Lect 5: Lee-Yang theorems of phase transitions

① Can Stat-mech describe phase transition?

No-phase transition at finite size

② Classification of phase transition

③ Simple example — molecular Zipper / zeros.

④ Yang-Lee theorem 1 and 2: — zeros and phase transitions

phase transition and density distribution of zeros

⑤ zeros on the unit circle —— unit circle theorem

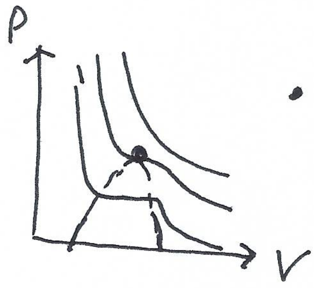
Ref: 1. Yang and Lee, Phy. Rev 87, 404 (1952)

2. Lee and Yang, Phy. Rev 87. 410 (1952)

3. P. H. ~~Ribe~~ Ribeiro dos Anjos, Phase transitions and zeros of the partition function (2016)

1. Thermodynamic phase

liquid-gas



- jump of specific volume
  latent heat
- critical temperaure

order-disorder

$\uparrow \uparrow \uparrow$ $\qquad$ $\uparrow \downarrow \uparrow$

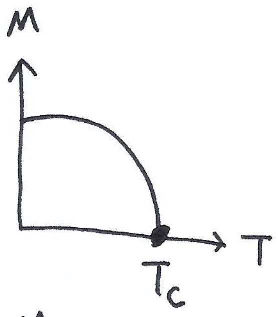
$\uparrow \uparrow \uparrow$ $\qquad$ $\downarrow \uparrow \downarrow$

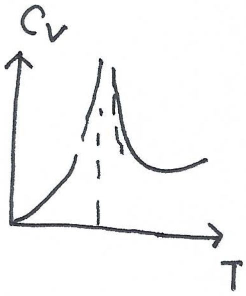
$T < T_c$ $\qquad$ $T > T_c$

$M \neq 0$ $\qquad$ $M = 0$

order parameter

$$M = \frac{1}{N} \sum_i \langle \sigma_i \rangle$$





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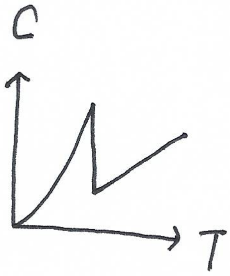
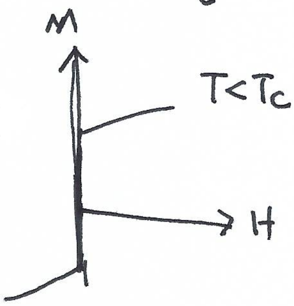
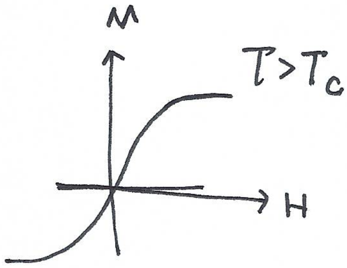






- continuous transition
- no latent heat

Phase transitions are location of singurlarities!

2. State-mech

$$Z(\beta, V) = \sum_i g_i \, e^{-\beta \varepsilon_i}$$, all ~~ther~~ terms are regular.

- If for a finite system, $F = -\frac{1}{\beta} \ln Z(\beta, V)$ is also regular, no phase transition

- F is always continuous, but its derivations do not.

$$\begin{cases} P = \dfrac{1}{V} \ln \Theta \\ n = \dfrac{\partial}{\partial y} \dfrac{1}{V} \ln \Theta \end{cases}$$

liquid-gas ~~transition~~, P is continuous but n is not! latent heat

$$\cancel{S = -\frac{\partial \Omega}{\partial T}, \quad C_V = -T \frac{\partial^2 \Omega}{\partial T^2} \quad S = -\partial}$$

Mayer cluster expansion.

- magnetic system

$$M = -\frac{\partial F}{\partial H}, \quad \chi = \frac{\partial M}{\partial H} = -\left.\frac{\partial^2 F}{\partial H^2}\right|_{H=0}$$ diverge.

$$S = -\frac{\partial F}{\partial T}, \quad C_V = -T \frac{\partial^2 F}{\partial T^2}$$

Stat-mech

- $$Z_N(\beta, V) = \int d\Omega \; e^{-\beta(K+V)} \qquad d\Omega = \frac{d^3x_1 \cdots d^3x_N \, d^3p_1 \cdots d^3p_N}{N! \; h^{3N}}$$

$$K = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} \phi_{ij}$$

$$Z_N(\beta, V) = \frac{1}{N! \, \lambda_T^{3N}} Q_N(\beta, V), \qquad \lambda_T = \frac{h}{\sqrt{2m\pi k_B T}}$$

$$Q_N = \int d^3r_1 \cdots d^3r_N \; e^{-\beta \sum_{i<j}^{N} \phi_{ij}}$$

$$\textcircled{H}(z, \beta, V) = \sum_{N=0}^{\infty} z^N Z_N(\beta, V) \quad \text{where} \quad z = e^{\beta\mu}$$

$$= \sum_{N=0}^{\infty} y^N \frac{Q_N}{N!} \qquad y = z/\lambda_T^3$$

The grand potential $\Omega = -\frac{1}{\beta} \ln \textcircled{H}$

$\Omega = F - N\mu, \; = G - PV - N\mu$ where Gibbs $G = F + PV$

$dG = -S\,dT + V\,dp + \mu\,dN \Rightarrow \mu = \left(\frac{\partial G}{\partial N}\right)_{T,p}$ since T, p are intensive

$\mu = f(T, p) \Rightarrow G = N\mu + \text{const}$

$$\Rightarrow \Omega = -PV \Rightarrow \boxed{\frac{P}{k_B T} = \lim_{V\to\infty} \frac{1}{V} \ln \textcircled{H}}$$

$$= -\frac{1}{\beta} \ln \textcircled{H}$$

$$N = -\frac{\partial \ln \textcircled{H}}{\partial(\beta\mu)} = -z \frac{\partial \ln \textcircled{H}}{\partial z} = -\frac{\partial \ln \textcircled{H}}{\partial \ln y}$$

$$\rightarrow \boxed{n = \lim_{V\to\infty} \frac{\partial}{\partial \ln y} \frac{1}{V} \ln \textcircled{H}}$$

