Estructura de la Materia 2

Clase 15 - Teoría

Docentes

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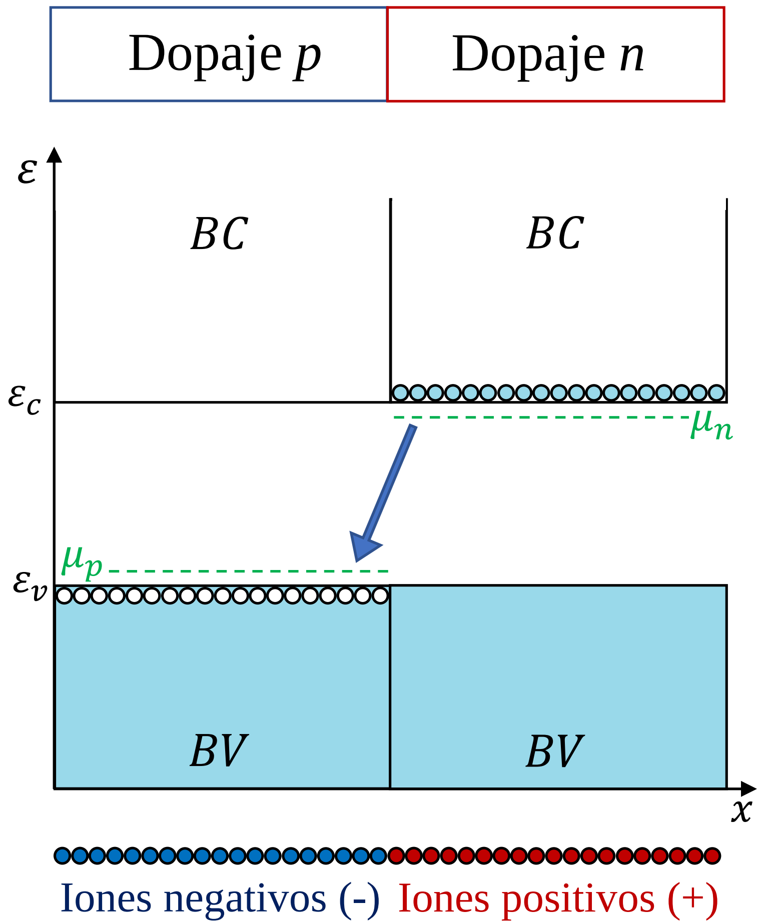
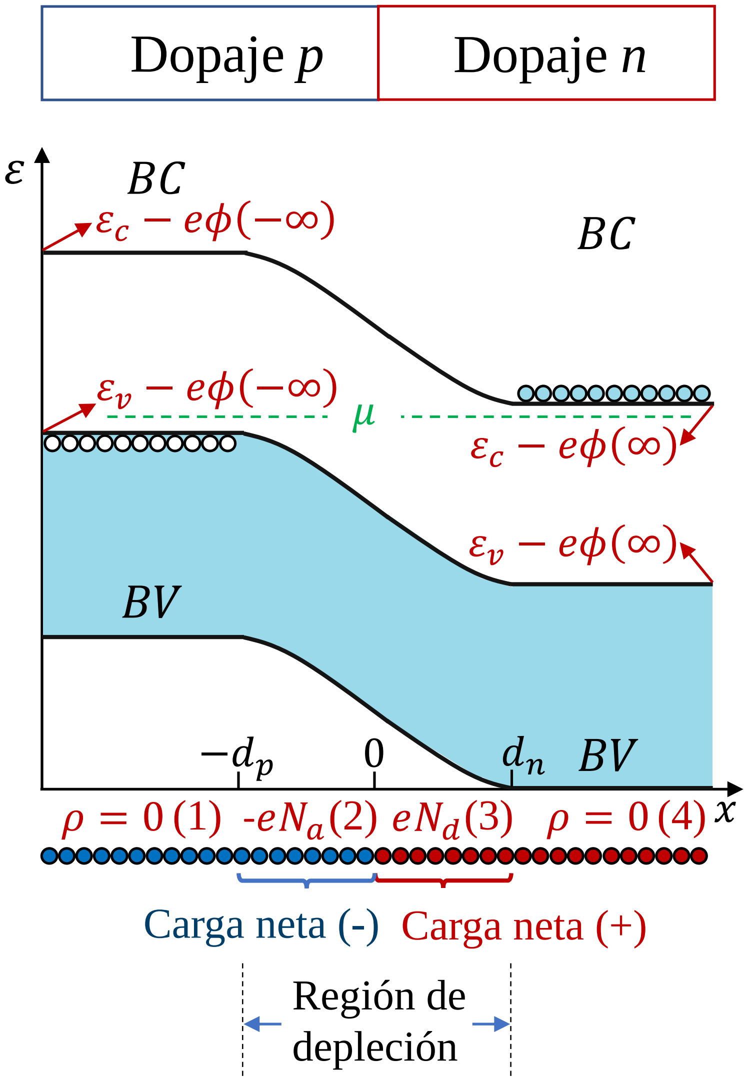
Repaso

