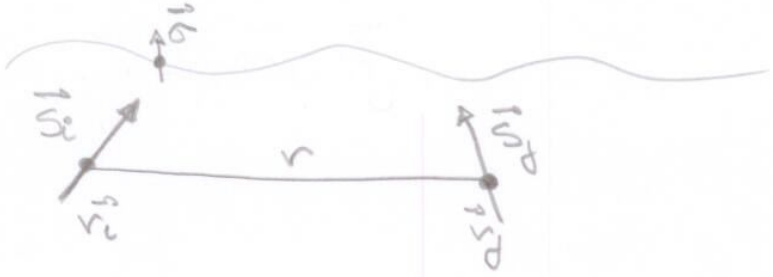
Magnetismo

(1) Magnetismo localizado - Terras raras.



$$\bar{J}(\vec{r}_i - \vec{r}_e)\, \bar{S}_i . \vec{\sigma}$$

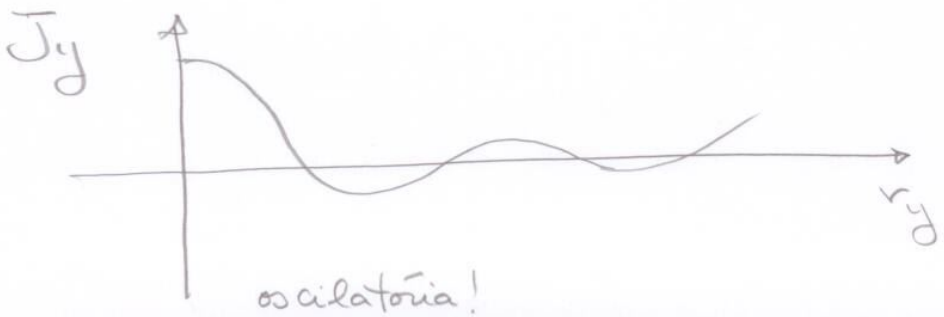
Em segunda ordem de teoria de perturbação

$$\mathcal{H} = -\sum J_{ij}\, \vec{S}_i . \vec{S}_j$$

$$J_{ij} = \frac{4\bar{J}^2 m k_F^4}{(2\pi)^3} \frac{k_F r \cos k_F r - \operatorname{sen} k_F r}{(k_F r)^4}$$

$$k_F r \gg 1$$

$$J_{ij} = \frac{4\bar{J}^2 m k_F^4}{(2\pi)^3} \frac{\cos k_F r}{(k_F r)^3}$$



oscilatória!

$$\mathcal{H} = -J \sum_{j} \vec{S}_i \cdot \vec{S}_j \qquad J \text{ (primeiros vizinhos)}$$

$$= -\sum_j \vec{h}_j \cdot \vec{S}_j \qquad \vec{h}_j = J \sum_i \vec{S}_i$$

Aproximação de campo médio

$$m = \chi_0 h$$

$$h = h_{ext} + h_{eff}$$

$$\boxed{h_{eff} = Jz\langle S \rangle \equiv \lambda m} \qquad \lambda = Jz$$

$$m = \chi_0 (h_{ext} + \lambda m)$$

$$m(1 - \lambda \chi_0) = \chi_0 h_{ext}$$

$$m = \chi h_{ext}$$

$$\chi = \frac{\chi_0}{1 - \lambda \chi_0}$$

$\chi_0 = C/T$ para momentos localizados

$$\chi = \frac{C/T}{1 - \lambda C/T} = \frac{C/T}{\frac{T - \lambda C}{T}} = \frac{C}{T - \lambda C}$$

$$\lambda C = T_c \Rightarrow \chi = \frac{C}{T - T_c}$$

Para eletrons itinerantes

$$\chi_0 = g\mu_B^2 \rho(E_F)$$

$$\chi = \frac{g\mu_B^2 \rho(E_F)}{1 - g\mu_B^2 \lambda \rho(E_F)}$$

$$\lambda = U/g\mu_B^2$$

$$m = \frac{g\mu_B^2 \rho(E_F)}{1 - U\rho(E_F)} h_{ext}$$

Modelo de Ising - Campo médio

$$\mathcal{H} = -J \sum_{ij} S_i^z S_j^z$$

$$= -\sum_j h_j S_j^z \qquad h_j = J \sum_i S_i^z$$

campo médio $h_j = Jzm = h$

Consideramos $S^z = \pm 1/2$ $\qquad \mathcal{H}_{CM} = -Jzm S_j^z$

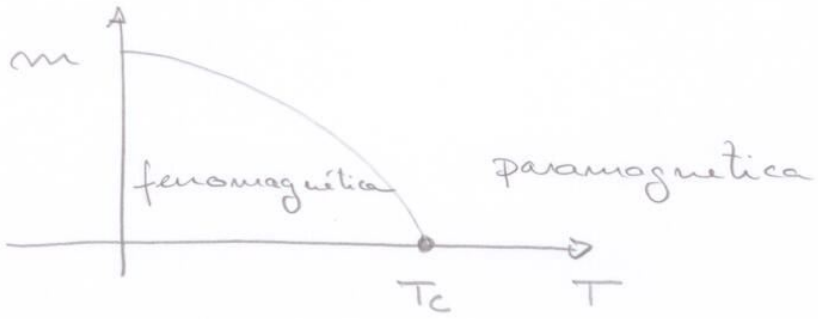
$$m = \langle S_j^z \rangle = \frac{\sum_{S^z} P(S_j^z) S_j^z}{\sum_{S^z} P(S_j^z)} = \frac{P(1/2)\,1/2 + P(-1/2)(-1/2)}{P(1/2) + P(-1/2)}$$

