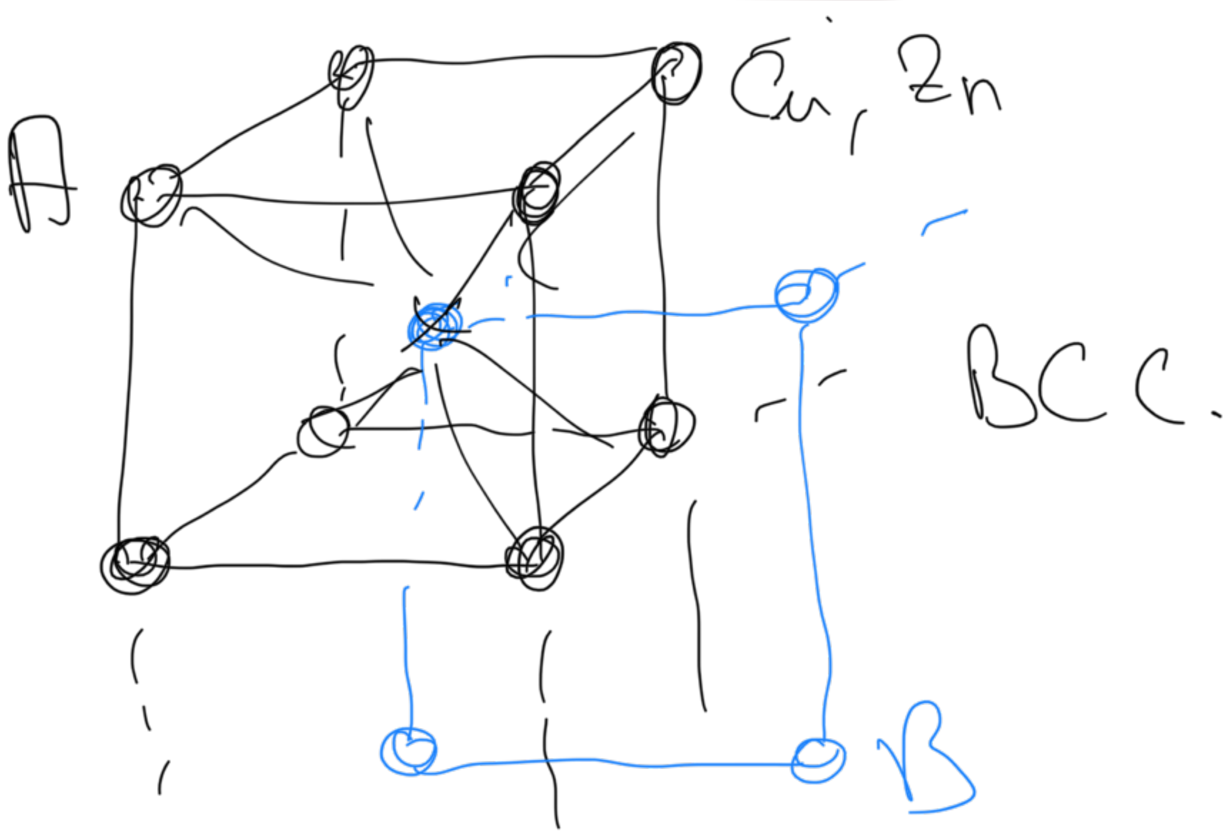
3) El Modelo de Ising en mezclas binarias



$$\varepsilon_{Cu-Zn} < \varepsilon_{Cu-Cu}, \varepsilon_{Zn-Zn}$$

$$E = N_{Cu-Cu}\,\varepsilon_{Cu-Cu} + N_{Zn-Zn}\,\varepsilon_{Zn-Zn} + N_{Zn-Cu}\,\varepsilon_{Zn-Cu}$$

N átomos, $\frac{N}{2}$ átomos de Cu

" " " Zn

los $\frac{N}{2}$ átomos de Cu $\rightarrow 8 \times \frac{N}{2}$ ligaduras que tem Cu-Cu ou Zn-Zn

$$4N = N_{Cu-Zn} + 2N_{Cu-Cu}$$

igual $4N = N_{Cu-Zn} + 2N_{Zn-Zn}$

$$\Rightarrow N_{Zn-Zn} = N_{Cu-Cu} = 2N - \frac{N_{Cu-Zn}}{2}$$

$$E = \boxed{2N\left[\varepsilon_{Cu-Cu} + \varepsilon_{Zn-Zn}\right]} \rightarrow \text{cte.}$$

$$+ N_{Cu-Zn}\left(\varepsilon_{Cu-Zn} - \frac{\varepsilon_{Cu-Cu} + \varepsilon_{Zn-Zn}}{2}\right)$$

definimos

$$\underset{i \in A}{\sigma_i} = \begin{cases} +1 & \text{si Cu} \\ -1 & \text{si Zn} \end{cases}$$

et

$$\underset{i \in B}{\sigma_i} = \begin{cases} -1 & \text{si Cu} \\ +1 & \text{si Zn} \end{cases}$$

$$H = -J \sum \sigma_i \sigma_j$$

$$\sum_{\langle i,j\rangle}$$

$$= -J N_{Cu-Zn} + J\left(N_{Cu-Cu} + N_{Zn-Zn}\right)$$

$$= -2J N_{Cu-Zn} + \underbrace{4NJ}_{cte.}$$

def $J = \dfrac{\varepsilon_{Cu-Cu} + \varepsilon_{Zn-Zn}}{2} - \dfrac{\varepsilon_{Cu-Zn}}{2} > 0$

