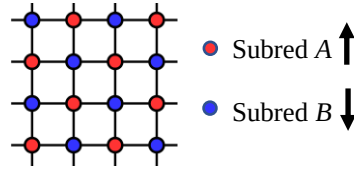


Magnetismo: Antiferromagnetismo; Dominios

Antiferromagneto: Interacción a primeros vecinos

$$\mathcal{H} = -\frac{J_{int}}{2} \sum_{\langle i,j \rangle} \bar{S}_i \cdot \bar{S}_j + g_L \mu_B \bar{H} \cdot \sum_i \bar{S}_i, \quad J_{int} < 0$$



Campo medio

Para el sitio i,A : $\mathcal{H}_{i,A} = \bar{S}_{i,A} \cdot [-J_{int} z \langle \bar{S}_{j,B} \rangle + g_L \mu_B \bar{H}] = \bar{S}_{i,A} \cdot g_L \mu_B \bar{H}_{ef,B}$; $\bar{H}_{ef,B} = \bar{H} - \frac{J_{int}}{g_L \mu_B} z \langle \bar{S}_{j,B} \rangle$

Nº de coordinación

Para el sitio i,B : $\mathcal{H}_{i,B} = \bar{S}_{i,B} \cdot [-J_{int} z \langle \bar{S}_{j,A} \rangle + g_L \mu_B \bar{H}] = \bar{S}_{i,B} \cdot g_L \mu_B \bar{H}_{ef,A}$; $\bar{H}_{ef,A} = \bar{H} - \frac{J_{int}}{g_L \mu_B} z \langle \bar{S}_{j,A} \rangle$

$$\bar{H} = H \hat{z} \rightarrow m_{A,B} = \frac{g_L \mu_B}{2} \left[(2S+1) \coth \left(\frac{\beta g_L \mu_B H_{ef,B,A} (2S+1)}{2} \right) - \coth \left(\frac{\beta g_L \mu_B H_{ef,B,A}}{2} \right) \right]$$

$$\xrightarrow{g_L \mu_B H_{ef} \ll k_B T} m_{A,B} = \frac{(g_L \mu_B)^2}{3k_B T} S(S+1) H_{ef,B,A} = \frac{(g_L \mu_B)^2}{3k_B T} S(S+1) \left(H + \frac{z J_{int}}{(g_L \mu_B)^2} m_{B,A} \right)$$

$$\rightarrow m_A = m_B = m \rightarrow m \left(1 - \frac{z J_{int}}{3k_B T} S(S+1) \right) = \frac{(g_L \mu_B)^2}{3k_B T} S(S+1) H$$

$$\rightarrow m = \frac{(g_L \mu_B)^2}{3k_B T - z J_{int} S(S+1)} S(S+1) H$$

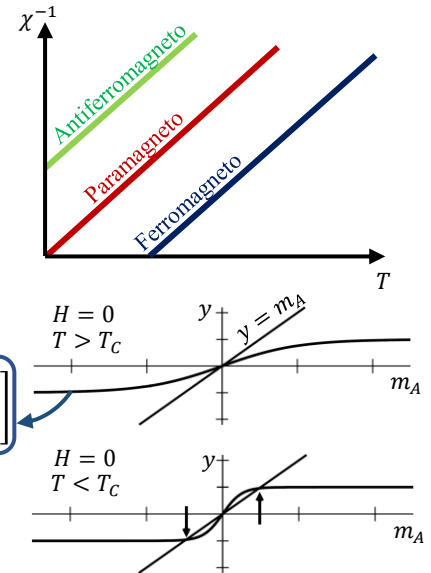
$$\rightarrow \chi = \frac{N}{V} \frac{(g_L \mu_B)^2}{3k_B (T + T_C)} S(S+1), \quad \text{con } T_C = -\frac{z J_{int} S(S+1)}{3k_B}$$

Por otro lado, analizando a campo nulo:

$$m_{A,B} = \frac{g_L \mu_B}{2} \left[(2S+1) \coth \left(\frac{\beta (2S+1) z J_{int}}{2 g_L \mu_B} m_{B,A} \right) - \coth \left(\frac{\beta z J_{int}}{2 g_L \mu_B} m_{B,A} \right) \right]$$

$$\rightarrow m_A = -m_B \quad (\coth \text{ es una función impar y } J_{int} < 0)$$

→ Magnetización espontánea (para cada subred) cuando $T < T_C$



Anisotropía magnetocristalina

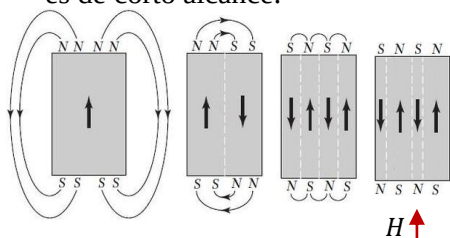
Debido al entorno anisotrópico de los átomos en una red cristalina, existen direcciones preferenciales para la orientación de los espines incluso en ausencia de campo magnético.