$$P(1/2) = e^{-\frac{\beta J z m}{2}} \quad ; \quad P(-1/2) = e^{\frac{\beta J z m}{2}}$$

$$\beta = 1/k_B T$$

$$m = (1/2)\left[\frac{e^{-\beta J z m/2} - e^{\beta J z m/2}}{e^{\beta J z m/2} + e^{-\beta J z m/2}} \right]$$

$$\boxed{m = \frac{1}{2} \tanh\left(\frac{\beta J z m}{2}\right)}$$



$T = 0$, $\tanh \infty = 1 \Rightarrow m = 1/2$

$T \to T_c$, $m \to 0$, $\tanh x \simeq x$

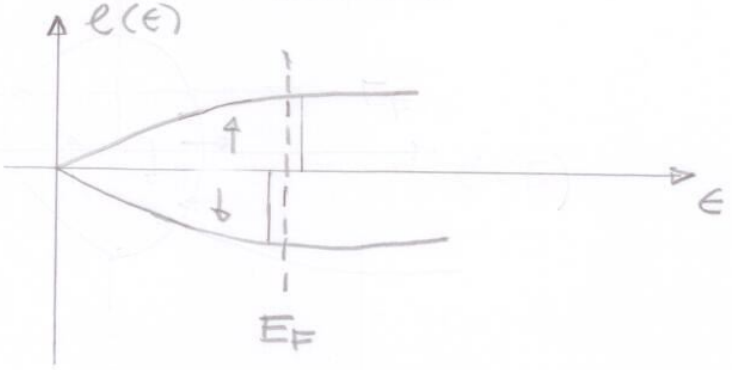
$$m = \frac{1}{2} \frac{J z m}{k_B T_c}$$

$$\boxed{k_B T_c = \frac{J z}{2}}$$

Ferromagnetismo, elétrons itinerantes

modelo de Hubbard

$$\mathcal{H} = \underbrace{\sum_{k,\sigma} \epsilon_k n_{k\sigma}}_{\text{energia cinética}} + \underbrace{U \sum_i n_{i\uparrow} n_{i\downarrow}}_{\text{repulsão coulombiana}}$$



Fase paramagnética $\quad n_{i\uparrow} = n_{i\downarrow}$

ou $\quad n_{0\uparrow} = n_{0\downarrow} = n/2$

Vamos transferir δn eletrons da banda de spin ↓ para a banda de spin ↑.

O custo de energia cinética é

$$\Delta E_{cin} = \delta\epsilon\, \delta n = \delta\epsilon \cdot \ell(E_F)\delta\epsilon$$
$$= \ell(E_F)\,\delta\epsilon^2 > 0$$

O custo de energia de interação é

$$\Delta E_{int} = U(n_0 + \delta n)(n_0 - \delta n) - U n_0^2$$
$$= -U\delta n^2 = -U\,\ell(E_F)^2 \delta\epsilon^2 < 0$$

A variação total de energia é

$$\Delta E_{tot} = \Delta E_{cin} + \Delta E_{int} = e(E_F)(\delta\epsilon)^2 - U e^2(E_F)(\delta\epsilon)^2$$

$$= e(E_F)(\delta\epsilon)^2 \left[1 - U e(E_F)\right]$$

que vai ser positivo ou negativo dependendo se $1 - U e(E_F)$ é maior ou menor que zero

$$1 - U e(E_F) = 0$$

instabilidade ferromagnética!

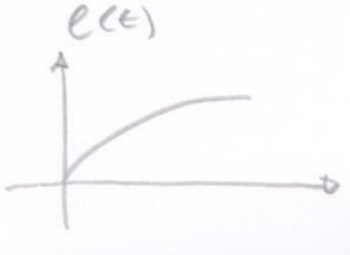
Densidade de estados

$$\epsilon(k) = k^2/2m \qquad e_k\,dk = e_\epsilon\,d\epsilon$$

$$e_k\,dk = \frac{V}{(2\pi)^3}\,4\pi k^2\,dk \qquad e_\epsilon = e(\epsilon) = \frac{e_k\,dk}{d\epsilon}$$

$$d\epsilon/dk = k/m \;;\; k = \sqrt{2m\epsilon} \qquad e(\epsilon) = \frac{e_k}{d\epsilon/dk}$$

$$e(\epsilon) = \frac{V}{(2\pi)^3}\frac{4\pi k^2}{d\epsilon/dk} = \frac{V}{(2\pi)^3}\frac{4\pi\, 2m\epsilon}{\sqrt{2m\epsilon}/m}$$



$$e(\epsilon) = \frac{Vm}{2\pi^2}\sqrt{2m\epsilon} = \frac{V\sqrt{2}}{2\pi^2}m^{3/2}\epsilon^{1/2}$$