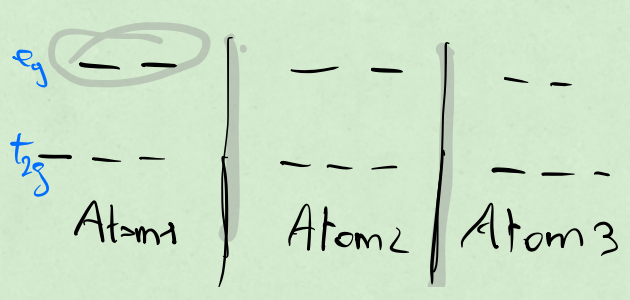
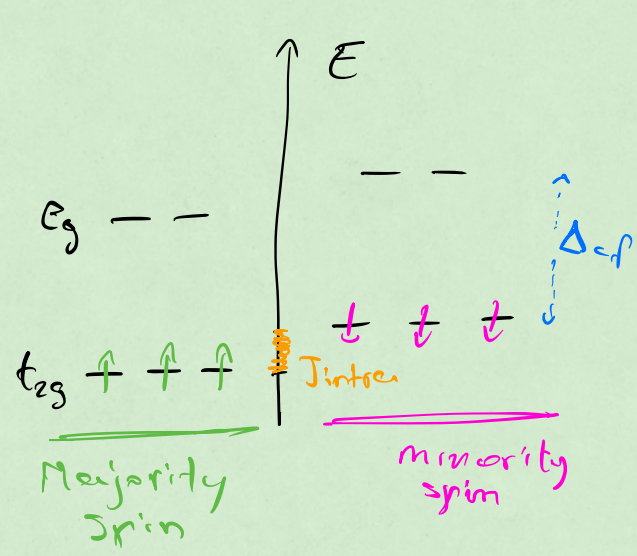
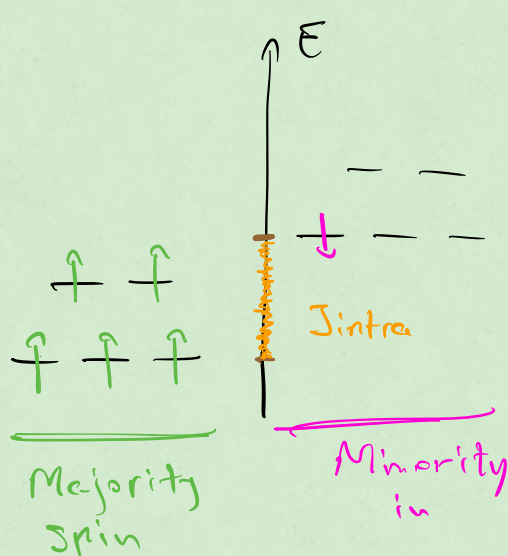
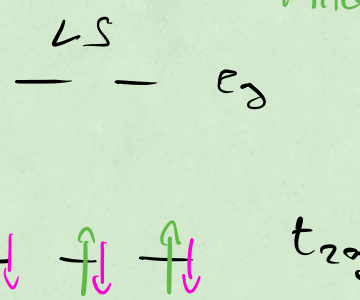
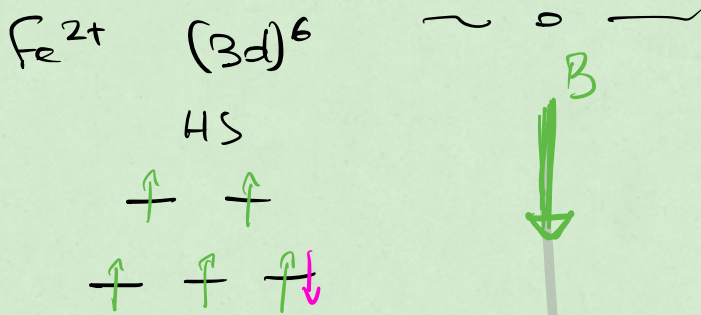


