Mean-field approximation (page 142)

Starting point reformulates partition function

in terms of local magnetic field $h_i \equiv \sum_{k \in (ik)} s_k$



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

$$= \sum_{\{s_i\}} \exp\left[\beta \sum_{(ij)} s_i s_j + \beta H \sum_i s_i\right]$$

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

Factor F corrects for double-counting link $s_i s_j$ in both h_i and h_j

Wrap up

Interacting theories can exhibit **phase transitions**

Interacting means ΔE_i from change in *i*th 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

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

Wrap up

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

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

Magnetization $|m| = \frac{|M|}{N} = \frac{|n_+ - n_-|}{n_+ + n_-}$ characterizes different 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 $\frac{d|m|}{dT}$ discontinuous