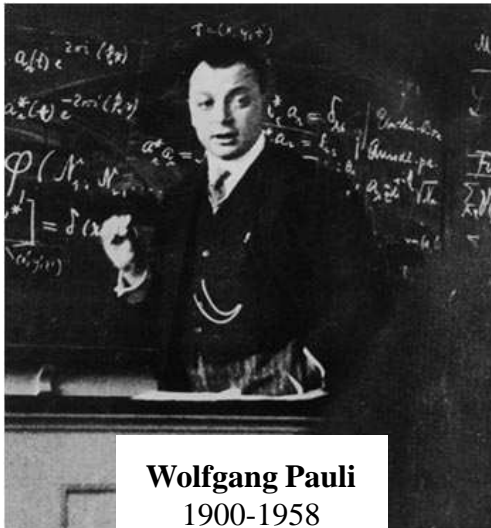


Intercambio

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

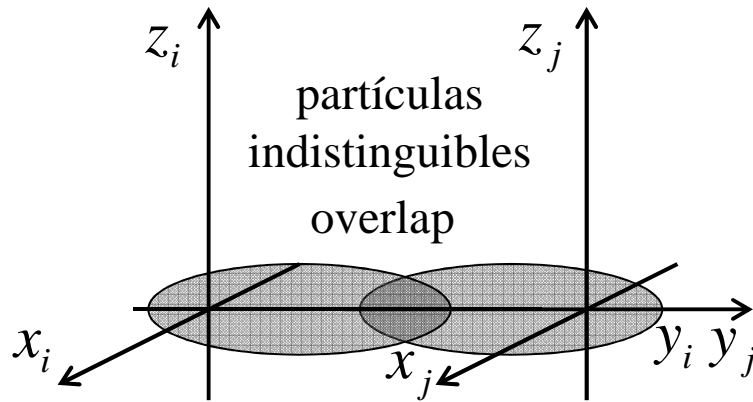
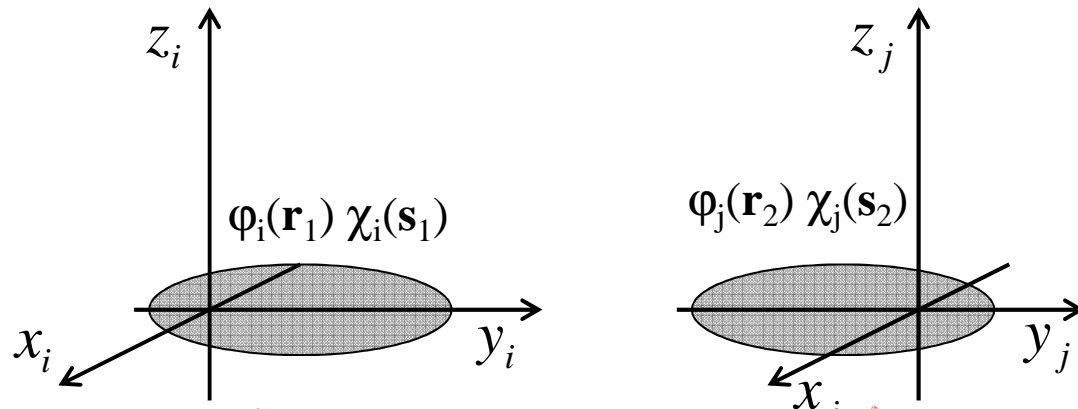
Bosones:

$s=0, 1, 2, 3\dots$

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:

$s=1/2, 3/2, 5/2\dots$



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

Estado de dos fermiones

factor espacial

factor de espín

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

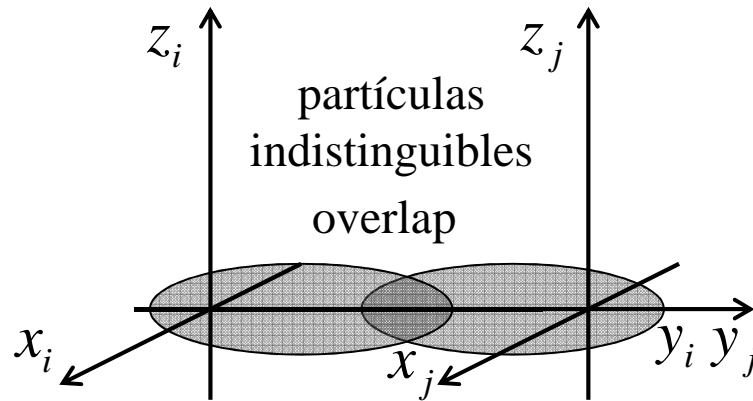
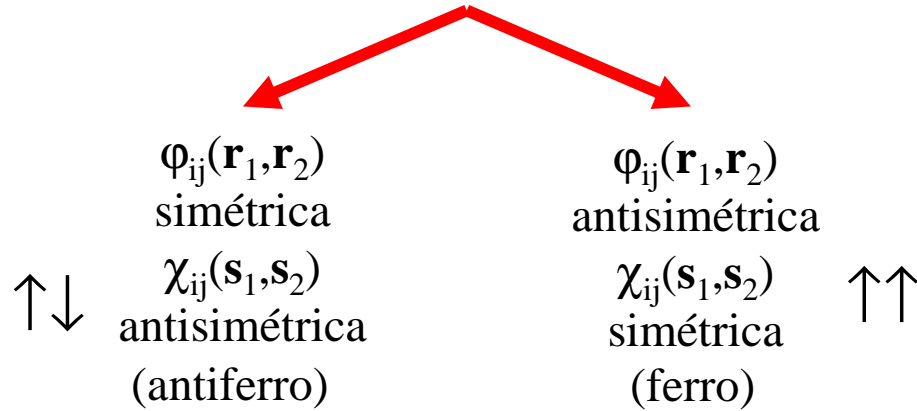
$$\chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