	S	$\mu_{th} [\mu_B]$	μ^{exp}
Fe^{2+}	2	4	2.2
Co^{2+}	$3/2$	3	1.7
Ni^{2+}	1	2	0.6

- th.
- assumed HS
 - quenching of L

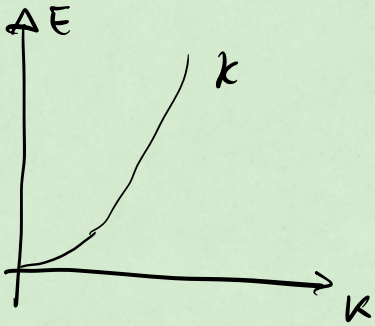
LOCAL MOM. MAGNETISM



Separated atoms



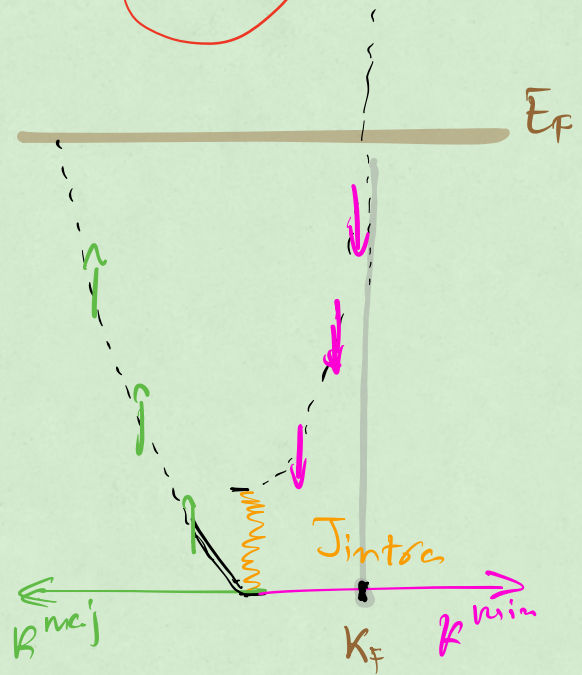
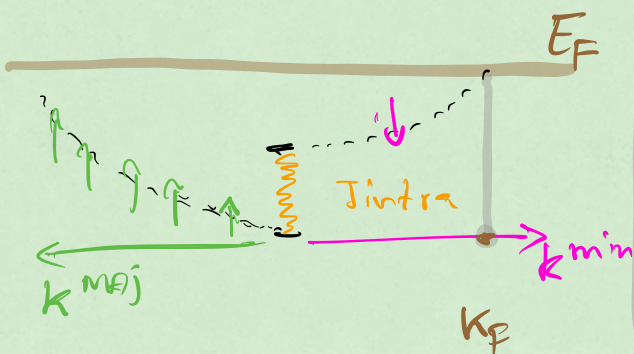
ITINERANT MAGNETISM



How do I split bands to recreate HS vs LS configuration

HS

LS



$$k_F^{HS} > k_F^{LS}$$

High DOS
"flat" band

low DOS
"parabolic" band

Lecture 7.11.2022

$$E_{\text{ech}} = - J_{\text{intra}} P \dots \text{spin polarization } (n_{\uparrow} - n_{\downarrow})$$

$$D^{\text{maj}}(E) = D_0 \left(E + \frac{J_{\text{intra}} P}{2} \right)$$

$$D^{\text{min}}(E) = D_0 \left(E - \frac{J_{\text{intra}} P}{2} \right)$$

$$N = \int_0^{E_F(P)} (D^{\text{maj}} + D^{\text{min}}) dE$$

$$P = \int_0^{E_F(P)} (D^{\text{maj}} - D^{\text{min}}) dE$$

(E_F, P) unknowns

DOS(E) and any given energy range gives the number of levels in that range; thus $\text{DOS}(E)dE$ is the number of levels lying between the energies E and $E + dE$, and $1/\text{DOS}(E)$ is the average energy separation of adjacent levels in that range. The DOS as a function of energy, shown in figure 3.2.b for manganese, can be obtained from the band structure in momentum space. As a rule of thumb, a peaked density of state (flat band) corresponds to a more localized character of the electron, while a smeared out density of state (parabolic band) corresponds to electrons with more itinerant character.

