Lecture 22 - WiSe2022/2023

Thursday, January 5, 2023 6:59 PM

3.5. Exchange interaction between itinerant (mobile) electrons

- Important for descriptions of ferromagnets (Ni, Co, Fe)

↳ collective exchange interaction between e^- + a whole e^- gas

step #1 : exchange interaction between two free e^-

- two e^- (i and j), pair wave function, plane waves $\phi = e^{i \cdot k \cdot r}$, same spin

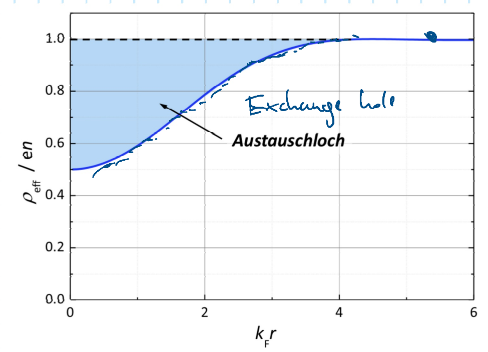
$$\psi_{ij} = \frac{1}{\sqrt{2}\,V}\left[e^{i \cdot k_i \cdot r_i} \cdot e^{i \cdot k_j \cdot r_j} - e^{i k_i \cdot r_j} \cdot e^{i \cdot k_j \cdot r_i}\right]$$

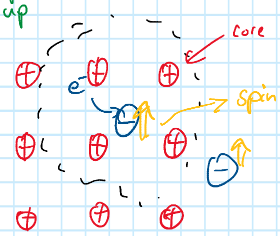
Probability

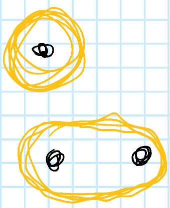
$$|\psi_{ij}|^2 \, dr_i^3 \, dr_j^3 = \frac{1}{V^2}\left[1 - \cos\left\{(k_i - k_j)\cdot(r_i - r_j)\right\}\right] dr_i^3 \, dr_j^3$$

$r_i = r_j$

$$\rho_{eff}(\vec{r}) = \underbrace{\frac{e\,n}{2}\left\{1 - 9 \cdot \frac{\left[\sin(k_F \cdot r) - k_F \cdot r \cdot \cos(k_F \cdot r)\right]^2}{(k_F \cdot r)^6}\right\}}_{\Uparrow \text{ spin up}} + \underbrace{\frac{e \cdot n}{2}}_{\Downarrow \text{ spin down}}$$







⇒ e^- less shielded by any other e^-

↳ see more positive cores

↳ Higher binding energy

→ good for Coulomb interaction

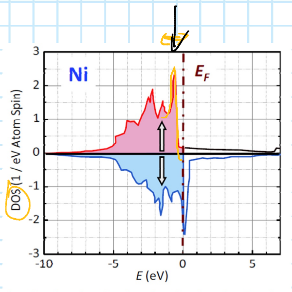
↳ BUT: trapped in a whole

↳ Higher kinetic energy

- Can have a positive or negative energy contribution $[\Delta E_{pot} + \Delta E_{kin}]$

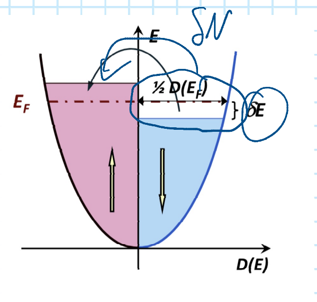
- ΔE_{kin} : $\delta p \sim \frac{\hbar}{\delta x} \sim \hbar k_F \Rightarrow \Delta E_{kin} \propto \frac{\delta p^2}{2m^*} \propto \frac{k_F^2}{m^*}$

ΔE_{pot} : $U \propto \frac{1}{r} \propto k_F$



$\Delta E_{pot} > \Delta E_{kin} \rightarrow m^*$ large $\rightarrow$ flat bands
$\rightarrow$ DOS high $\rightarrow$ conduction bands 3d, 4f, 5f

Step #2 : Band ferromagnetism in metals (Stoner criterion)



$\rightarrow$ Assume that the e^- levels renormalize due to e^- correlations of e^- with the same spin

$\hookrightarrow$ some $\downarrow$ will switch to $\uparrow$

$\hookrightarrow$ kinetic Energy change: $\delta N = \frac{1}{2} \cdot D(E_F) \cdot \delta E$

$$\Delta E_{kin} = \frac{\delta N}{V} \cdot \delta E = \frac{1}{2V} \cdot D(E_F) \cdot \delta E^2$$

$\hookrightarrow$ potential energy :

$$N_{\uparrow\downarrow} = \frac{N}{2} \pm \delta N \quad ; \quad n_{\uparrow/\downarrow} = \frac{n}{2} \pm \delta n \qquad n = \frac{N}{V}$$

- Magnetization

$$M_A \overset{?}{=} -\frac{1}{2} \cdot g \cdot \mu_B \cdot \left[n_\uparrow - n_\downarrow\right] = -\mu_B \cdot \frac{D(E_F)}{V} \cdot \delta E$$

- imagine M_A is creating a fictious inner „molecular B-field"

$$B_A = \cdot \mu_0 \cdot \lambda \cdot M_A$$

λ: molecular field constant

$$\Delta E_{pot} = -\int_0^{B_A} M \cdot dB = -\mu_0 \cdot \lambda \int_0^{M_A} M \cdot dM = -\frac{1}{2} \cdot \mu_0 \cdot \lambda \cdot M_A^2$$

$$\Delta E_{pot} = \underbrace{-\frac{1}{2} \mu_0 \cdot \lambda \cdot \mu_B^2}_{-\frac{1}{4} U} \left[\frac{D(E_F)}{V} \cdot \delta E\right]^2$$

$$U = \frac{1}{V} \cdot 2 \cdot \mu_0 \cdot \mu_B^2 \cdot \lambda$$

$$\Delta E = \Delta E_{kin} + \Delta E_{pot} = \frac{1}{2V} \cdot D(E_F) \cdot [\delta E]^2 \cdot \Big[\underbrace{1 - \frac{1}{2} \cdot U \cdot D(E_F)}_{1/[\cdot]\ :\ \text{Stoner factor}} \Big]$$

$$\boxed{\frac{1}{2} U D(E_F) > 1}$$

↳ FM requires a high U and/or a high DOS