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

antisimétrica

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

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

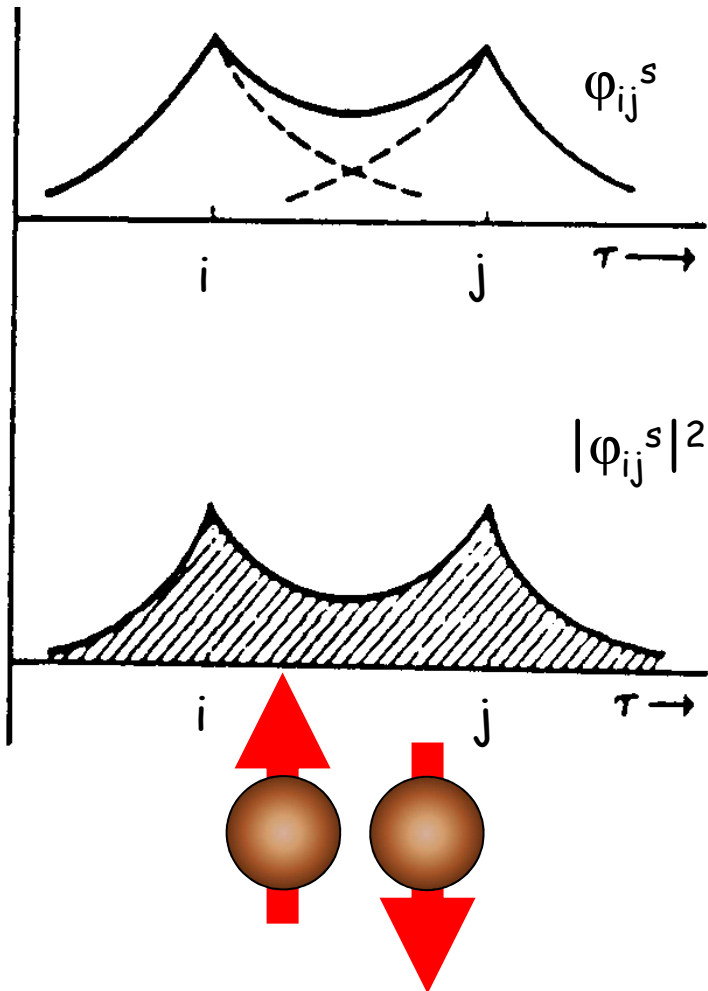


$$\Psi_{ij}(1,2) = \varphi_{ij}(\mathbf{r}_1, \mathbf{r}_2) \chi_{ij}(\mathbf{s}_1, \mathbf{s}_2)$$

Factor espacial

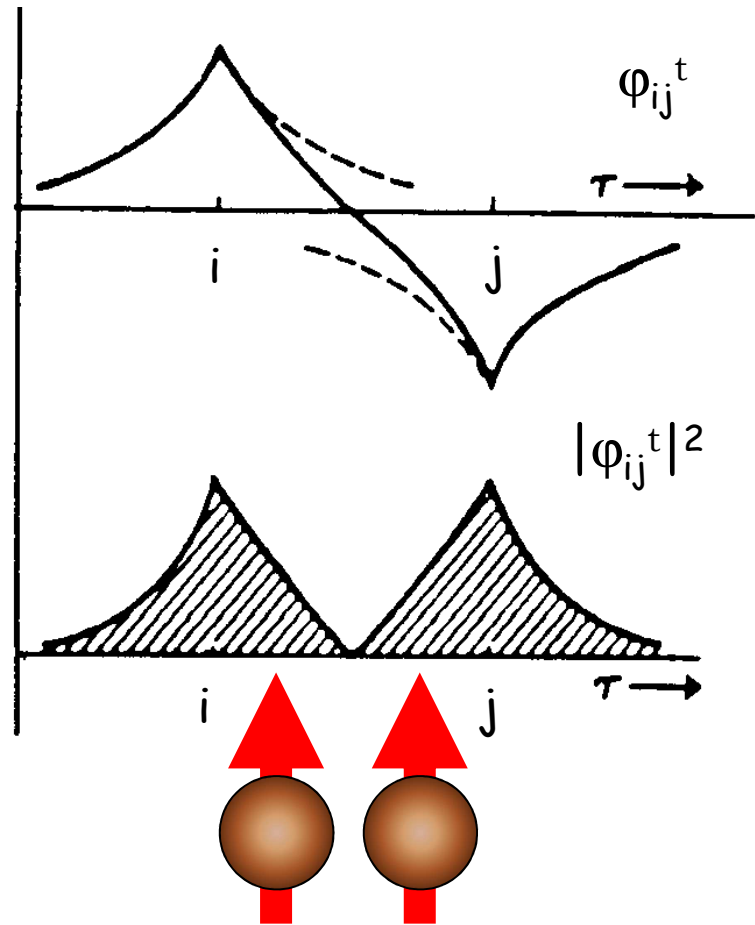
$$\varphi_{ij}^s = \frac{1}{\sqrt{2}} \{ \varphi_i(\vec{r}_1) \varphi_j(\vec{r}_2) + \varphi_i(\vec{r}_2) \varphi_j(\vec{r}_1) \}$$

(simétrico)



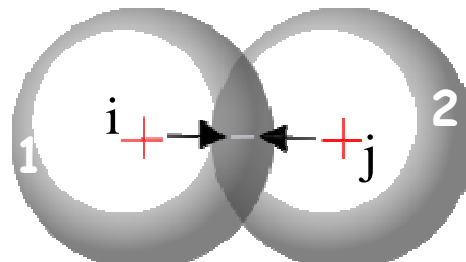
$$\varphi_{ij}^t = \frac{1}{\sqrt{2}} \{ \varphi_i(\vec{r}_1) \varphi_j(\vec{r}_2) - \varphi_i(\vec{r}_2) \varphi_j(\vec{r}_1) \}$$

(antisimétrico)



