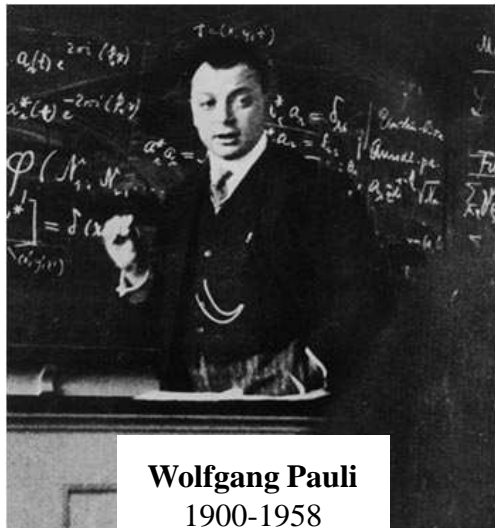


Intercambio

Orden magnético de corto alcance. Interacción de intercambio

Electrones **1 y 2** de dos átomos vecinos **i,j**.

Spin-statistics theorem



Fierz

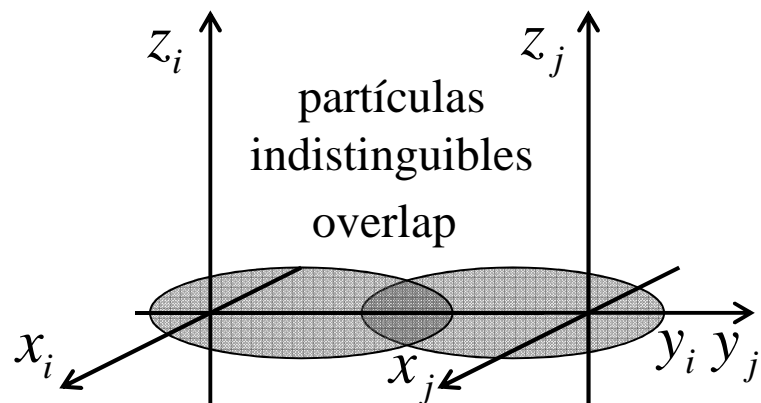
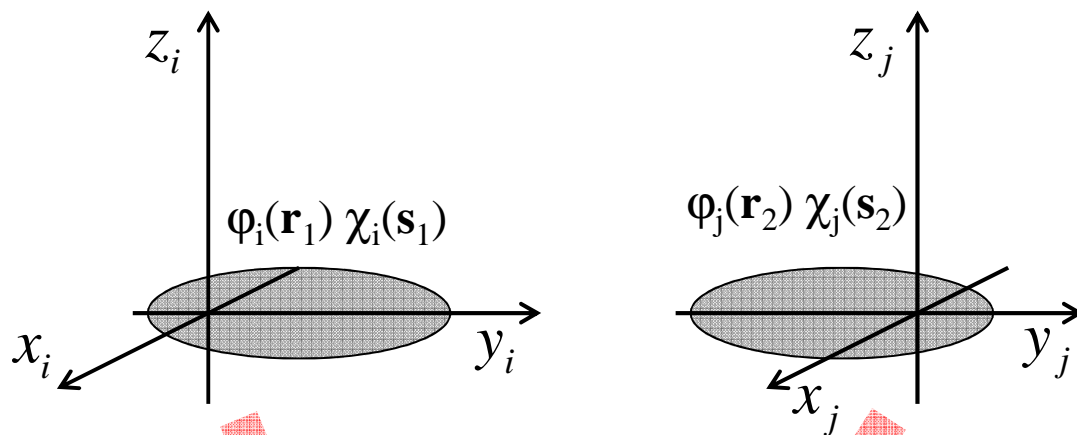
Pauli

Schwinger

Feynman

El estado de un sistema de partículas idénticas de espín entero no cambia cuando dos partículas son intercambiadas: tienen estados simétricos. Las partículas con estados simétricos se llaman **bosones**.

El estado de un sistema de partículas idénticas de espín semientero cambia de signo cuando dos partículas son intercambiadas: tienen estados antisimétricos. Las partículas con estados antisimétricos se llaman **fermiones**.



$$\Psi_{ij}(1,2) = \varphi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

Estado de dos fermiones

factor espacial	factor de espín
-----------------	-----------------

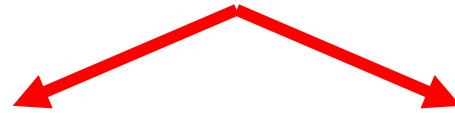
$\varphi_{ij}(\mathbf{r}_1, \mathbf{r}_2)$	$\chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$
--	---

$$\Psi_{ij}(1,2) = \varphi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

antisimétrica

electrones $\rightarrow \Psi_{ij}(1,2)$ antisimétrica

$$\Psi_{ij}(1,2) = \phi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

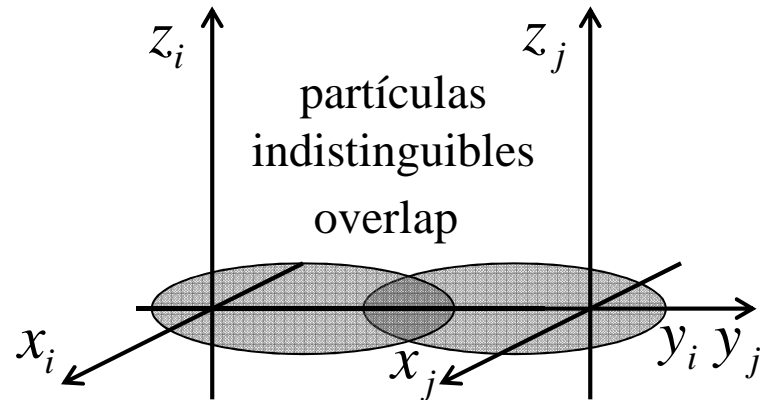


$\phi_{ij}(\mathbf{r}_1, \mathbf{r}_2)$
simétrica

$\chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$
antisimétrica

$\phi_{ij}(\mathbf{r}_1, \mathbf{r}_2)$
antisimétrica

$\chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$
simétrica



$$\Psi_{ij}(1,2) = \phi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

Factor de espín

$$\chi_{ij}^s = \frac{1}{\sqrt{2}} \{ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \}$$

$$S = 0$$

Singlete
(antisimétrico)

$$\chi_{ij}^t = \left\{ \begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}} [|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] \\ |\downarrow\downarrow\rangle \end{array} \right\}$$

$$S = 1$$

Triplete
(simétrico)

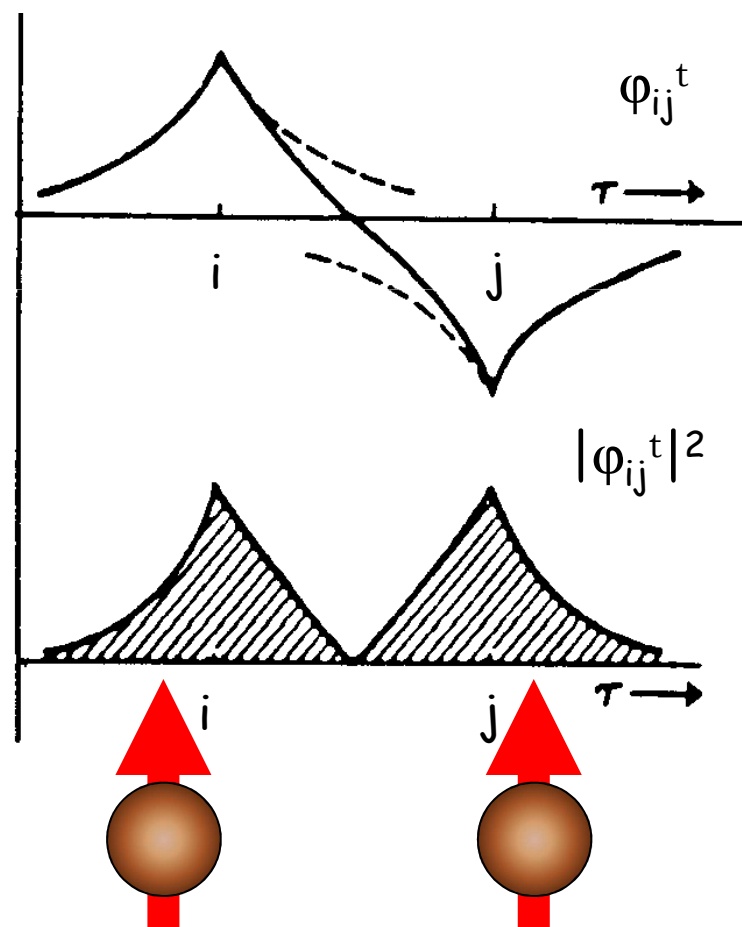
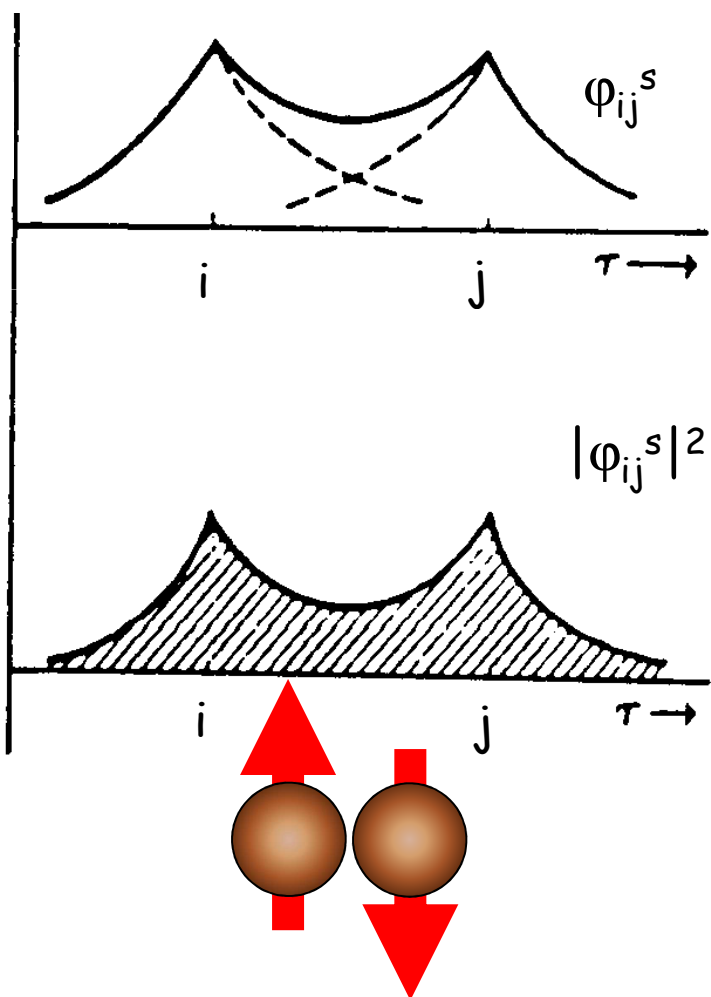
Factor espacial

$$\varphi_{ij}^s = \frac{1}{\sqrt{2}} \{ \varphi_i(\vec{r}_1) \varphi_j(\vec{r}_2) + \varphi_i(\vec{r}_2) \varphi_j(\vec{r}_1) \}$$

(simétrico)

$$\varphi_{ij}^t = \frac{1}{\sqrt{2}} \{ \varphi_i(\vec{r}_1) \varphi_j(\vec{r}_2) - \varphi_i(\vec{r}_2) \varphi_j(\vec{r}_1) \}$$