Mayer cluster expansion

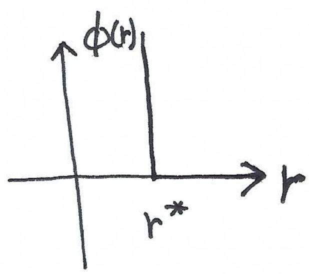
$$\Theta(z,\beta V) = \sum_{N=0}^{\infty} z^N Z_N(\beta, V) \qquad z = e^{\beta\mu}$$

$$Z_N(\beta, V) = \int d\Omega\, e^{-\beta(K+V)} \qquad d\Omega = \frac{d^3x_1 \cdots d^3x_N\, d^3p_1 \cdots d^3p_N}{N!\,(2\pi\hbar)^{3N}}$$

$$K = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} \phi_{ij}$$

$$Z_N(\beta, V) = \frac{1}{N!\,\lambda_T^{3N}}\, Q_N(\beta, V) \qquad \lambda_T = \frac{h}{\sqrt{2m\pi k_B T}}$$

$$Q_N = \int d^3r_1 \cdots d^3r_N\, e^{-\beta \sum_{i<j}^{N} \phi_{ij}} \qquad \text{define } f_{ij} = e^{-\beta\phi_{ij}} - 1 = \begin{cases} -1 & r \to 0 \\ 0 & r > r^* \end{cases}$$



$$e^{-\beta \sum_{i<j} \phi_{ij}} = \prod_{i<j} (1 + f_{ij})$$

$$= 1 + \sum_{i<j} f_{ij} + \sum_{i<j} \sum_{k<l} f_{ij} f_{kl} + \cdots$$

$$Q_N = \int d^3r_1 \cdots d^3r_N \left(1 + \sum_{i<j} f_{ij} + \cdots\right) = \left[\int d^3r\right]^N + \frac{N(N-1)}{2} V^{N-2} \int dr_1 dr_2\, f_{12}$$

$$\frac{N!}{(N-2)!\,(1!)^{N-2}\, 1!\,(2!)^1}$$

$$= \frac{N!}{N!} (b_1 V)^N + \frac{N!}{(N-2)!\,2!} (b_1 V)^{N-2} \overset{(2!)}{(b_2 V)} + \cdots\cdots$$

$$b_1 = \frac{1}{V}\int dr = 1, \qquad b_2 = \frac{1}{2!\,V} \int f_{12}\, dr_1 dr_2 = \frac{1}{2!} \int f_{12}\, dr_{12}$$

1 $\qquad$ 1 — 2

Viral expansion : $\dfrac{PV}{Nk_BT} = \sum_{l=1}^{\infty} \dfrac{a_l(T)}{(V/N)^{l-1}}$

It can be proved $a_1 = b_1 = 1$

$$a_2 = -b_2 = -2\pi \int_0^{\infty} (e^{-u(r)/kT} - 1) r^2 dr$$

$$= b - a/k_BT$$

$$\Rightarrow \frac{PV}{Nk_BT} = \left[1 + \frac{N}{V}\left(b - \frac{a}{k_BT}\right)\right]$$

$$P = \frac{Nk_BT}{V}\left(1 + \frac{N}{V}b\right) - \left(\frac{N}{V}\right)^2 a \Rightarrow (P + n^2 a) \approx \frac{Nk_BT}{V} \frac{1}{1 - \frac{N}{V}b}$$

$$\Rightarrow (P + n^2 a)(V - Nb) = Nk_BT$$

$P = P_{kinetic} -$ collision . attraction

$\sim P_{kin} - n^2 a$

$V_{occ} = V - Nb$, $P_{kin} V_{occ} = Nk_BT$

$\rightarrow (P + n^2 a)(V - Nb) = Nk_BT$

$\boxed{\text{Van der Waals Eq.}}$

②

$$Q_N(\beta,V) = \sum{}' \frac{N!}{\prod_l m_l!\,(l!)^{m_l}} \prod_l (b_l\, l!\, V)^{m_l}$$

m_1 : 1-particle clust

m_2 2-particle cluster

m_3 3-particle cluster

$$= N! \sum_{\{m_l\}}{}' \prod_{l=1} \frac{1}{m_l!} (b_l V)^{m_l}$$

$$\text{Ⓗ}(z,\beta,V) = \sum_{N=0}^{\infty} \frac{z^N}{\lambda_T^{3N}} \sum_{\{m_l\}}{}' \frac{1}{m_l!} (b_l V)^{m_l}$$

$$= \prod_{l=1}^{\infty} \left[\sum_{m_l=0}^{\infty} \frac{1}{m_l!} \left[\left(\frac{z}{\lambda_T^3}\right)^l b_l V \right]^{m_l} \right]$$

$$= \prod_{l=1}^{\infty} \exp\left(\left(\frac{z}{\lambda_T^3}\right)^l b_l V \right)$$

$$\Rightarrow \ln \text{Ⓗ} = \sum_{l=1}^{\infty} \left(\frac{z}{\lambda_T^3}\right)^l b_l V$$

$$\Rightarrow \frac{1}{V} \ln \text{Ⓗ} = \sum_{l=1}^{\infty} b_l y^l, \quad \text{where } y = z/\lambda_T^3 = e^{\beta\mu}/\lambda_T^3$$

$$\boxed{\frac{P}{k_B T} = \lim_{V\to\infty} \frac{1}{V} \ln \text{Ⓗ} = \sum_{l=1}^{\infty} b_l y^l}$$

$$N = -\frac{\partial \ln \text{Ⓗ}}{\partial(\mu\beta)} = -\frac{\partial \ln \text{Ⓗ}}{\partial \ln z} = -z\frac{\partial \ln \text{Ⓗ}}{\partial z} = \sum_{l=1}^{\infty} l\, y^l b_l V$$

$$\Rightarrow \boxed{n = \lim_{V\to\infty} \frac{\partial \ln \text{Ⓗ}}{\partial \ln y} \frac{1}{V} = \sum_{l=1}^{\infty} l\, b_l y^l}$$

$n = \frac{N}{V}$

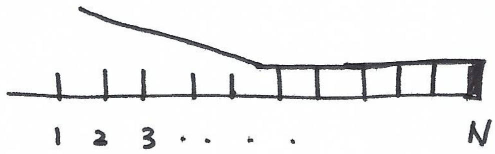
$\frac{1}{v}$

specific volume

§ Simple example — molecular zipper

① open from left to right

② if the k-th link is open, then it contribute an energy ε



Single ended molecular Zipper

③ if the k-th link is closed, then $\varepsilon = 0$.