Evaluación de la energía potencial

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

$$U = \frac{q^2}{4\pi\epsilon_0} \left(\frac{1}{r_{ij}} - \frac{1}{r_{i1}} - \frac{1}{r_{i2}} - \frac{1}{r_{j1}} - \frac{1}{r_{j2}} + \frac{1}{r_{12}} \right)$$


Valor esperado de U

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

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

(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)

en el estado singlete:

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

en el estado triplete:

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

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

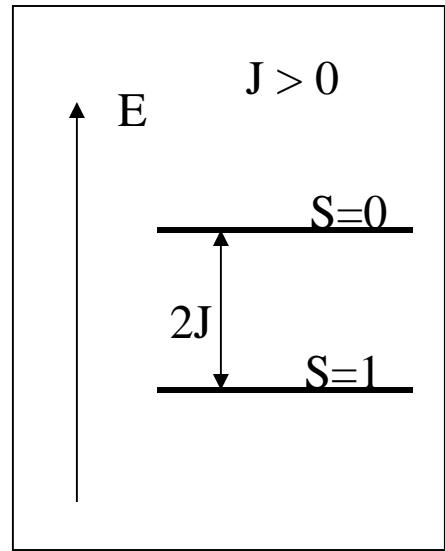
Término directo

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

Término de intercambio

diferencia de energía entre ambos estados:

$$E_s - E_t = 2J_{ij}$$

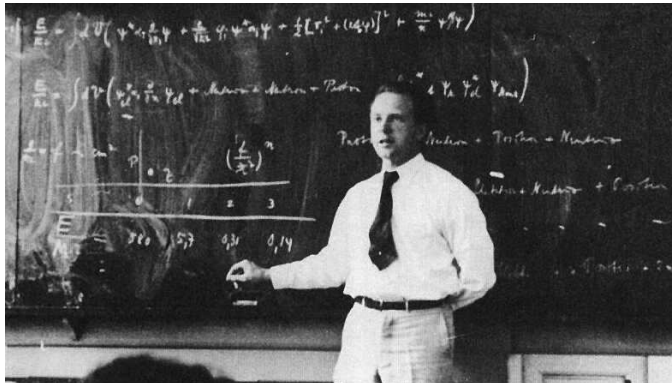


Sistema de dos estados

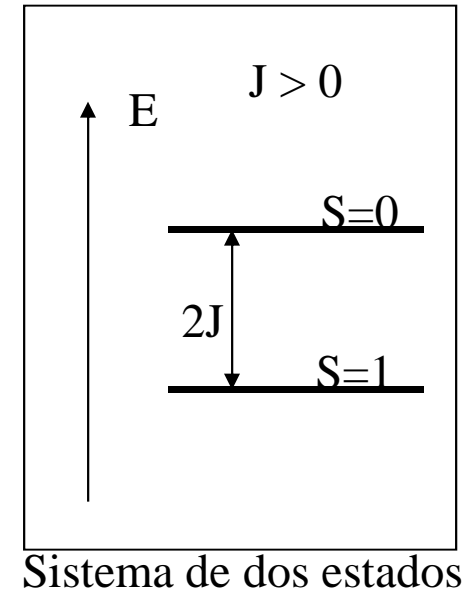
Operador Hamiltoniano de espín

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

Hamiltoniano
de Heisenberg



Werner Heisenberg (1901 - 1976)



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

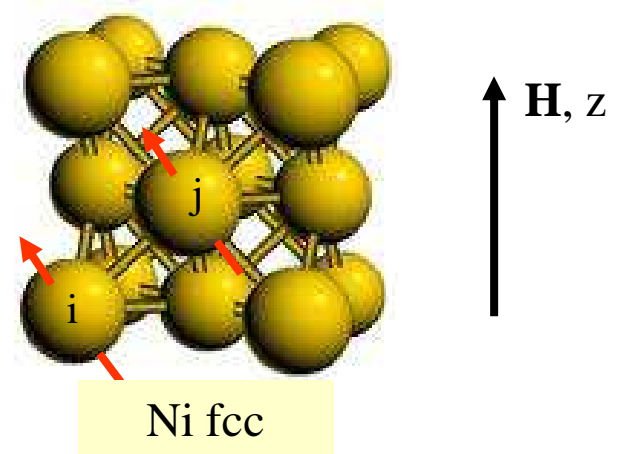
(a) Ferromagnetismo

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

Consideramos dos contribuciones a la energía

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

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



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

intercambio Zeeman

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

$$E = -\mu_0 \sum_i \mu_i \cdot \vec{H}_{ef}$$

$$E = -\mu_0 \sum_i \mu_i \cdot \vec{H}_{ef}$$

Campo de Weiss

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

\vec{H}_{Weiss}



Scanned at the American
Institute of Physics

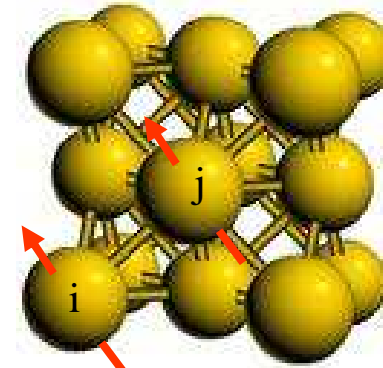
Pierre Weiss (1865-1940)