(antisimétrico)



Evaluación de la energía potencial

núcleo-núcleo
núcleo-electrón
núcleo-electrón
núcleo-electrón
núcleo-electrón
electrón-electrón

$$U = \alpha \left(\frac{1}{r_{ij}} - \frac{1}{r_{i1}} - \frac{1}{r_{i2}} - \frac{1}{r_{j1}} - \frac{1}{r_{j2}} + \frac{1}{r_{12}} \right)$$

Valor esperado de U

$$E_S = \langle U \rangle_S = \langle \varphi_{ij} | U | \varphi_{ij} \rangle = \int_{\text{todo el espacio}} \varphi_{ij}^*(\vec{r}_1, \vec{r}_2) U \varphi_{ij}(\vec{r}_1, \vec{r}_2) dV_1 dV_2$$

en el estado singlete:

(llamamos $\varphi_i(\vec{r}_1) = \varphi_{i1}$)

$$E_s = \langle U \rangle_s = \int \varphi_{ij}^{s*}(\vec{r}_1, \vec{r}_2) U \varphi_{ij}^s(\vec{r}_1, \vec{r}_2) dV_1 dV_2$$

todo el espacio

$$E_s = K_{ij} + J_{ij}$$

$$K_{ij} = \int \varphi_{i1}^* \varphi_{j2}^* U \varphi_{i1} \varphi_{j2} dV_1 dV_2$$

Término directo

$$J_{ij} = \int \varphi_{i1}^* \varphi_{j2}^* U \varphi_{i2} \varphi_{j1} dV_1 dV_2$$

Término de intercambio

en el estado triplete:

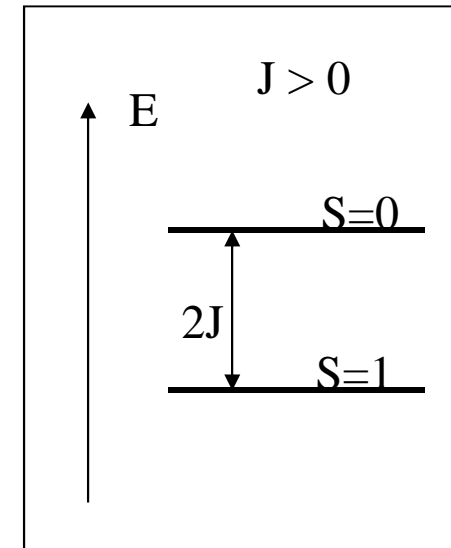
$$E_t = \langle U \rangle_t = \int \varphi_{ij}^{t*}(\vec{r}_1, \vec{r}_2) U \varphi_{ij}^t(\vec{r}_1, \vec{r}_2) dV_1 dV_2$$

*todo el
espacio*

$$E_s = K_{ij} - J_{ij}$$

diferencia de energía entre ambos estados:

$$E_s - E_t = E(s = 0) - E(s = 1) = 2J_{ij}$$

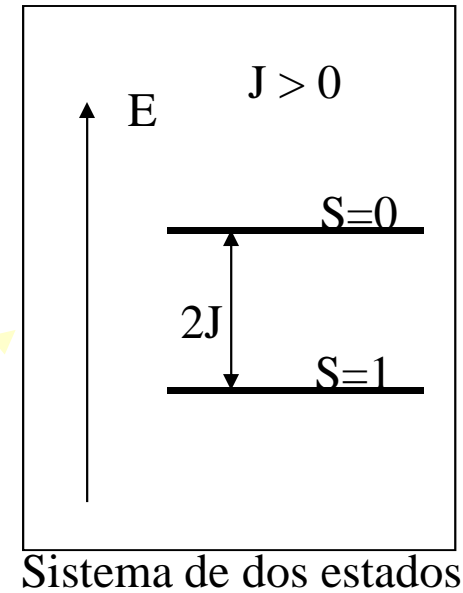


Sistema de dos estados

Operador Hamiltoniano de espín

$$\mathcal{H}_{spin} = 2J_{ij} \vec{s}_i \cdot \vec{s}_j$$

Hamiltoniano
de Heisemberg



Valor típico de J en materiales con
elementos 3d (Cr, Mn, Fe, Co Ni)

$$J_{ij} \approx 10^{-21} \text{ Joules}$$

Alcance espacial de la interacción de intercambio

$$\psi(r, \theta, \phi) = R(r)P(\theta)F(\phi)$$

Función de onda electrónica

$$R_{n,l}(r) = r^l L_{n,l} e^{-r/na_0}$$

Polinomio de Laguerre (át. H)

$$J(r) \approx e^{-\alpha r}$$

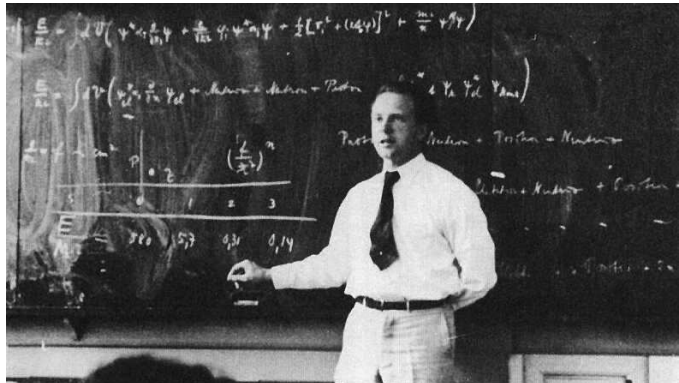
Interacción de corto alcance

Operador Hamiltoniano de espín



Paul Dirac (1902 - 1984)

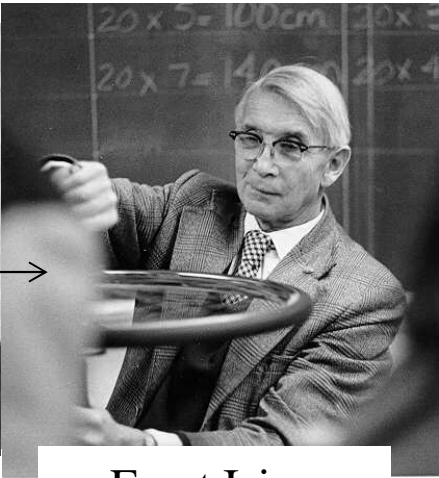
Hamiltoniano de Heisemberg

$$\mathcal{H}_H = -2J_{ij} \vec{s}_i \cdot \vec{s}_j$$


Werner Heisenberg (1901 - 1976)

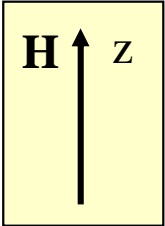


Wilhelm Lenz (1888 - 1957)



Ernst Ising (1900 - 1998)

Hamiltoniano de Ising

$$\mathcal{H}_I = -2J_{ij} s_{iz} s_{jz}$$


Empleo muy difundido en física y otras áreas del conocimiento

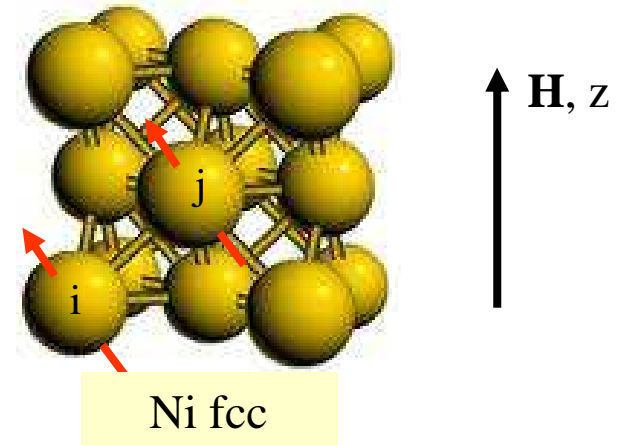
(a) Ferromagnetismo

Análisis simple del Ferromagnetismo. Teoría del campo molecular para electrones localizados en un sólido elemental.

Consideramos dos contribuciones a la energía

$$E = - \sum_{ij} J_{ij} \vec{s}_i \cdot \vec{s}_j - \sum_i \mu_0 g \mu_B \vec{s}_i \cdot \vec{H}$$

$J_{ij} > 0 \Rightarrow$ ferromagnetismo



$$E = - \sum_{ij} \overset{\text{intercambio}}{J_{ij}} \vec{s}_i \cdot \vec{s}_j - \sum_i \overset{\text{Zeeman}}{\mu_0 g \mu_B} \vec{s}_i \cdot \vec{H}$$

$$E = -\mu_0 g \mu_B \sum_i \vec{s}_i \cdot \left(\sum_j \frac{J_{ij} \vec{s}_j}{\mu_0 g \mu_B} + \vec{H} \right)$$

$$E = -\mu_0 g \mu_B \sum_i \vec{s}_i \cdot \vec{H}_{ef}$$

$$E = -\mu_0 g \mu_B \sum_i \vec{s}_i \cdot \vec{H}_{ef}$$

Campo de Weiss

$$\vec{H}_{ef} = \sum_i \frac{J_{ij} \vec{s}_j}{\mu_0 g \mu_B} + \vec{H}$$

\vec{H}_{Weiss}



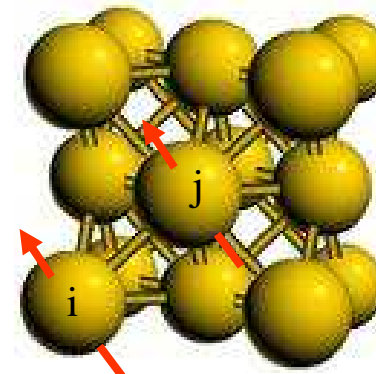
Scanned at the American
Institute of Physics

Pierre Weiss (1865-1940)

Limitando la suma a
los primeros vecinos

$$\vec{H}_{Weiss} = \sum_j \frac{J_j \vec{s}_j}{\mu_0 g \mu_B} \approx \frac{p J_j \langle s \rangle_z}{\mu_0 g \mu_B} \hat{u}_z$$

$$p = 12$$



Ni fcc

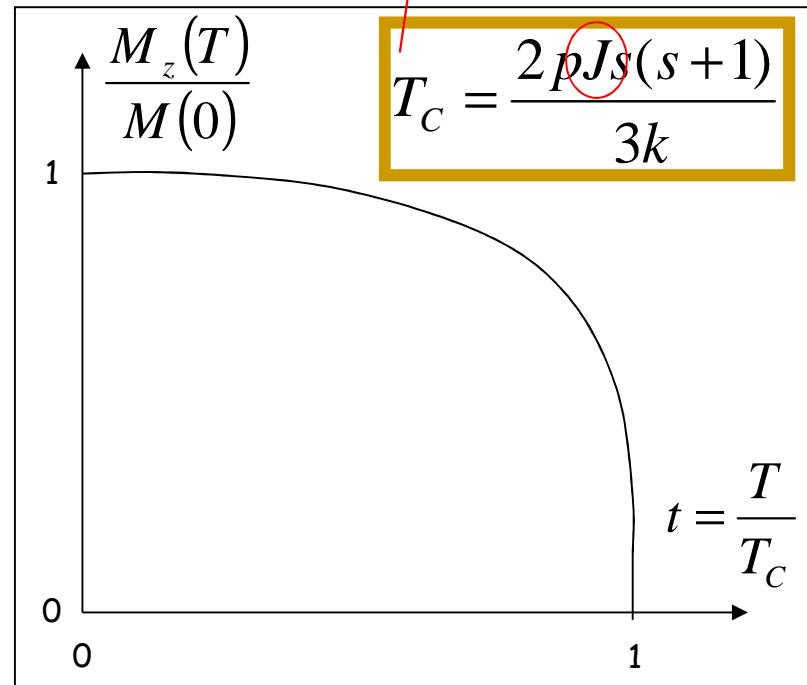
$$H_w^i = \frac{2pJ \langle s_z \rangle}{\mu_0 g \mu_B} \longleftrightarrow \begin{cases} \approx 6.4 \times 10^8 \text{ A/m} \\ \approx 800 \text{ Tesla} \end{cases}$$