The zipper only has N. configurations: no-link open; the first link open; the first and second link open. We can further impose an degeneracy "g" for each open link

$$Z = 1 + g e^{-\beta\varepsilon} + g^2 e^{-2\beta\varepsilon} + \cdots g^{N-1} e^{-(N-1)\beta\varepsilon} = \frac{1 - e^{-N\beta\varepsilon} g^N}{1 - e^{-\beta\varepsilon} \cdot g}$$

define $z = g e^{-\beta\varepsilon}$ $\Rightarrow$ $Z(z) = \dfrac{1 - z^N}{1 - z}$

The fraction of open link $\dfrac{\langle n \rangle}{N} = \dfrac{1}{N Z} \sum_n n z^n = \dfrac{z}{N} \dfrac{1}{Z} \sum_{n=0}^{N} \dfrac{\partial}{\partial z} z^n$

$$= \frac{z}{N} \frac{\partial \ln Z}{\partial z}$$

$$\ln Z = \cancel{1 - z^N}\ \ln(1 - z^N) - \ln(1 - z)$$

$$\frac{\partial \ln Z}{\partial z} = \frac{-N z^{N-1}}{1 - z^N} + \frac{1}{1 - z} \quad \Rightarrow \quad \frac{\langle n \rangle}{N} = \frac{1}{N} \frac{z}{1 - z} - \frac{z^N}{1 - z^N}$$

as $N \to \infty$, $\rho = \dfrac{\langle n \rangle}{N} = \begin{cases} 0 & \text{if } z < 1 \\ 1/2 & \text{if } z = 1 \\ 1 & \text{if } z > 1 \end{cases}$

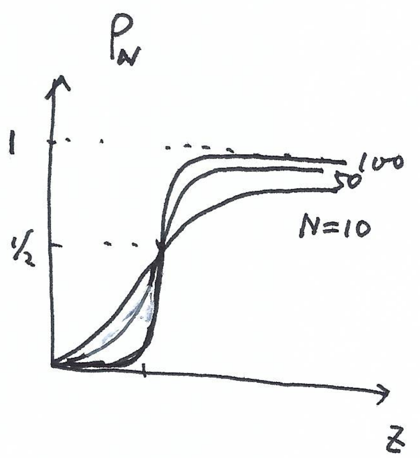
At $z = 1 \Rightarrow \rho = \dfrac{\langle n \rangle}{N} = \dfrac{1}{N} \dfrac{1 + 2 + \cdot N-1}{1 + 1 + \cdot\cdot} = \dfrac{1}{N^2} \dfrac{N(N-1)}{2} \rightarrow 1/2.$

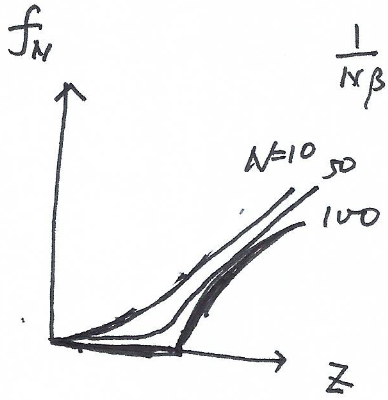
free energy $f_N = \frac{1}{N\beta} \ln Z_N = \frac{1}{N\beta}\left[\ln(1-z^N) - \ln(1-z)\right]$ ③

as $N \to \infty$.

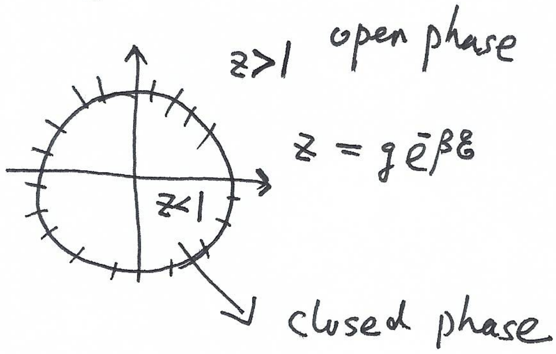
$$f(z) = \lim_{N\to\infty} \frac{1}{N\beta} \ln Z_N = \begin{cases} 0 & z \le 1 \\ \frac{1}{\beta}\ln z & \text{if } z > 1 \end{cases}$$

$$\frac{1}{N\beta} \ln \frac{z^N}{z-1} \to \frac{1}{N\beta}\ln z^N = \frac{1}{\beta}\ln z$$





zeros of partition function



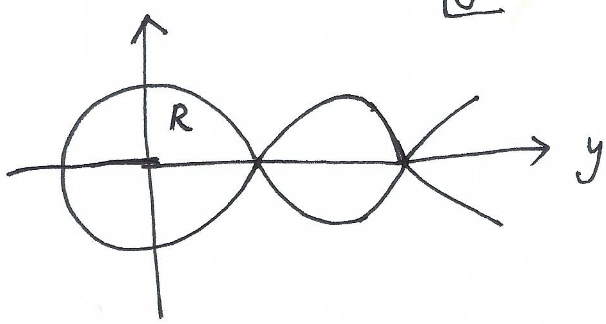
$\boxed{\text{Theorem 1}}$ For all $y>0$, $V^{-1} \ln \Theta_V$ approaches the limit as $V \to \infty$. This limit is independent of the shape of V. and is a continuous, monotonically increasing function of y.

Roughly speaking $\frac{P}{k_B T}$ exists in the limit $V \to \infty$, and increase as increasing chemical potential (fix $k_B T$)

$$\Theta_V = \prod_{i=1}^{M} \left(1 - \frac{y}{y_i}\right)$$ ← assume # of particles in V is finite

y's are roots of Θ_V, and their distribution in the complex plane give the analytic behavior of thermodynamic functions in the y-plane.

$\boxed{y}$



$\boxed{\text{Theorem 2}}$

In the complex y plane, in a region R, ~~...~~ free of roots. In this region as $V \to +\infty$

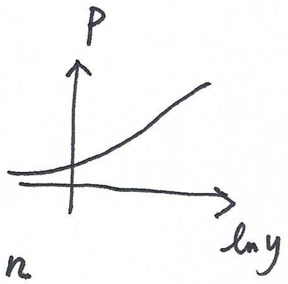
$$\frac{1}{V} \ln \Theta, \quad \frac{\partial}{\partial \ln y} \frac{1}{V} \ln \Theta, \quad \left(\frac{\partial}{\partial \ln y}\right)^2 \left(\frac{1}{V} \ln \Theta\right) \cdots$$

approaches limits, and they are analytic wrt y. ~~The two limits~~

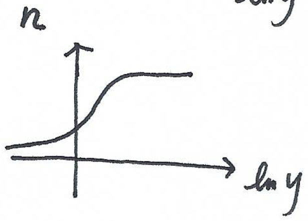
$\lim_{V \to \infty}$ and $\frac{\partial}{\partial \log y}$ commute, and then $n = \frac{\partial}{\partial \ln y}\left(\frac{P}{k_B T}\right)$.

This means that inside R, it's one phase.