Juntura semiconductora *p-n*: Equilibrio térmico



Suponemos impurezas totalmente ionizadas en cada semiconductor.



$$e\Delta\phi \overset{\mu_p = \mu_n = \mu}{=} E_g + k_B T \ln\left[\frac{N_d N_a}{N_c P_v}\right] \sim E_g$$

$$\nabla^2\phi = \frac{d^2\phi}{dx^2} = -\frac{4\pi\rho(x)}{\epsilon} \quad \text{(Poisson)}$$

$$\phi = \begin{cases} \phi(\infty) & (1) \\ \phi(\infty) - \dfrac{2\pi e N_d}{\epsilon}(x - d_n)^2 & (2) \\ \phi(-\infty) + \dfrac{2\pi e N_a}{\epsilon}(x + d_p)^2 & (3) \\ \phi(-\infty) & (4) \end{cases}$$

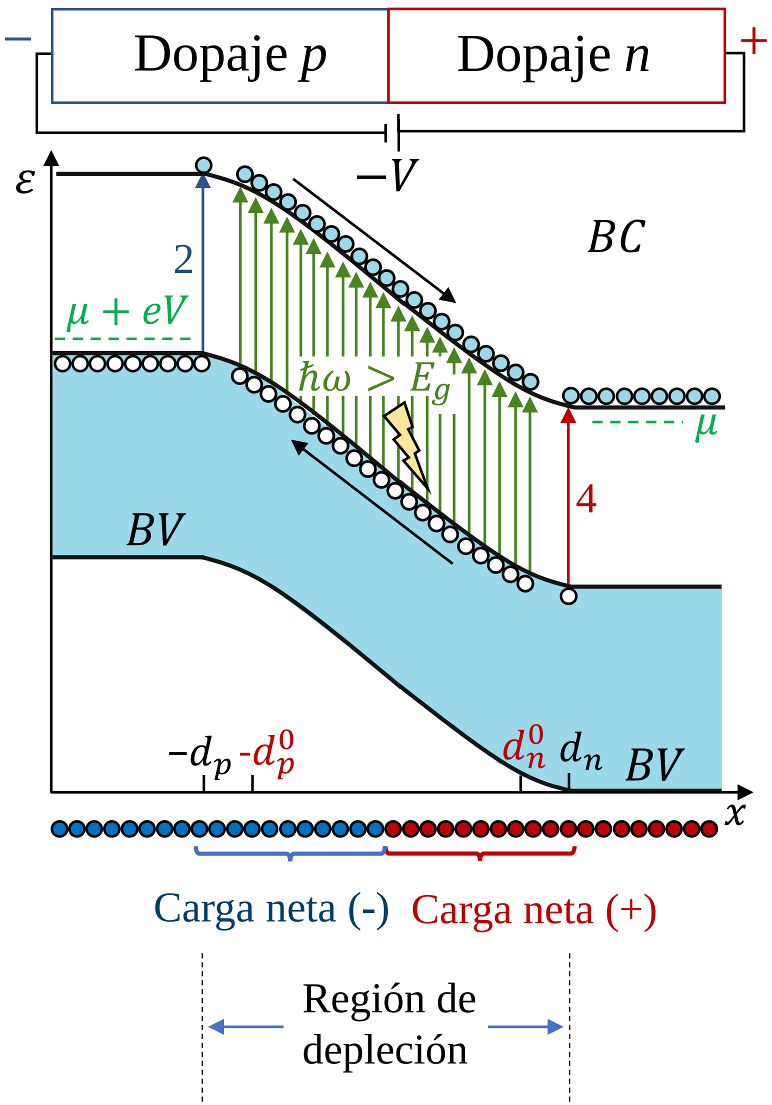
Continuidad de ϕ, ϕ' en $x = 0$:

$$\rightarrow N_d d_n = N_a d_p$$

$$\rightarrow d_{n,p} = \left[\frac{(N_a/N_d)^{\pm 1}}{N_d + N_a}\frac{\epsilon\Delta\phi}{2\pi e}\right]^{1/2}$$

Repaso

Juntura semiconductora *p-n*: Potencial externo



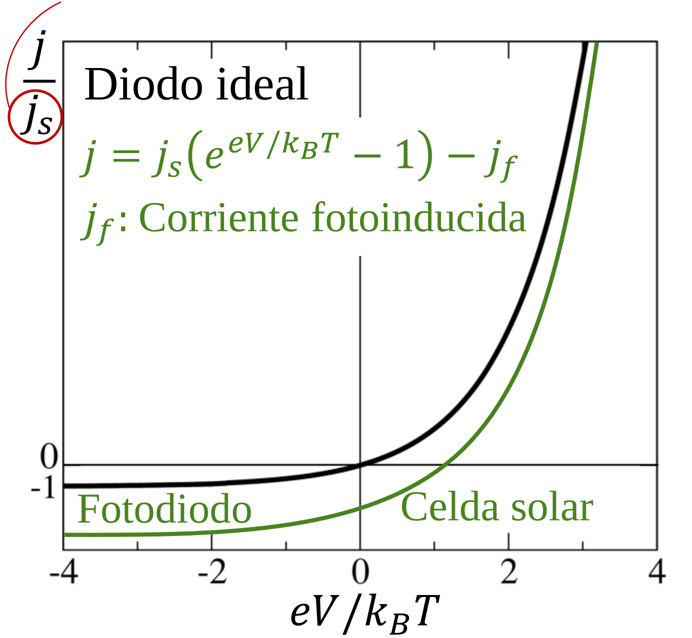
$$V \neq 0 \rightarrow \Delta\phi = (\Delta\phi)_0 - V$$

