Lecture 20 - Phase transitions Pt 3

$$\mathcal{H}_{Ising} = -\sum_{\langle ij \rangle} \frac{J}{2} s_i s_j - \sum_{i=1}^{N} h s_i$$

$$m = \langle s_i \rangle = \frac{1}{N} \left\langle \sum s_i \right\rangle$$

$$= \frac{1}{N} \frac{\partial \log Z}{\partial (\beta h)}$$

$$Z = \sum_{s_1, s_2, s_3 \ldots s_N = \pm 1} e^{-\beta \mathcal{H}(s_1, s_2, \ldots, s_N)}$$

$$\delta s_i = s_i - m \Rightarrow s_i = \delta s_i + m$$

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^{N} s_i$$

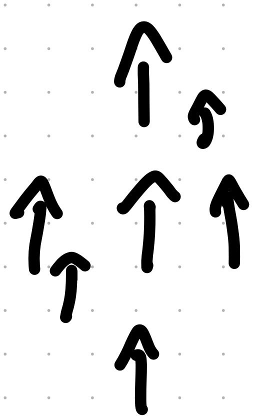
$$= -\frac{J}{2} \sum_{\langle i,j \rangle} [\delta s_i + m][\delta s_j + m] - h \sum_{i=1}^{N} s_i$$

$$\underbrace{\delta s_i \delta s_j}_{\text{aprox} \approx 0} + m \delta s_i + m \delta s_j + m^2$$

$$\langle \delta s_i \delta s_i \rangle \simeq \mathrm{Var}(s_i) \approx 0$$

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle}\left(m^2 + m(s_i - m) + m(s_j - m)\right) - h\sum s_i$$

$$= +\sum_{\langle i,j\rangle}\frac{m^2 J}{2} - \frac{mJ}{2}\sum_{\langle i,j\rangle}(s_i + s_j) - h\sum_{i=1}^{N} s_i$$



$$\#\ \text{neighbors} = 2d = z \leftarrow \text{coordination number}$$

$$\sum (x_i + x_j) = \sum_{i=1}^{N} x_i + \sum_{j=1}^{N} x_j$$

$$= 2 \sum_{i=1}^{N} x_i$$

$$\sum_{i=1}^{N} \sum_{j=1}^{3} s_i = 3 \sum_{i=1}^{N} s_i$$

$$H_{MF} = Nz(Jm^2) - (h + 2mJz) \sum_{i=1}^{N} s_i$$

$$Z = \sum_{s_1, s_2, \ldots s_N} e^{-\beta \left[NzJm^2 - (h + 2mJz \sum_{i=1}^{N} s_i) \right]}$$

$$Z = e^{-\beta J m^2 N z}\left[\sum_{s_i=\pm 1} e^{\beta(h+2mJz)s_i}\right]^N$$

$$\underbrace{e^{\beta(h+2mJz)} + e^{-\beta(h+2mJz)}}_{2\cosh\left[\beta(h+2mJz)\right]}$$

$$\langle s_i\rangle = \frac{k_B T}{N}\frac{\partial \log Z}{\partial h} = k_B T \frac{\partial}{\partial h}\left[\log \cosh\left[\beta(h+2mJz)\right]\right]$$