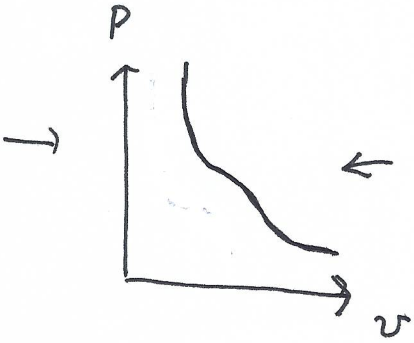
Case (1): Roots of $\Theta_V(y) = 0$ do not close in onto the positive axis of y as $V \to \infty$.



$$n = \frac{\partial}{\partial \ln y}\left(\frac{P}{k_BT}\right)$$

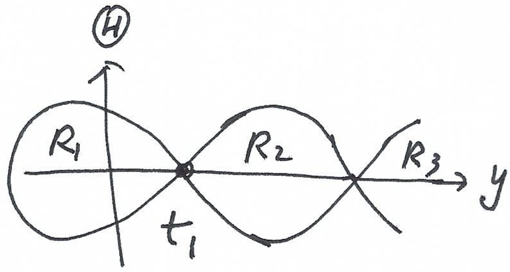


n is also an incresing function of ln y



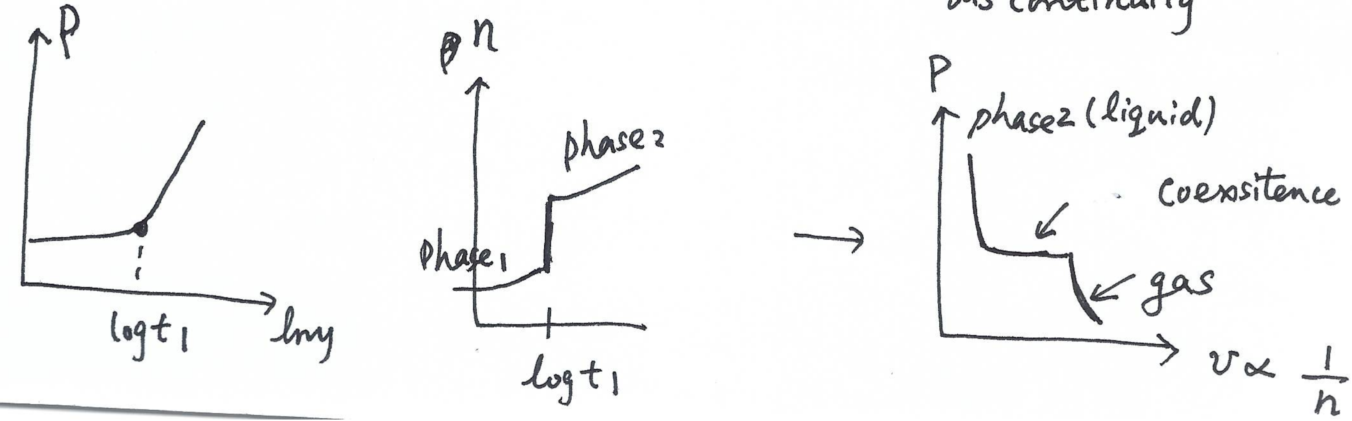
isotherm P increas analytically as v decrease.

a single phase.



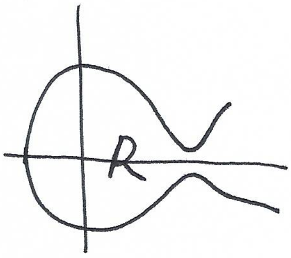
Case (2) Within each region $R_{1,2,3}$ free of roots, P/k_BT and n are analytic increasing function of y. On isotherm P increas as v decrease.

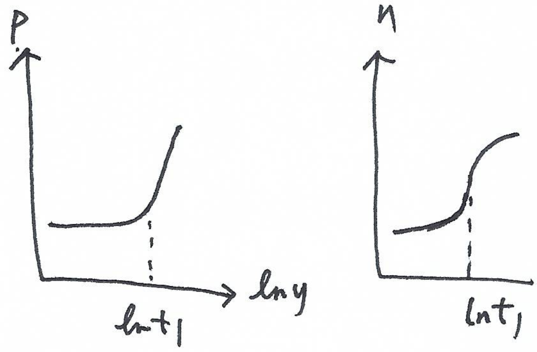
At point $y = t_1$, P is continous (Theorem 1), but n has a discontinuity; n increases as across the discontinuity

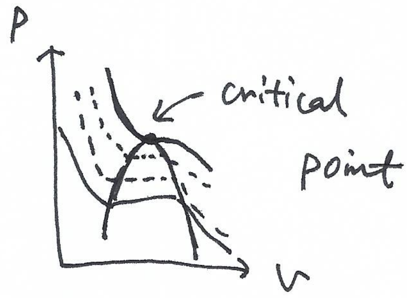


As ~~temperature~~ changes, $H(z, \beta, V)$ changes, and so does t_1

t_1 will moves along y-axis. At a certain T_c, such that t_1 doesnot exist anymore







More on Zeros

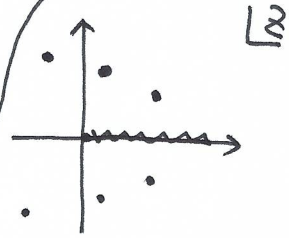
(*) Partition function zeros.

z could be fugacity $z = e^{\beta\mu}$ for grand canonical ensemble.

Assume partition function can be written as a polynomial in terms of variable z. ← which control the phase transition.

$$Z_N(z) = \sum_{n=0}^{N} a_n z^n = a_N \prod_n (z - r_n)$$

Since $a_n \geq 0$, $\Big\{$ Z_N has no roots along the positive axis of z. r_n and $\bar{r}_n$ appear in pairs → there could be root on negative axis.

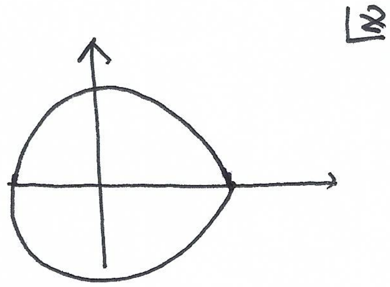


Then $f_N(z) = \frac{1}{N} \ln Z_N$

$$= \frac{\ln a_N}{N} + \sum_{n=1}^{N} \frac{1}{N} \ln(z - r_n)$$

★ There should be no singularity as z moves along the positive axis $z > 0$, This means no phase transition in finite systems

(*) As $N \to \infty$, # of zeros grow and can accumulate in curves (e.g. unit circle)



Zero can approach the positive real axis as $N \to \infty$. seperating two phases!