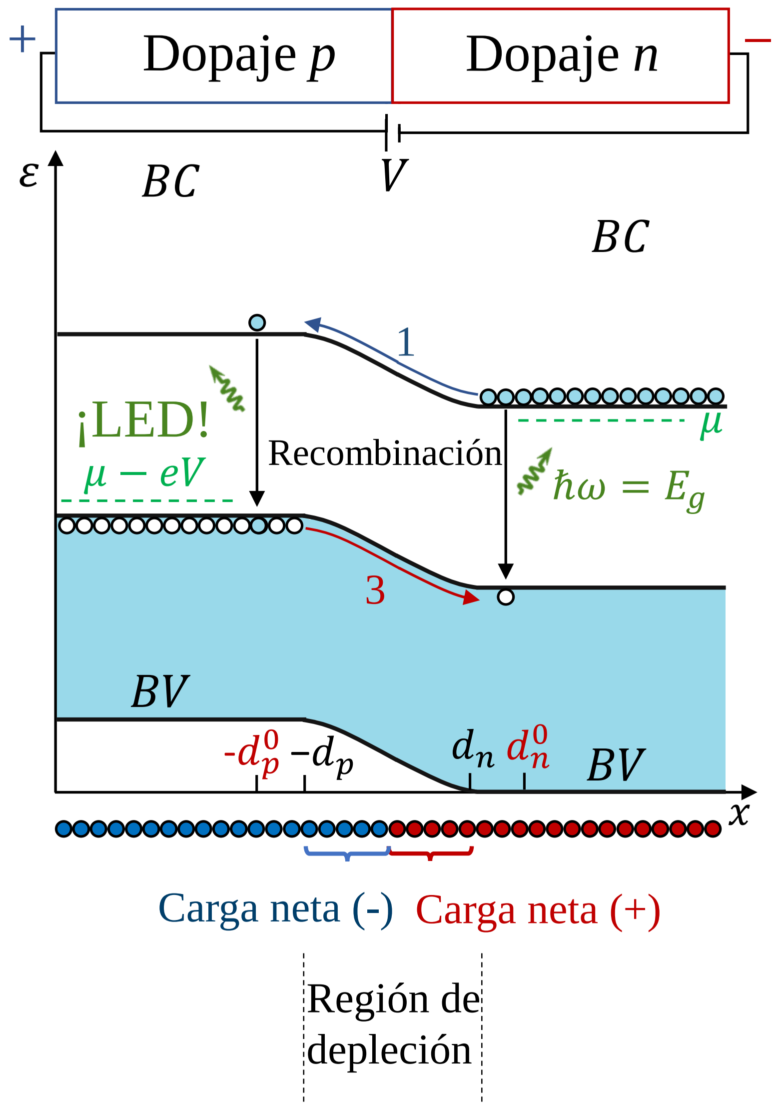
$$d_{n,p}(V) = d_{n,p}(0)\sqrt{1 - V/(\Delta\phi)_0}$$

$$(1)\ J_e^{rec} \propto e^{-\frac{e\Delta\phi}{k_BT}} \quad (2)\ J_e^{gen} \propto e^{-\frac{E_g}{k_BT}}$$

$$(3)\ J_h^{rec} \propto e^{-\frac{e\Delta\phi}{k_BT}} \quad (4)\ J_h^{gen} \propto e^{-\frac{E_g}{k_BT}}$$

$$j = \left[e\left(J_e^{gen} + J_h^{gen}\right)\right]\left(e^{eV/k_BT} - 1\right)$$