Temperatura de Curie

$$H_{ef} = \sum_j \frac{J_{ij} \langle s_z \rangle}{\mu_0 g \mu_B} + H$$

$$\langle \mu_z \rangle = \mu B_J \left(\frac{\mu_0 g \mu_B s H_{ef}}{kT} \right)$$

$$\mu_0 g \mu_B \langle s_z \rangle = \mu B_J \left(\frac{\mu_0 g \mu_B s H_{ef}}{kT} \right)$$



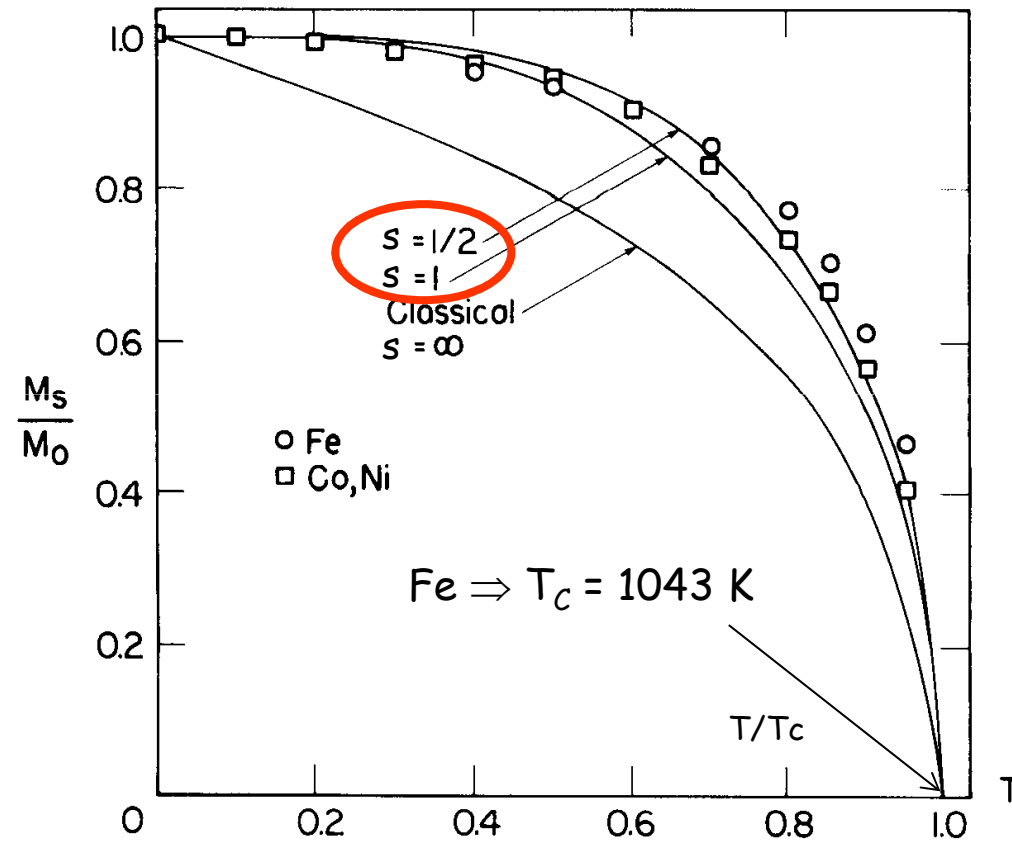
Ecuación trascendente para $\langle s_z \rangle$, $\langle \mu_z \rangle$ ó M_z

$$T_c = \frac{2pJs(s+1)}{3k}$$

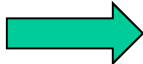
Temperaturas de Curie

Material	Curie temperature (K)
Fe	1043
Co	1388
Ni	627
Gd	293
Dy	85
CrBr ₃	37
Au ₂ MnAl	200
Cu ₂ MnAl	630
Cu ₂ MnIn	500
EuO	77
EuS	16.5
MnAs	318
MnBi	670
GdCl ₃	2.2
Fe ₂ B	1015
MnB	578

Ejemplo: estimación del spin s y la integral de intercambio J para el Fe bcc (α)



Ejemplo: estimación del spin s y la integral de intercambio J para el Fe bcc (α)

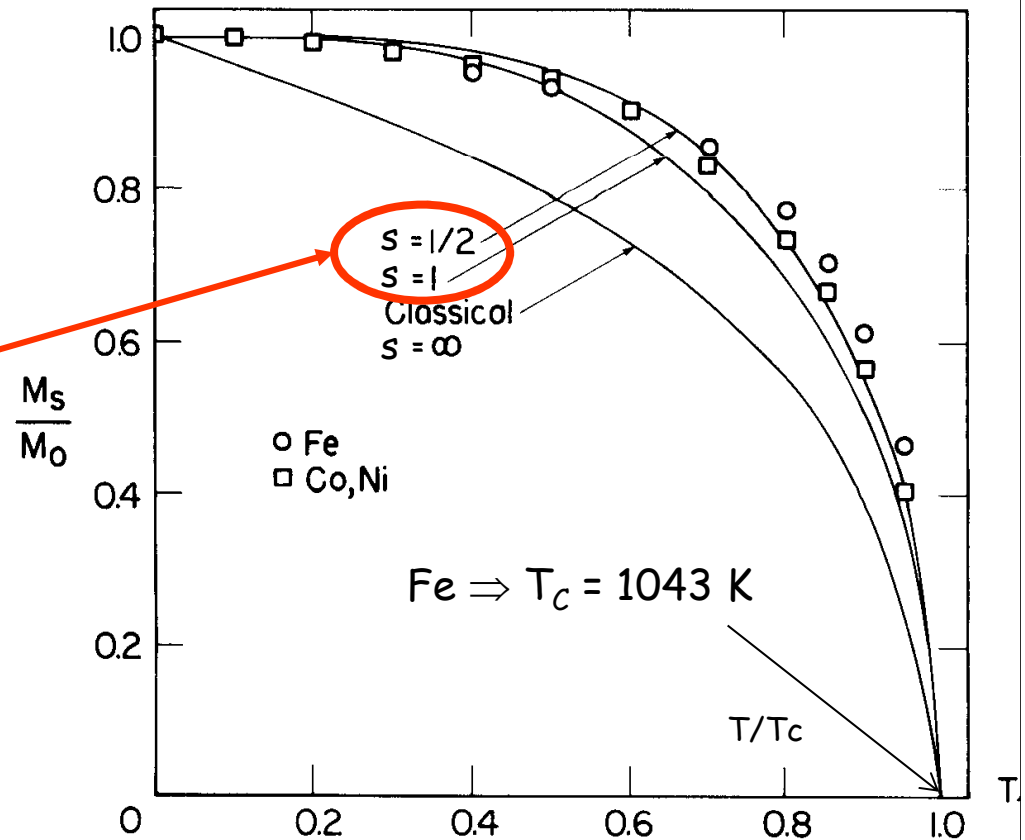


$$J = \frac{3kT_C}{2ps(s+1)}$$

(1) s_{Fe} ?

(1a) M_S vs T

$s_{Fe} \approx 0.5 - 1.0$

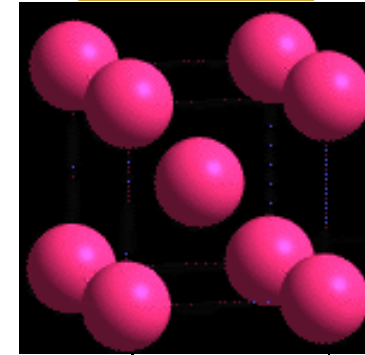


$s_{Fe}?$

(1b) valor de M_S a 0 K

$$M_S = 2.198 \text{ Tesla}$$

bcc-Fe



$$a = 2.865 \text{ \AA}$$

$$\mu_{at} = M_S \frac{V_{cel}}{2} = M_S \times \frac{a^3}{2} = \frac{2.198}{4\pi \times 10^{-7}} \left(\frac{A}{m} \right) \times \frac{(2.865)^3}{2} \times 10^{-30} m^3 = 2.065 \times 10^{-23} Am^2 = 2.23 \mu_B$$

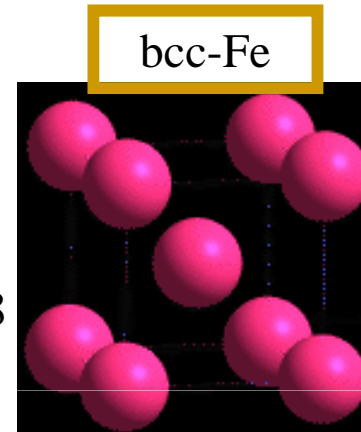
$$\mu_{at} = g s_{Fe} \mu_B = 2 s_{Fe} \mu_B$$

$$s_{Fe} \approx 1.115$$

$$J = \frac{3kT_C}{2ps(s+1)}$$

→ 1043K
→ 1.115

p = 8



$$J_{\alpha-Fe} \approx \frac{3 \times 1.38 \times 10^{-23} \text{ (Joule / K)} \times 1043 \text{ K}}{2 \times 8 \times 1.115 \times 2.115} = 1.21 \times 10^{-21} \text{ Joule}$$

$J_{\alpha-Fe} \approx 1.21 \times 10^{-21} \text{ Joule}$

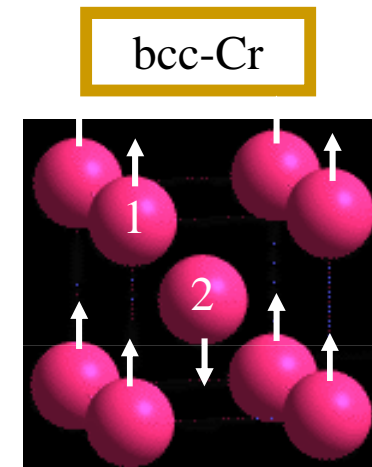
(b) Antiferromagnetismo

Análisis simple del Antiferromagnetismo. Teoría del campo molecular para electrones localizados en un sólido elemental.

$$E = - \sum_{i,j}^{N,p} J_{ij} \vec{s}_i \cdot \vec{s}_j - \sum_i^N \mu_0 g \mu_B \vec{s}_i \cdot \vec{H}$$

acoplamiento con primeros, o con primeros y segundos vecinos

Ejemplo, Red bcc: sólo dos subredes 1 y 2, p primeros vecinos (1) y p' segundos vecinos (2)