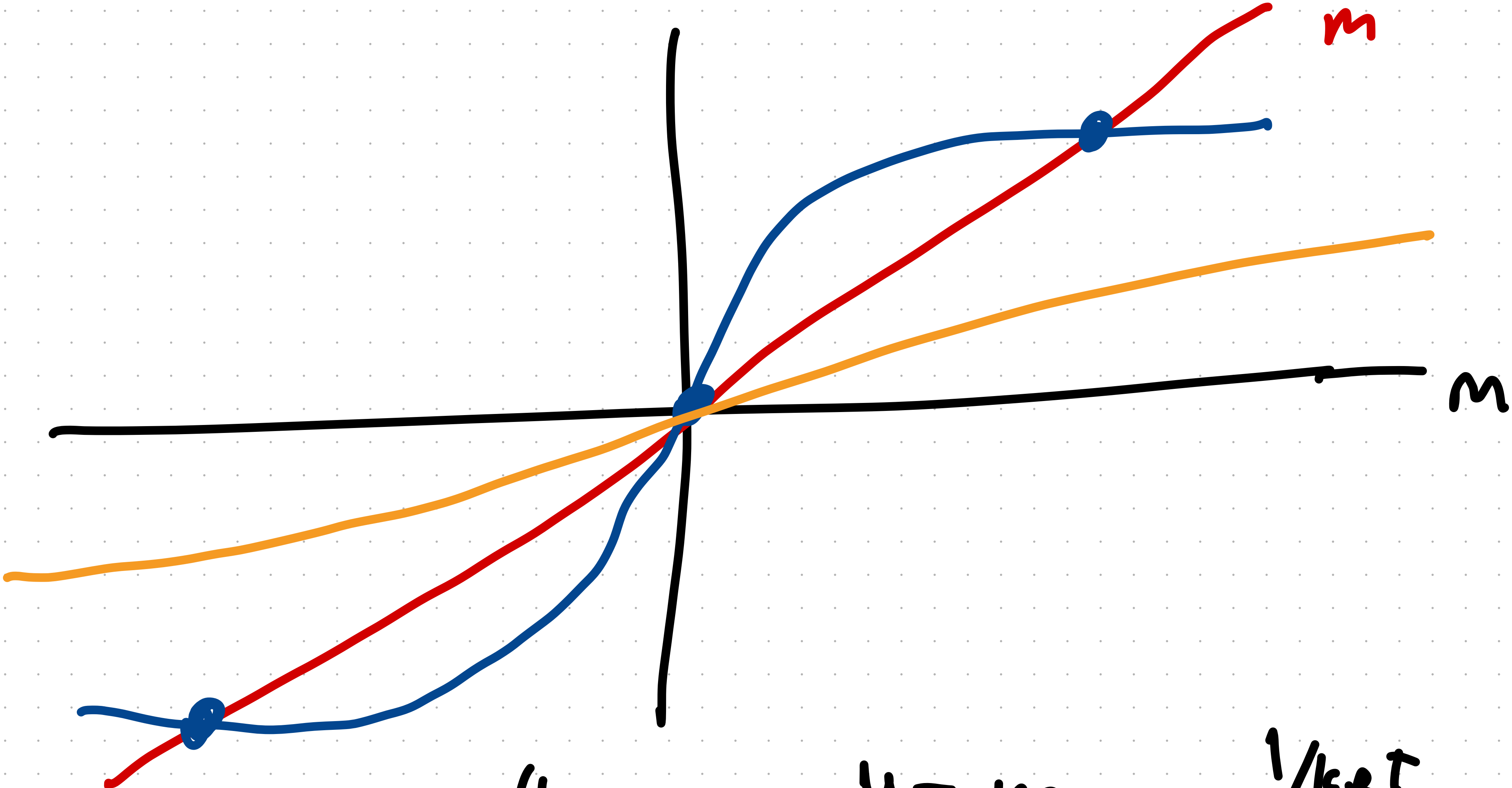
$$\langle s_i \rangle = k_B T \frac{\partial}{\partial h}\left[\log\left[\cosh[\beta(h+2mJz)]\right]\right]$$