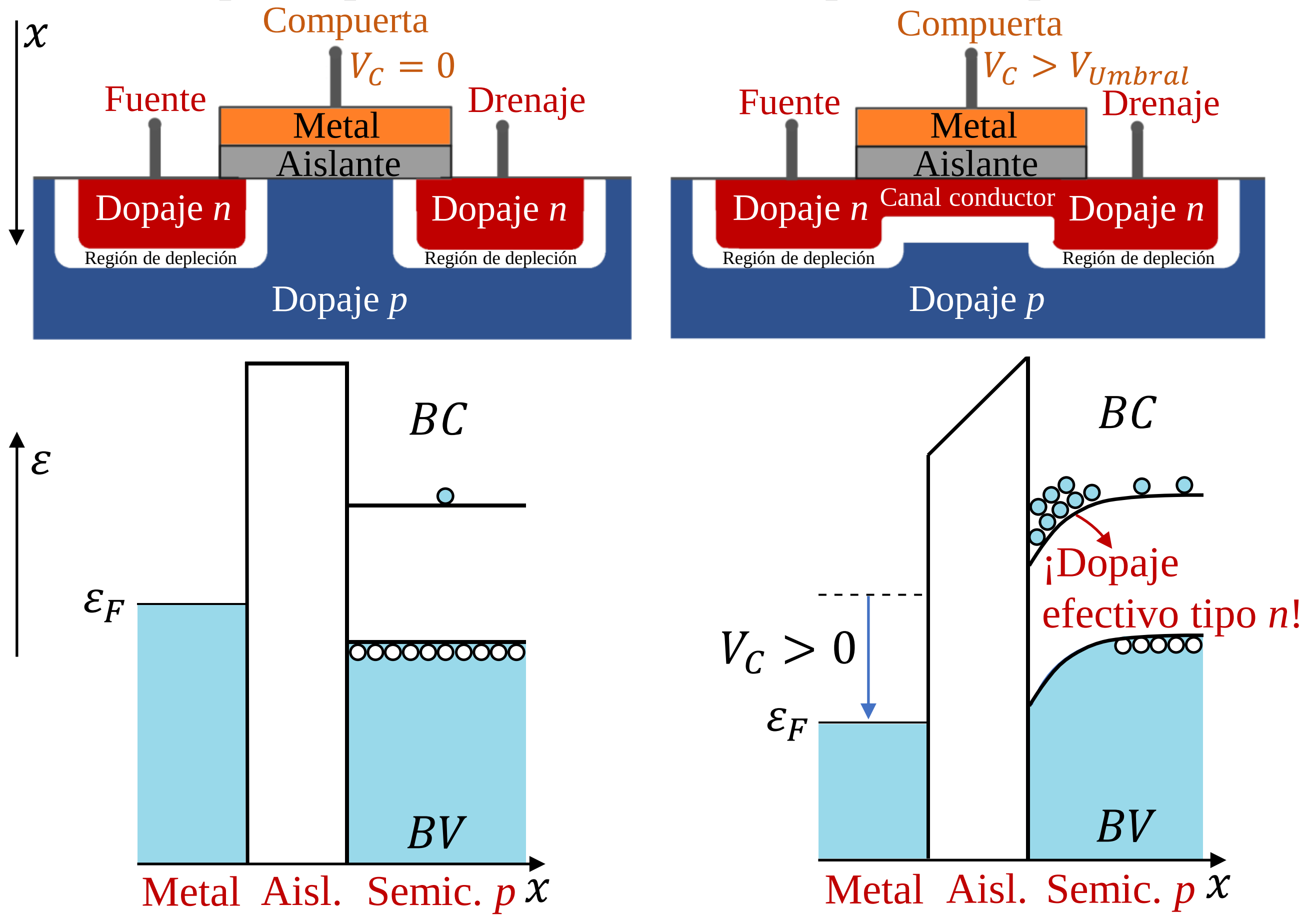




Transistor y pozos cuánticos

Transistor de efecto de campo (MOSFET)

Se utiliza principalmente como interruptor o amplificador.

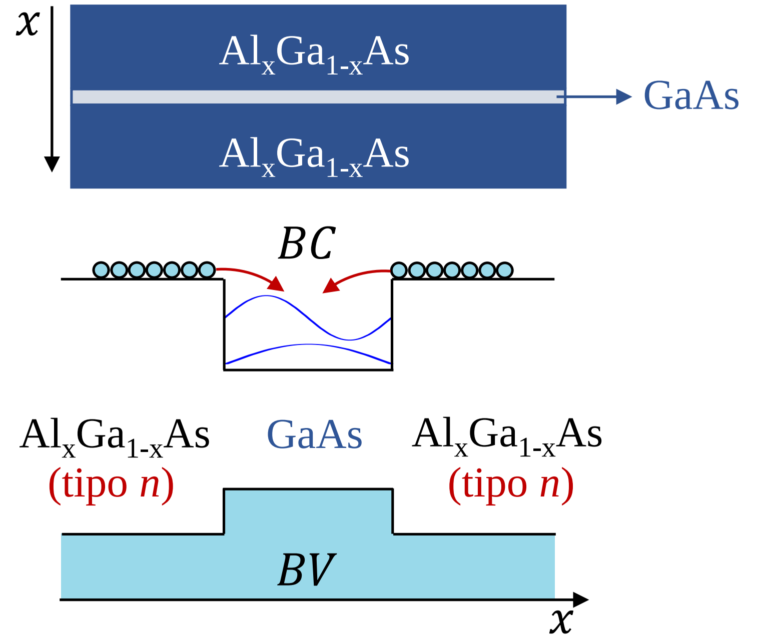


Al aumentar V_C por encima de V_{umbral}, sea crea un canal de conducción, cuyo tamaño (y resistencia) depende de V_C.

