

Duality

①

- Ising model can be solved exactly in 2D (Onsager)
- before its solution: Kramers and Wannier have shown that 2D Ising model undergoes a phase transition $\Rightarrow$ located critical point

Duality for Square lattice Ising model

Ising model, square lattice

$$\sigma_i = \pm 1$$

$$Z_N = \sum_{\sigma_1} \dots \sum_{\sigma_N} \exp \left[K \underbrace{\sum_{\langle i,j \rangle} \sigma_i \sigma_j}_{\text{horizontal bonds}} + K \underbrace{\sum_{\langle i,k \rangle} \sigma_i \sigma_k}_{\text{vertical bonds}} \right]$$

- partition function can be written in two equivalent forms
- Low-temperature representation.

if all spins parallel, contribution to Z_N is

$$\exp[KH + KH]$$

- H - number of horizontal bonds
- number of vertical bonds

if we have r horizontal bonds connecting anti-parallel spins

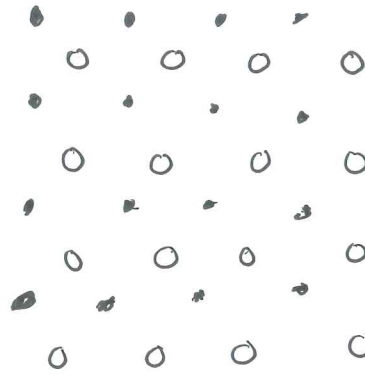
s vertical bonds connecting anti-parallel spins

$$\text{contribution to } Z_N \quad \exp[K(H-2r) + K(H-2s)]$$

construction of dual lattice

square lattice points: $\downarrow$ ($\bullet$)

dual lattice points: $\downarrow$ ($\circ$)



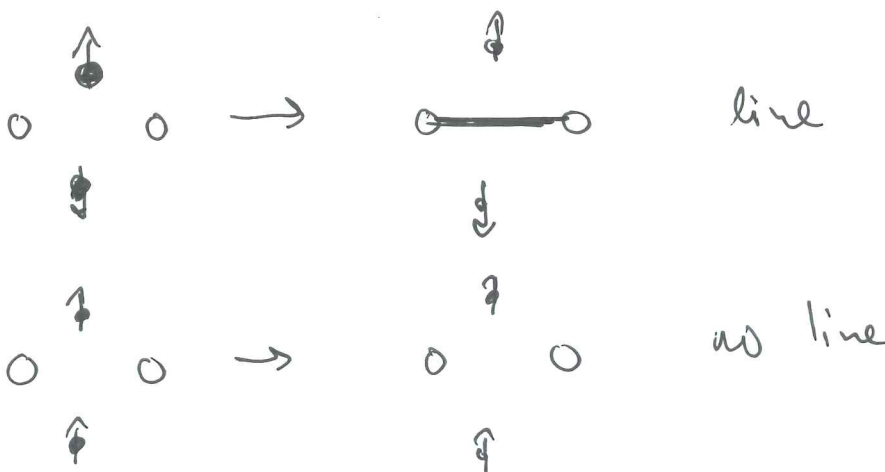
- dual lattice points are
on the faces of squares
constructed by connecting
nearest neighboring lattice points of $\downarrow \Rightarrow$



On dual lattice one can represent the spin configurations
of $\downarrow$ as polygons:

for neighboring spins $\Rightarrow$ - if two spins are anti-parallel, line connecting
dual lattice points which bisect line between
spins $\Rightarrow$ thick line
- if spins are parallel $\Rightarrow$ no line

i.e.



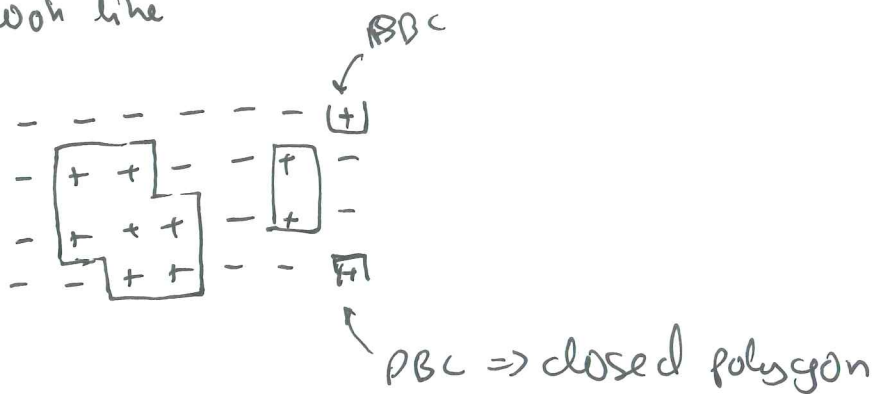
this procedure will divide lattice into polygons