Niquel

Limitando la suma a
los primeros vecinos

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

primeros vecinos
 $p = 12$

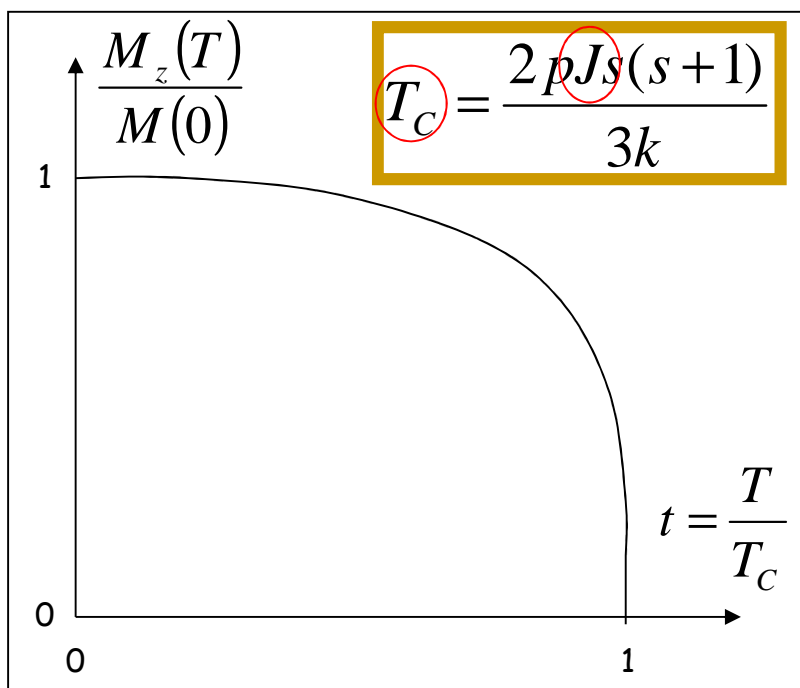


Ni fcc

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

Temperatura de Curie

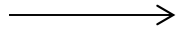
T_C es proporcional a J



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

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



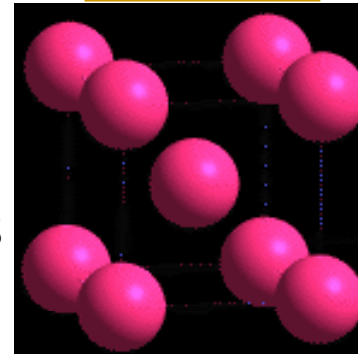
$$s_{\text{Fe}} \approx 1.115$$

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

bcc-Fe

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

Arrows indicate the following substitutions:
- $3kT_C$ is substituted with 1043K
- $ps(s+1)$ is substituted with 1.115
- p is substituted with 8

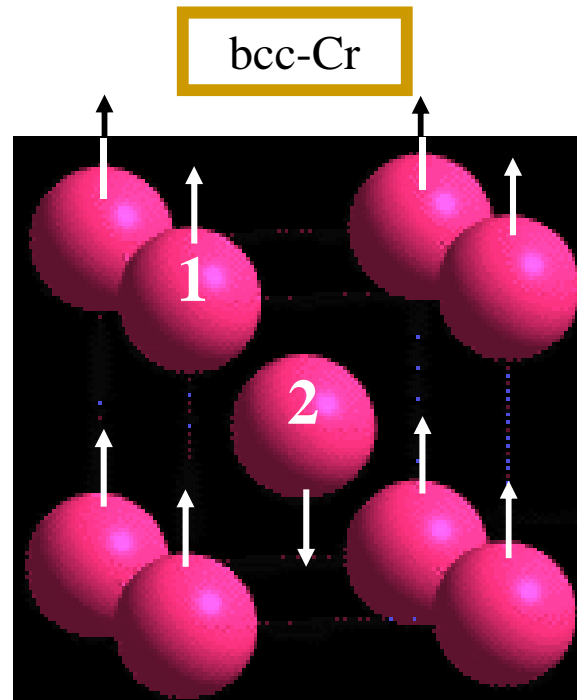


$$J_{\alpha\text{-Fe}} \approx \frac{3 \times 1.38 \times 10^{-23} (\text{Joule} / \text{K}) \times 1043 \text{K}}{2 \times 8 \times 1.115 \times 2.115} = 1.21 \times 10^{-21} \text{ Joule}$$

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

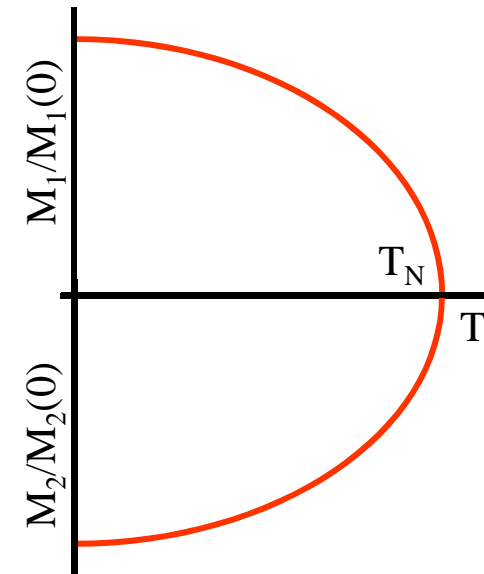
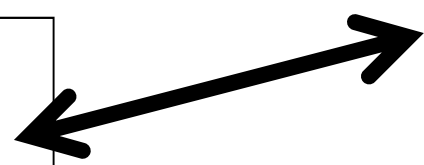
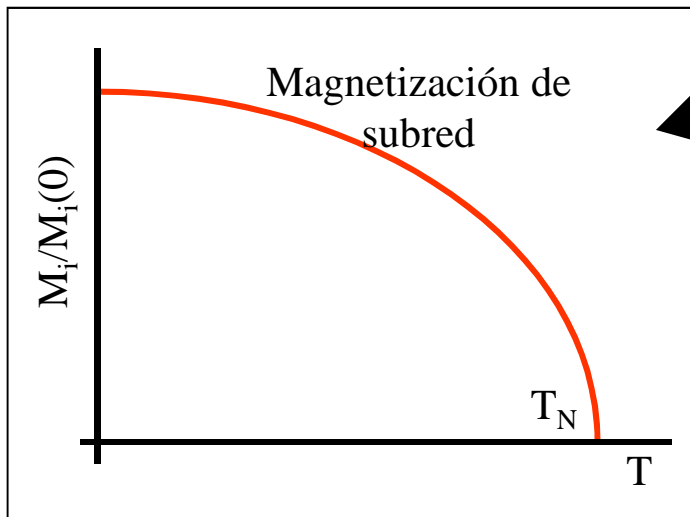
(b) Antiferromagnetismo