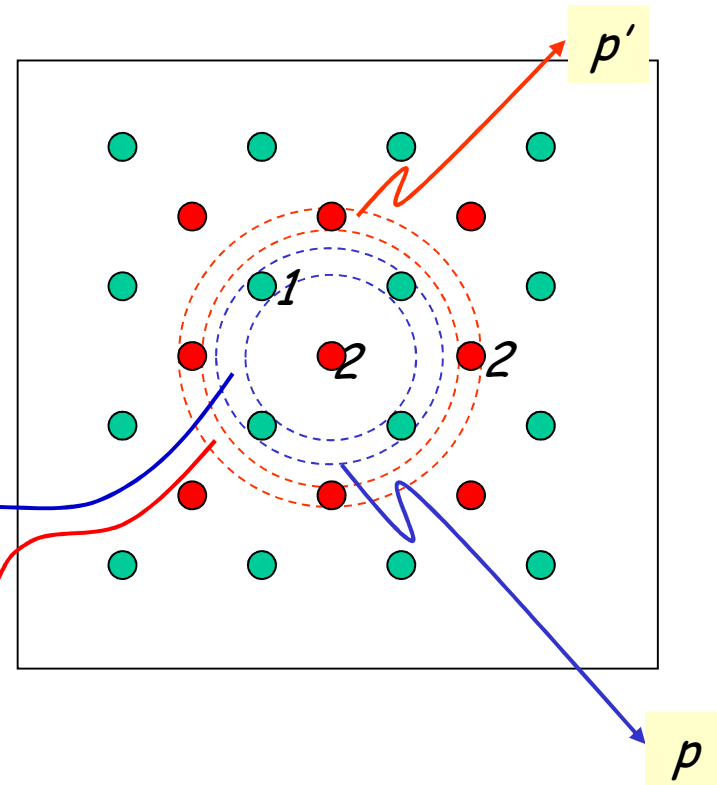


Subredes 1 y 2

Para fijar ideas nos
ubicamos en un punto de
la subred 2

(a) intercambio $J < 0$ entre
primeros vecinos

(b) J' , acoplamiento entre
segundos vecinos (de la misma
subred-2), $|J| \gg |J'|$

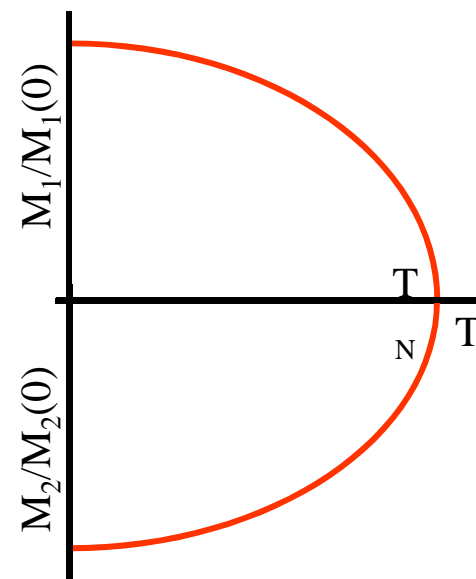
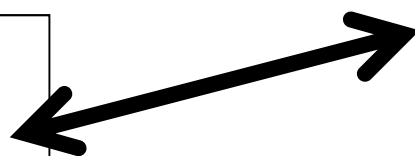
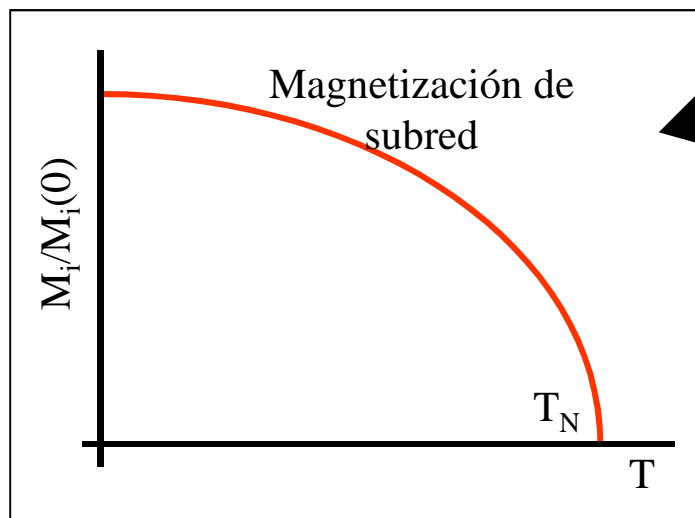


$$H_{Weiss}^{(2)} = \frac{2}{\mu_0 g \mu_B} (pJ \langle s_1 \rangle + p' J' \langle s_2 \rangle)$$

Campo de Weiss sobre
momentos de la subred 2

$$H_{Weiss}^{(1)} = \frac{2}{\mu_0 g \mu_B} (pJ \langle s_2 \rangle + p' J' \langle s_1 \rangle)$$

Campo de Weiss sobre
momentos de la subred 1



$$M_i \neq 0$$

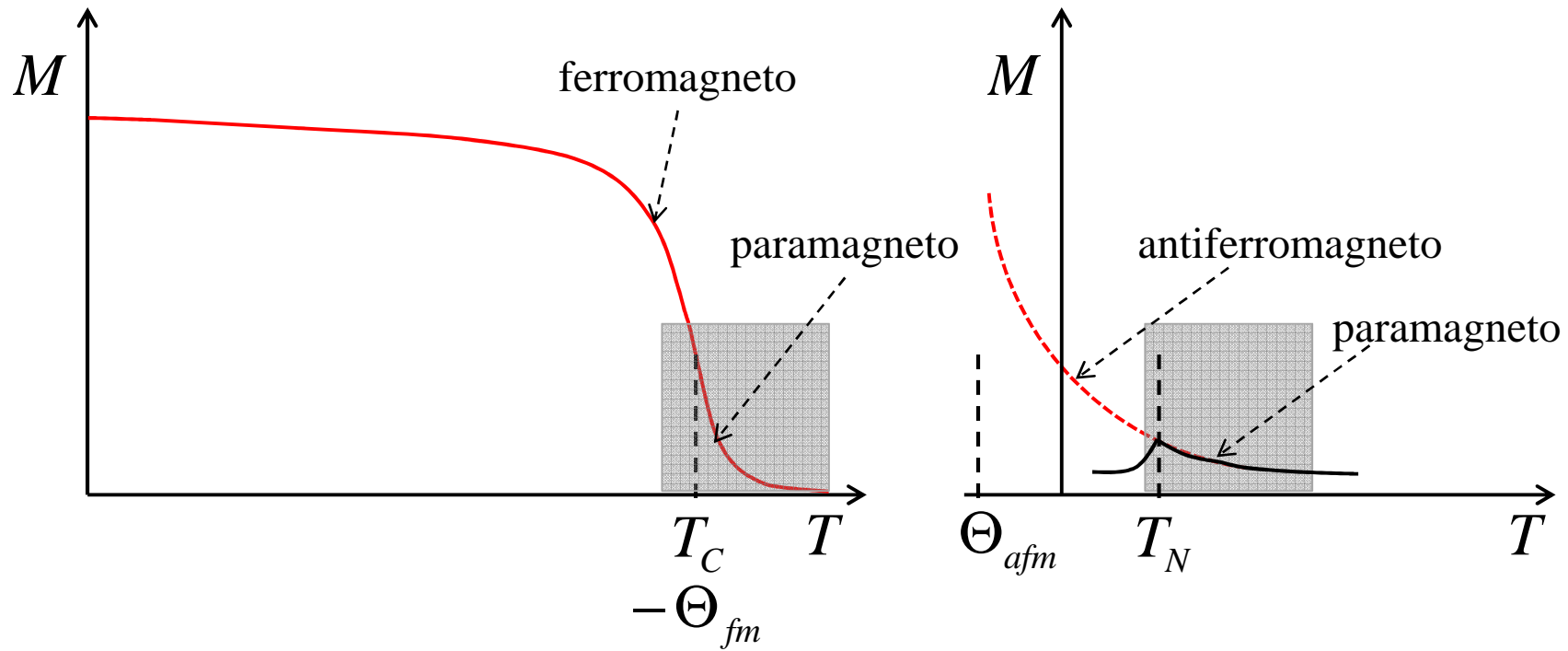
$$M_1 + M_2 = 0$$



$$\vec{M}_2 = -\vec{M}_1$$

$$T_N = \frac{2(pJ)_{ef} s(s+1)}{3k} = \frac{2(-pJ + p'J')s(s+1)}{3k}$$

$$J < 0, \quad |J| \gg |J'| \Rightarrow T_N > 0$$



Ley de Curie-Weiss

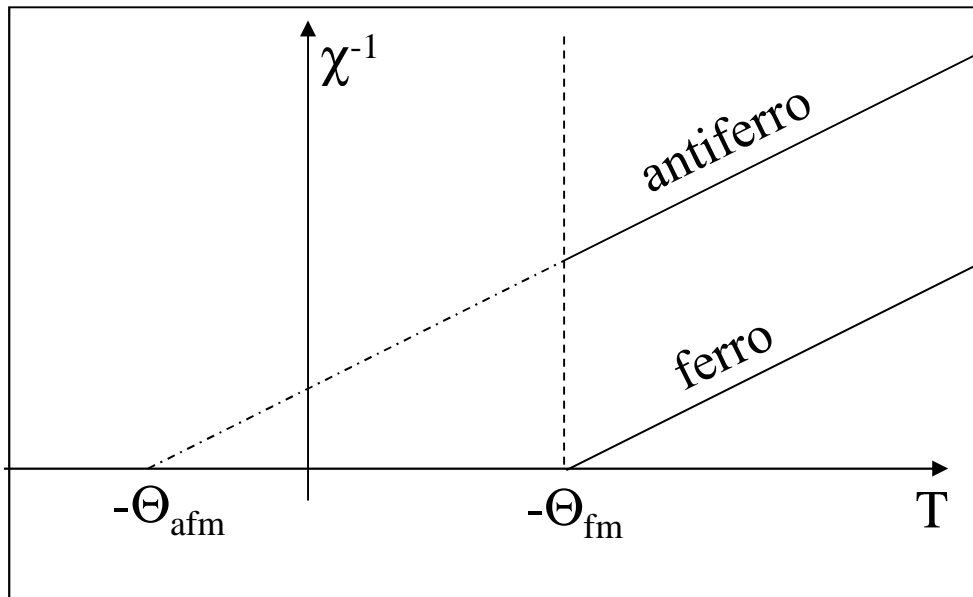
$$\chi_{inic} = \frac{C}{T + \Theta}$$

$$\Theta_{afm} = -\frac{2s(s+1)(pJ + p'J')}{3k} > 0$$

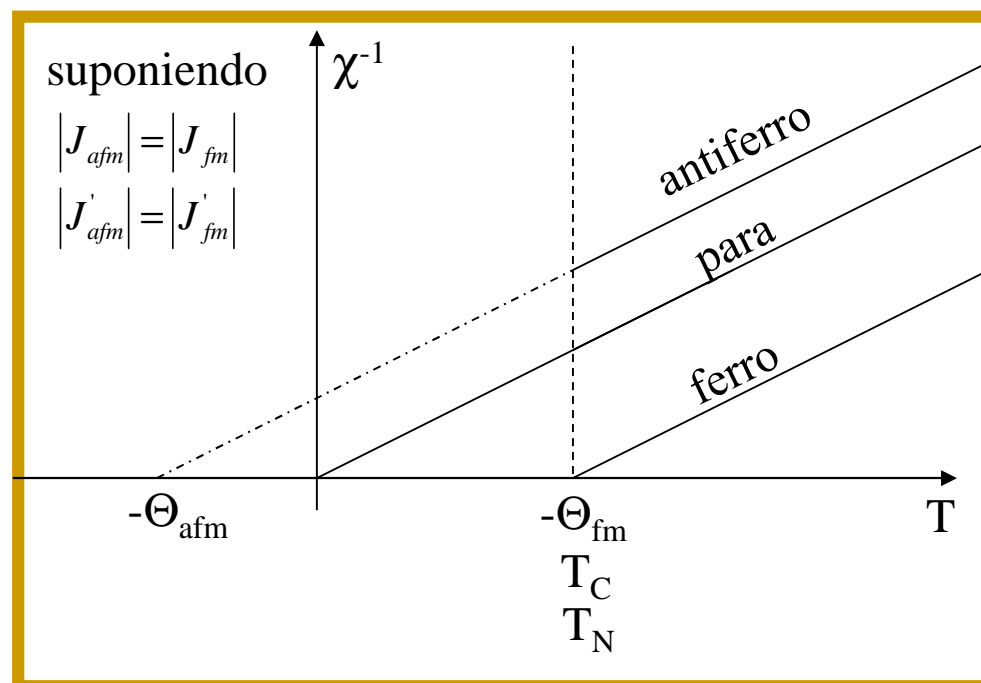
$$\Theta_{fm} = -\frac{2s(s+1)(pJ + p'J')}{3k} < 0$$