- there will be r vertical lines
 s horizontal lines

r and s are even numbers

(5)

typically a configuration with lines (dual representation) would look like



partition function may be written

$$\begin{aligned} Z_N &= 2 \exp[M(K+K)] \sum_P \exp(-2Kr - 2Ks) \\ &= 2 \exp[2MK] \sum_P \exp[-2K(r+s)] \end{aligned}$$

this two originates from the fact that negating all spins leads to an energetically equivalent configuration

$\sum_P$ - denotes summation over all closed polygons

High-temperature representation

$$\begin{aligned} \exp[K\sigma_i\sigma_j] &= \cosh K + \sinh K \sigma_i \sigma_j \\ &= \cosh K (1 + \tanh K \sigma_i \sigma_j) \end{aligned}$$

$$Z_N = (\cosh K)^{2M} \sum_{\sigma_1, \dots, \sigma_N} \prod_{\langle i,j \rangle} (1 + \tanh K \sigma_i \sigma_j) \prod_{\langle i,j \rangle} (1 + \tanh K \sigma_i \sigma_j)$$

horizontal bonds
vertical bonds

product for Z_N can be expanded

(9)

$$Z_N = (\cosh K)^{2N} \sum_{\sigma_i} \dots \prod_{\sigma_i, \sigma_j} (1 + v \sigma_i \sigma_j) \prod_{(i,j)} (1 + v \sigma_i \sigma_j)$$

from each bond contribution $(1 + v \sigma_i \sigma_j)$
we can take either the 1 or the $v \sigma_i \sigma_j$
 $\Downarrow$ no line represent by line
we will have terms like

$$v^r \sigma_1^{n_1} \sigma_2^{n_2} \sigma_3^{n_3} \dots$$

~~n_i indi~~

n_i - number of lines which have site i as an endpoint

Since $\sigma_i = \pm 1$ only those terms contribute for which

n_i are all even (other ones are zero)

$$\Downarrow \quad \Downarrow \quad \Downarrow$$

$$Z_N = 2^N (\cosh K)^{2N} \sum_P v^r v^s$$

$\sum_P$ - sum over closed polygons on lattice L

for PBC: $n = N$ we have

$$Z_N = 2^N (\cosh K)^{2N} \sum_P v^r v^s$$

$$v = \tanh K$$

high-temperature: $Z_N = 2^N (\cosh K)^{2N} \sum_P v^{(r+s)}$ $v = \tanh K$

low - $\sum_P$ - sum over closed polygons on dual lattice L^*

low-temperature: $Z_N = 2 \exp[2NK] \sum_P w^{(r+s)}$ $w = \exp(-2K)$

$\sum_P$ - sum over closed polygons on dual lattice L^*

critical point can be determined by considering the dimensionless free energy in the two representations (high-T, low-T) (5)

$$\mathcal{F} = - \lim_{N \rightarrow \infty} \frac{\ln Z_N}{N}$$

from low-T expansion $\mathcal{F}(K) = -2K - \mathcal{Q}(w)$

$$w = \exp(-2K)$$

$$\mathcal{Q}(w) = \sum_p w^{r+s}$$

from high-T expansion $\mathcal{F}(K) = -\ln 2 \cosh^2 K - \mathcal{Q}(v)$

$$v = \tanh K$$

we can define K^* : $\tanh K^* = e^{-2K}$ and then

eliminate $\mathcal{Q}(v) = \mathcal{Q}(w)$

$$\begin{aligned} \Downarrow \quad \Downarrow \\ \mathcal{F}(K^*) &= \mathcal{F}(K) + 2K - \ln 2 \cosh^2 K^* \\ &= \mathcal{F}(K) + \ln \tanh K^* - \ln 2 \cosh^2 K^* \\ &= \mathcal{F}(K) - \ln 2 \sinh K^* \cosh K^* \\ &= \mathcal{F}(K) - \ln \sinh 2K^* \end{aligned}$$

critical point occurs at $K = K^* = K_c$

$$\Rightarrow \ln \sinh 2K^* = 0$$

$$\sinh 2K^* = 1$$

$$K_c = 0.44068694 \dots$$

Back to Ideal Quantum Gases

- collection of identical particles $\Rightarrow$ regarded as indistinguishable
 $\Rightarrow$ statistics (as we have seen already) plays a crucial role