$\Rightarrow H_{Ising} = E_{Cu-Zn} + cte.$

4] Modelo de Heisenberg

en cada sitio $\vec{S}_i = \begin{pmatrix} S^x_i \\ S^y_i \\ S^z_i \end{pmatrix}$, $\vec{S}_i \cdot \vec{S}_i = 1$

$$\boxed{H = -\sum_{i,j} J_{i,j}\, \vec{S}_i \cdot \vec{S}_j}$$

→ Simetría, grupo de simetría

O(3) ...

$O(3)$ $M \in O(3)$ $M^T M = \mathbb{1}$

$(\det M)^2 = 1 \Rightarrow \det M = \pm 1$

$SO(3) \subset O(3)$ tq $M^T M = \mathbb{1}$
$\det M = 1$

$SO(3) \rightarrow$ grupo de rotaciones.

$\rightarrow$ $\vec{S} \rightarrow -\vec{S}$ $\begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix} \rightarrow \begin{pmatrix} -S^x \\ S^y \\ S^z \end{pmatrix}$

$\notin SO(3)$

$\in O(3)$

obs si es en Mecánica Cuántica

$\vec{S}_i \rightarrow$ espines $\vec{S}^2 = \hbar^2 s(s+1)$

$[S^a, S^b] = i\hbar \epsilon^{abc} S^c \rightarrow SO(3)$

$$H(\vec{h}) = -\sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$$

simetría $SO(2) \rightarrow$ rotaciones alrededor de $\vec{h}$

$$\vec{M} = \sum_i \langle \vec{S}_i \rangle$$

$$Z = \int \prod_i d^2\vec{S}_i \, e^{-\beta H}$$

$$\langle O \rangle = \frac{1}{Z} \int \prod_i d^2\vec{S}_i \, e^{-\beta H} \, O$$

Si C.B.P. $\Rightarrow$ todos los sitios son equivalentes

$$\vec{M} = N\vec{m} \qquad \vec{m} = \langle \vec{S}_i \rangle \;\; \forall i$$

<u>Funciones de correlación:</u>

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle_c = \langle \vec{S}_i \cdot \vec{S}_j \rangle - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle$$

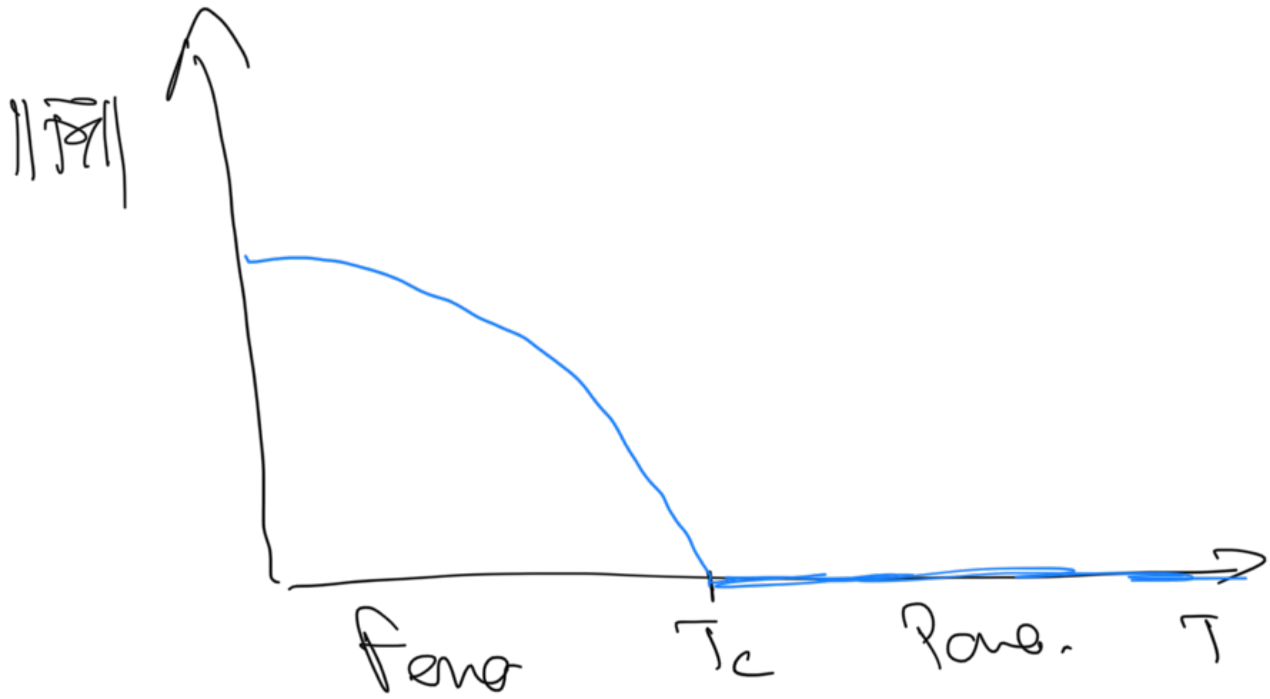
$$M^\alpha = \sum_i \langle S_i^\alpha \rangle$$