Pozos cuánticos

GaAs y AlAs son semiconductores de *gap* directo con E_g^{GaAs} = 1.4 eV y E_g^{AlAs} = 2.7 eV. Aleaciones $Al_xGa_{1-x}As$ tienen E_g intermedios.

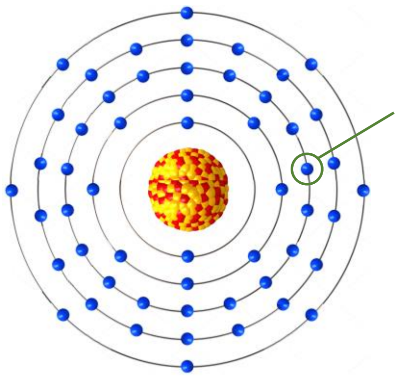
→ Heteroestructuras de $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ pueden formar pozos cuánticos.



Utilizando $Al_xGa_{1-x}As$ tipo *n*(*p*), e^-(h^+) "caen" al pozo creando un gas bidimensional de e^-(h^+).

Magnetismo

Magnetismo localizado



Vector potencial

Factor giromagnético

$$\mathcal{H}_{at} = \frac{\bar{p}^2}{2m_e} + V(\bar{r}) \xrightarrow{\text{Agregamos } \bar{H}} \mathcal{H} = \frac{\left(\bar{p} + \frac{e}{c}\bar{A}\right)^2}{2m_e} + g\mu_B \bar{H}\cdot\bar{\sigma} + V(\bar{r})$$

Espín

$\bar{l} = \bar{r}\times\bar{p}/\hbar$

$\bar{A} = \bar{H}\times\bar{r}/2$

$= e\hbar/2m_e c$

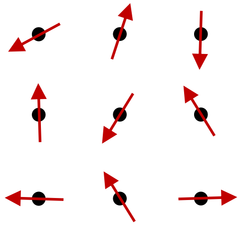
$$\mathcal{H} = \mathcal{H}_{at} + \mu_B \bar{H}\cdot(g\bar{\sigma} + \bar{l}) + \frac{e^2}{8m_e c^2}|\bar{H}\times\bar{r}|^2$$

Es siempre positivo y aumenta la energía

Factor de Landé

Sumando sobre todos los e⁻

$$\Delta\mathcal{H} = \mu_B \bar{H}\cdot\underbrace{(g\bar{S} + \bar{L})} + \frac{e^2}{8m_e c^2}\sum_i |\bar{H}\times\bar{r}_i|^2 = \underbrace{\mu_B g_L \bar{H}\cdot\bar{J}}_{\text{Paramagnetismo}} + \underbrace{\frac{e^2}{8mc^2}\sum_i |\bar{H}\times\bar{r}_i|^2}_{\text{Diamagnetismo}}$$



Se calcula con reglas de Hund

> 0: Feromagneto

< 0: Antiferromagneto

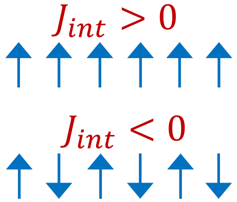
Agregamos J_{int}

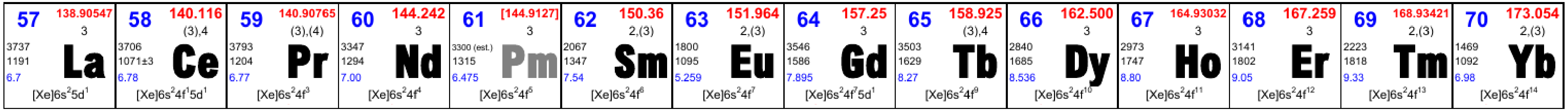
(Despreciamos diamagnetismo)

$$\Delta\mathcal{H}_{cristal} = \mu_B g_L \bar{H}\cdot\sum_m \bar{J}_m - \frac{J_{int}}{2}\sum_{m,n}\bar{J}_m\bar{J}_n$$

Corre sobre sitios de la red

Se usa para iones de tierras raras por orbitales localizados 4*f*.





57	58	59	60	61	62	63	64	65	66	67	68	69	70
138.90547	140.116	140.90765	144.242	[144.9127]	150.36	151.964	157.25	158.925	162.500	164.93032	167.259	168.93421	173.054
3	(3),4	(3),(4)	3	3	2,(3)	2,(3)	3	(3),4	3	3	3	2,(3)	2,(3)
3737	3706	3793	3347	3300 (est.)	2067	1800	3546	3503	2840	2973	3141	2223	1469
1191	1071±3	1204	1294	1315	1347	1095	1586	1629	1685	1747	1802	1818	1092
6.7	6.78	6.77	7.00	6.475	7.54	5.259	7.895	8.27	8.536	8.80	9.05	9.33	6.98
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
[Xe]6s^{2}5d^1	[Xe]6s^{2}4f^{1}5d^1	[Xe]6s^{2}4f^3	[Xe]6s^{2}4f^4	[Xe]6s^{2}4f^5	[Xe]6s^{2}4f^6	[Xe]6s^{2}4f^7	[Xe]6s^{2}4f^{7}5d^1	[Xe]6s^{2}4f^9	[Xe]6s^{2}4f^{10}	[Xe]6s^{2}4f^{11}	[Xe]6s^{2}4f^{12}	[Xe]6s^{2}4f^{13}	[Xe]6s^{2}4f^{14}