Bose-Einstein or Fermi-Dirac

- use grand canonical ensemble $\Rightarrow$ allows particle number to fluctuate

- in quantum case:
$$\Xi_{\mu}(T, V) = \text{Tr} \left\{ e^{-\beta(\hat{H}_0 - \mu \hat{N})} \right\}$$

- consider gas in box with sides $L \Rightarrow V = L^3$

$$\vec{p} = \hbar \vec{k} = \hbar \left(\frac{2\pi m_x}{L}, \frac{2\pi m_y}{L}, \frac{2\pi m_z}{L} \right)$$

n_x, n_y, n_z range from $-\infty, \infty$

- energy levels:
$$\epsilon_{\vec{n}} = \frac{2\hbar^2}{m} \frac{\pi^2}{L^2} (m_x^2 + m_y^2 + m_z^2)$$

- kinetic energy operator:
$$\hat{H}_0 = \sum_{\vec{n}} \epsilon_{\vec{n}} \hat{n}_{\vec{n}}$$

- number operator:
$$\hat{N}_0 = \sum_{\vec{n}} \hat{n}_{\vec{n}}$$

summation $\sum_{\vec{n}} \rightarrow$ ranges over all possible values of $\vec{n}$

- grand partition function for bosons

$$\Xi_{\mu}(T, V) = \prod_{\vec{n}} \left[\sum_{n_{\vec{n}}=0}^{\infty} e^{-\beta(\epsilon_{\vec{n}} - \mu n_{\vec{n}})} \right]$$

- grand partition function for fermions

$$\Xi_{\mu}(T, V) = \prod_{\vec{n}} \left[\sum_{n_{\vec{n}}=0}^1 e^{-\beta(\epsilon_{\vec{n}} - \mu n_{\vec{n}})} \right]$$

Bose-Einstein Gases

- assuming spin $s=0$

$$\Xi_{BE}(T, V, \mu) = \prod_{\vec{n}} \left(\sum_{n_{\vec{n}}=0}^{\infty} e^{-\beta n_{\vec{n}} (\epsilon_{\vec{n}} - \mu)} \right) = \prod_{\vec{n}} \frac{1}{1 - e^{-\beta(\epsilon_{\vec{n}} - \mu)}}$$

- grand potential Ω_{BE}

$$\Omega_{BE}(T, V, \mu) = -k_B T \ln [\Xi_{BE}(T, V, \mu)] = k_B T \sum_{\vec{n}} \ln [1 - e^{-\beta(\epsilon_{\vec{n}} - \mu)}]$$

- average number of particles in gas:

$$\langle N \rangle = - \frac{\partial \Omega_{BE}}{\partial \mu} = \frac{1}{T} \sum_{\vec{n}} \frac{e^{-\beta(\epsilon_{\vec{n}} - \mu)}}{1 - e^{-\beta(\epsilon_{\vec{n}} - \mu)}} = \sum_{\vec{n}} \frac{1}{e^{\beta(\epsilon_{\vec{n}} - \mu)} - 1} = \sum_{\vec{n}} \langle n_{\vec{n}} \rangle$$

$$\langle n_{\vec{n}} \rangle = \frac{z}{e^{\beta \epsilon_{\vec{n}}} - z} \quad z = e^{\beta \mu}$$

- system can undergo a phase transition

* exponential $e^{\beta \epsilon_{\vec{n}}}$ can range: $1 \leq e^{\beta \epsilon_{\vec{n}}} \leq \infty$

* fugacity $z = e^{\beta \mu}$ can range: $0 \leq z \leq 1$

otherwise $\langle n_{\vec{n}} \rangle$ could be negative

$\Downarrow$
chemical potential $\mu \leq 0$ $\Uparrow$ (or in general ~~smallest~~
 $\mu \leq \epsilon_{\min}$)

* consider state with quantum number $\vec{n} = \vec{0} \Rightarrow \epsilon_{\vec{0}} = 0$

$$\langle n_{\vec{0}} \rangle = \frac{z}{1 - z}$$

for $z \rightarrow 1$ $\langle n_{\vec{0}} \rangle \rightarrow \infty \Rightarrow$ occupation can become

macroscopic $\Rightarrow$ phase transition

thermodynamic quantities available from Z_N / Ω

average particle number:

$$\langle N \rangle = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} \left(\frac{z}{\exp\left(\frac{p}{2m}\right) (p_1^2 + p_2^2 + p_3^2)} - z \right)$$