Stoner criterion

Let us go back to the explanation of metallic ferromagnetism. We sketch in the following the main ideas behind the Stoner-Wohlfarth-Slater model, which is an extension of band theory to include the effect of an intra-atomic exchange interaction. These two ingredients allow establishing a condition for the existence of an imbalance between majority and minority spins in itinerant electrons. Defining the polarization P with respect to some spin quantization axis³ as the difference between the number of majority- and minority-spin electrons $P = N^{\text{maj}} - N^{\text{min}}$, one can express the exchange contribution to the electron-gas energy as

$$E_{\text{exch}} = -J_{\text{intra}}P. \quad (3.1)$$

In the equation above J_{intra} can be identified with the intra-atomic exchange interaction responsible for the first Hund's rule in atoms. Let $D_0(E)$ be the density of states per atom common to both spin channels in the absence of spin imbalance. Then we apply an opposite shift to the energy of electrons with majority and minority spin to account for the exchange energy given in Eq. (3.1) (see Fig. 3.3):

$$D^{\text{maj}}(E) = D_0 \left(E + \frac{1}{2} J_{\text{intra}} P \right)$$

$$D^{\text{min}}(E) = D_0 \left(E - \frac{1}{2} J_{\text{intra}} P \right).$$

At this point the problem is defined by the following pair of equations

$$\begin{cases} N = \int_0^{E_F(P)} \left[D_0 \left(E + \frac{1}{2} J_{\text{intra}} P \right) + D_0 \left(E - \frac{1}{2} J_{\text{intra}} P \right) \right] dE \\ P = \int_0^{E_F(P)} \left[D_0 \left(E + \frac{1}{2} J_{\text{intra}} P \right) - D_0 \left(E - \frac{1}{2} J_{\text{intra}} P \right) \right] dE, \end{cases} = F(P) \quad (3.2)$$

³To help visualization the spin quantization direction has been defined in Fig. 3.3 along the direction of an external magnetic field.

