Chap 8:

Origins of Ferromagnetism: Exchange

$\Rightarrow$ Spin-Symmetry $\Rightarrow$ Atomic picture

$\Leftrightarrow$ Rare Earths

$\longrightarrow$ Homogeneous e^- gas: "Metal"

$\Rightarrow$ Indep. Model: Pauli - PARAmagn.

$\Rightarrow$ HF: $\Rightarrow$ Chap. 6

X

$$\left(\frac{E}{N}\right)^{HF} = \frac{36.1\,eV}{\left(\frac{r_s}{a_B}\right)^2} - \frac{12.5\,eV}{\left(\frac{r_s}{a_B}\right)}$$

$\frac{N}{V} \Rightarrow$

$$\Rightarrow \frac{r_s}{a_B} = \left(\frac{3}{4\pi}\left(\frac{V}{N}\right)\right)^{1/3}$$

$$\Rightarrow E = N\left\{78.2\,eV\left(\frac{N}{V}\right)^{2/3} - 20.1\,eV\left(\frac{N}{V}\right)^{1/3}\right\}$$

$$N = N^{+} + N^{-}$$

$$= N \left\{ 78.2\,\mathrm{eV} \left[\left(\frac{N^+}{V}\right)^{2/3} + \left(\frac{N^-}{V}\right)^{2/3} \right] - 20.1\,\mathrm{eV} \left[\left(\frac{N^+}{V}\right)^{1/3} + \left(\frac{N^-}{V}\right)^{1/3} \right] \right\}$$

$$E(N^+) + E(N^-)$$

$$\Rightarrow N,\; P = \frac{N^+ - N^-}{N} \begin{cases} \to \pm 1 & M_S \gg 0 \\ \to 0 & M_S = 0 \end{cases}$$

$$= N \cdot T \cdot \left\{ \frac{1}{2}\left[(1+P)^{5/3} + (1-P)^{5/3} \right] - \frac{5}{4}\,\alpha \left[(1+P)^{4/3} + (1-P)^{4/3} \right] \right\}$$

$$N^+ = \frac{N}{2}(P+1)$$

$$N^- = \frac{N}{2}(P-1)$$

historical Notation

$\to$ Bloch

$$\alpha \to \frac{1}{10}\left(\frac{V}{N}\right)^{1/3}$$

$\alpha = ?$ Ferromagnetic state?

$$\Rightarrow \Delta \doteq E(N,P) - E(N,P=0)$$

$$= NT\left\{\frac{1}{2}\left[(1+P)^{5/3} + (1-P)^{5/3} - 2\right] - \frac{5}{4}\alpha\left[(1+P)^{4/3} + (1-P)^{4/3} - 2\right]\right.$$

$$\overset{!}{<} 0$$

$$\underbrace{\alpha > \alpha_c = 0.905}$$

$$\left(\frac{r_s}{a_0}\right) \gtrsim 5.45$$

$\to$ Cs Ferromagnet

$\to$ Fe, Ni, Co NOT?

Metals: $1.8 < \quad) \quad < 5.6$

$\to$ Even in improved theories (XC) $\to$ results even wronger

$\Rightarrow$ Homo. e^- gas is wrong!

$\Rightarrow$ Band description:

DFT-Formalism: $n(r) = n^+(r) + n^-(r)$

$$m(r) = \left(n^+(r) - n^-(r)\right)\mu_B$$

$\to$ DFT-LDA (spin polarized)

gives right results: Fe, Ni, Co Ferromagnets

$\Rightarrow$ DFT: xc-potential: Taylor-Expansion

$$V_{xc} \approx \frac{\delta E_{xc}(n^+, n^-)}{\delta m} \approx V_{xc}^0(n, m=0) + \tilde{V}(r)\, m(r)$$

$$= V_{xc}^0 \pm \frac{1}{2} I\, M$$

$\hookrightarrow I$ ... Stoner parameter $\rightarrow$ X integrals

$$M = \int \cancel{\#}\, dr\; m(r)$$

$$\Rightarrow \varepsilon_i^{+/-} = \varepsilon_i^0 \pm \frac{1}{2} I M$$

$$N^{+/-}(E) = \sum_i \int_{BZ} d\vec{k}\; \delta(E - \varepsilon_i(\vec{k}))$$

$$= N^0(E \pm \tfrac{1}{2} I M)$$

$$N = \int_0^{\varepsilon_F} [N^0(E + \tfrac{1}{2} I M) + N^0(E - \tfrac{1}{2} I M)]\, d\varepsilon$$

$$M = \int_0^{\varepsilon_F} [\quad M \quad - \quad M\;]\, d\varepsilon$$

$F(M) \stackrel{!}{=} M \rightarrow$ Self-consistently

$$F(0) = 0 \qquad\qquad F(\pm\infty) = \pm\infty$$

$$F(-M) = F(+M) \quad F'(M) \geq 0$$

Slope larger 1 at $M=0$ $\Rightarrow$ spontaneous $M_S \neq 0$

$$J \cdot N^0(\varepsilon_F) > 1$$

Fe, Ni, Co

DFT

$\underbrace{\text{STONER Criteria}}$

Descriptors

"Find something simple to describe something complex"

Magnetic Domain Structure: Macroscopic

short ranged χ

long range dipoles