$$\chi = \frac{C}{T + \Theta}$$

$$\chi^{-1} = \frac{T + \Theta}{C}$$



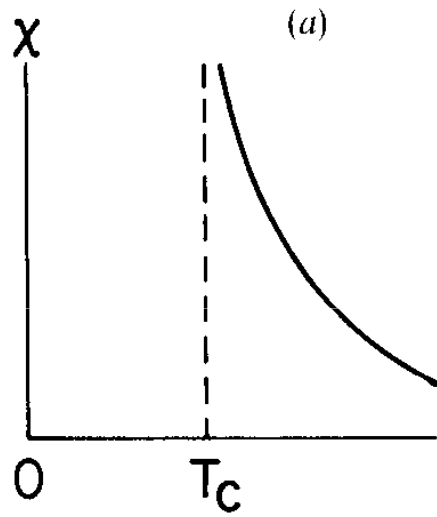
antiferro	ferro	para
$J \leq 0; J \gg J' $	$J \geq 0; J \gg J' $	$J = J' = 0$
$\Theta_{afm} = -\frac{2s(s+1)(pJ + p'J')}{3k} > 0$	$\Theta_{fm} = -\frac{2s(s+1)(pJ + p'J')}{3k} < 0$	$\Theta_{pm} = 0$
$T_N = \frac{2s(s+1)(p'J' - pJ)}{3k} > 0$	$T_C = \frac{2s(s+1)(p'J' + pJ)}{3k} > 0$	$T_{Cr}^{pm} = 0$
$T_N \neq \Theta_{afm}$	$T_C = -\Theta_{fm}$	



Ley de Curie-Weiss

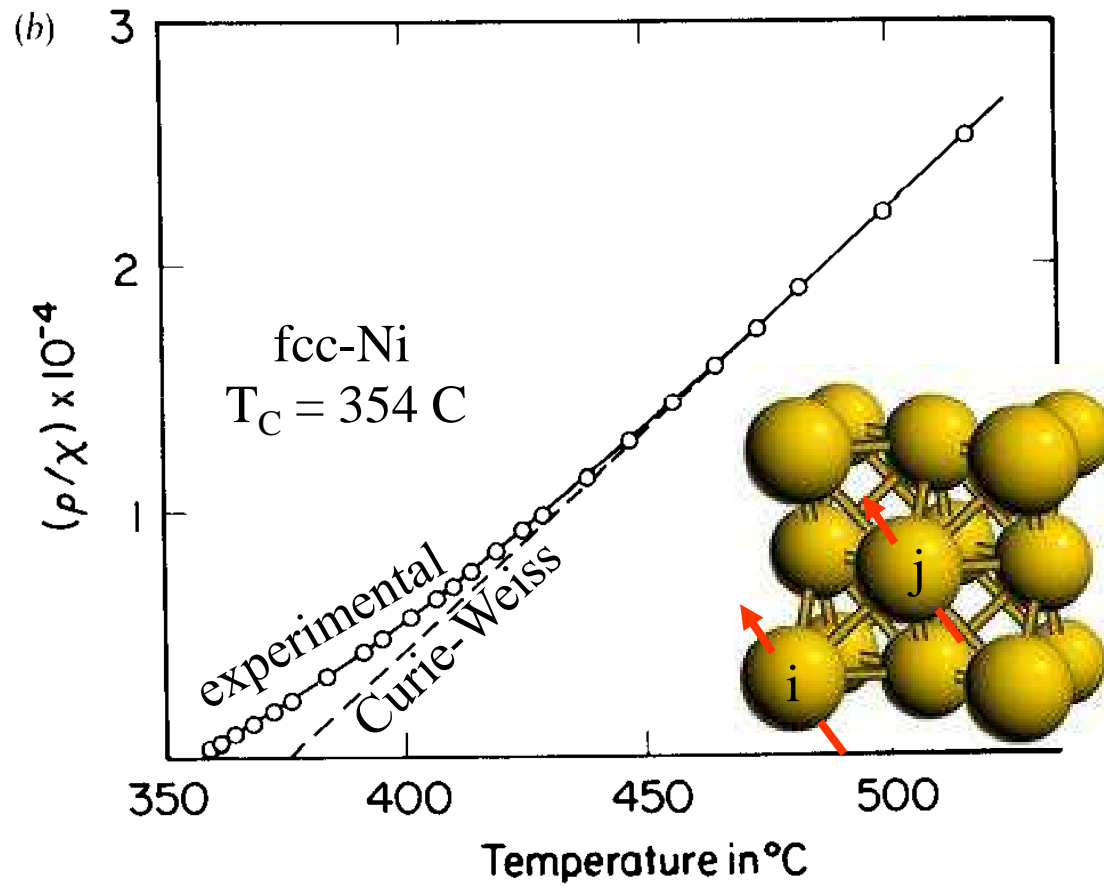
$$\chi = \frac{C}{T + \Theta}$$

ferromagneto

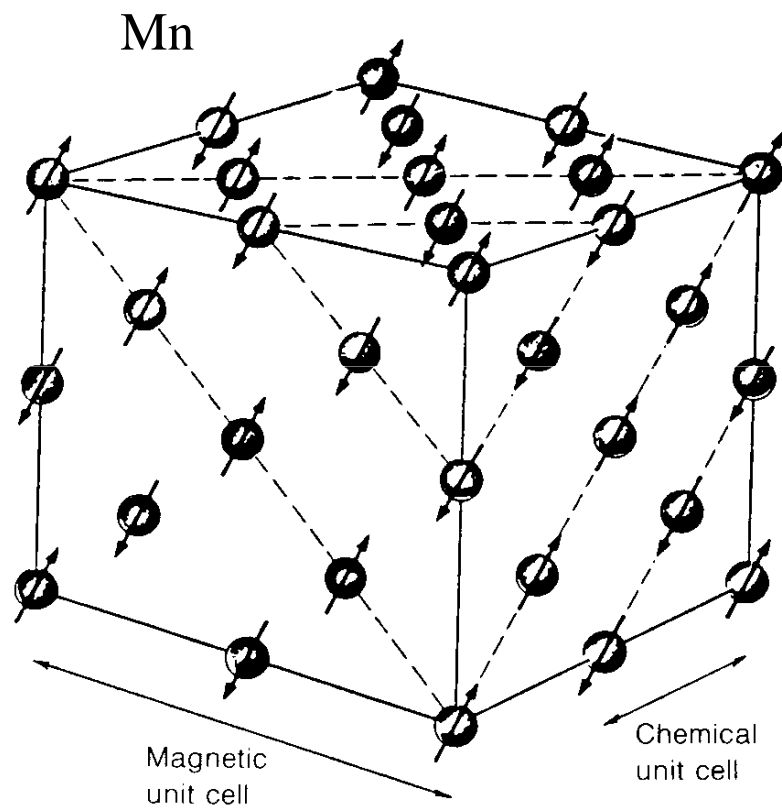
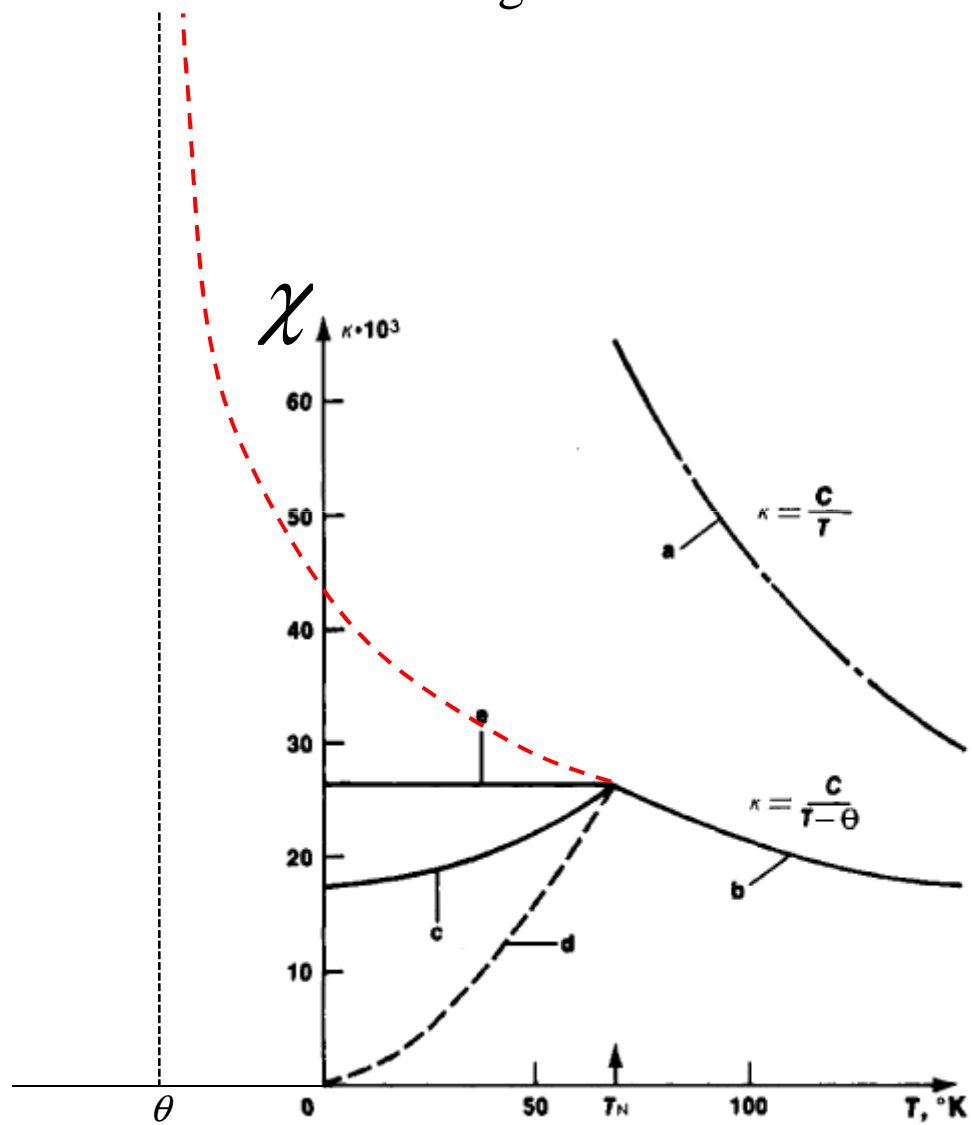


$$\chi = \frac{C}{T - T_C}$$

Curie-Weiss Law
($T > T_C$)