Susceptibilidad magnética

$$\chi^{\alpha\beta} = \frac{\partial M^\alpha}{\partial h^\beta} = \delta^{\alpha\beta} \frac{\partial M^1}{\partial h^1}$$

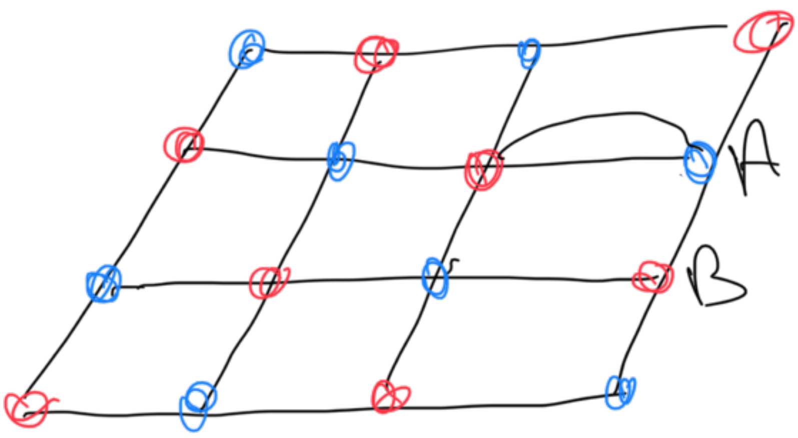
$\Rightarrow$ para $d = 1, 2$ $\Rightarrow$ no hay fase ordenada.

$\Rightarrow$ para $d \geq 3$



<u>obs</u>

Modelos antiferromagnéticos.



Red bipartita.

Ising:

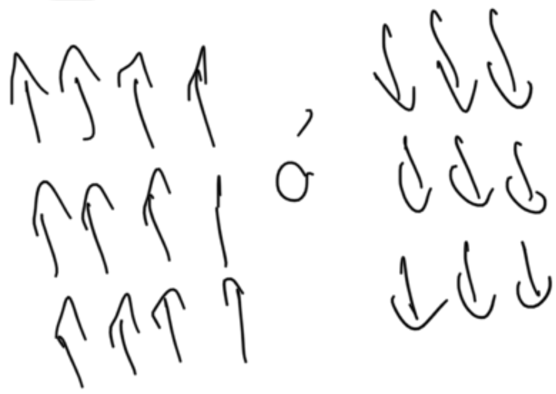
$$H = -J \sum_{<ij>}' \sigma_i \sigma_j \qquad J > 0$$

ahora $H = +J \sum \sigma_i \sigma_j \qquad J > 0$

$\langle i,j \rangle$

Config de más baja energía:

$-J$ Ferro

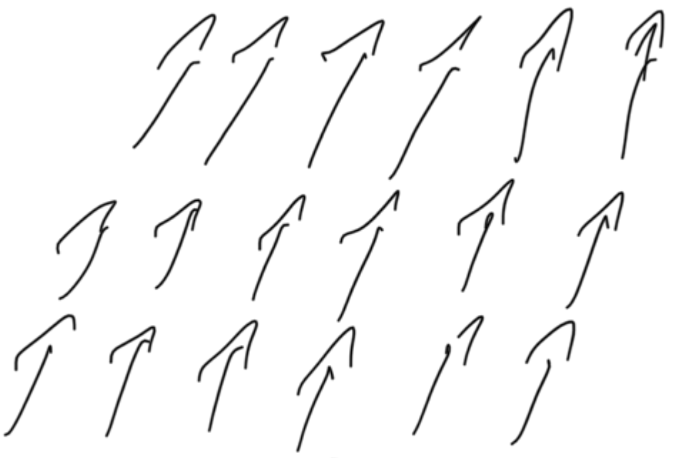


$+J$ AF.

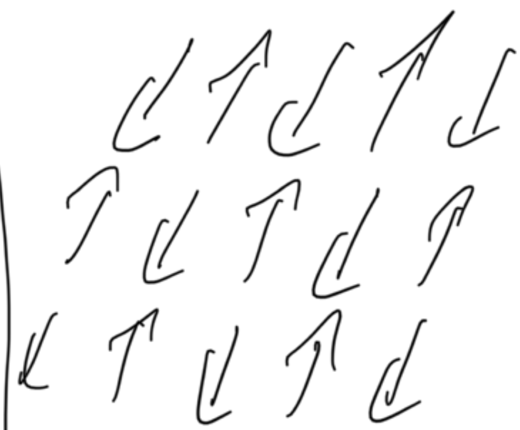
orden de Néel

Heisenberg.