$$P = F(P) \quad \rightarrow \quad \begin{cases} y = F(P) \\ y = P \end{cases}$$

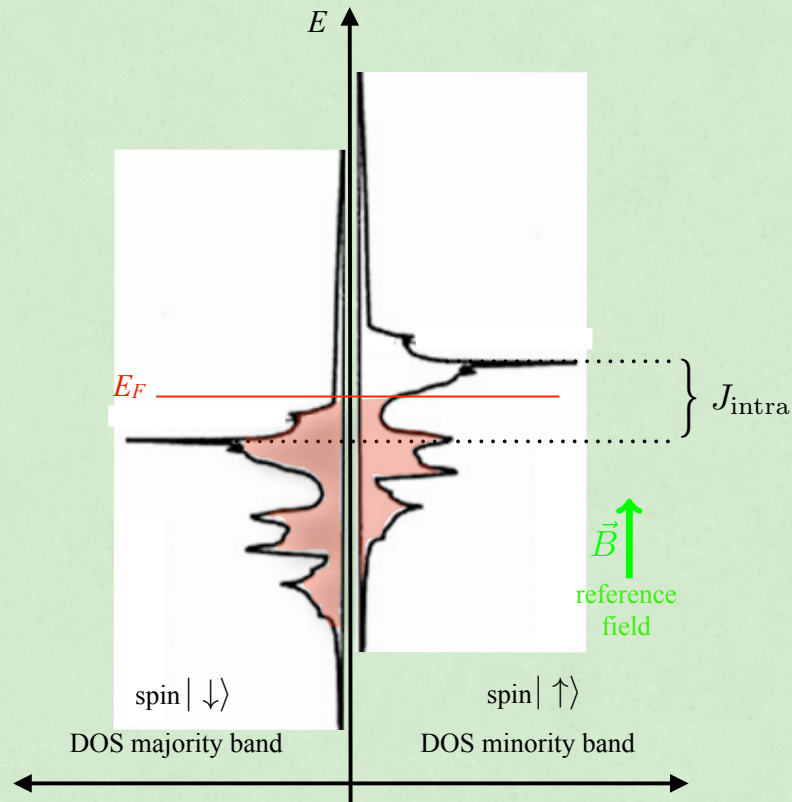


Figure 3.3: Pictorial representation of the Stoner-Wohlfarth-Slater model in terms of the density of states (DOS) of d electrons. The red-shaded area indicates filled electron states below the Fermi energy E_F , while empty states above E_F are shown without shadowing. The spin states with the largest number of electrons are called “majority spins” and the corresponding band is the “majority band”; the term “minority” is used for the other electron spins and band. The centers of the majority and minority d bands, assumed to be reasonably localized, are separated by the splitting produced by the intra-atomic exchange interaction J_{intra} . Since the labels “spin-up” and “spin-down” are only meaningful in conjunction with a quantization direction, an external field defines this quantization axis.

in which the unknowns are the spin polarization P and the Fermi energy $E_F(P)$. We will come back to the dependence of E_F on P later on. Practically, the core levels are not relevant in this problem because the electrons occupying those levels are all paired in spin singlets and, thus, do not contribute to the spin imbalance. Therefore, $N = N^{\text{maj}} + N^{\text{min}}$ can be identified with the number of electrons in the outer shell of a magnetic atom. Ideally, one can imagine solving the first equation to obtain $E_F(P)$ and insert this quantity in the second one. In this way, one would end up dealing with a self-consistent equation for the unknown P qualitatively similar to the equation of state of a ferromagnet obtained with the mean-field approximation: $P = F(P)$. The function $F(P)$ has the following important properties:

1. $F(0) = 0$
2. $F(-P) = -F(P)$, i.e. $E_F(-P) = E_F(P)$
3. $F(\pm\infty) = \pm P_{\text{Hund}}$ and $-P_{\text{Hund}} < F(P) < +P_{\text{Hund}}$
4. $F'(0) = (dF/dP)_{P=0} \geq 0$.

P_{Hund} is the largest attainable polarization of the electron gas and corresponds to the magnetic moment obtained applying the first Hund's rule to the considered metal⁴. Under these conditions, the graphical solution of the implicit equation for P evidences two possible scenarios. For $F'(0) < 1$, the equation $P = F(P)$ has only the solution $P = 0$ (curve a in Fig. 3.4). For $F'(0) > 1$, the equation has three solutions: $P = 0$ and two solutions with finite P of opposite sign (marked with open circles on the curves b and c in Fig. 3.4). The last ones generally provide non-integer values of P . In this case it can be shown that the $P = 0$ solution maximizes the total energy, while the two solutions with opposite sign are the minima of the energy associated with a finite spin imbalance in the ground state. In particular, the atomic magnetic moment is related to the spin imbalance by the equation

$$\mu = \frac{1}{2}g\mu_B P, \quad (3.3)$$

where P is a solution of the equation $P = F(P)$. Various solutions of this equation are qualitatively summarized in Fig. 3.4, where they are indicated with \bar{P} to help distinguish between different cases. A finite polarization is

⁴To be precise, by P_{Hund} we mean the polarization that the atom in a solid would have without taking into account the itinerant character of conduction electrons. Therefore, P_{Hund} shall generally be smaller than the free-ion value because of the quenching of the orbital momentum operated by the crystal field.