Una posibilidad sería: $\mathcal{H} = -\frac{J_{int}}{2} \sum_{\langle i,j \rangle} \bar{S}_i \cdot \bar{S}_j - \kappa \sum_i (S_i^z)^2$ (Puede pensarse en un cristal tetragonal elongado en la dirección $\hat{z}$)

Dominios magnéticos (ferromagneto)

Si bien la interacción dipolar magnética es despreciable frente a la interacción de intercambio, se torna apreciable cuando se tienen suficientes átomos, como ocurre en un material macroscópico ($\sim 10^{23}$ átomos).

Esto sucede porque la interacción dipolar magnética es de largo alcance, mientras que la de intercambio es de corto alcance.



Energía magnetostática: $\frac{1}{8\pi} \int H^2 dV$

Formar dominios magnéticos disminuye la energía total del sistema.

La región entre dominios recibe el nombre de "pared de dominio".

Aplicar un campo magnético externo desplaza paredes de dominio.

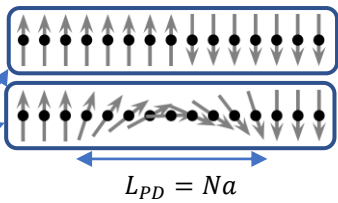
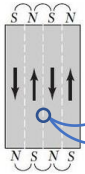


https://en.wikipedia.org/wiki/Magnetic_domain

0.1 mm

Magnetismo: Dominios e histéresis

Pared de dominio



$$E_{int} = -J_{int} \bar{S}_i \cdot \bar{S}_j = -J_{int} S^2 \cos(\theta_i - \theta_j) \approx -J_{int} S^2 \left(1 - \frac{(\delta\theta)^2}{2}\right)$$

$$\Delta E_{int} = J_{int} S^2 (\delta\theta)^2 / 2 = J_{int} S^2 (\pi/N)^2 / 2$$

$$E_{int}^{PD} = N J_{int} S^2 (\pi/N)^2 / 2 = J_{int} S^2 \pi^2 / 2N$$

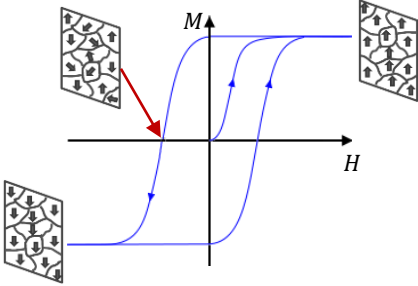
$$E_{ani} = -\kappa (S_i^z)^2 = -\kappa [S \cos \theta_i]^2 \rightarrow \Delta E_{ani} = \kappa S^2 (1 - \cos^2 \theta_i) \rightarrow E_{ani}^{PD} = \sum_i \kappa S^2 \sin^2 \theta_i$$

$$\rightarrow E_{ani}^{PD} = \kappa S^2 \int_0^\pi \sin^2 \theta d\theta \left(\frac{N}{\pi}\right) = \frac{N}{\pi} \kappa S^2 \int_0^\pi \frac{1 - \cos(2\theta)}{2} d\theta = \frac{N}{\pi} \kappa S^2 \left(\frac{\theta}{2} - \frac{\sin(2\theta)}{4}\right) \Big|_0^\pi = \frac{N \kappa S^2}{2}$$

$$\rightarrow E_{Total}^{PD} = \frac{J_{int} S^2 \pi^2}{2N} + \frac{N \kappa S^2}{2} \rightarrow \frac{\partial E_{Total}^{PD}}{\partial N} = 0 = -\frac{J_{int} S^2 \pi^2}{2N^2} + \frac{\kappa S^2}{2} \rightarrow \frac{J_{int} \pi^2}{N^2} = \kappa$$

$$\rightarrow N = \pi \sqrt{J_{int}/\kappa} \rightarrow E_{Total,min}^{PD} = \pi S^2 \sqrt{J_{int} \kappa} \quad (\text{Notar que si un cristal es extremadamente pequeño, puede resultar conveniente formar un monodominio})$$