Magnetismo

Magnetismo itinerante: Orden magnético a campo nulo

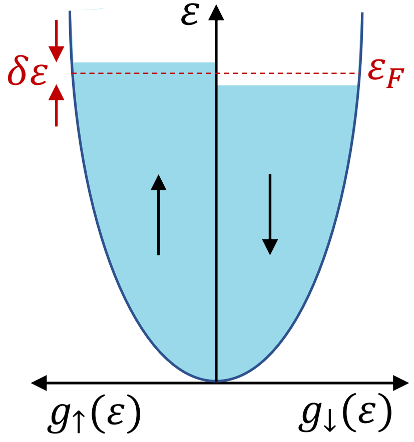
$$\mathcal{H} = \mathcal{H}_{Tight-Binding} + \mathcal{H}_{Hubbard} \qquad \mathcal{H}_{Hubbard} = U\sum_i n_{i\uparrow}n_{i\downarrow}$$

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 ↑ (↓) en el sitio i

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



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

Aproximo: $$Un_{i\uparrow}n_{i\downarrow} = \frac{U}{4}(n_{i\uparrow}+n_{i\downarrow})^2 - \frac{U}{4}(n_{i\uparrow}-n_{i\downarrow})^2 \approx \frac{U}{4}\overbrace{\langle n_{i\uparrow}+n_{i\downarrow}\rangle}^{\text{N° medio de e}^-\text{ por sitio: } x}{}^2 - \frac{U}{4}\overbrace{\langle n_{i\uparrow}-n_{i\downarrow}\rangle}^{=(\rho_\uparrow-\rho_\downarrow)v}{}^2$$

Magnetización: $$M = -\frac{g}{2}\mu_B(\rho_\uparrow-\rho_\downarrow) = -\frac{g\mu_B\delta\varepsilon}{4}g(\varepsilon_F) \rightarrow \frac{E_{Hubbard}}{V} = \boxed{\frac{U}{4}\frac{x^2}{v} - \frac{U}{v}\left(\frac{Mv}{g\mu_B}\right)^2}$$

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

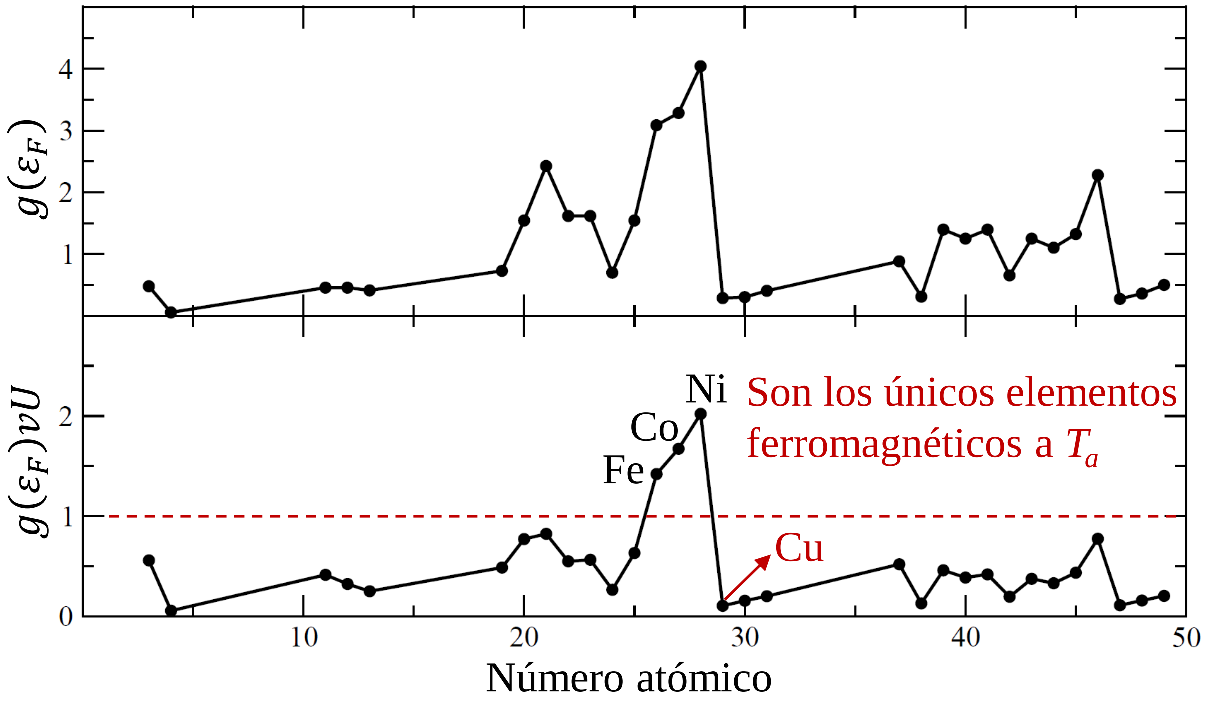
$$\approx \frac{\overset{= K(M=0)}{\enclose{circle}{K_0}}}{V} + \frac{g(\varepsilon_F)}{2}\left\{\left[\frac{(\varepsilon_F+\delta\varepsilon/2)^2}{2} - \frac{\varepsilon_F^2}{2}\right] - \left[\frac{\varepsilon_F^2}{2} - \frac{(\varepsilon_F-\delta\varepsilon/2)^2}{2}\right]\right\} = \frac{K_0}{V} + \frac{g(\varepsilon_F)}{2}\left(\frac{\delta\varepsilon}{2}\right)^2 = \boxed{\frac{K_0}{V} + \frac{g(\varepsilon_F)}{2}\left(\frac{2M}{g\mu_B g(\varepsilon_F)}\right)^2}$$