- convert summation to an integral, but points

at $p_1=0, p_2=0, p_3=0$ have to be removed

explicitly

$$\sum_{\vec{p}} \sim \int d\vec{p} = \frac{V}{(2\pi\hbar)^3} \int d\vec{p} = \frac{4\pi V}{(2\pi\hbar)^3} \int_0^{\infty} p^2 dp$$

- explicitly add contribution back in

$$\langle N \rangle = \frac{z}{1-z} + \frac{4\pi V}{(2\pi\hbar)^3} \int_0^{\infty} p^2 dp \left(\frac{z}{\exp\left(\frac{p^2}{2m}\right)} - z \right)$$

$$\Omega = k_B T \ln(1-z) + \frac{4\pi V}{(2\pi\hbar)^3} \int_0^{\infty} p^2 dp \ln[1 - z \exp(-p^2/2m)]$$

- transform to dimensionless variables:

$$x^2 = \frac{p^2}{2m}$$

$$\langle N \rangle = \frac{z}{1-z} + \frac{4V}{\lambda_T^3 \sqrt{\pi}} \int_0^{\infty} x^2 dx \left(\frac{z}{e^x - z} \right)$$

$$\Omega = k_B T \ln(1-z) + \frac{4k_B T V}{\lambda_T^3 \sqrt{\pi}} \int_0^{\infty} x^2 dx \ln[1 - z e^{-x}]$$

$$\lambda_T = \left(\frac{2\pi\hbar^2}{m k_B T} \right)^{1/2}$$

Since $PV = -Q$

$\Downarrow$

$$P = - \frac{Q}{V} = - \frac{k_B T \ln(1-z)}{V} + \frac{k_B T}{\lambda_T^3} g_{5/2}(z) - \tilde{I}_P(z, \frac{\lambda_T \sqrt{\pi}}{L})$$

$$g_{5/2}(z) = - \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 dx \ln(1 - z e^{-x^2}) = \sum_{\alpha=1}^{\infty} \frac{z^\alpha}{\alpha^{5/2}}$$

$$\tilde{I}_P(z, a) = \frac{4 k_B T}{\lambda_T^3 \sqrt{\pi}} \int_0^a x^2 dx \ln(1 - z e^{-x^2})$$

to show that $g_{5/2}(z) = \sum_{\alpha=1}^{\infty} \frac{z^\alpha}{\alpha^{5/2}}$: expand integrand in powers of z , integrate each term

average particle number:

$$\langle n \rangle = \frac{\langle N \rangle}{V} = \frac{1}{V} \frac{z}{1-z} + \frac{1}{\lambda_T^3} g_{3/2}(z) - \tilde{I}_n(z, \frac{\lambda_T \sqrt{\pi}}{L})$$

$$g_{3/2}(z) = z \frac{d}{dz} g_{5/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 dx \cdot \left(\frac{z}{e^{x^2} - z} \right) = \sum_{\alpha=1}^{\infty} \frac{z^\alpha}{\alpha^{3/2}}$$

$$\tilde{I}_n(z, a) = \frac{4}{\sqrt{\pi} \lambda_T^3} \int_0^a x^2 dx \left(\frac{z}{e^{x^2} - z} \right)$$

$$\lim_{a \rightarrow 0} \tilde{I}_n(z, a) = \lim_{a \rightarrow 0} \tilde{I}_P(z, a) = 0$$

$\Downarrow$

$$P = - \frac{k_B T \ln(1-z)}{V} + \frac{k_B T}{\lambda_T^3} g_{5/2}(z)$$

$$\langle n \rangle = \frac{1}{V} \frac{z}{1-z} + \frac{1}{\lambda_T^3} g_{3/2}(z)$$

$g_{5/2}(z), g_{3/2}(z)$ — well-behaved functions of z

functions: $-\frac{1}{V} \ln(1-z)$, $\frac{1}{V} \frac{z}{1-z}$

fix $\langle n \rangle, T$ let $V \rightarrow \infty$ $z \rightarrow 1$

in neighborhood of $z = 1 - \frac{1}{n_0 V} \Rightarrow z = 1 - \frac{1}{n_0 V}$

$$\lim_{V \rightarrow \infty} -\frac{1}{V} \ln\left(\frac{1}{n_0 V}\right) \rightarrow 0$$

$$\lim_{V \rightarrow \infty} \frac{1}{V} \frac{\left(1 - \frac{1}{n_0 V}\right) n_0 V}{1} \rightarrow n_0$$

$$P = \begin{cases} \frac{k_B T}{\lambda_T^3} g_{5/2}(z) & \text{if } z < 1 \\ \frac{k_B T}{\lambda_T^3} g_{5/2}(1) & \text{if } z = 1 \end{cases}$$