Histéresis en ferromagnetos



Para un grano cristalino: $\frac{\Delta E}{V} = g_L \mu_B \rho \bar{S} \cdot \bar{H} - \kappa \rho S_{eje-grano}^2 + \text{cte}$

Densidad de espines
Componente a lo largo de eje-grano

$$\rightarrow \frac{\Delta E}{V} = -\bar{M} \cdot \bar{H} - \kappa \frac{M_{eje-grano}^2}{(g_L \mu_B)^2 \rho} = -\bar{M} \cdot \bar{H} - \kappa' M_{eje-grano}^2$$

$$\bar{H} = H \hat{z} \rightarrow \frac{\Delta E}{V} = -|M||H| \cos \theta - \kappa' |M|^2 \cos^2(\theta - \phi) \quad \phi = 0 \quad \hat{z} \text{ Eje grano}$$

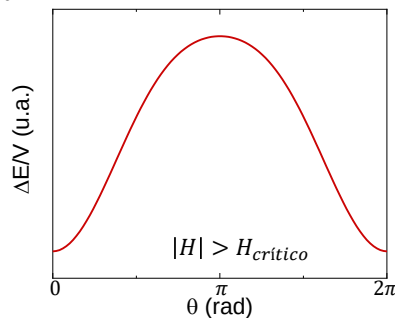
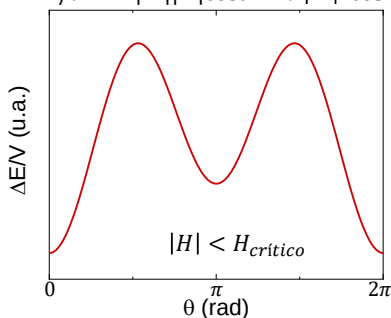
ΔE es mínimo cuando $\bar{M}$ y $\bar{H}$ son paralelos, y puede existir un mínimo relativo cuando son antiparalelos.

$$\frac{\partial(\Delta E)}{\partial \theta} = 0 \rightarrow -|M||H| \sin \theta - 2\kappa' |M|^2 \cos \theta \sin \theta = 0 \rightarrow \theta = 0, \pi, \arccos\left(-\frac{|H|}{2\kappa'|M|}\right)$$

$H_{crítico} = 2\kappa'|M|$ $\rightarrow$ Si $|H| < H_{crítico}$ existe un mínimo relativo, además del mínimo absoluto

Si $\bar{M}$ apunta en la dirección $-\hat{z}$ y se aplica un campo en la dirección $\hat{z}$ $\rightarrow$ Debe ser suficientemente grande ($> H_{crítico}$) para rotar a los espines.

$$\Delta E/V = -|M||H| \cos \theta - \kappa' |M|^2 \cos^2 \theta$$



Magnetismo: Ferromagnetismo itinerante

Magnetismo itinerante: Orden magnético a campo nulo

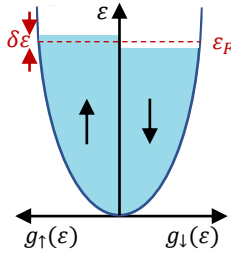
$$\mathcal{H} = \mathcal{H}_{\text{Tight-Binding}} + \mathcal{H}_{\text{Hubbard}} \quad \mathcal{H}_{\text{Hubbard}} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

i : Corre sobre sitios de la red

U : Costo energético por tener $2e^-$ en el mismo sitio

$n_{i\uparrow}(n_{i\downarrow})$: N° de e^- con espín $\uparrow(\downarrow)$ en el sitio i

¿Conviene tener $\rho_{\uparrow} \neq \rho_{\downarrow}$?



$$\begin{cases} \epsilon_{F,\uparrow} = \epsilon_F + \delta\epsilon/2 \\ \epsilon_{F,\downarrow} = \epsilon_F - \delta\epsilon/2 \end{cases} \rightarrow \rho_{\uparrow} - \rho_{\downarrow} = \int_0^{\epsilon_F + \frac{\delta\epsilon}{2}} \frac{g(\epsilon)}{2} d\epsilon - \int_0^{\epsilon_F - \frac{\delta\epsilon}{2}} \frac{g(\epsilon)}{2} d\epsilon \approx \delta\epsilon \frac{g(\epsilon_F)}{2}$$