Magnetismo

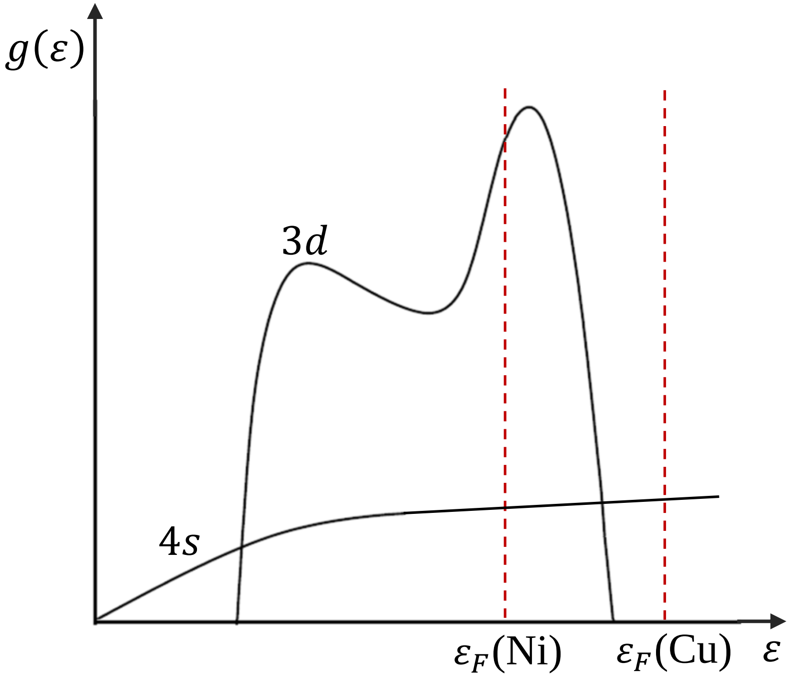
Magnetismo itinerante: Orden magnético a campo nulo

$$\frac{E}{V}=\frac{K+E_{Hubbard}}{V}=\frac{K_0+\overset{=\,E_{Hubbard}(M=0)}{\boxed{U_0}}}{V}+\frac{1}{2g(\varepsilon_F)}\left(\frac{2M}{g\mu_B}\right)^2-\frac{U}{v}\left(\frac{Mv}{g\mu_B}\right)^2=\frac{\overset{=\,E(M=0)}{\boxed{E_0}}}{V}+\left(\frac{M}{g\mu_B}\right)^2\left[\frac{2}{g(\varepsilon_F)}-vU\right]$$