More formal development:

$$f_N(z) = \frac{1}{N}\ln a_N + \sum_{n=1}^{N}\frac{1}{N}\ln(z - x_n - iy_n) \qquad r_n = x_n + iy_n$$

$$= \frac{1}{N}\ln a_N + \int_{\mathbb{R}^2} \rho_N(x,y)\ln(z - x - iy)\,dx\,dy \qquad \int dx\,dy\,\rho(x,y) = 1.$$

where $\rho_N(x,y) = \frac{1}{N}\sum_{n=1}^{N}\delta(x-x_n)\delta(y-y_n). \xrightarrow{N\to\infty} \rho(x,y),$

Consider the thermodynamic limit. $f(z) = \lim_{N\to\infty} f_N(z)$, we may write

$$f(z) = \int_{\mathbb{R}^2} \rho(x,y)\ln(z-x-iy)\,dx\,dy + \text{const}.$$

$f(z)$ is analytic at $\rho(x,y)=0$. Define $f(z) = \underset{\text{real}}{\phi(z)} + i\,\underset{\text{imaginary}}{\psi(z)}$

$$\phi(z) = \mathrm{Re}\, f(z) = \int_{\mathbb{R}^2} \rho(x,y)\ln|z-x-iy|\,dx\,dy$$

$$\psi(z) = \mathrm{Im}\, f(z) = \int_{\mathbb{R}^2} \rho(x,y)\arg(z-x-iy)\,dx\,dy$$

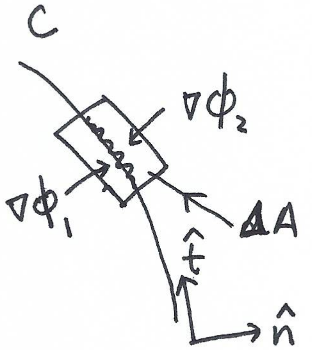
$$\Rightarrow \begin{cases} \dfrac{\partial\phi}{\partial x} = \dfrac{\partial\psi}{\partial y} \\[2ex] \dfrac{\partial\phi}{\partial y} = -\dfrac{\partial\psi}{\partial x} \end{cases} \quad \text{Cauchy-Riemann condition.}$$

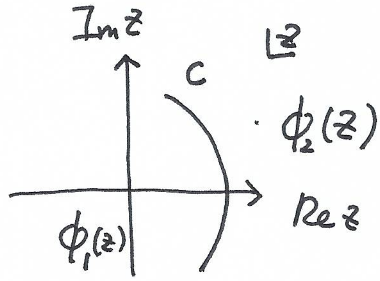
$$\nabla\phi\cdot\nabla\psi = 0 \longrightarrow \nabla\phi \perp \nabla\psi$$

$\nabla^2\phi = \nabla^2\psi = 0$ if $\rho(z) = 0$ (not at singular point!).

$$\nabla^2 \ln|x+iy| = 2\pi\delta(x)\delta(y) \Rightarrow \boxed{\begin{aligned}\nabla^2\phi(z) &= 2\pi\int_{\mathbb{R}^2}\rho(x,y)\,\delta(x-x_0)\delta(y-y_0)\,dx\,dy \\ &= 2\pi\rho(z)\end{aligned}}$$

Suppose in the complex plane of z, we have $\phi_1(z)$ and $\phi_2(z)$ expressions, but they need to be continous at the phase boundary C





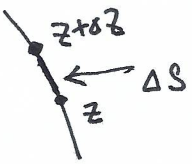
Consider an arc length ΔS inside a small area ΔA. Defin $\lambda(s)$ as the line density of zeros along C

$$\int_{\Delta A} \rho(x,y)\,dx\,dy = \lambda(s)\,\Delta S$$

$$\int_{\text{along the loop}} \nabla\phi\cdot\hat{n}(z)\,ds = \int_{\Delta A} \nabla^2\phi(z)\,dx\,dy = 2\pi\lambda(s)\,\Delta S$$

$$\nabla\phi\cdot\hat{n}(z) = \nabla\psi\cdot\hat{t}(z) \Rightarrow \int_{\Delta A} \nabla\psi\cdot\hat{t}(z)\,ds = 2\pi\lambda(s)\,\Delta S$$

$$\Rightarrow \left[\left(\psi_2(z+\Delta z)-\psi_2(z)\right)-\left(\psi_1(z+\Delta z)-\psi_1(z)\right)\right] = 2\pi\lambda(z)\,\Delta S$$



$$\frac{d}{ds}\left[\psi_2(z)-\psi_1(z)\right]\cdot\frac{1}{2\pi} = \lambda(z)$$

$z(s)$ along the boundary, s is the arclength $\Rightarrow$ $\boxed{\lambda(s) = \frac{1}{2\pi}\frac{d}{dz}\left(\psi_2(z)-\psi_1(z)\right)\cdot\frac{dz}{ds}}$

Zxample: Zipper, N-1 root uniformly distributes on the unit circle

$$p(z) = \frac{1}{N}\sum_{n=1}^{N-1} \delta(x-\cos\theta_n)\,\delta(y-\sin\theta_n) = \frac{1}{2\pi}\,\delta(|z|-1)$$

circumferences

$$\Rightarrow \boxed{\lambda(\theta) = \frac{1}{2\pi}}$$ ← normalization along the unit circle.

The dimensionless free engy. $\beta f(z) = \begin{cases} 0 & |z|<1 \\ \ln z & |z|>1 \end{cases}$

$$\Rightarrow \begin{cases} \phi_1 = 0, \quad \psi_1 = 0 \\ \phi_2 = \ln|z|, \quad \psi_2 = \arg(z) \end{cases}$$

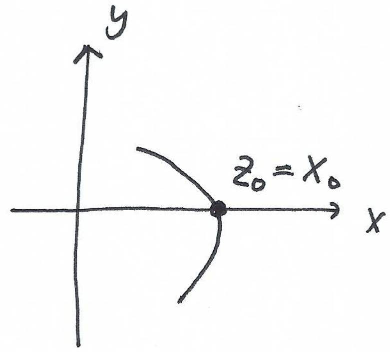
$$\Rightarrow \frac{d}{dr}\phi_2\Big|_{|z|=1} - \frac{d}{dr}\phi_1\Big|_{|z|=1} = 1 = 2\pi\lambda(\theta)$$

$$\boxed{\frac{d}{d\theta}\psi_2\Big|_{|z|=1} - \frac{d}{d\theta}\psi_1\Big|_{|z|=1} = 1}$$

Nature of phase transitions

Consider an example that a phase transition occurs at $z_0 > 0$

free energy is analytic on either side of z_0



$$f_1(z) = f_1(z_0) + a_1(z-z_0) + b_1(z-z_0)^2 + \cdots$$

$$f_2(z) = f_2(z_0) + a_2(z-z_0) + b_2(z-z_0)^2 + \cdots$$

$\Rightarrow f_1(z_0) = f_2(z_0)$

$$\Rightarrow \phi_1(z) = \phi(x_0) + a_1(x-x_0) + b_1[(x-x_0)^2 - y^2] + \cdots$$