N° medio de e^- por sitio: $x = (\rho_{\uparrow} - \rho_{\downarrow})v$

$$\text{Aproximo: } U n_{i\uparrow} n_{i\downarrow} = \frac{U}{4} (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{4} (n_{i\uparrow} - n_{i\downarrow})^2 \approx \frac{U}{4} \langle n_{i\uparrow} + n_{i\downarrow} \rangle^2 - \frac{U}{4} \langle n_{i\uparrow} - n_{i\downarrow} \rangle^2$$

$$\text{Magnetización: } M = -\frac{\mathcal{H}}{2} \mu_B (\rho_{\uparrow} - \rho_{\downarrow}) = -\frac{\mathcal{H} \mu_B \delta\epsilon}{4} g(\epsilon_F) \rightarrow \frac{E_{\text{Hubbard}}}{V} = \frac{U}{4} \frac{x^2}{v} - \frac{U}{v} \left(\frac{Mv}{\mathcal{H} \mu_B} \right)^2$$

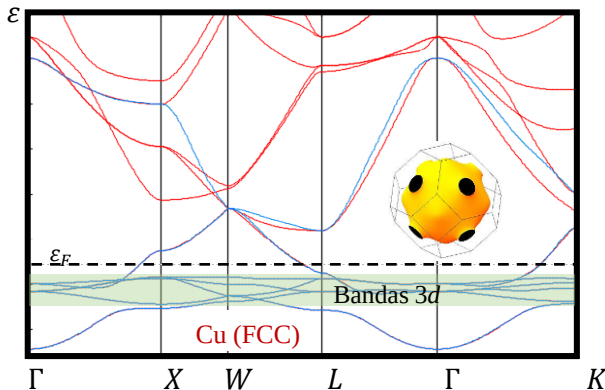
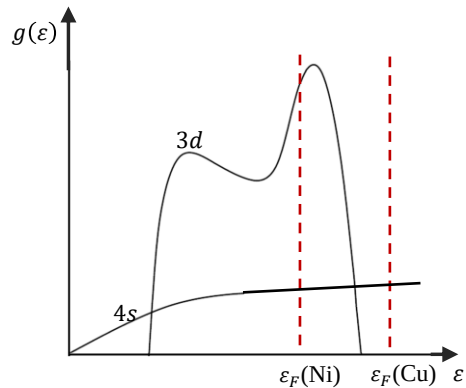
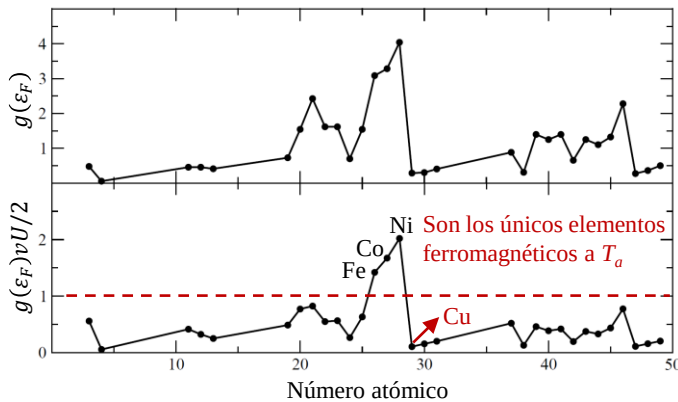
$$\text{E cinética: } \frac{K}{V} = \int_0^{\epsilon_F + \frac{\delta\epsilon}{2}} \epsilon \frac{g(\epsilon)}{2} d\epsilon + \int_0^{\epsilon_F - \frac{\delta\epsilon}{2}} \epsilon \frac{g(\epsilon)}{2} d\epsilon = 2 \int_0^{\epsilon_F} \epsilon \frac{g(\epsilon)}{2} d\epsilon + \int_{\epsilon_F}^{\epsilon_F + \frac{\delta\epsilon}{2}} \epsilon \frac{g(\epsilon)}{2} d\epsilon - \int_{\epsilon_F - \frac{\delta\epsilon}{2}}^{\epsilon_F} \epsilon \frac{g(\epsilon)}{2} d\epsilon$$

$$\approx \frac{K_0}{V} + \frac{g(\epsilon_F)}{2} \left\{ \left[\frac{(\epsilon_F + \delta\epsilon/2)^2}{2} - \frac{\epsilon_F^2}{2} \right] - \left[\frac{\epsilon_F^2}{2} - \frac{(\epsilon_F - \delta\epsilon/2)^2}{2} \right] \right\} = \frac{K_0}{V} + \frac{g(\epsilon_F)}{2} \left(\frac{\delta\epsilon}{2} \right)^2 = \frac{K_0}{V} + \frac{g(\epsilon_F)}{2} \left(\frac{2M}{\mathcal{H} \mu_B g(\epsilon_F)} \right)^2$$