$$= k_B T \cdot \frac{1}{\cosh[\;]} \cdot \sinh[\;] \cdot \beta$$

$$\underline{m} = \tanh[\beta(\underline{h}+2mJz)]$$

no analytical solution

is there spontaneous magnetization at $h=0$



graphically

$$y = m$$

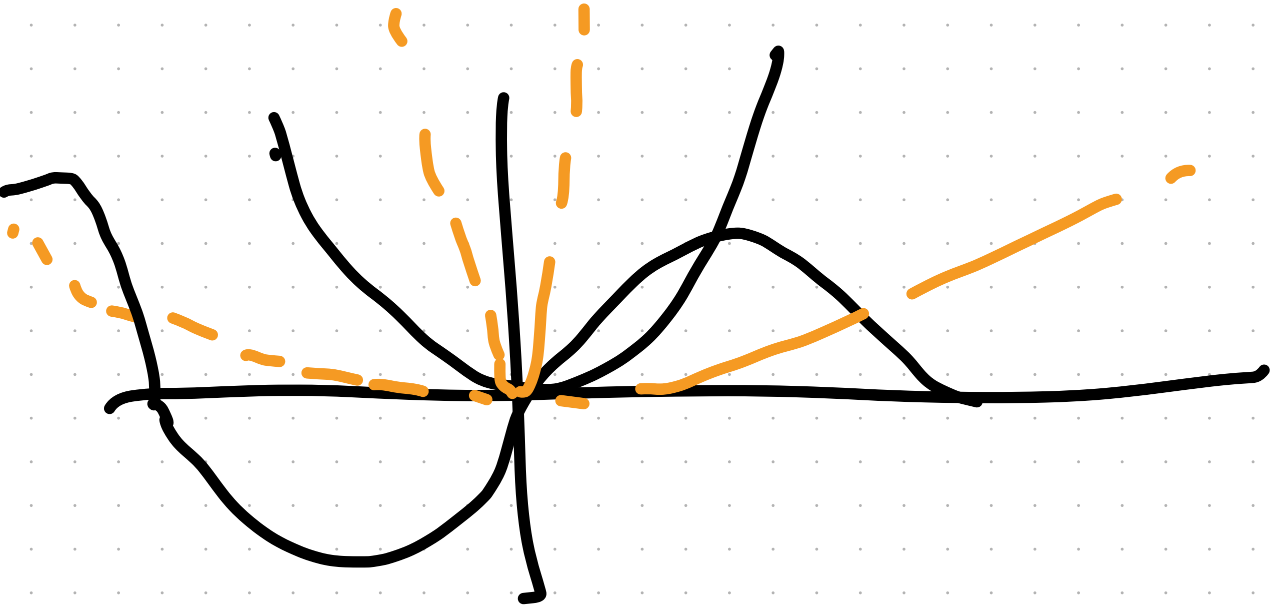
$$\frac{1}{k_B T}$$

$$x = \tanh(\beta\, 2 m J z)$$

low T 3 solutions

high T 1 solution

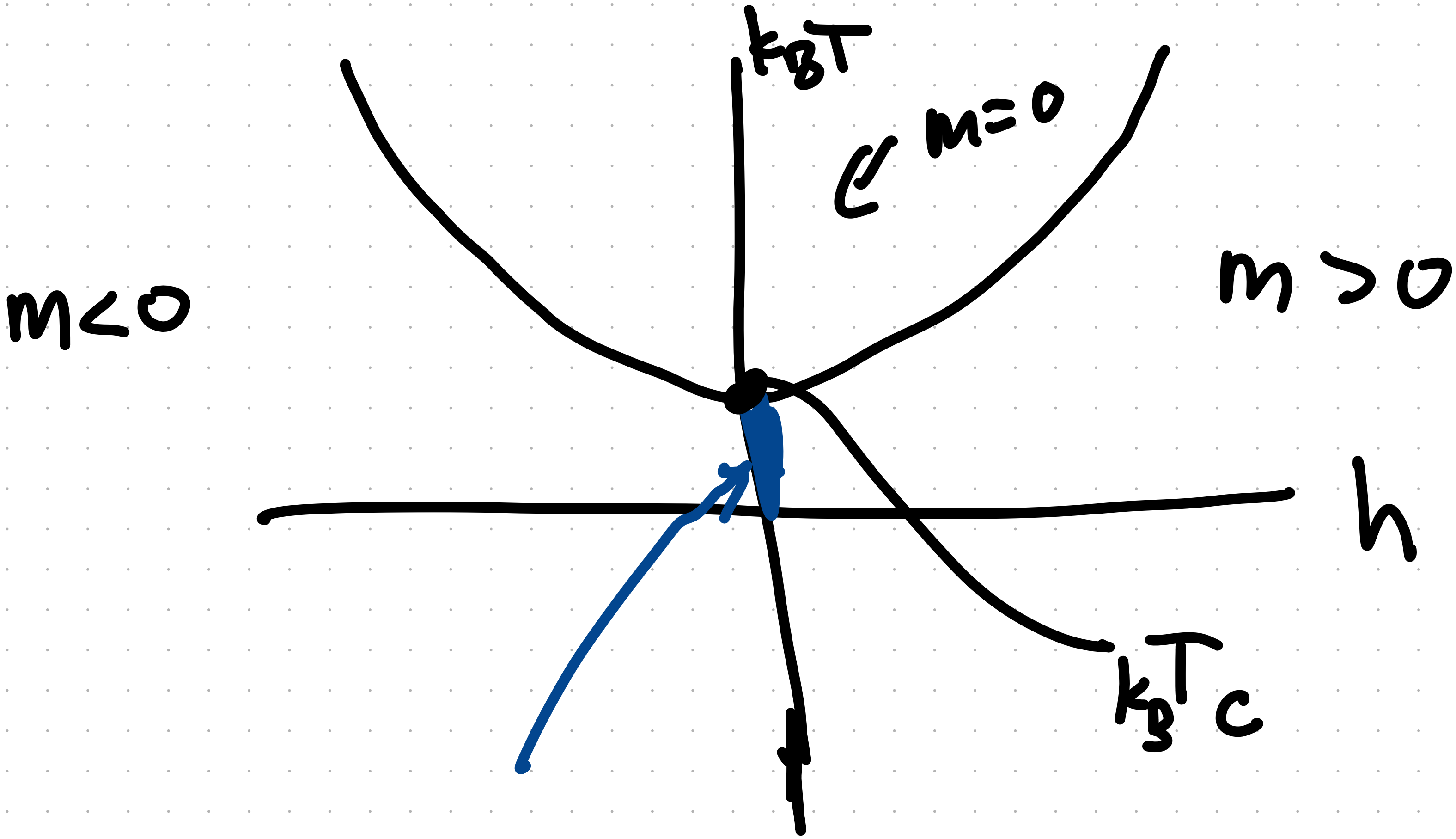
$$\sin(x) = a x^2$$



$2\beta J z = 1$ separates 2 cases

$$k_B T_c = 2 J z$$

$$k_B T_c = 2Jz$$



$|m|>0, \; h=0$

$$k_B T_c = 4Jd$$