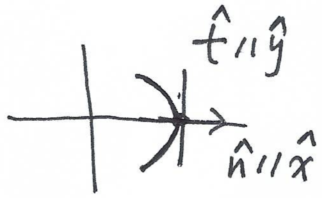
$$\phi_2(z) = \quad 1 \to 2.$$

★ first order phase transition : $a_1 \neq a_2$, $b_1 \neq b_2$

$$a_1(x-x_0) + b_1[(x-x_0)^2 - y^2] = a_2(x-x_0) + b_2[(x-x_0)^2 - y^2]$$

$$\Rightarrow y^2 = (x-x_0)^2 + \frac{a_2-a_1}{b_2-b_1}(x-x_0) \leftarrow \text{boundary curve}$$

This is a hyperbola $\quad \tilde{y}^2 = \tilde{x}^2 + \Delta^2$



Smoothly passes the transition point :

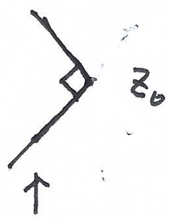
$$\boxed{\lambda(s) = \frac{1}{2\pi}\left(\frac{d}{dx}\phi_1 - \frac{d}{dx}\phi_2\right)\Bigg|_{x=x_0} = \frac{a_2-a_1}{2\pi}}$$

The density of zeros is finite at the 1st order phase transition !

⊛ 2nd order transition

$$a_1 = a_2 \ , \ b_1 \neq b_2 \quad \Rightarrow \quad (x-x_0)^2 - y^2 = 0 \qquad y = \pm(x-x_0)$$

on the curve $y = x - x_0$, Check the imaginary part



$$\psi_1((1+i)y) = \psi(x_0) + ay + 2b_1(x-x_0)y$$

$$= \psi(x_0) + ay + 2b_1 y^2 + \cdots$$

$$\psi_2((1+i)y) = \psi(x_0) + ay + 2b_2 y^2 + \cdots$$

The arc length s between z_0 and $z - z_0 = x + iy$ along the boundary.

$$s^2 = 2y^2 \quad \Rightarrow \quad \lambda(s) = \frac{1}{2\pi}\frac{d}{ds}(\psi_2 - \psi_1) = \frac{1}{2\pi}\frac{d}{ds}(b_2 - b_1)s^2 \Big|$$

$$= s(b_2 - b_1)/\pi$$

This means that the density of zeros decays linerly to zero.

⊛ higher order transition

$$\text{if} \quad f_1(z) = f(z_0) + a_1^{(1)}(z-z_0) + a_2^{(1)}(z-z_0)^2 + \cdots$$

$$f_2(z) = f(z_0) + a_1^{(2)}(z-z_0) + a_2^{(2)}(z-z_0)^2 + \cdots$$

If $a_i^{(1)} = a_i^{(2)}$ for $i = 1, 2, \cdots n-1$, but $a_n^{(1)} \neq a_n^{(2)}$ we have

$$z - z_0 = s e^{i\alpha} \Rightarrow$$ real part of $f(z)$ should be continuouse along the boundary

$$\Rightarrow \quad a_n^{(1)} \cos n\alpha = a_n^{(2)} \cos n\alpha$$

$$\left\{ a_n^{(1)} \neq a_n^{(2)} \right. \quad \Rightarrow \boxed{\alpha = \pi/2n}$$

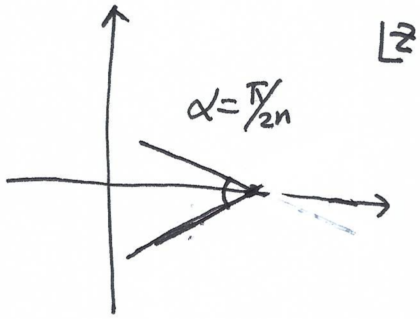
(14) (7)

$\cancel{s^2 = y^2}$

$\alpha = \pi/2n$

$$\lambda(s) = \frac{1}{2\pi} \frac{d}{ds} (a_n^{(2)} - a_n^{(1)}) \sin n\alpha \cdot s^n$$

$$\lambda(s) = \frac{1}{2\pi} (a_n^{(2)} - a_n^{(1)})\, n\, s^{n-1} \quad \sim s^{n-1}$$



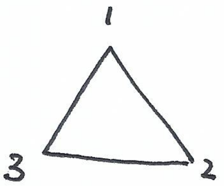
§ Zeros on the unit circle for the Ising model

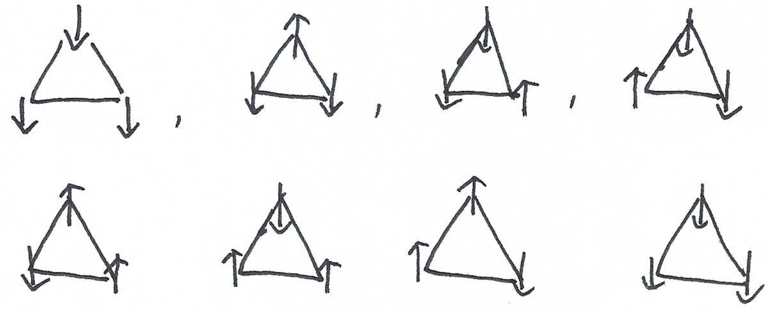
$$H = - \sum_{\langle ij\rangle} \underbrace{(\sigma_i \sigma_j - 1)}_{J_{ij}/2} - \sum_i h_i \frac{(\sigma_i + 1)}{2}$$

Define $A_{ij} = e^{-\beta J_{ij}}$, $\quad z_i = e^{-h_i\beta}$ - fugacity

If all the sites spin down, then $H = 0$. For at site i, flip spin ↓ to ↑, then a contriubtion $z_i = e^{-h_i}$ appears. For a bond anti-fermon configunation, it contributes $A_{ij} = e^{-\beta J_{ij}}$

Example 3-site





$$\mathcal{Z}_3(z_1 z_2 z_3) = 1 + z_1 A_{12} A_{13} + z_2 A_{21} A_{23} + z_3 A_{31} A_{32}$$
$$+ z_1 z_2 A_{13} A_{23} + z_2 z_3 A_{21} A_{31} + z_3 z_1 A_{32} A_{12} + z_1 z_2 z_3$$

$0 < A_{ij} < 1$, if set $h_1 = h_2 = h_3$, then $z_1 = z_2 = z_3$.

$$\mathcal{Z}_3(z, z z) = 1 + \alpha z + \alpha z^2 + z^3 = (z+1)(z^2 + \alpha z + 1)$$

$\alpha = A_{12}A_{13} + A_{12}A_{23} + A_{13}A_{23}$, $\Rightarrow$ $z_1 = -1$

$$z_{2,3} = \cancel{\frac{-\alpha + i\sqrt{4-}}{2}} \; -\frac{\alpha}{2} \pm i\sqrt{1-\left(\frac{\alpha}{2}\right)^2}$$

All the roots lie in the unit circle!