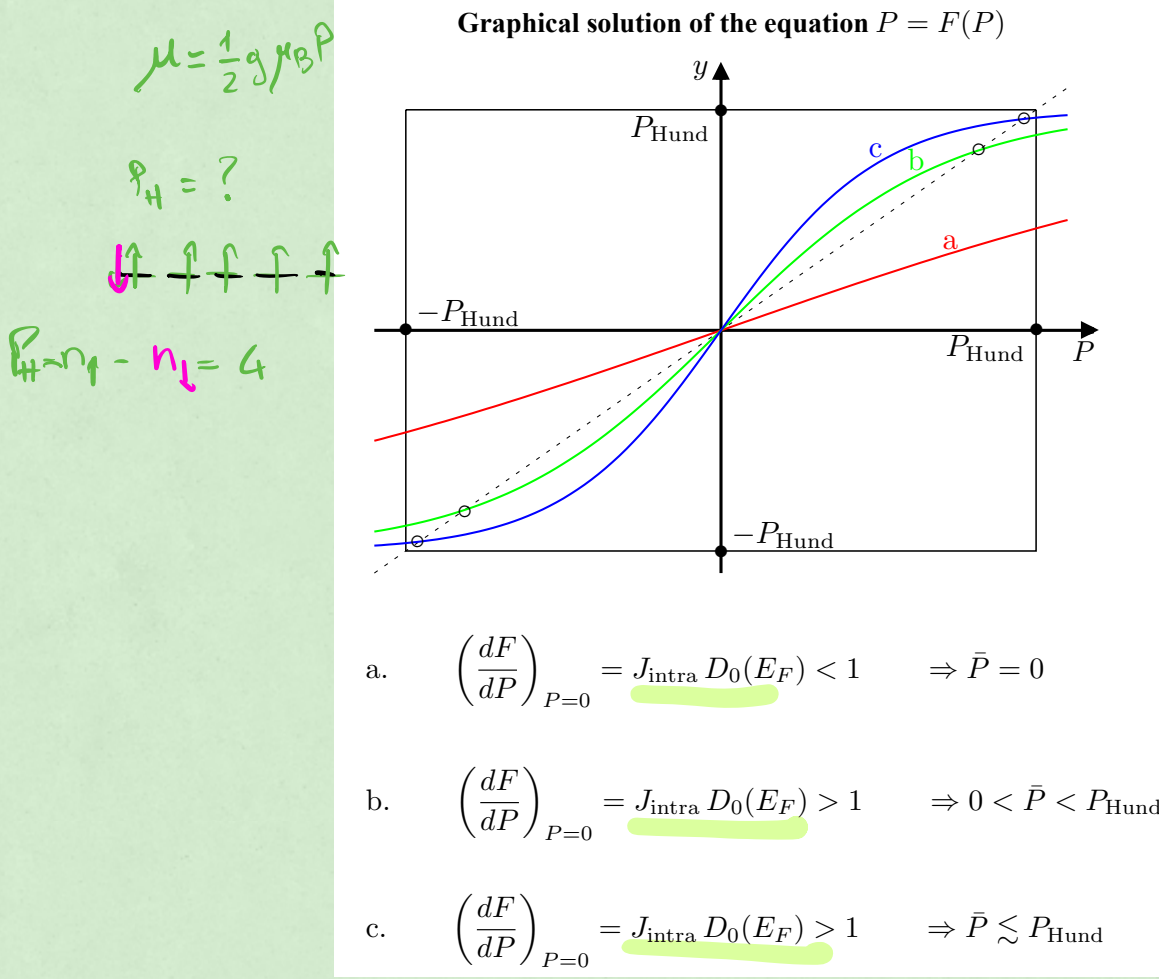
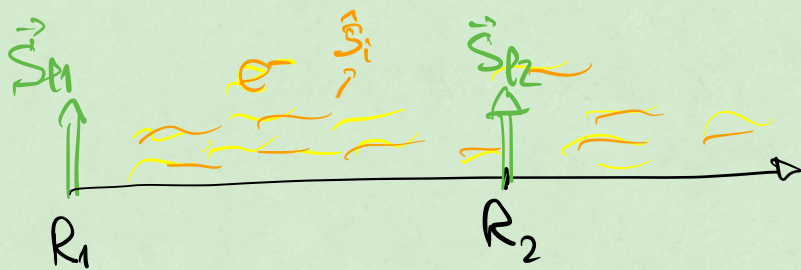