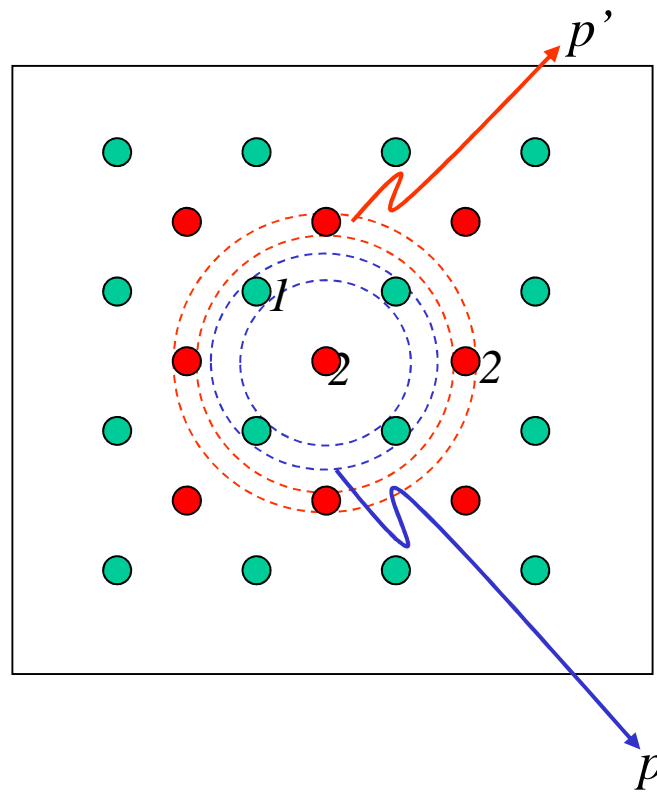


antiferromagneto



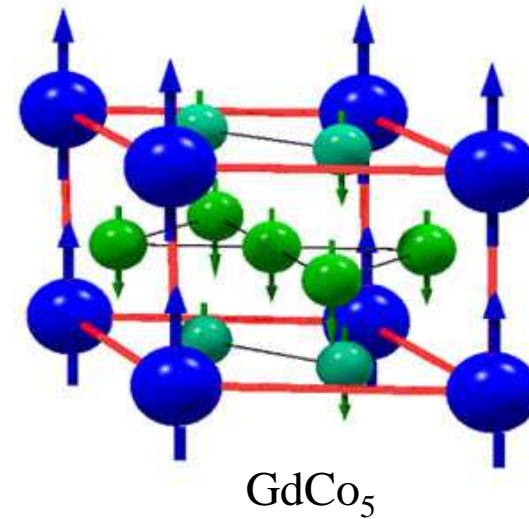
(c) Ferrimagnetismo

Ferrimagnetismo



$$s_1 \neq s_2$$

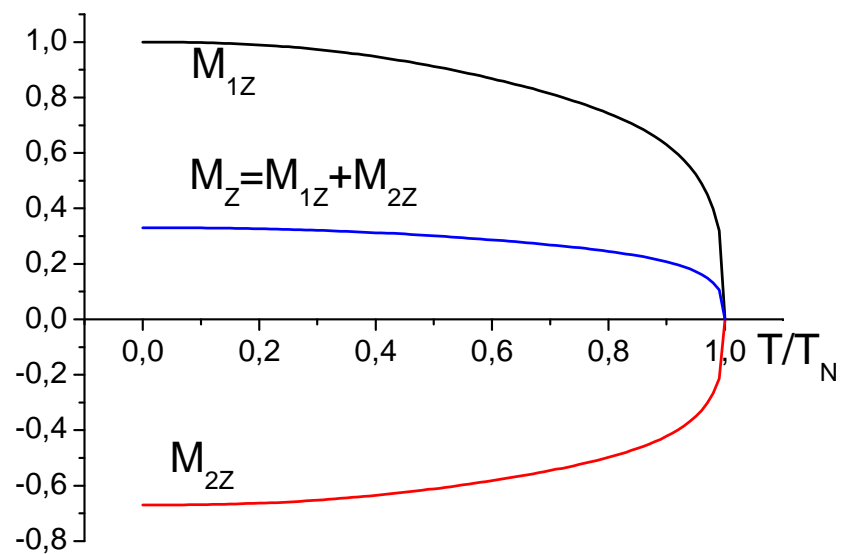
Ferrimagneto: momento opuesto y diferente en cada subred



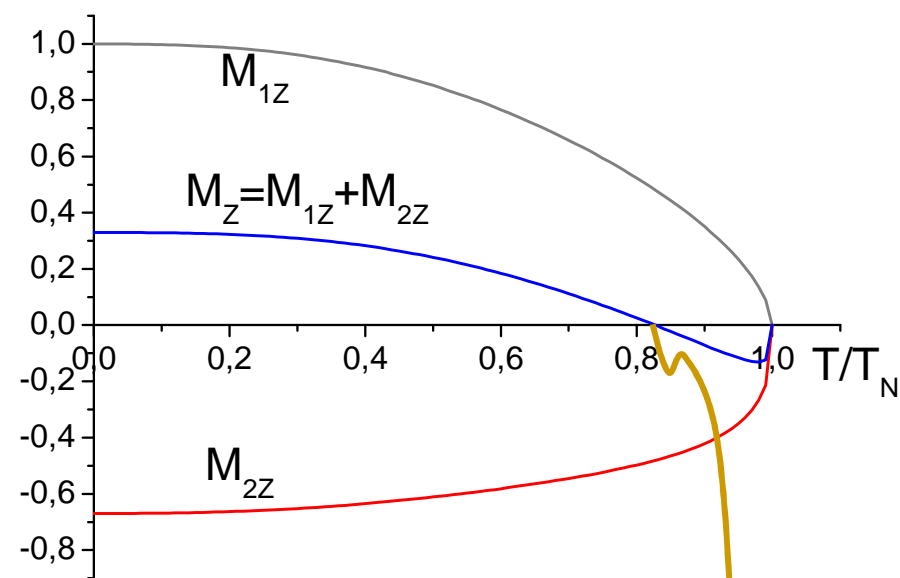
$$H_{Weiss}^{(2)} = \frac{2}{\mu_0 g \mu_B} (pJ \langle s_1 \rangle + p'J' \langle s_2 \rangle)$$

$$H_{Weiss}^{(1)} = \frac{2}{\mu_0 g \mu_B} (pJ \langle s_2 \rangle + p'J' \langle s_1 \rangle)$$

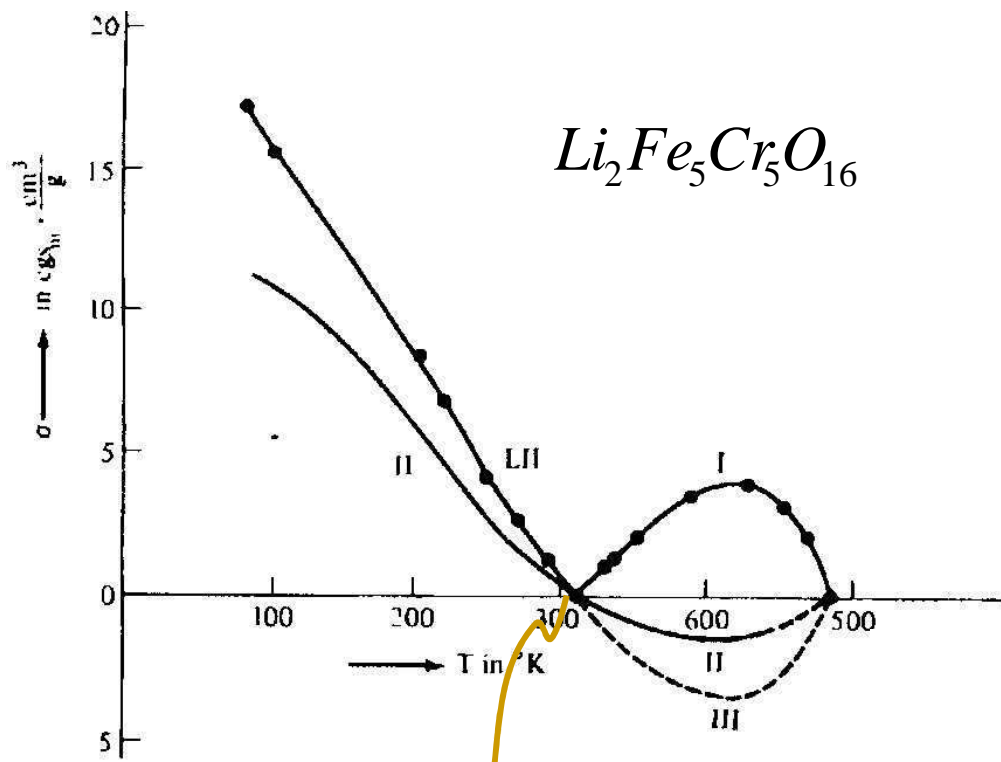
Sub-redes con comportamiento térmico similar



