

Chap 8:

Origine of Ferromagnetism: Exchange

\Rightarrow Spin-Symmetry \Rightarrow Atomic picture

\leftrightarrow Rare Earths

\rightarrow Homogeneous e^- gas: "Metal"

\Rightarrow Indep. Model: Pauli - P&R magn.

\Rightarrow HF: \Rightarrow Chap. 6

$$\left(\frac{\bar{E}}{N}\right)^{HF} = \frac{30.1 \text{ eV}}{\left(\frac{r_s}{a_0}\right)^2} - \overset{x}{\frac{12.5 \text{ eV}}{\left(\frac{r_s}{a_0}\right)}}$$

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

$$\Rightarrow \frac{r_s}{a_0} = \left(\frac{3}{4\pi} \left(\frac{V}{N}\right)^{1/3}\right)$$

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

$$N = N^+ + N^-$$

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

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

$$\Rightarrow N, P = \frac{N^+ - N^-}{N} \begin{cases} \pm 1 & M_s \geq 0 \\ 0 & M_s = 0 \end{cases}$$

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

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

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

↓ historical notation
→ Bloch

$$\rightarrow \frac{1}{10} \left(\frac{V}{N} \right)^{1/3} \rightarrow \alpha = ? \text{ Ferromagnetic state?}$$

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

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

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

$$\leq 0$$

$$d > d_c = 0.905$$

$$\left(\frac{r_s}{a_B} \right) \approx 5.45$$

Metals: $1.8 < \dots < 5.6$

Cs Ferromagnet
 Fe, Ni, Co NOT

Even in improved theories (XC) → results even wronger

⇒ Homo. e^- gas is wrong!

⇒ Band description:

$$\text{DFT-Formalism: } n(r) = n^+(r) + n^-(r)$$

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

→ DFT-LDA (spin polarized)

gives right results: Fe, Ni, Co ferromagnets

⇒ DFT: xc-potential: Taylor-Expansion

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

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

↪ ... Stoner parameter → X integrals
 $M = \int dr m(r) \leftarrow$

$$\Rightarrow \mathcal{E}_i^{\pm} = \mathcal{E}_i^0 \pm \frac{1}{2} \mathcal{I} M$$

$$N^{\pm}(E) = \sum_i \int_{BZ} d\vec{k} \delta(E - \mathcal{E}_i(\vec{k}))$$

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

$$N = \int_0^{\mathcal{E}_F} [N^0(E + \frac{1}{2} \mathcal{I} M) + N^0(E - \frac{1}{2} \mathcal{I} M)] dE$$

$$\hat{M} = \int_0^{\mathcal{E}_F} [\quad] dE$$

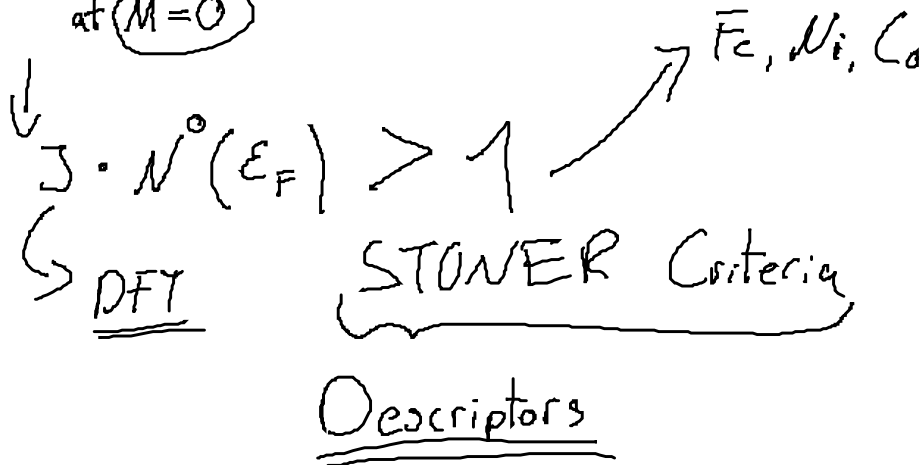
$F(M) \hat{=} M \rightarrow$ Self-consistently

$$F(0) = 0$$

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

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

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



"Find something simple to describe something complex"

Magnetic Domain Structure: Macroscopic