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



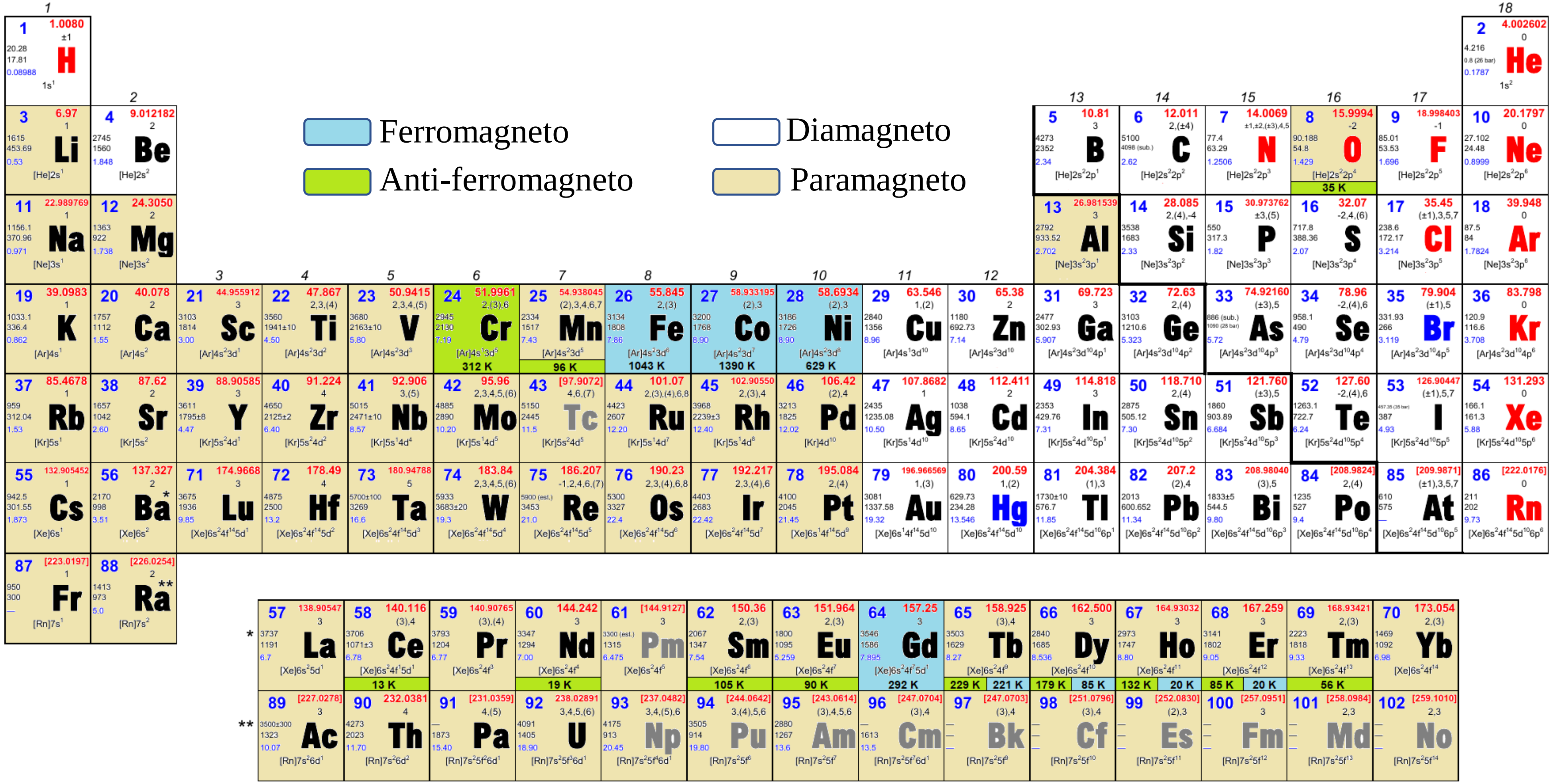
Son los únicos elementos ferromagnéticos a T_a



Magnetismo

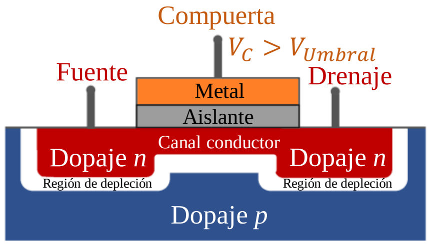
Magnetismo en la tabla periódica

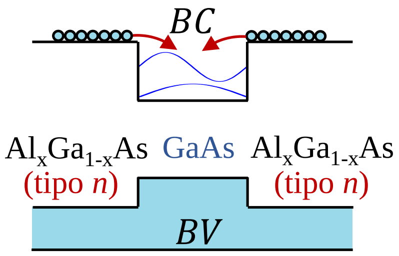
Considerando todas las contribuciones, se obtiene un comportamiento dominante.

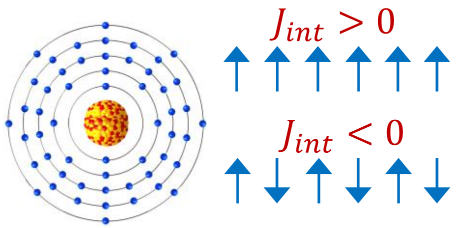


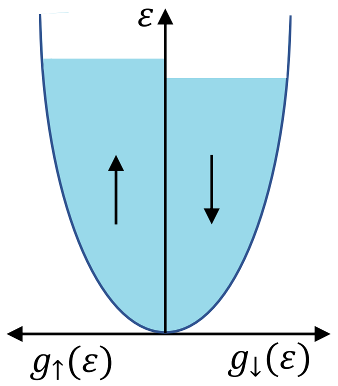
Resumen

- Transistor y pozos cuánticos
- Magnetismo localizado
- Ferromagneto/Anti-ferromagneto/Paramagneto/Diamagneto
- Magnetismo itinerante
- Hamiltoniano de Hubbard y Criterio de Stoner









Programa de la materia

- Red cristalina y red recíproca ✓
- Difracción de rayos X ✓
- Cohesión en sólidos ✓
- Vibraciones, fonones y propiedades térmicas ✓
- Electrones en sólidos ✓
- Semiconductores ✓
- Introducción a magnetismo ✓