In 2d turns out that

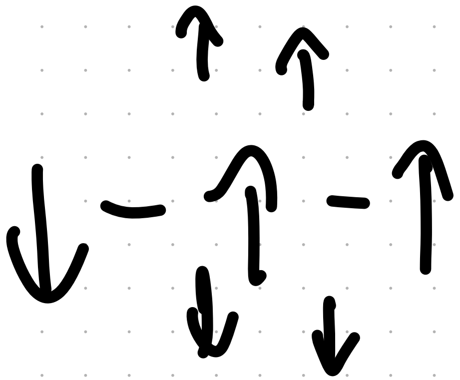
$k_B T_c = 2.269 J$

mf $= 2Jz = 8J$

mf model over estimates this temp neglecting fluctuations

MFT becomes better as $d \to \infty$

Ising model - MFT exact in 4 dimensions

) as $d \uparrow$ $z \uparrow$

$d \to \infty$ infinite neighbours

$$f(m,\beta) \underset{MF}{\approx} -\frac{k_B T}{N} \ln Z_{MF}$$

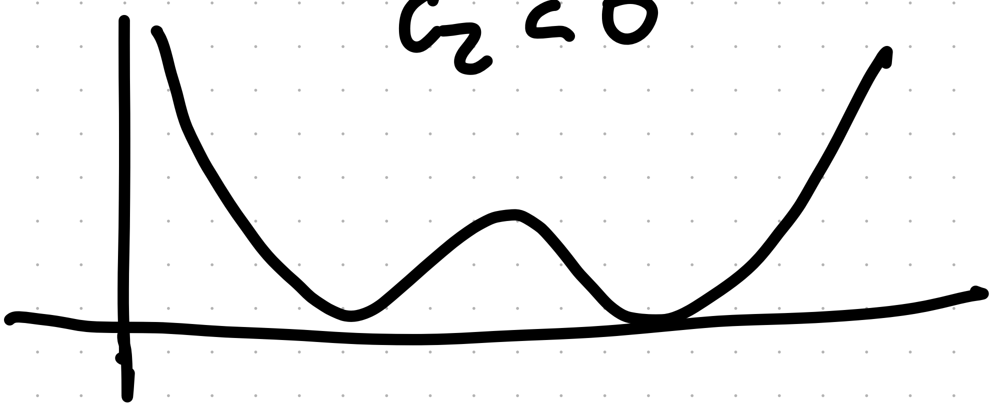
field

$$= J m^2 z - \frac{1}{\beta} \log\left[2\cosh\left(\cancel{h} + 2mJz\right)\beta\right]$$