Sub-redes con diferente comportamiento térmico

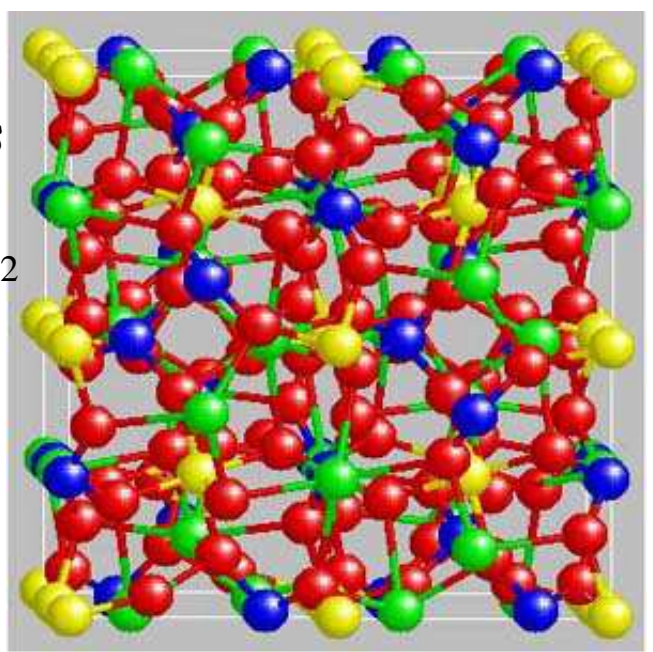


Punto de compensación



Punto de compensación

garnets
 $\text{Y}_3\text{Fe}_5\text{O}_{12}$



garnets de tierras raras

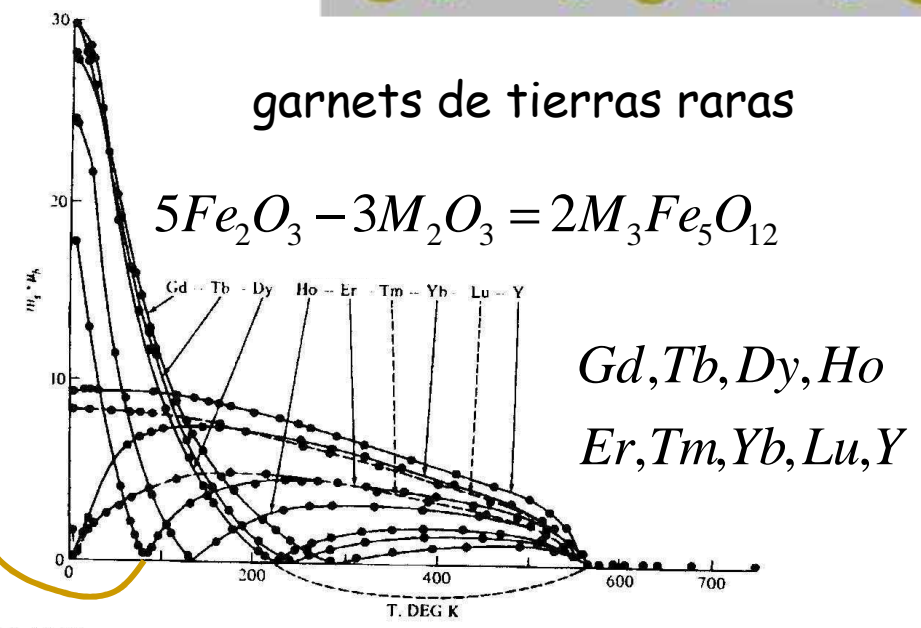
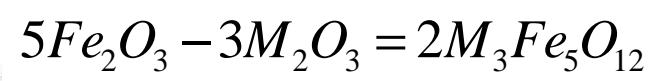
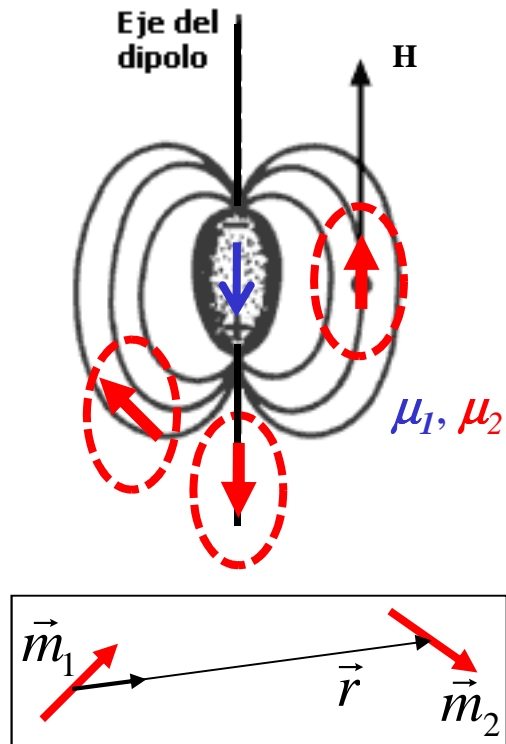


Figure 11.13-Temperature dependencies of the magnetic moments of the rare earth garnets. Note the occurrence of a compensation point in several of the curves. From Bertaut F., and Pauthenet,R., Proc. IEE, 104, Suppl.#5, 261,(1957)

Ordenamiento magnético por interacción dipolar



$$U_{dip} = \frac{\mu_0}{4\pi r^3} [\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_2 \cdot \hat{r})]$$

$$U_{dip} \approx \frac{\mu_0}{4\pi r^3} \mu_1 \mu_2$$

entre momentos atómicos:

$$U_{dip} \approx \frac{\mu_0}{4\pi r^3} \mu_1 \mu_2$$

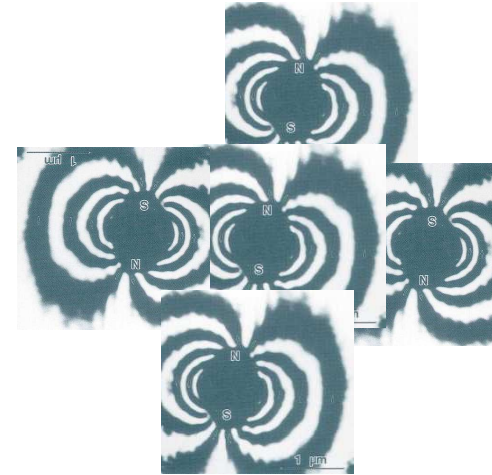
$$\mu_1 \approx \mu_2 \approx \mu_B \approx 10^{-23} \text{ Am}^2$$

$$r \approx 0.2 \text{ nm} = 2 \times 10^{-10} \text{ m}$$

$$U_{dip} \approx \frac{4\pi \times 10^{-7}}{4\pi \times 8 \times 10^{-30}} \times 10^{-46} \text{ Joules} = 1.25 \times 10^{-24} \text{ Joules} = 0.78 \times 10^{-5} \text{ eV}$$

Podemos comparar esta interacción con la de intercambio (*exch*)

$$U_{exch} \approx 2J_{exch} = 10^{-21} \text{ Joules} = 0.63 \times 10^{-2} \text{ eV}$$



Considerando que

$$T_{Cr} \approx \alpha U$$



$$\frac{(T_{Cr})_{dip}}{(T_{Cr})_{exch}} \approx \frac{U_{dip}}{U_{exch}} \approx 10^{-3} \xrightarrow{T_{exch} < 10^3 K} (T_{Cr})_{dip} < 1K$$

Sólo pueden esperarse efectos de ordenamiento dipolar a escala atómica a temperaturas muy bajas

Interacción dipolar entre NPs

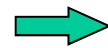
Cómo depende U_{dipolar} de $\langle r \rangle$ y $\langle d \rangle$?

$$|U_{\text{dip}}| \approx \frac{\mu_0}{4\pi r^3} \mu_i \mu_j$$

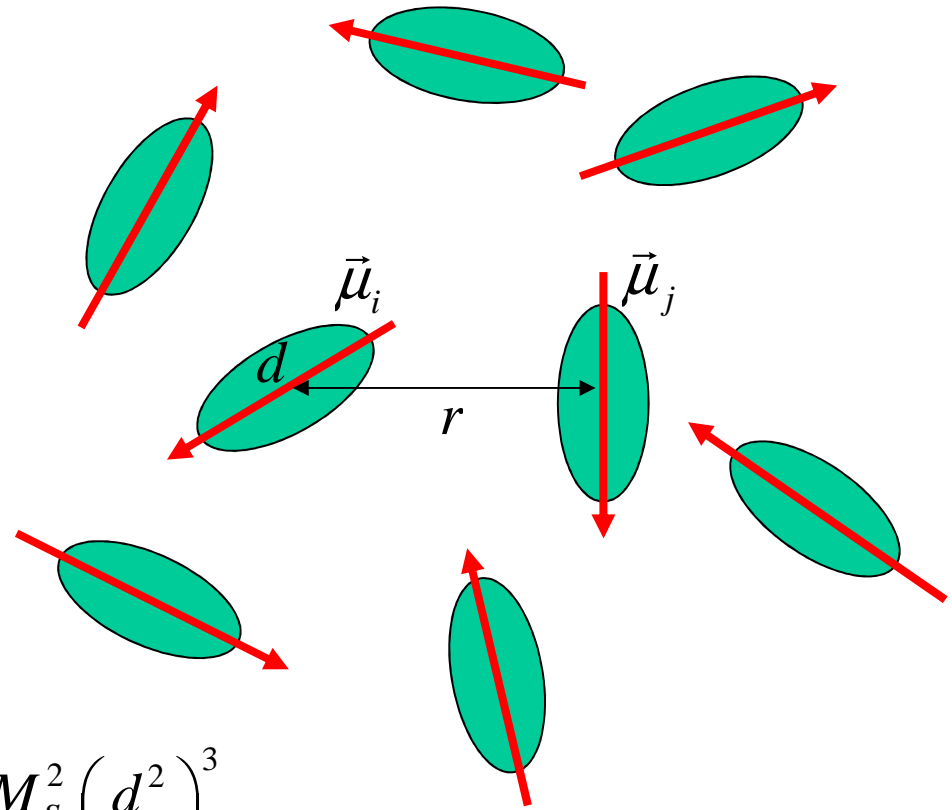
$$\mu_i \approx \mu_j \approx \mu = M_S V_p = M_S \pi d^3 / 6$$

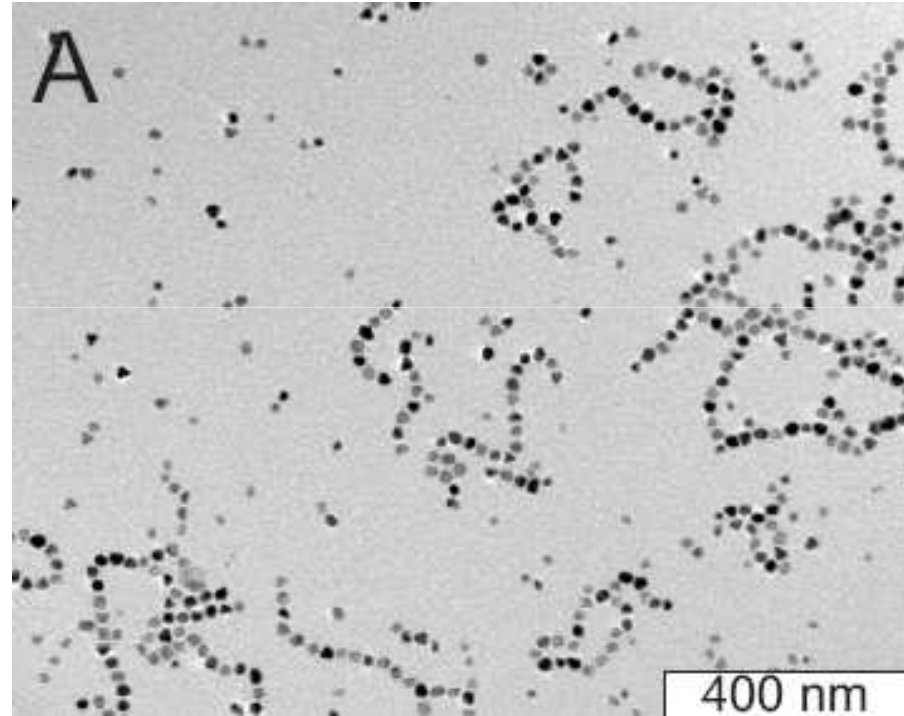
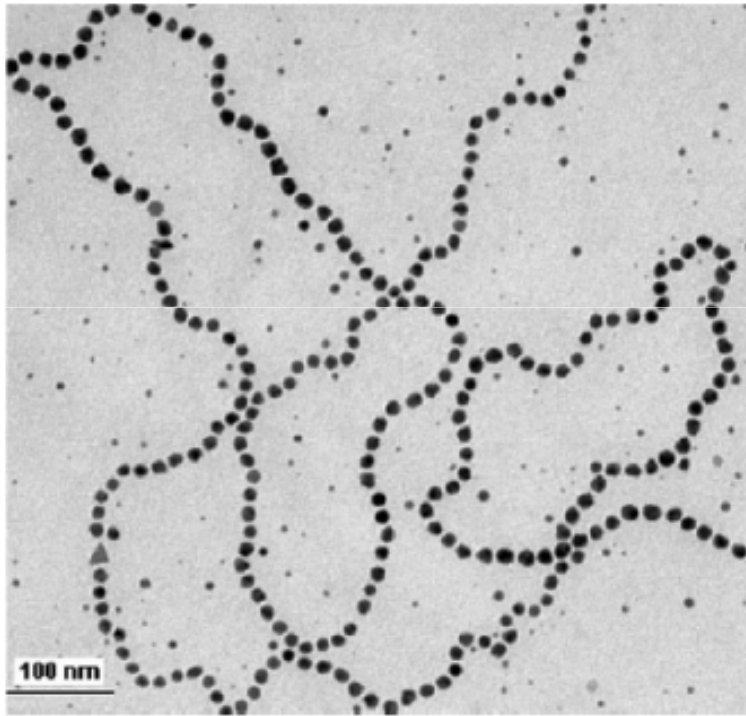
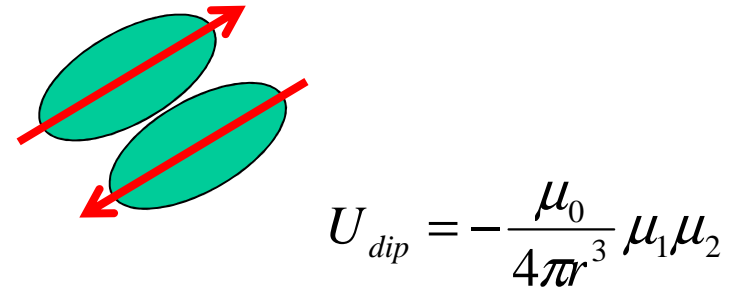
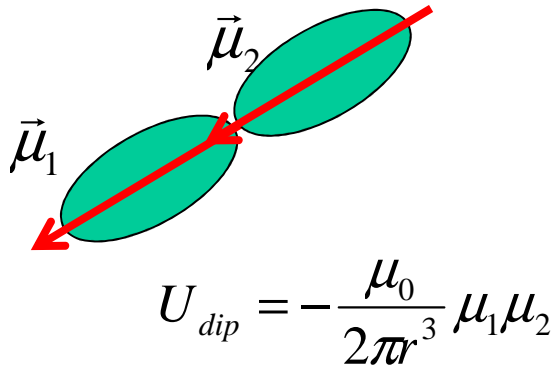
$$|U_{\text{dip}}| \approx \frac{\mu_0 \mu^2}{4\pi r^3} = \frac{\mu_0 (M_S \pi d^3 / 6)^2}{4\pi r^3} \approx \frac{\pi \mu_0 M_S^2}{144} \left(\frac{d^2}{r} \right)^3$$