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



Subredes 1 y 2

Ejemplo, Red bcc: dos subredes 1 y 2, $p = 8$
primeros vecinos (1) y $p' = 6$ segundos vecinos (2)



$$M_i \neq 0$$

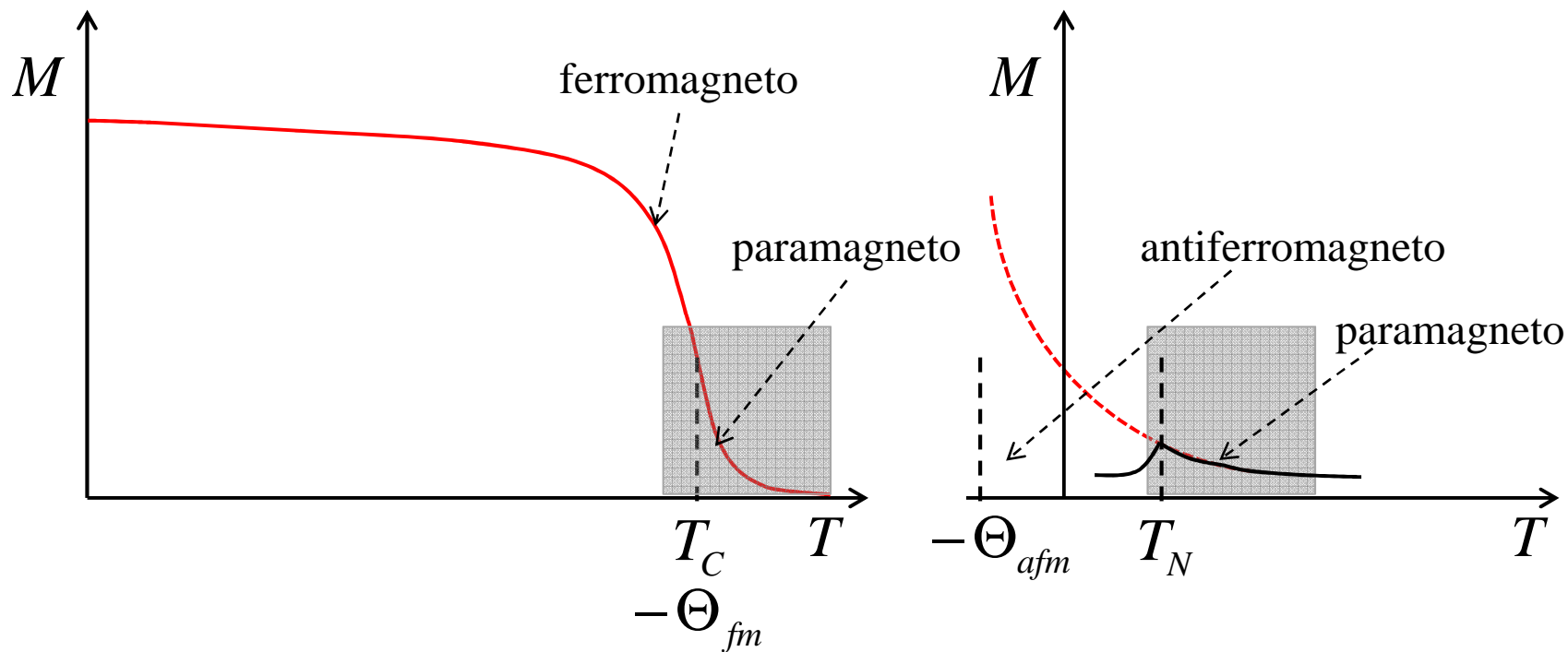
$$M_1 + M_2 = 0$$



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

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

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



Ley de Curie-Weiss

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

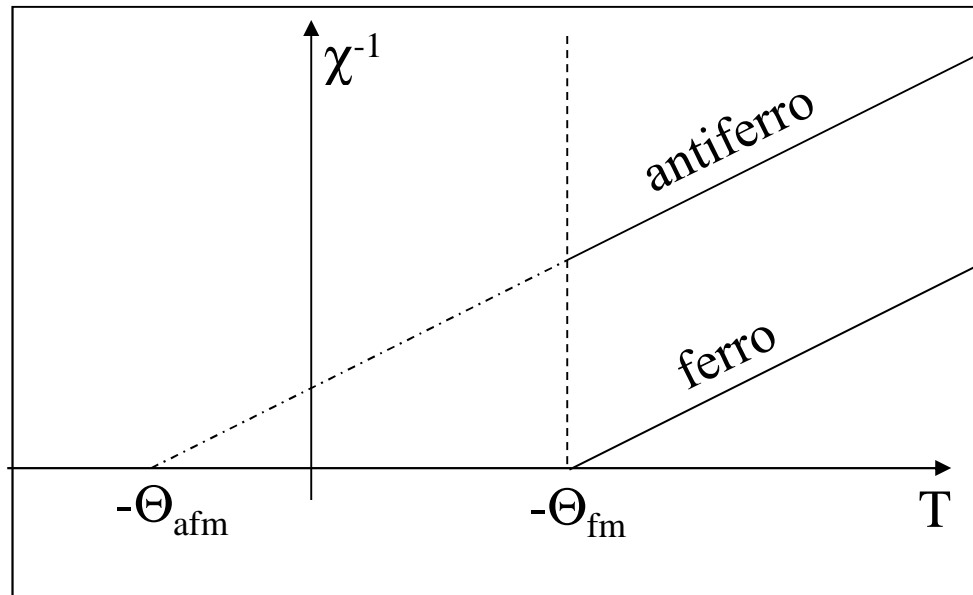
$$\Theta_{afm} = -\frac{2s(s+1)(pJ + p'J')}{3k} > 0$$