§ 1D Ising model with Periodic boundary condition

transfermatrix method

$$Z = \sum_{\sigma_i = \pm 1, \cdots \pm N} e^{\beta J/2 \sum_{i=1}^{N} (\sigma_i \sigma_{i+1} - 1) + \frac{\beta h}{4} \sum_{i=1}^{N} (\sigma_i + \sigma_{i+1} + 1 + 1)}$$

$$= \sum_{\{\sigma_i\}} T_{\sigma_1 \sigma_2} T_{\sigma_2 \sigma_3} \cdots T_{\sigma_N \sigma_1}$$

$$T_{\sigma_i \sigma_{i+1}} = e^{\beta J/2 (\sigma_i \sigma_{i+1} - 1) + \frac{\beta h}{4} (\sigma_i + \sigma_{i+1} + 2)}$$

$$\rightarrow \begin{pmatrix} e^{\beta h} & e^{-\beta J + \frac{\beta h}{2}} \\ e^{-\beta J + \frac{\beta h}{2}} & 1 \end{pmatrix} = \begin{pmatrix} z & A z^{1/2} \\ A, z^{1/2} & 1 \end{pmatrix} = A^{1/2} z^{1/2} \begin{pmatrix} A^{-1/2} z^{1/2} & A^{1/2} \\ A^{1/2} & A^{-1/2} z^{-1/2} \end{pmatrix}$$

$$Z = \mathrm{tr}\, T^N = (\lambda_+^N + \lambda_-^N)(Az)^{\frac{N}{2}}$$

~~eigenvalues~~

$$\cancel{\det \begin{pmatrix} \lambda - z & -Az^{1/2} \\ -Az^{1/2} & \lambda - 1 \end{pmatrix} = (\lambda - z)(\lambda - 1) - A^2 z = 0}$$

$$\cancel{\lambda^2 - (z+1)\lambda + z(1 - A^2) = 0 \Rightarrow}$$

$$\det \begin{pmatrix} \lambda - A^{-1/2} z^{1/2} & -A^{1/2} \\ -A^{1/2} & \lambda - A^{-1/2} z^{-1/2} \end{pmatrix} = 0$$

$$\lambda^2 - A^{-1/2}(z^{1/2} + z^{-1/2})\lambda + (A^{-1} - A) = 0$$

$$\Delta = A^{-1}(z + z^{-1} + 2) - 4A^{-1} + 4A$$

$$= A^{-1}(z^{1/2} - z^{-1/2})^2 + 4A$$

$$\lambda_\pm = \frac{1}{2}\left[A^{-1/2}(z^{1/2} + z^{-1/2}) \pm \sqrt{A^{-1}(z^{1/2} - z^{-1/2})^2 + 4A} \right)$$

zeros $\Rightarrow$ $\lambda_+^N + \lambda_-^N = 0$

$$\Rightarrow \frac{\lambda_+}{\lambda_-} = e^{i\frac{\pi}{N} + i2\pi\frac{n}{N}} = e^{i\alpha_n}, \quad n = 1, 2, \cdots N$$

$$\lambda_\pm = R e^{i\theta_\pm}$$

$$\Rightarrow \begin{cases} \lambda_+ + \lambda_- = R(e^{i\theta_+} + e^{i\theta_-}) = A^{-1/2}(z^{1/2} + z^{-1/2}) \\ \lambda_+\lambda_- = R^2 e^{i(\theta_+ + \theta_-)} = A^{-1} - A \end{cases}$$

$A = e^{-\beta J}$ is real $\Rightarrow$ $A^{-1} - A > 0 \Rightarrow \theta_- = -\theta_+ \Rightarrow R^2 = A^{-1} - A$

$0 < A < 1$ $\qquad R = A^{-1/2}(1-A^2)^{1/2}$

$$\Rightarrow \quad z^{1/2} + z^{-1/2} = A\, 2R\cos\theta_+$$

$$= 2A^{1/2}(1-A^2)^{1/2}\cos\theta_+$$

$z^2 + 2\sigma z + 1 = 0 \qquad \propto \sigma = A^{1/2}(1-A^2)^{1/2} < 1$

$\Rightarrow z = -\sigma \pm i\sqrt{1-\sigma^2} \quad \Rightarrow \quad |z| = 1.$

Let's write $z = e^{i\theta}$

$$\Rightarrow \lambda_\pm = \frac{1}{2}\left[A^{-1/2}\, 2\cos\frac{\theta}{2} \pm \sqrt{A^{-1}\left(2i\sin\frac{\theta}{2}\right)^2 + 4A}\right]$$

$$= A^{-1/2}\left[\cos\frac{\theta}{2} \pm i\sqrt{\sin^2\frac{\theta}{2} - A^2}\right]$$

$$A = \sin\frac{\theta_0}{2} \Rightarrow \lambda_\pm = \frac{1}{\sqrt{\sin\frac{\theta_0}{2}}}\left(\cos\frac{\theta}{2} \pm i\sqrt{\sin^2\frac{\theta}{2} - \sin^2\frac{\theta_0}{2}}\right)$$

$$|\lambda_\pm| = \frac{1}{\sqrt{\sin\frac{\theta_0}{2}}}\left(1 - \sin^2\frac{\theta_0}{2}\right) = \frac{1-A^2}{\sqrt{A}}$$

19 ⓐ

$$\frac{\cos\frac{\theta_n}{2} + i\left(\sin^2\frac{\theta_n}{2} - \sin^2\frac{\theta_0}{2}\right)^{1/2}}{\cos\frac{\theta_n}{2} - i\left(\sin^2\frac{\theta_n}{2} - \sin^2\frac{\theta_0}{2}\right)^{1/2}} = e^{i\alpha_n} \quad . \quad \alpha_n = \frac{\pi}{N} + 2\pi\frac{n}{N}$$

$$\Rightarrow \cos\alpha_n = \frac{\cos^2\frac{\theta_n}{2} - \left(\sin^2\frac{\theta_n}{2} - \sin^2\frac{\theta_0}{2}\right)}{1 - \sin^2\frac{\theta_0}{2}} = \frac{\cos\theta_n + \sin^2\frac{\theta_0}{2}}{\cos^2\frac{\theta_0}{2}}$$

$$2\cos^2\frac{\alpha_n}{2} = 1 + \cos\alpha_n = \frac{1+\cos\theta_n}{\cos^2\frac{\theta_0}{2}} = \frac{2\cos^2\frac{\theta_n}{2}}{\cos^2\frac{\theta_0}{2}}$$