Figure 3.4: The dashed straight line indicates the bisectrix $y = P$. Solid lines indicate representative functions $y = F(P)$ obtained (qualitatively) for different values of $J_{\text{intra}} D_0(E_F)$, which define the slope of the curves $y = F(P)$ at the origin (see Eq. (3.4)). Intersections of the straight line and the curves give the solutions to the equation $P = F(P)$ – here indicated with \bar{P} . Non-trivial solutions are marked with open circles. The red curve labeled with a does not fulfill the Stoner criterion in Eq. (3.5), therefore the only trivial solution $\bar{P} = 0$ is obtained. The other two curves labeled with b and c fulfill the criterion. The green curve (b) corresponds to a smaller value of $J_{\text{intra}} D_0(E_F)$, which yields an absolute value of the polarization \bar{P} significantly smaller than the maximal value P_{Hund} (marked with full dots on the axes). The blue curve (c) corresponds to a larger value of $J_{\text{intra}} D_0(E_F)$ for which the absolute value of the polarization \bar{P} approaches P_{Hund} .



$$H_{e-i} = - \underbrace{J_{\text{intra}} \hat{S}_{R1}}_{\text{parametric dependence}} \cdot \hat{S}_i(\underline{r}) \delta(\underline{r} - R_1)$$

$$H_{e-i} = g/\mu_B \vec{B}_{\text{eff}} \cdot \hat{S}_i(\underline{r})$$

Let's take $\underline{R}_1 = 0$

$$\vec{B}_{\text{eff}} \sim J_{\text{intra}} \vec{S}_{R1} \delta(\underline{r})$$

$$\hat{S}_i(\underline{r}) \sim J_{\text{intra}} \hat{S}_{R1} \int \chi(\underline{q}) e^{-i\underline{q} \cdot \underline{r}} d\underline{q}$$

conduction electrons (note the similarity with the assumption made in the calculation to estimate the magnetic anisotropy of Mn^{3+}). Under this hypothesis, the magnetic response of the conduction-electron gas is just the response to a δ -like excitation, which in the framework of magnetism is described by the susceptibility dependent on the wave vector $\chi(\underline{q})$:

$$\hat{\mathbf{s}}_i(\underline{r}) \propto J_{\text{intra}} \hat{\mathbf{S}}_l \int \chi(\underline{q}) e^{-i\underline{q}\cdot\underline{r}} d^d q. \quad (3.8)$$

The equation above relates the spatial dependence of the spin polarization of the electron gas surrounding a magnetic atom (“impurity”) to the susceptibility $\chi(\underline{q})$ of the gas itself. In order to provide an explicit dependence of $\hat{\mathbf{s}}_i$ on \underline{r} , one needs to know the expression of the susceptibility. Apart from constant prefactors – in which we are not interested – this is given by

$$\chi(\underline{q}) \propto \frac{1}{2} + \frac{k_F}{2q} \left(1 - \frac{q^2}{4k_F^2} \right) \ln \left| \frac{2k_F + q}{2k_F - q} \right|, \quad (3.9)$$

where k_F is the Fermi wave vector. Using a mathematical equivalence⁶ from Eq. (3.9) one obtains that

$$\int \chi(\underline{q}) e^{-i\underline{q}\cdot\underline{r}} d^d q \propto \frac{\sin(2k_F r) - 2k_F r \cos(2k_F r)}{(k_F r)^4}. \quad (3.11)$$