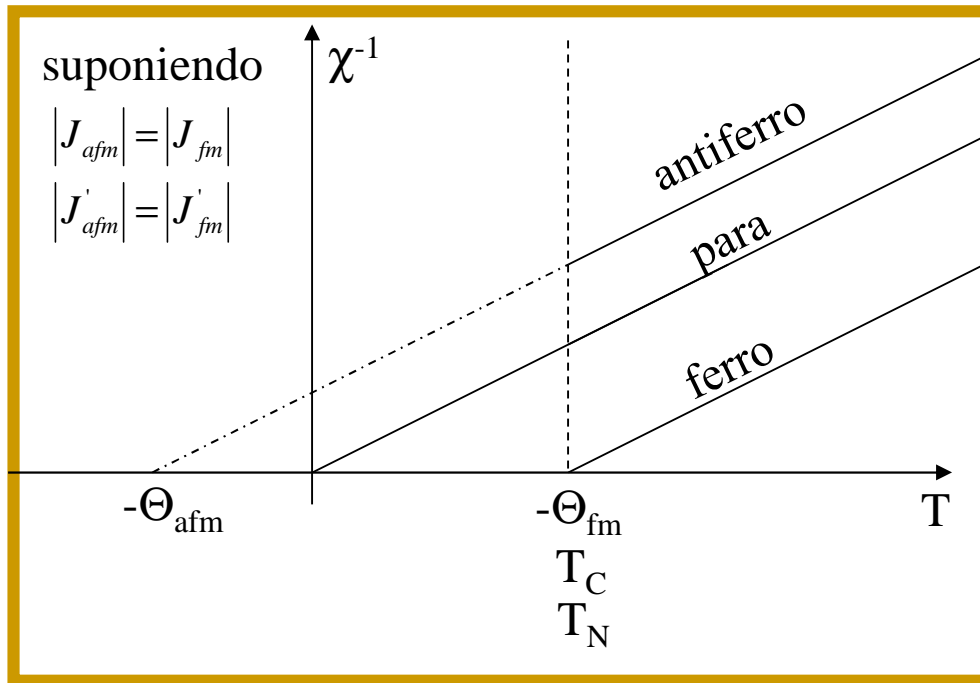
$$\Theta_{fm} = -\frac{2s(s+1)(pJ + p'J')}{3k} < 0$$

Por encima de la temperatura crítica:

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

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

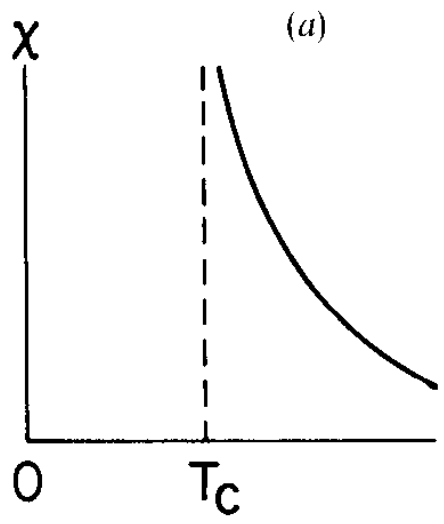




Ley de Curie-Weiss

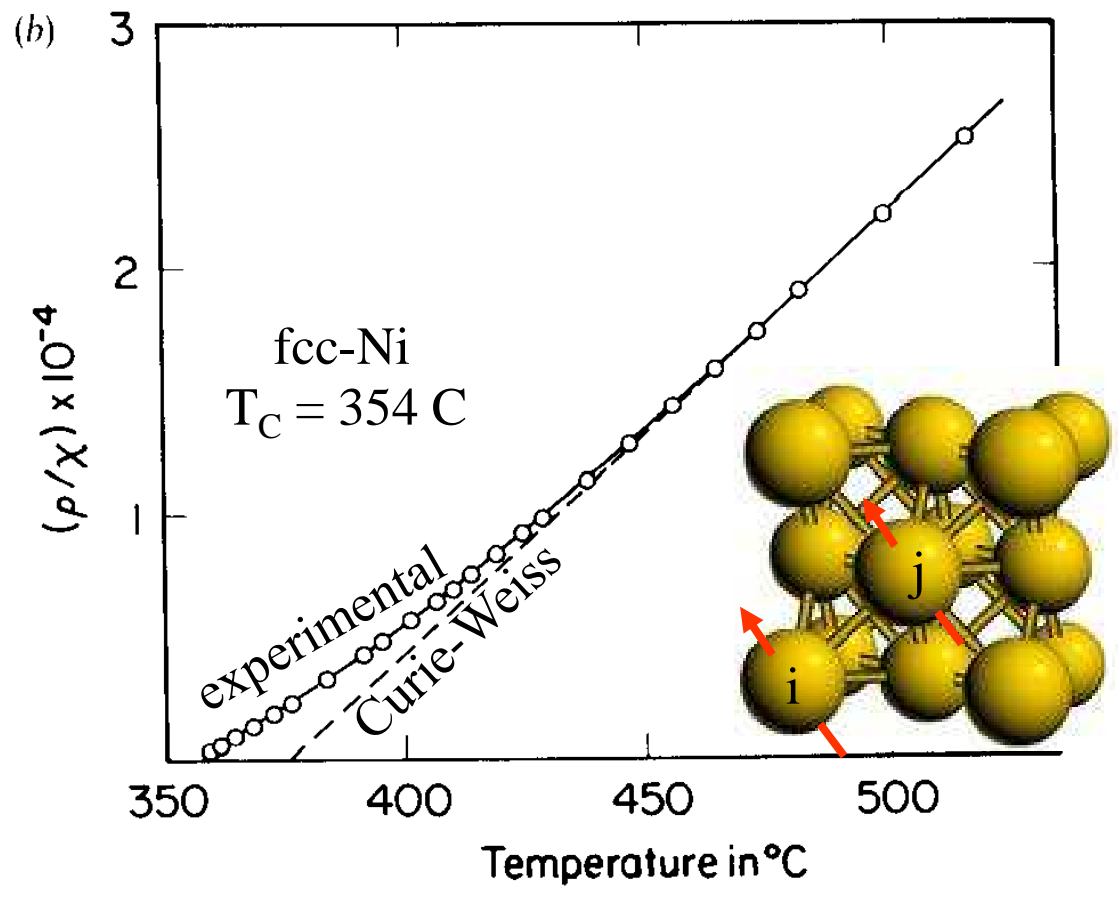
$$\chi = \frac{C}{T + \Theta}$$

ferromagneto



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

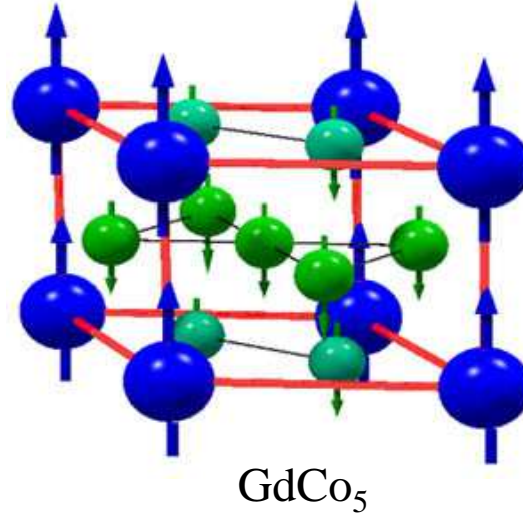
Curie-Weiss Law
($T > T_C$)



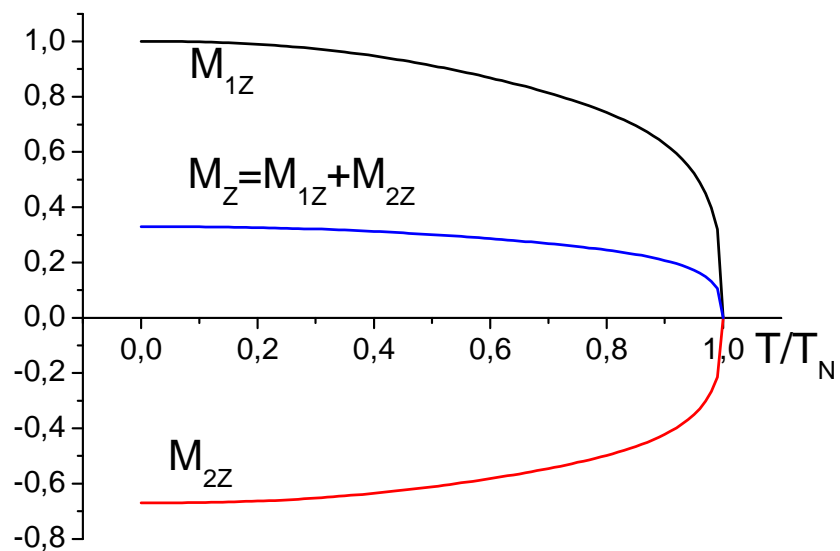
(c) Ferrimagnetismo

Ferrimagnetismo

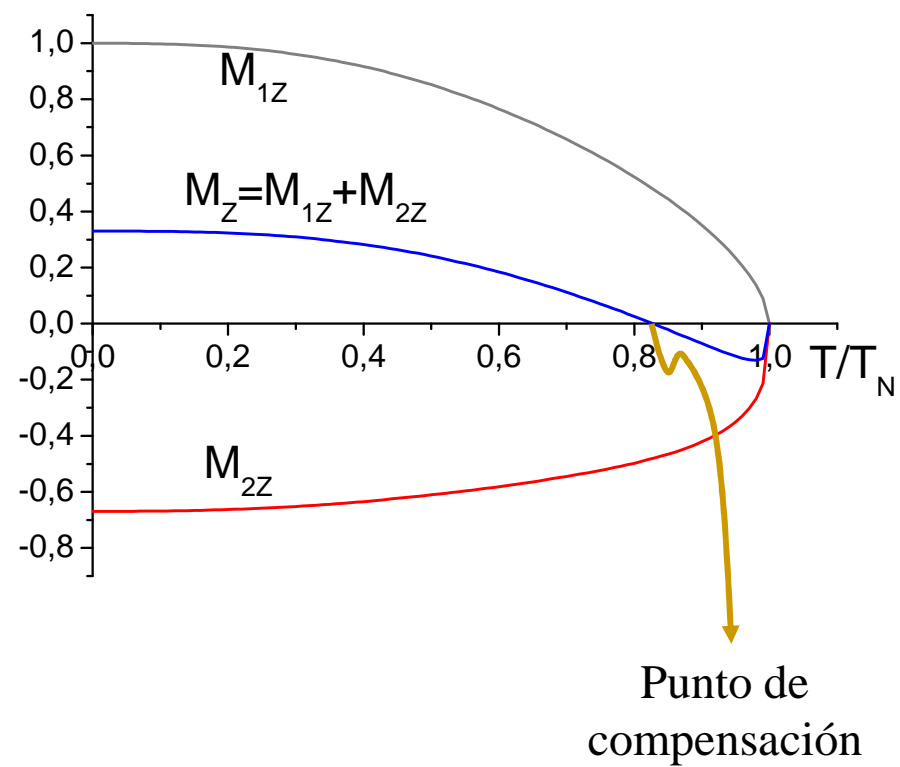
Ferrimagneto: momento
opuesto y diferente en
cada subred