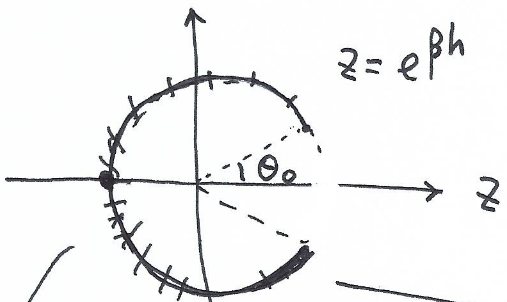
$$\Rightarrow \cos^2\frac{\alpha_n}{2} = \frac{\cos^2\frac{\theta_n}{2}}{\cos^2\frac{\theta_0}{2}} \quad \Rightarrow \quad \cos\frac{\theta_n}{2} = \cos\frac{\theta_0}{2}\cos\left(\frac{\pi}{2N} + \frac{n}{N}\pi\right)$$

$$z_1 = e^{i\theta_1} \quad \Rightarrow \cos\frac{\theta_1}{2} = \cos\frac{\theta_0}{2}\cos\left(\frac{3\pi}{2N}\right) \Rightarrow \theta_1 \to \theta_0 \text{ as } N \to +\infty$$

$$z_N = e^{i\theta_N} \quad \cos\frac{\theta_N}{2} \overset{\checkmark}{=} \cos\frac{\theta_0}{2}\cos\left(\frac{\pi}{2N}\right) \Rightarrow \frac{\theta_N}{2} \to \pi - \frac{\theta_0}{2} \quad N \to \infty$$

$$\theta_N \to \pi - \theta_0$$

$$\sin\frac{\theta_0}{2} = e^{-\beta J} > 0$$



Zeros on the unit circle.

$$\theta_n = \pi \Rightarrow \frac{\pi}{2N} + \frac{2n}{2N}\pi = \frac{\pi}{2}$$

$$(2n+1) = N$$

$$n \sim \frac{N}{2}$$

Define $\rho_N(\theta)$ as density of zeros along the unit circle.

$$\frac{n}{N} = \int_{\theta_0}^{\theta_n + 0^+} \rho_N(\theta)\, d\theta \qquad \text{let } N \to \infty$$

$$\cos\frac{\theta_n}{2} = \cos\frac{\theta_0}{2} \cos\left(\frac{n\pi}{N}\right)$$

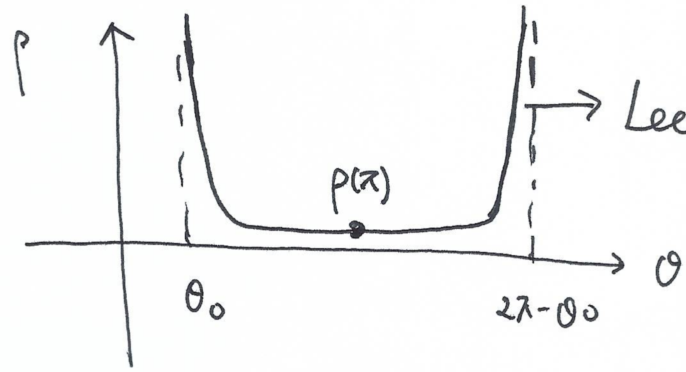
略去 n $\Rightarrow$ $$\cos\frac{\theta}{2} = \cos\frac{\theta_0}{2} \cos\left[\pi \int_{\theta_0}^{\theta} \rho(\theta)\, d\theta\right]$$

$$\frac{\partial}{\partial\theta} \cos\frac{\theta}{2} = \cos\frac{\theta_0}{2} \sin\left(\frac{n\pi}{N}\right) \pi\, \rho(\theta)$$

$$+\frac{1}{2}\sin\frac{\theta}{2} = \cos\frac{\theta_0}{2} \sqrt{1-\cos^2\left(\frac{n\pi}{N}\right)}\ \pi\, \rho(\theta)$$

$$\Rightarrow \rho(\theta) = \frac{\frac{1}{2\pi}\sin\frac{\theta}{2}}{\cos\frac{\theta_0}{2}\sqrt{1-\cos^2\frac{\theta}{2}/\cos^2\frac{\theta_0}{2}}} = \frac{1}{2\pi}\frac{\sin\frac{\theta}{2}}{\sqrt{\cos^2\frac{\theta_0}{2}-\cos^2\frac{\theta}{2}}}$$

$$= \begin{cases} \dfrac{1}{2\pi}\dfrac{\sin\frac{\theta}{2}}{\sqrt{\sin^2\frac{\theta}{2}-\sin^2\frac{\theta_0}{2}}} & \text{if } \theta \notin [-\theta_0, \theta_0] \\ 0 & \text{if } \theta \in [-\theta_0, \theta_0] \end{cases}$$



at Lee-Yang edge singularity

$$\rho(\pi) = \frac{1}{2\pi}\frac{1}{\sqrt{1-\sin^2\frac{\theta_0}{2}}} = \frac{1}{2\pi\sqrt{1-A^2}}$$

✓ elliptic integral ③

$$\int p(\theta)\, d\theta = \frac{1}{2\pi}\int_{\theta_0}^{2\pi-\theta_0} \frac{\sin\frac{\theta}{2}\, d\theta}{\sqrt{\sin^2\frac{\theta}{2} - \sin^2\frac{\theta_0}{2}}} \quad d\theta = \frac{1}{2\pi}\int_{x_0}^{1} \frac{x}{\sqrt{x^2 - x_0^2}} \frac{dx}{\sqrt{1-x^2}}$$

$x = \sin\frac{\theta}{2} \quad x_0 = \frac{\theta_0}{2}$

if $\beta \to \infty$, $A = 0$ $\Rightarrow$ $\boxed{p(\theta) = \frac{1}{2\pi}}$ First order transition

Theorem 3: Unit circle theorem, for the Ferromagnetic Ising model, the root of the partition function Z lies on the unit circle $|z| = 1$. This result is true independent of the lattice structure, range of J_{ij}, etc.
dimensionality and

$z = e^{-\beta h}$

$$F = -\frac{1}{\beta}\ln Z \Rightarrow \frac{-F}{N k_B T} = \frac{1}{N}\sum_i \ln(z - z_i)$$

$$\frac{-F}{N k_B T} = \int_0^{2\pi} d\theta\, p(\theta)\ln(z - e^{i\theta}) = \int_0^{\pi} d\theta\, p(\theta)\ln(z^2 - 2z\cos\theta + 1)$$

$e^{i\theta}$ and $e^{-i\theta}$ appear in pairs

$$M = -\frac{\partial F}{N \partial h} - 1/2 = -1/2 - \frac{\partial F/N\cdot\beta}{\partial(\beta h)} = -1/2 - \frac{\partial(-F/N\beta)}{\partial z}\cdot z$$

$$= -1/2 - 2z\int_0^{\pi} d\theta\, p(\theta)\, \frac{z - \cos\theta}{z^2 - 2z\cos\theta + 1}$$

$\Rightarrow$ [illegible] lattice gas