Si $d = r$ (partículas en contacto)

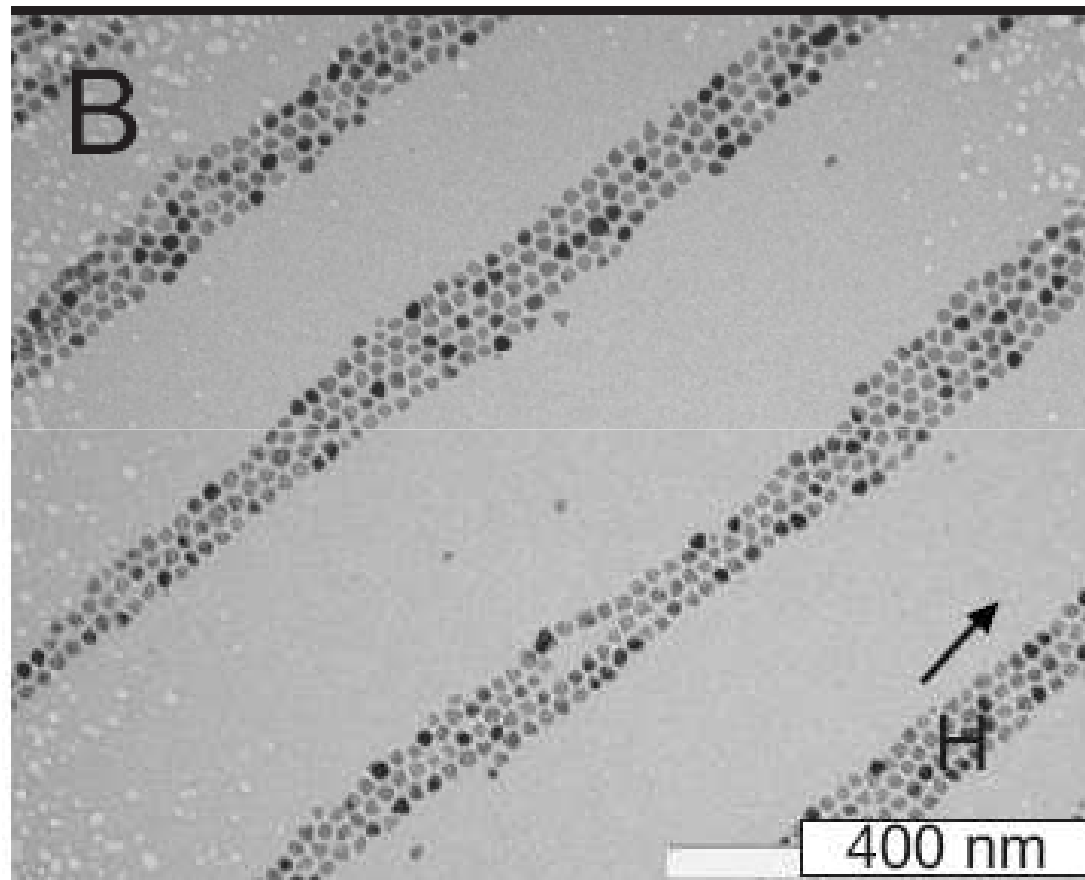
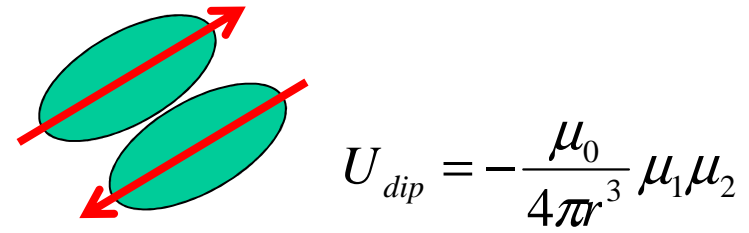
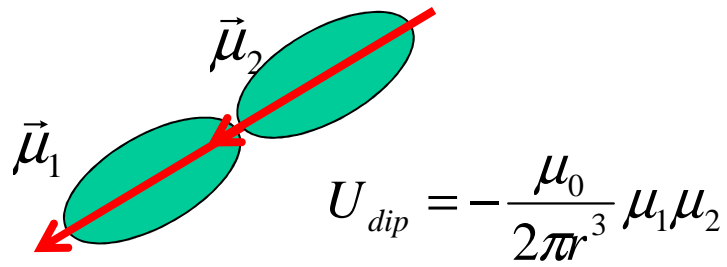


$$|U_{\text{dip}}| \approx \frac{\pi \mu_0 M_S^2}{144} d^3$$

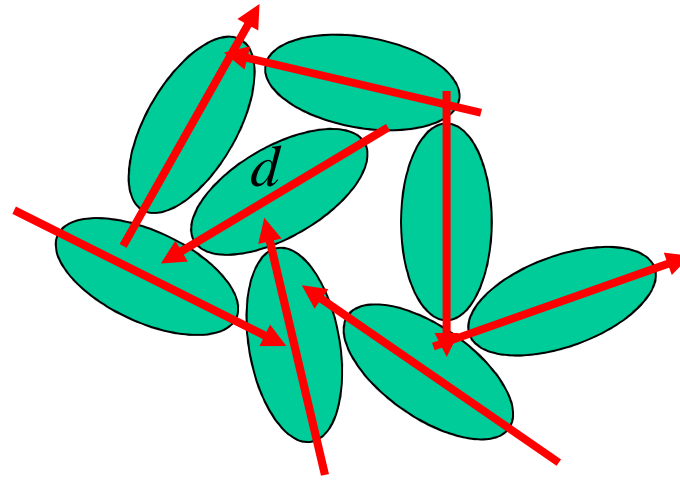




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Si $d = r$ (partículas en contacto) \rightarrow $|U_{dip}| \approx \frac{\pi\mu_0 M_S^2}{144} d^3$

magnetita $M_S^m \approx 90 \text{ emu/g} = 90 \text{ Am}^2 / \text{kg}$

$$M_S = M_S^m \rho \approx 4.5 \times 10^5 \text{ A/m}$$

$$d \approx 10 \text{ nm} = 1 \times 10^{-8} \text{ m}$$

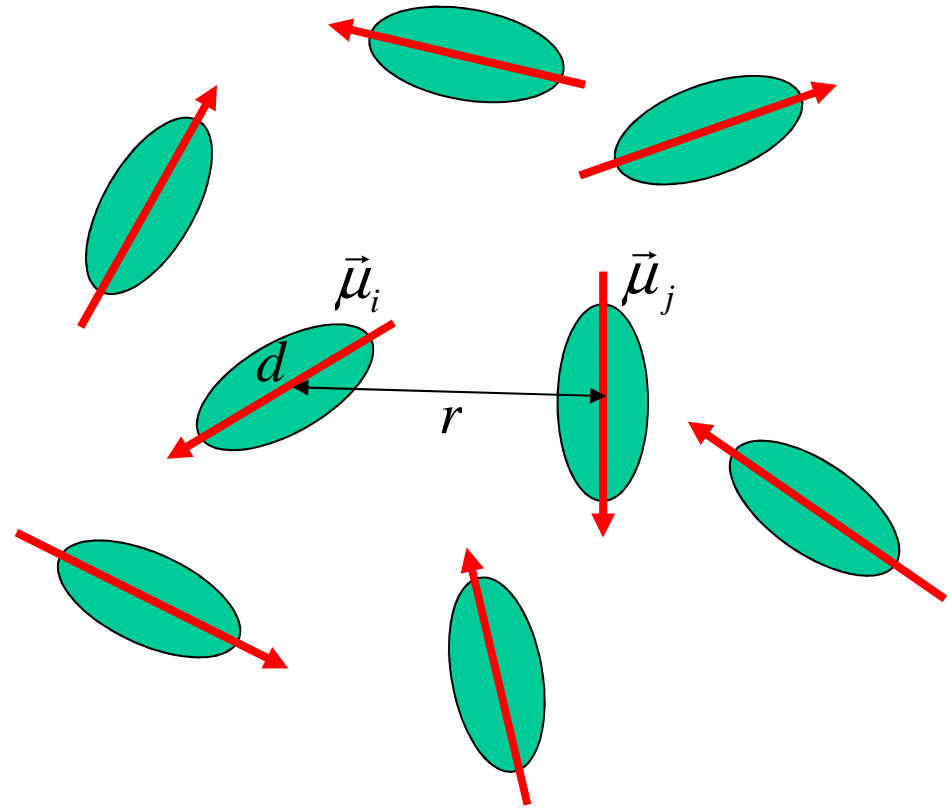
$$|U_{dip}| \approx 5.6 \times 10^{-21} \text{ J} \approx 3.5 \times 10^{-2} \text{ eV} \approx |U_{exch}|$$

Para qué relación $\langle r \rangle / \langle d \rangle$

será $U_{\text{Dipolar}} \ll U_{\text{Zeeman}}$?

$$|U_{\text{dip}}| \approx \frac{\mu_0}{4\pi r^3} \mu_i \mu_j$$

$$|U_Z| = \mu_0 \vec{\mu}_i \cdot \vec{H} \approx \mu_0 \mu_i H$$



$$\frac{|U_{\text{dip}}|}{|U_Z|} \approx \frac{M_S}{3H} \left(\frac{d}{r} \right)^3$$

$$\frac{|U_{\text{dip}}|}{|U_Z|} \ll 1 \Rightarrow \frac{r}{d} \gg \left(\frac{M_S}{3H} \right)^{1/3} \xrightarrow{M_S=10^6 \text{ Am}^{-1}, H=10^4 \text{ Am}^{-1}} \frac{r}{d} \gg 3.2$$



Fin módulo