Magnetismo itinerante: Orden magnético a campo nulo

$$\frac{E}{V} = \frac{K + E_{\text{Hubbard}}}{V} = \frac{K_0}{V} + \frac{E_{\text{Hubbard}}(M=0)}{V} + \frac{1}{2g(\epsilon_F)} \left(\frac{2M}{\mathcal{H} \mu_B} \right)^2 - \frac{U}{v} \left(\frac{Mv}{\mathcal{H} \mu_B} \right)^2 = \frac{E_0}{V} + \left(\frac{M}{\mathcal{H} \mu_B} \right)^2 \left[\frac{2}{g(\epsilon_F)} - vU \right]$$

$$\text{¿Cuándo conviene tener } M \neq 0? \rightarrow \frac{2}{g(\epsilon_F)} - vU < 0 \rightarrow g(\epsilon_F) > \frac{2}{vU} \rightarrow \frac{g(\epsilon_F)vU}{2} > 1 \quad (\text{Criterio de Stoner})$$



Magnetismo: Tabla periódica

Magnetismo en la tabla periódica

Considerando todas las contribuciones, se obtiene un comportamiento dominante.

(e⁻ de conducción: paramagnetismo de Pauli: $\chi_{Pauli} = \mu_B^2 g(\epsilon_F)$; diamagnetismo de Landau: $\chi_{Landau} = -\frac{1}{3} \chi_{Pauli}$)

1 1.0080 1 H [He]	2 4.002602 2 He [He]
3 6.94 3 Li [He]	4 9.012182 4 Be [He]
5 23.002891 5 Na [Ne]	6 24.304094 6 Mg [Ne]
7 39.0983 7 K [Ar]	8 39.0983 8 Ca [Ar]
9 58.932894 9 Sc [Ar]	10 58.932894 10 Ti [Ar]
11 88.905848 11 V [Ar]	12 50.9415 12 Cr [Ar]
13 54.938045 13 Mn [Ar]	14 55.845 14 Fe [Ar]
15 58.93274 15 Co [Ar]	16 58.93274 16 Ni [Ar]
17 63.546 17 Cu [Ar]	18 63.546 18 Zn [Ar]
19 65.38 19 Ga [Ar]	20 65.38 20 Ge [Ar]
21 72.63 21 As [Ar]	22 72.63 22 Se [Ar]
23 74.921595 23 Br [Ar]	24 78.96 24 Kr [Ar]
25 85.4678 25 Rb [Kr]	26 85.4678 26 Sr [Kr]
27 87.62 27 Y [Kr]	28 87.62 28 Zr [Kr]
29 88.905848 29 Nb [Kr]	30 91.224 30 Mo [Kr]
31 92.90638 31 Tc [Kr]	32 95.96 32 Ru [Kr]
33 101.07 33 Rh [Kr]	34 101.07 34 Pd [Kr]
35 106.42 35 Ag [Kr]	36 106.42 36 Cd [Kr]
37 112.411 37 In [Kr]	38 112.411 38 Sn [Kr]
39 118.710 39 Sb [Kr]	40 118.710 40 Te [Kr]
41 127.60 41 I [Kr]	42 127.60 42 Xe [Kr]
43 126.90547 43 Cs [Xe]	44 126.90547 44 Ba [Xe]
45 173.0547 45 Lu [Xe]	46 173.0547 46 Hf [Xe]
47 188.90784 47 Ta [Xe]	48 188.90784 48 W [Xe]
49 183.84 49 Re [Xe]	50 186.207 50 Os [Xe]
51 190.23 51 Ir [Xe]	52 192.225 52 Pt [Xe]
53 195.084 53 Au [Xe]	54 197.027 54 Hg [Xe]
55 200.59 55 Tl [Xe]	56 204.384 56 Pb [Xe]
57 207.2 57 Bi [Xe]	58 208.9804 58 Po [Xe]
59 209 59 At [Xe]	60 210 60 Rn [Xe]
61 223.01993 61 Fr [Rn]	62 223.01993 62 Ra [Rn]
63 227.0277 63 Ac [Rn]	64 227.0277 64 Th [Rn]
65 232.0377 65 Pa [Rn]	66 232.0377 66 U [Rn]
67 238.02891 67 Np [Rn]	68 238.02891 68 Pu [Rn]
69 244.04187 69 Am [Rn]	70 244.04187 70 Cm [Rn]
71 247.07031 71 Bk [Rn]	72 247.07031 72 Cf [Rn]
73 251.07958 73 Es [Rn]	74 251.07958 74 Fm [Rn]
75 252.08321 75 Md [Rn]	76 252.08321 76 No [Rn]