$-J$ (Ferro)



Ferro



Néel

obs para toda red bipartita
→ con 2 subláticas A y B

$$H_{Ferro} \longleftrightarrow H_{AF}$$

$$H = \sum J \, \sigma_i \sigma_j \longrightarrow \sum \sum \sigma_i \sigma_j$$

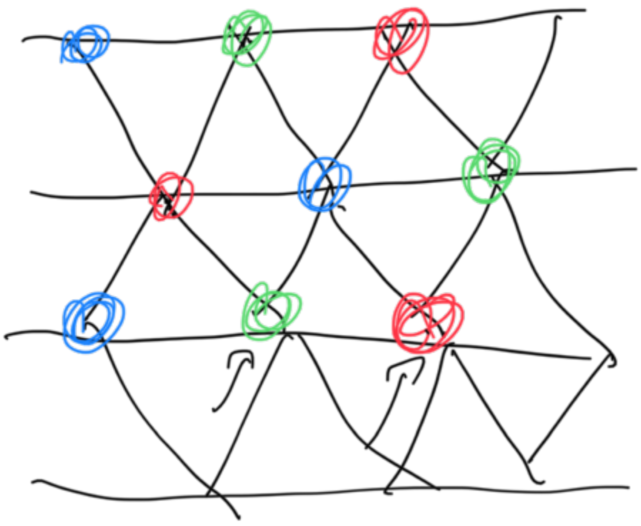
$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \rightarrow J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

$$\rightarrow \left(\begin{cases} \sigma_i \rightarrow \sigma_i & \text{si } i \in A \\ \sigma_i \rightarrow -\sigma_i & \text{si } i \in B \end{cases} \right)$$

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \rightarrow J \sum \vec{S}_i \cdot \vec{S}_j$$

$$\begin{cases} \vec{S}_i \rightarrow \vec{S}_i & \text{si } i \in A \\ \vec{S}_i \rightarrow -\vec{S}_i & \text{si } i \in B \end{cases}$$

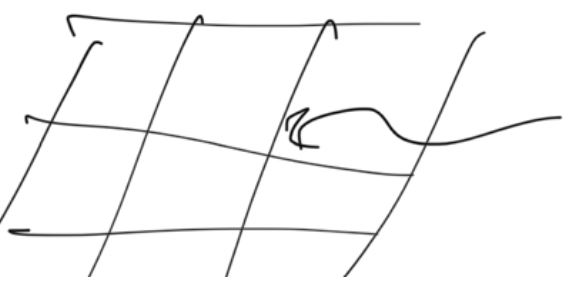
¿Y si la red no es bipartita?



para el modelo AF

→ Frustración

5] Modelo "XY"



sitios "i"

en cada sitio "i" $\longrightarrow \vec{S}_i = \begin{pmatrix} S^x_i \\ S^y_i \end{pmatrix}$

$$H = -J \sum_{\langle ij \rangle} \underline{\Delta^x S^x_i S^x_j + \Delta^y S^y_i S^y_j} + \cancel{\Delta^z S^z_i S^z_j}$$

$$\Delta^x = \Delta^y \gg \Delta^z$$

$$H = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j$$

grupo de simetría : $O(2)$
$SO(2)$

$$R = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \in SO(2)$$

$$SO(2) \sim U(1) \sim \{e^{i\theta}\}$$

$$\Psi = S_x + i S_y$$

$\sqrt{-1}$

$$\underline{\vec{S} \to R\vec{S}} \Leftrightarrow \underline{\Psi \to e^{i\theta}\Psi}$$

* transición metal - superconductor

J ... θ

$$H_{BCS} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k})\, C^{\dagger}_{\vec{k},\sigma} C_{\vec{k},\sigma}$$

$$+ \sum_{\vec{k},\vec{k}'} V(\vec{k},\vec{k}')\, C^{\dagger}_{\vec{k}\uparrow} C^{\dagger}_{-\vec{k}\downarrow} C_{\vec{k}'\downarrow} C_{-\vec{k}'\uparrow}$$

Simetría $U(1)$

$$\left|\begin{array}{l} C_{\vec{k},\sigma} \to e^{i\theta} C_{\vec{k},\sigma} \\ C^{\dagger}_{\vec{k},\sigma} \to e^{-i\theta} C^{\dagger}_{\vec{k},\sigma} \end{array}\right|$$

Superconductividad.

$$\langle C_{\vec{k},\downarrow} C_{-\vec{k}\uparrow} \rangle \neq 0$$

* Superfluidez.

He^4

$$H = \sum_{\vec{k}} \varepsilon(\vec{k})\, b^{\dagger}(\vec{k})\, b(\vec{k})$$

$$+ V_0 \sum_{\substack{\vec{k}_1+\vec{k}_2 \\ = \vec{k}_3+\vec{k}_4}} b^{\dagger}_{\vec{k}_1} b^{\dagger}_{\vec{k}_2} b_{\vec{k}_3} b_{\vec{k}_4}$$