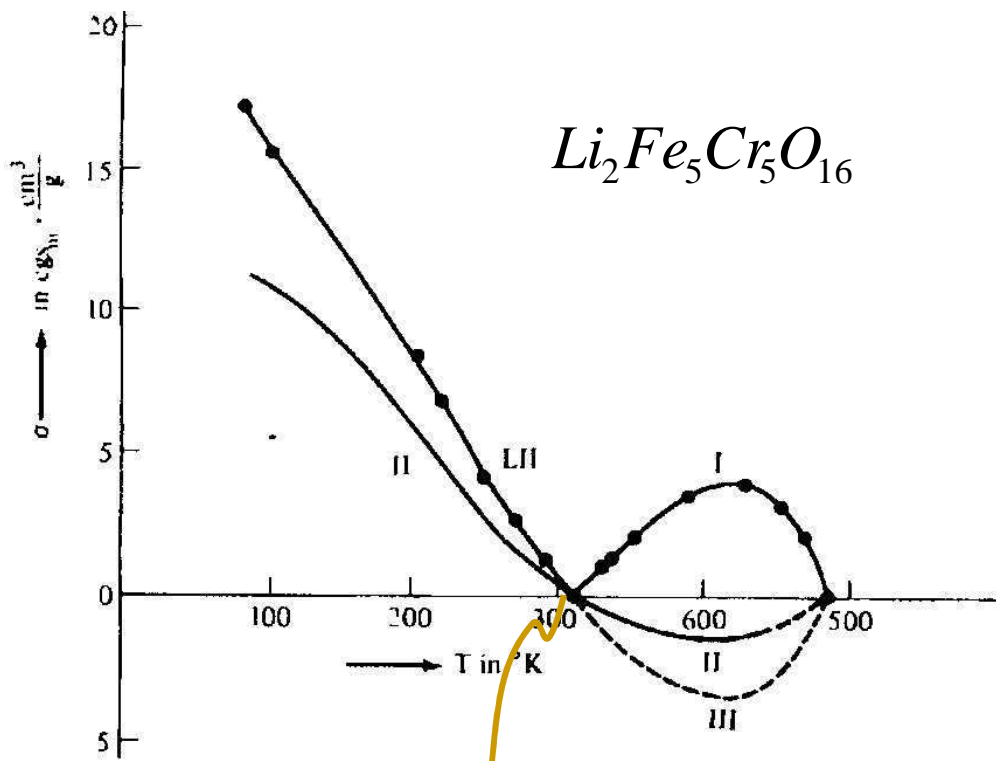


Sub-redes con comportamiento térmico similar

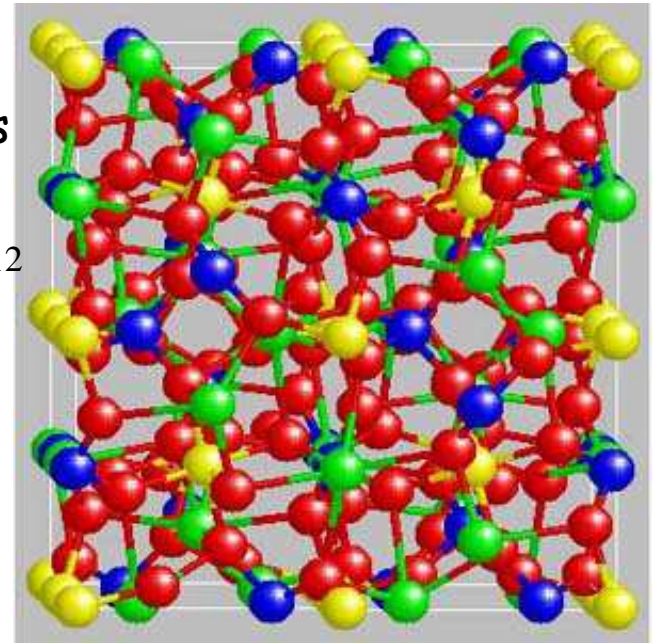
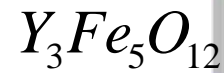


Sub-redes con diferente comportamiento térmico





garnets



Punto de compensación

garnets de tierras raras

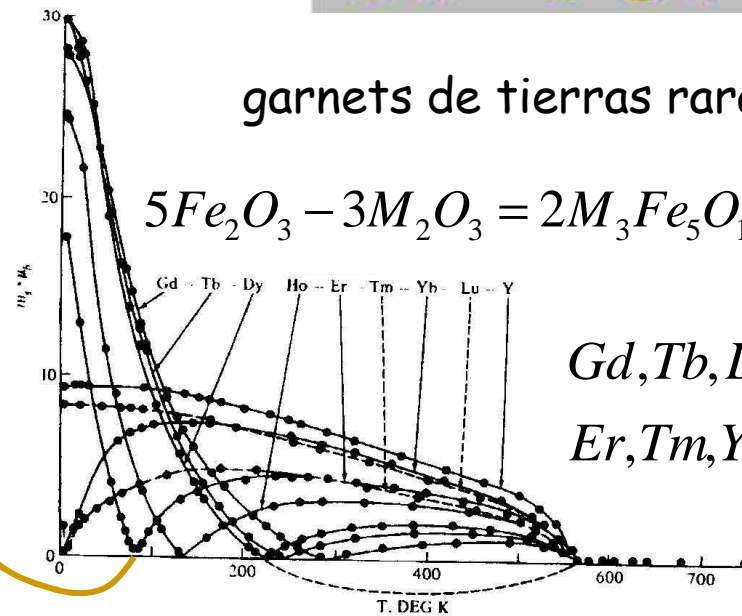
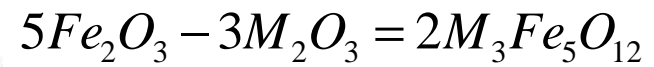


Figure 11.13-Temperature dependencies of the magnetic moments of the rare earth garnets. Note the occurrence of a compensation point in several of the curves. From Bertaut F., and Pauthenet, R., Proc. IEE, 104, Suppl.#5, 261,(1957)



Fin módulo

Fin módulo