$$\langle n \rangle = \frac{\langle N \rangle}{V} = \begin{cases} \frac{1}{\lambda_T^3} g_{3/2}(z) & \text{if } z < 1 \\ n_0 + \frac{1}{\lambda_T^3} g_{3/2}(z) & \text{if } z = 1 \end{cases}$$

in state ϵ_0 n_0 becomes macroscopic in size

to obtain critical temperature

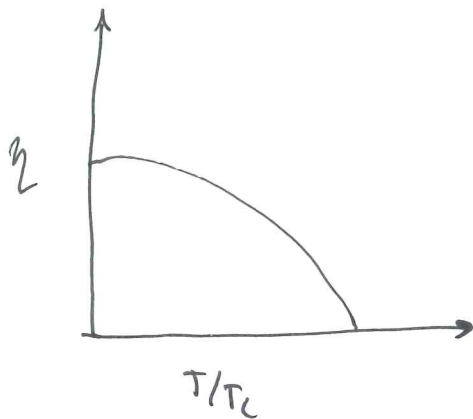
$$\langle n \rangle \lambda_T^3 = g_{3/2}(1)$$

$$\langle n \rangle_c = \frac{1}{\langle n_c \rangle} = \frac{g_{3/2}(1)}{\lambda_T^3} \sim A T^{3/2}$$

$$\text{or } T_c = \left(\frac{2\pi \hbar^2}{m k_B} \right) \left(\frac{\langle n \rangle}{g_{3/2}(1)} \right)^{2/3}$$

order parameter:

$$\eta = \frac{n_0}{\langle n \rangle} = 1 - \frac{g_{3/2}(1)}{\langle n \rangle \lambda_T^3} = 1 - \frac{\lambda_{T_c}^3}{\lambda_T^3} = 1 - \left(\frac{T}{T_c} \right)^{3/2}$$



since $P = \frac{k_B T}{\lambda_T^3} g_{5/2}(1)$ for $\eta = 1$

$\Rightarrow$ pressure is independent of volume below phase transition

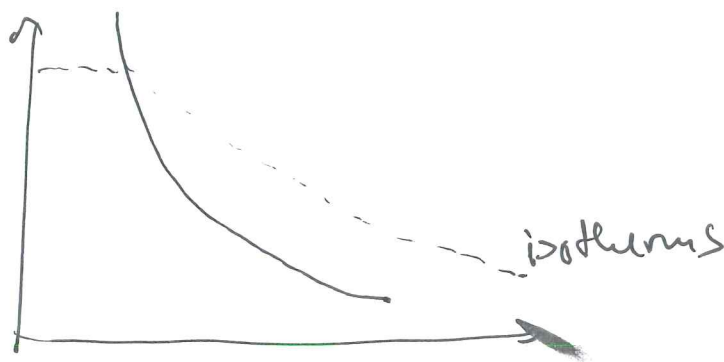
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$\Rightarrow$ coexistence curve:

$$P_c = \frac{k_B T_c}{\lambda_{T_c}^3} g_{5/2}(1) \sim T_c^{5/2}$$

$$\text{since } \langle V \rangle_c \sim \frac{1}{T_c^{3/2}} \Rightarrow T_c = \frac{1}{\langle V_c \rangle^{2/3}}$$

$$P_c \sim \frac{1}{\langle V_c \rangle^{5/3}} \Rightarrow \text{coexistence curve}$$



entropy:

given by $-\frac{\partial \Omega}{\partial T} = -\frac{\partial PV}{\partial T}$

$$P V = \frac{k_B T}{\lambda_T^3} g_{5/2}(z) V$$

$$S = \frac{5}{2} \frac{k_B}{\lambda_T^3} g_{5/2}(z) V$$

$$= \frac{5}{2} \frac{k_B g_{5/2}(z) g_{5/2}(z)}{\lambda_T^3 g_{3/2}(z)} V$$

$$= \frac{5}{2} k_B \frac{\langle n \rangle g_{5/2}(1)}{g_{3/2}(1)} V = \frac{5}{2} k_B \langle N \rangle \frac{g_{5/2}(1)}{g_{3/2}(1)}$$

$$\frac{S}{N} = \frac{5}{2} k_B \frac{g_{5/2}(1)}{g_{3/2}(1)}$$

$\Rightarrow$ entropy per particle in normal phase at T_c

$\Rightarrow$ condensed particles carry no entropy

~~latent heat~~ $\rightarrow$

latent heat $L = T \Delta S = \frac{5}{2} k_B T_c \frac{g_{5/2}(1)}{g_{3/2}(1)}$