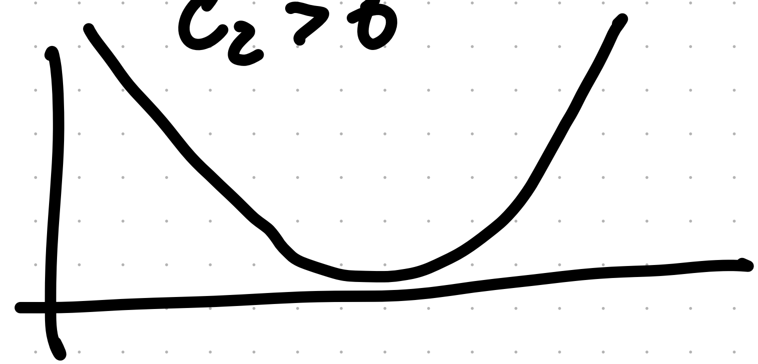
$$f(0,\beta) \underset{m\approx 0}{\approx} \underline{c_0 + c_2 m^2 + c_4 m^4}$$

$$c_2 = Jz - 2J^2 z^2 \beta \leftarrow 2Jz\beta = 1$$

$c_2 < 0$

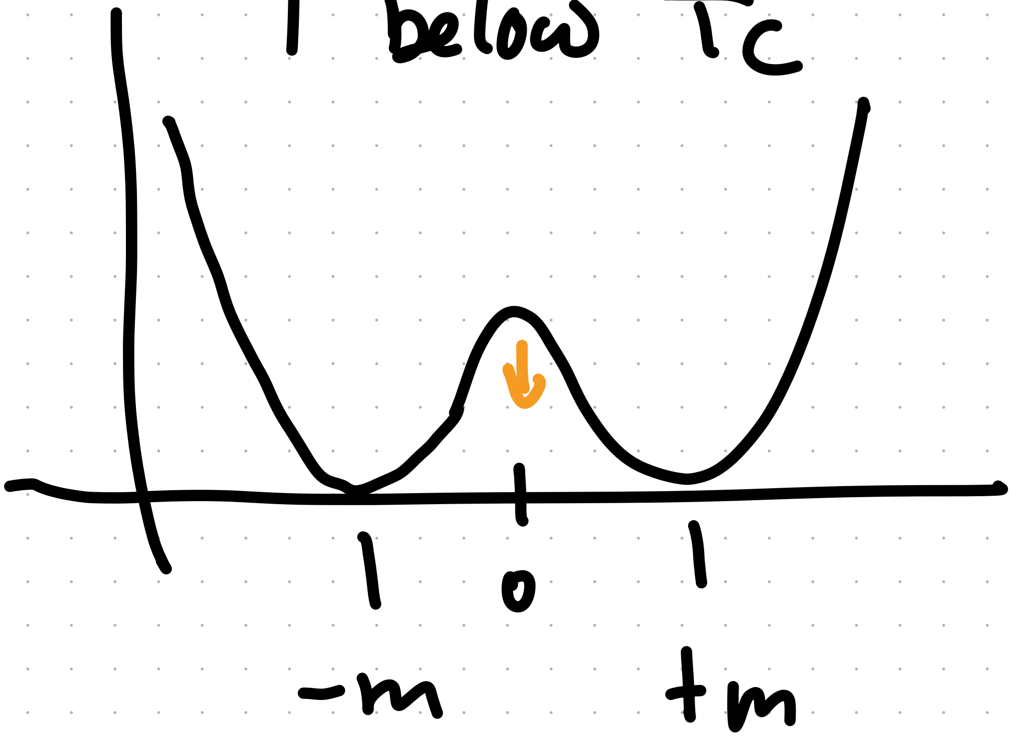


$c_2 > 0$

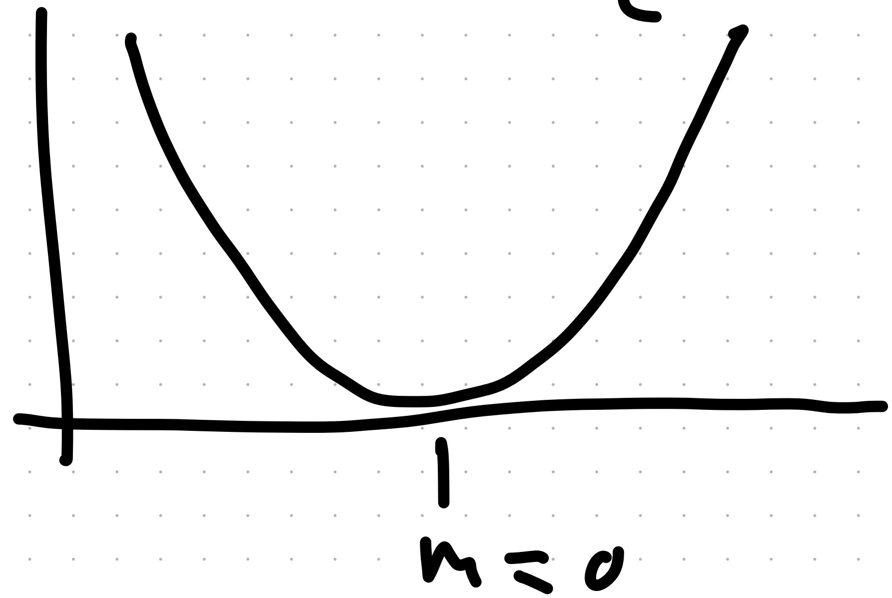


Shape of free energy near a critical point