$b \to e^{i\theta} b$

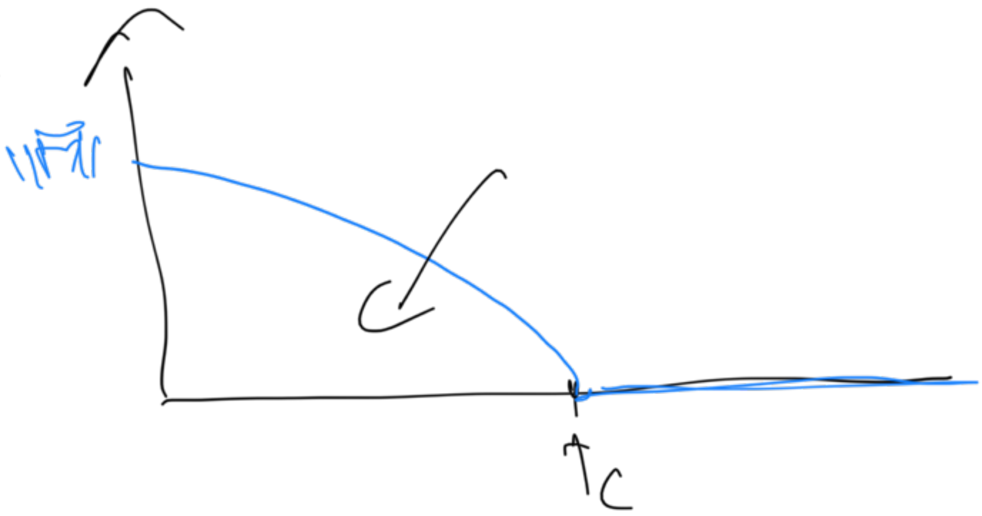
$b^{\dagger} \to e^{-i\theta} b^{\dagger}$

$b^{\dagger} \to c$

$\sim 2{,}14\ K \Rightarrow$ condensación de BE.

$$\langle b(h=0)\rangle \neq 0$$

$3 \geq d$



$d=1 \Rightarrow$ no hay transición de fase

$d=2 \to$ Fase B.K.T.

II Aproximación de Campo Medio

Ising. N espines.

$$H(h) = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i$$

El caso $J=0$

$$Z = \sum e^{-\beta H} = \sum e^{+h\beta\sum_i \sigma_i}$$

$\{\sigma\}$ $\qquad$ $\{\sigma\}$

$$= \sum_{\{\sigma\}} \prod_i e^{+\beta h \sigma_i} = \prod_i \left(\sum_{\sigma_i = \pm 1} e^{+\beta h \sigma_i} \right)$$

$\sigma_1 = \pm 1, \sigma_2 = \pm 1, \sigma_3 = \pm 1 \ldots$

$$Z = Z_1^N \quad \text{donde} \quad Z_1 = \sum_{\sigma = \pm 1} e^{+\beta h \sigma}$$

$$\Rightarrow Z = 2\,\mathrm{ch}(\beta h)$$

$$\langle \sigma_i \rangle = \frac{1}{Z} \sum_{\{\sigma\}} e^{-\beta H} \sigma_i$$

$$= \frac{1}{Z_1 \cancel{Z_2} \cdots \cancel{Z_N}} \cancel{Z_2} \cancel{Z_3} \cdots \cancel{Z_N} \sum_{\sigma_1 = \pm 1} e^{+\beta h \sigma_1} \sigma_1$$

$$= \frac{1}{Z_1} \underbrace{\sum_{\sigma_1 = \pm 1} e^{+\beta h \sigma_1} \sigma_1} = \frac{1}{Z_1} 2\,\mathrm{sh}(\beta h)$$

$$\Rightarrow \langle \sigma_1 \rangle = \frac{2\,\mathrm{Sh}(\beta h)}{2\,\mathrm{ch}(\beta h)} = \mathrm{tgh}(\beta h)$$

$$m = \mathrm{tgh}(\beta h)$$

el caso $J \neq 0$

$$H = -J \sum_{\langle ij\rangle} \boxed{\sigma_i\sigma_j} - h\sum_i \sigma_i$$

todos os sítios equivalentes.

$$m = \langle\sigma_i\rangle \quad ; \quad \sigma_i = m + \delta\sigma_i$$

$$\sigma_i\sigma_j = (m+\delta\sigma_i)(m+\delta\sigma_j)$$
$$= m^2 + m(\delta\sigma_i + \delta\sigma_j) + \cancel{\delta\sigma_i\delta\sigma_j}$$

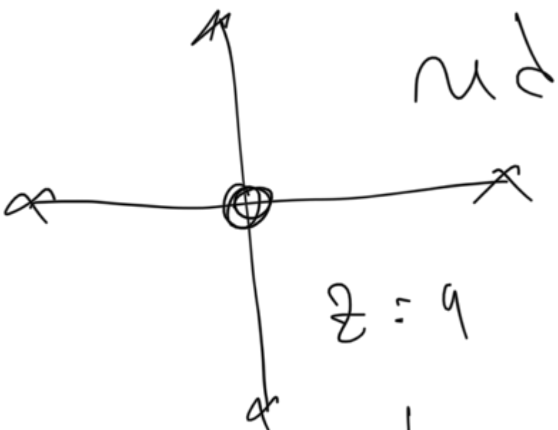
Aprox. de C.M.