Combined with Eq. (3.8), the last expression tells us that when a localized magnetic moment is introduced into a metal, the spins of conduction electrons develop an oscillating polarization in the vicinity of the local moment⁷. The polarized conduction electrons, in turn, shall produce an effective field on the magnetic moment localized at another lattice site, by virtue of Eq. (3.6) itself. This eventually leads to an effective exchange coupling between the spins $\hat{\mathbf{S}}_{l1}$ and $\hat{\mathbf{S}}_{l2}$ associated with two localized magnetic moments in the metal

$$\mathcal{H}_{\text{RKKY}} = -J_{\text{RKKY}} \hat{\mathbf{S}}_{l1} \cdot \hat{\mathbf{S}}_{l2} \quad (3.12)$$

with

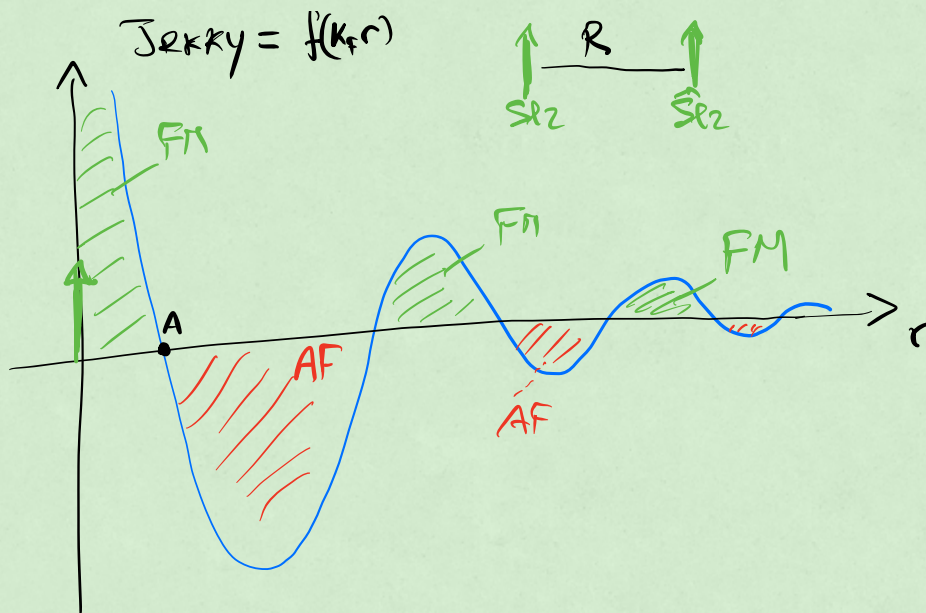
$$J_{\text{RKKY}} = J_0 \frac{2k_F R \cos(2k_F R) + \sin(2k_F R)}{(k_F R)^4}. \quad (3.13)$$

typo!

⁶The equivalence of interest is

$$\ln \left| \frac{2k_F + q}{2k_F - q} \right| = 2 \int_0^\infty \frac{\sin(2k_F x) \sin(qx)}{x} dx. \quad (3.10)$$

⁷These spin-density oscillations have the same form as the Friedel charge-density oscillations that result when an electron gas screens out a charge impurity.



$$J(k_F r) = 0 \quad k_F r_A = \dots \pi = \text{const.}$$

$$\frac{2\pi}{\lambda_F} \cdot r_A = \text{const.} \Rightarrow r_A = \alpha \lambda_F$$

if $R < r_A$ FM coupling 😊

if $R > r_A$ AF coupling (up to the next node!)

Physical meaning

$$\left. \begin{array}{l} \lambda_F \sim \frac{1}{k_F} \\ k_F^3 \sim N_{e, \text{band}} \end{array} \right\} \Rightarrow \lambda_F \sim \frac{1}{(N_{e, \text{band}})^{1/3}}$$