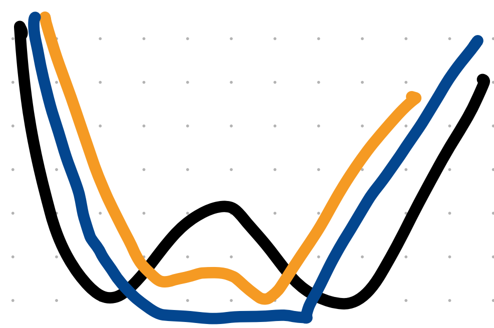
T below T_c



T above T_c



as $T \to T_c$ from below

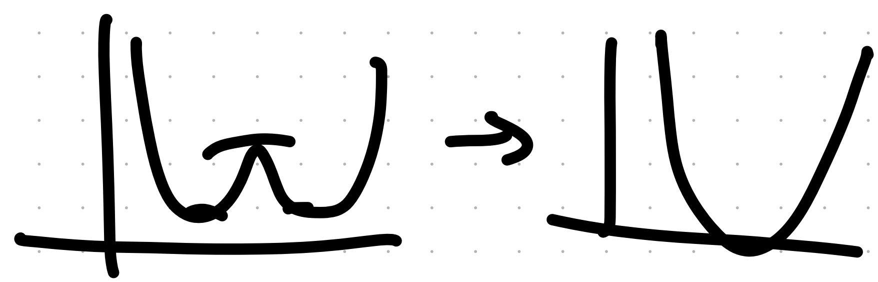


Physics – guess free energy shape

$$f(\beta, m) \propto c_0 + \cancel{c_1 m} + c_2 m^2 + \cancel{c_3 m^3} + c_4 m^4 + \cancel{\ldots}$$

$\uparrow$ order parameter)