$$\delta\sigma_i = \sigma_i - m$$

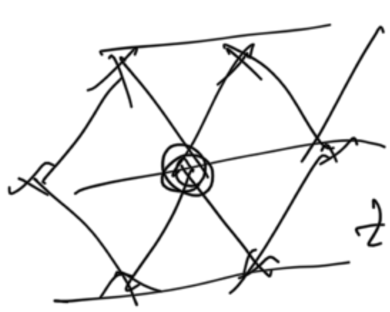
$$\Rightarrow \sigma_i\sigma_j = m(\sigma_i+\sigma_j) - m^2 + \cancel{\delta\sigma_i\delta\sigma_j}$$

$$H = -J\sum_{\langle ij\rangle}{}'(-m^2) - mJ\sum_{\langle ij\rangle}{}'(\sigma_i+\sigma_j) - h\sum_i \sigma_i$$

nº de z vizinhos por sítio



$z = 4$



$z = 6$

$$\sum_{\langle ij\rangle} = \frac{z}{2}N \qquad \sum_{\langle ij\rangle}\sigma_i = \frac{z}{2}\sum_i \sigma_i$$

$$H = \frac{Nm^2Jz}{2} - Jzm\sum_i\sigma_i - h\sum_i\sigma_i$$

$$H = \frac{Nm^2Jz}{2} - h_{eff}\sum_i \sigma_i$$

$$h_{eff} = h + Jz\underbrace{m}_{\langle\sigma_i\rangle}$$

$$Z = \sum_{\{\sigma\}} e^{-\beta H} = (Z_{1eff})^N$$ donde

$$Z_{1eff} = \sum_{\sigma=\pm 1} e^{-\frac{\beta m^2 Jz}{2} + \beta h_{eff}\sigma}$$

$$= e^{-\frac{\beta m^2 Jz}{2}}\, 2\,\mathrm{ch}(\beta h_{eff}) =$$

$$Z = (Z_{1eff})^N = e^{-\beta F}$$

$$F = \frac{Nm^2Jz}{2} - k_B T N \ln\left(2\,\mathrm{ch}(\beta h_{eff})\right)$$

$$\langle \sigma \rangle = \frac{1}{z_{eff}} \sum_{\sigma=\pm 1} e^{\frac{\beta m^2 J z}{2} + \beta h_{eff} \sigma} \sigma$$

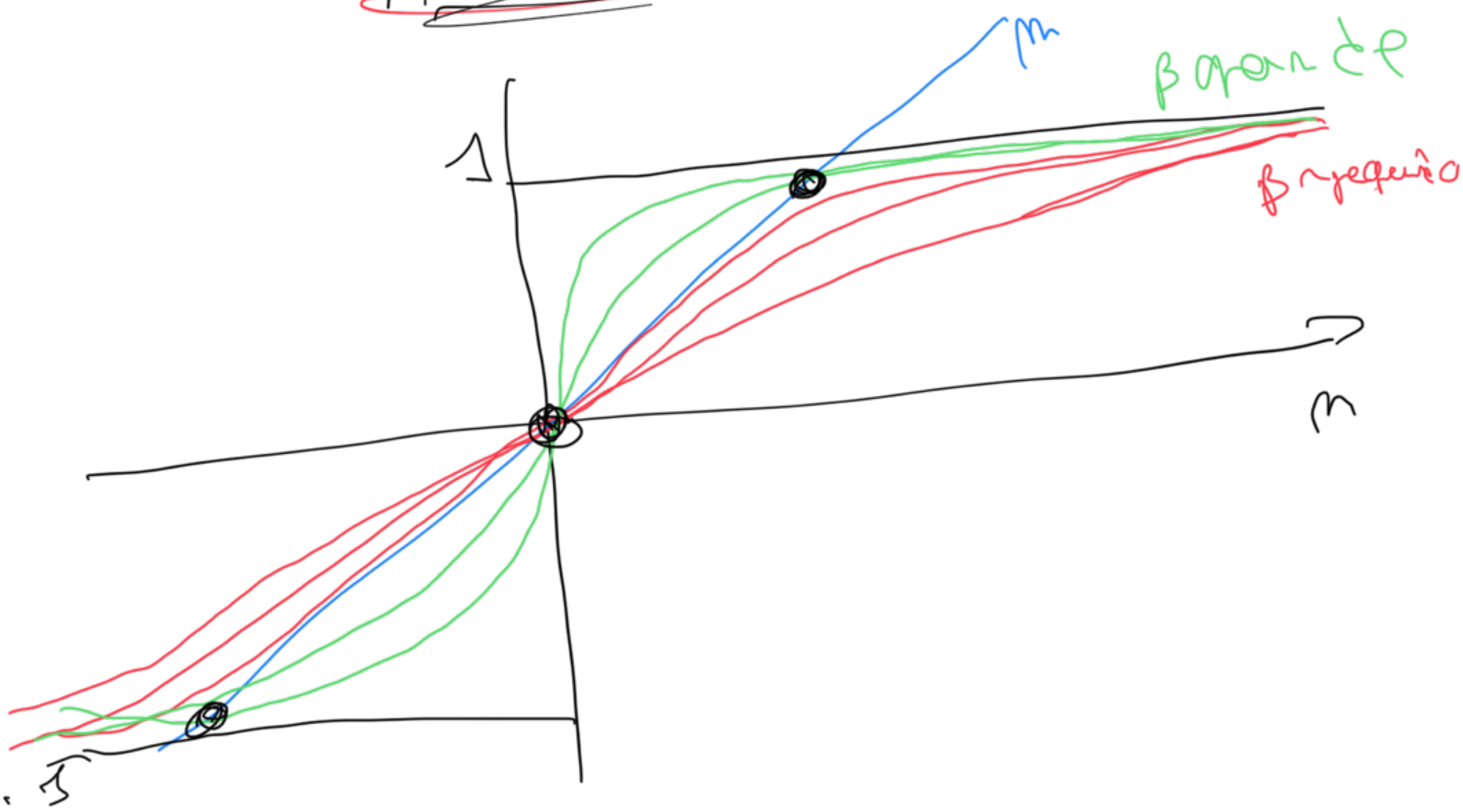
$$= tgh [\beta h_{eff}]$$

$$m \Rightarrow \underline{m = tgh [\beta (J z m + h)]}$$

ecuación de auto-consistencia de la aproximación de C.M.

$$\boxed{h = 0}$$

$$\boxed{m = tgh [\beta J z m]}$$



si β pequeño: el único cruce

m = 0 ⇒ Parag

es para $m=0$ ...

Si β grande

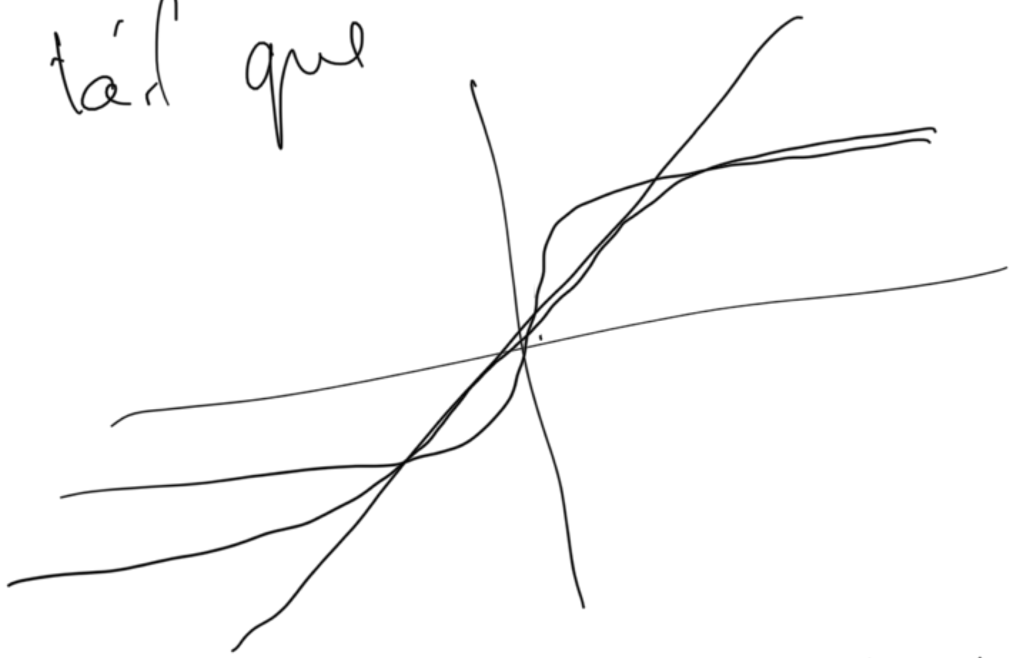
$\rightarrow$ 3 cruces $m=0\,,\ \pm m_0$

$$\frac{F}{N} = \frac{Jzm^2}{2} - k_BT\ln 2 - k_BT\ln\left[1+\frac{(\beta zJm)^2}{2}\right]$$

$$\simeq cte + \frac{Jz}{2}\left(1-\frac{zJ}{k_BT}\right)m^2 + \mathcal{O}(m^4)$$

$\rightarrow$ β crítico $\rightarrow$ T crítica T_c

es tal que



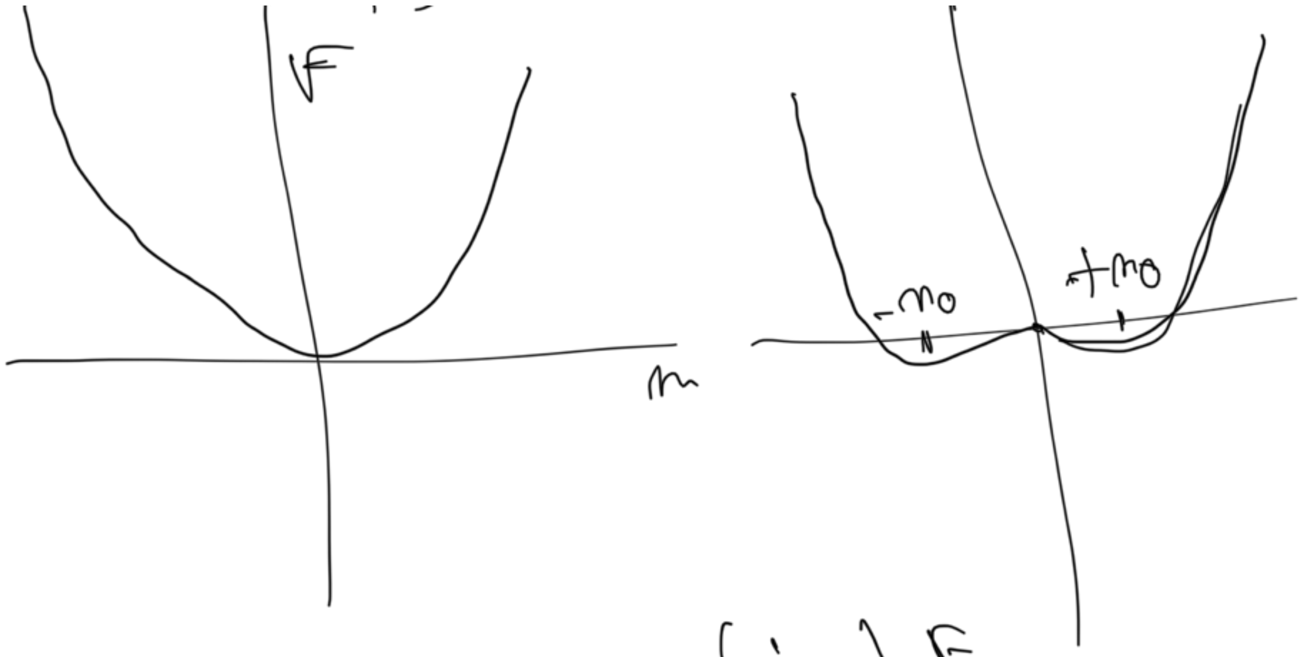
$\operatorname{tgh}[\beta zJm]$ tiene pendiente 1