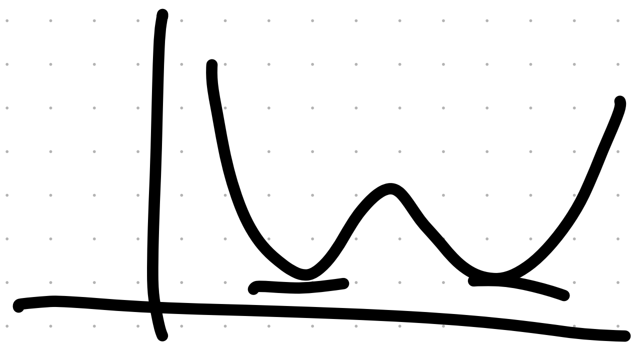
symmetric under no field, no odd terms



ask where this transition happens where min/max

$$\frac{\partial f(\beta,m)}{\partial m} = 0 = 2m\,c_2 + 4m^3 c_4$$

$$m_0 = \pm\sqrt{-\frac{c_2}{2c_4}}$$



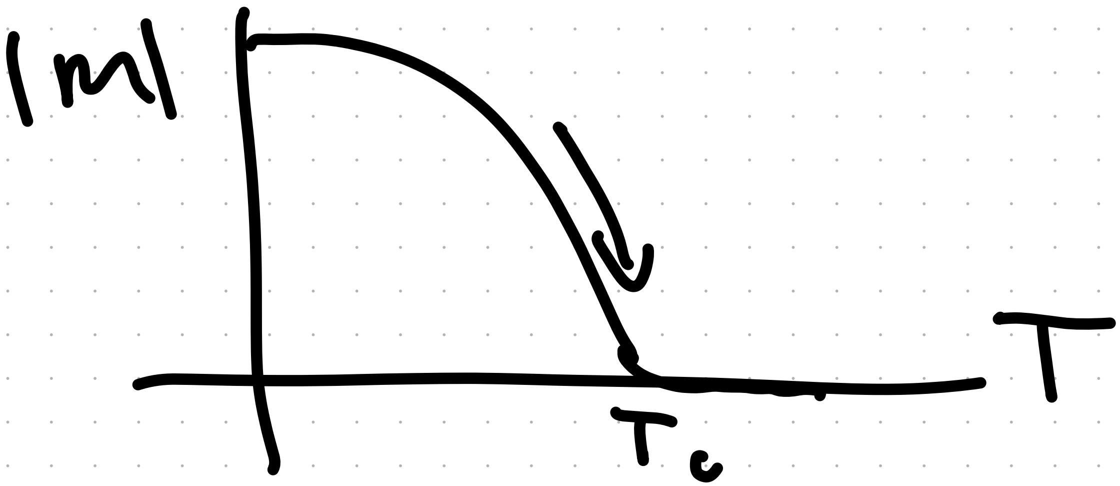
$$c_2 = Jz - 2J^2 z^2 \beta$$

$$= \frac{1}{2\beta_c} - \frac{\beta}{2\beta_c^2}$$

$$\beta_c = \frac{1}{2Jz}$$

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

$T \to T_c$ from below



$$m = \pm \sqrt{\frac{T_c}{2T}\frac{(T_c - T)}{c_4}} \sim$$

$$|m| \sim (T_c - T)^{1/2}$$

critical exponent (becomes exact)

Characterize system close to a transition by exponents:

$$C_V = \left(\frac{\partial \varepsilon}{\partial T}\right) \sim |T - T_c|^{-\alpha}$$

$$K_T = -\frac{1}{v}\left(\frac{\partial v}{\partial P}\right) \sim |T - T_c|^{-\gamma}$$

$$P - P_c \sim (\rho - \rho_c)^{\delta} \operatorname{sign}(\rho - \rho_c)$$

$$\rho_L - \rho_G \sim |T_c - T|^{\beta}$$

(m)

Table 16.1

$$K_T \sim \chi = \frac{\partial m}{\partial h}$$

$$P \sim h = \partial A / \partial m$$

$$C_v = C_v = \frac{\partial \varepsilon}{\partial T}$$

$$\rho_L - \rho_G = m$$

By looking at derivatives of free energy — connect exponents

Scaling Relation - Ben Widom

Eg $2 - \alpha = 2\beta + \gamma$

MF ising model

$\alpha = 0, \ \beta = \frac{1}{2}, \ \gamma = 1, \ \delta = 3$ ⇐

Measured: $\alpha = 0.1, \ \beta = 0.34$

$\gamma = 1.35, \ \delta = 4.2$

Van der Waals

Universality

$$U(x) = \frac{1}{4}(x-a)^2(x+a)^2$$

$$\frac{du}{dx} = \frac{1}{4}\Big[2(x-a)(x+a)^2 + 2(x+a)(x-a)^2\Big]$$

$$= \frac{1}{2}\Big[(x+a)\big[(x-a)^2 + (x-a)(x+a)\big]\Big]$$

$$= \frac{1}{2}\Big[(x+a)(x-a)\big[(x-a) + (x+a)\big]\Big]$$

$$= x(x+a)(x-a)$$