si $m\rightarrow 0$

$\operatorname{tgh}(\beta_c zJm) \simeq \beta_c zJm \sim m$

$\Rightarrow \beta_c = \dfrac{1}{zJ} \Rightarrow \boxed{T_c = \dfrac{zJ}{k_B}}$

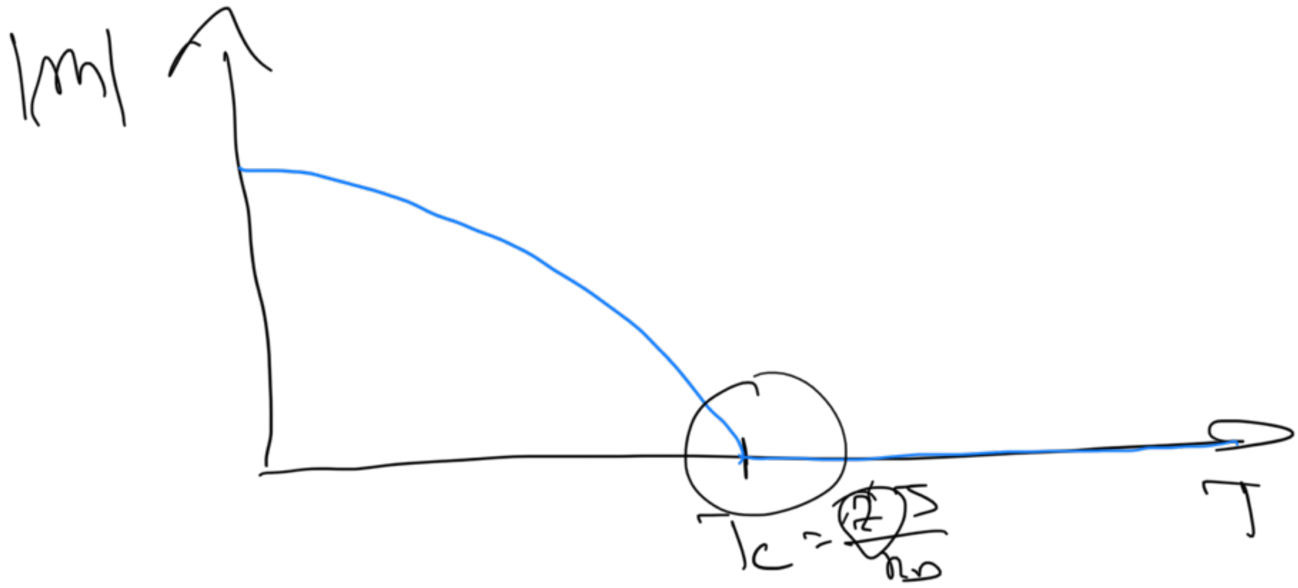
$T>T_c$ $\qquad$ $T<T_c$



mínimo de F

$m = \pm m_0$

→ Transição Ferro $T_c = \dfrac{zJ}{k_B}$



$$m = \operatorname{tgh}\left[\frac{Jzm}{k_B T}\right] \qquad m \text{ pequeno}$$

$$\cancel{m} \simeq \frac{Jz\cancel{m}}{k_B T} - \frac{1}{3}\left(\frac{Jz}{k_B T}\right)^3 m^{\cancel{3}\,2} + \dots$$

$$\Rightarrow 1 = \frac{Jz}{k_B T} - \frac{1}{3}\left(\frac{Jz}{k_B T}\right)^3 m^2 + \dots$$

$$\Rightarrow \frac{Jz}{k_B T_c} = \frac{Jz}{k_B T} - \frac{1}{3}\left(\frac{Jz}{k_B T}\right)^3 m^2$$

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

$$\Rightarrow \frac{m^2}{3} = \left(\frac{k_B T}{3z}\right)^3 \left(\frac{3z}{k_B}\right)\left(\frac{T_c - T}{T_c T}\right)$$

$$\Rightarrow m \simeq \text{cte} \sqrt{T_c - T} \sim |t|^\beta$$

$$\boxed{\beta = \frac{1}{2}}$$

1-D

$$z = 2$$