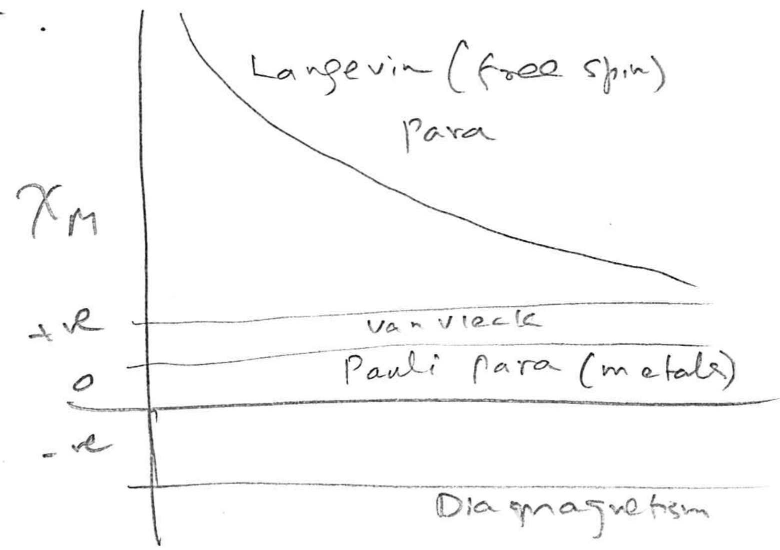
Pauli paramagnetism

Using Classical mechanics, $M = N\mu_B^2 B / k_B T$ (Anil)

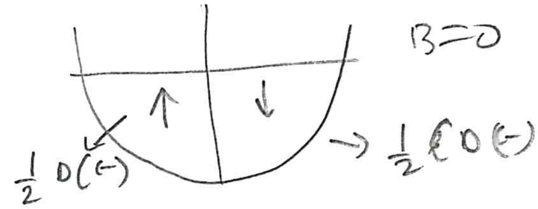
Instead it is observed magnetism of non-ferro material is independent of T.



Most electrons cannot respond to external field because states are already occupied. Only electrons within $k_B T$ can respond. Only a fraction $T/T_F \sim 0.01$ contribute to spin susceptibily.

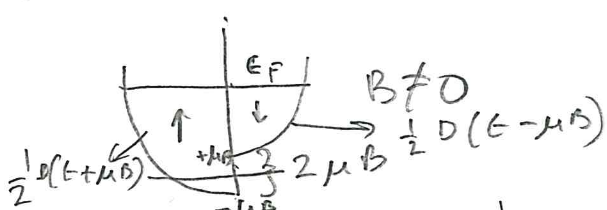
$$M = \frac{N\mu^2 B}{k_B T}\left(\frac{T}{T_F}\right) = \frac{N\mu^2 B}{k_B T_F}$$

Better derivation: Assume $T \ll T_F$ and $\mu B \ll \epsilon_F$



$$N_+ = \frac{1}{2}\int_{-\mu B}^{\epsilon_F} d\epsilon\, f(\epsilon)\, D(\epsilon + \mu B)$$

$$\approx \frac{1}{2}\int_0^{\epsilon_F} d(\epsilon)\, f(\epsilon)\, D(\epsilon) + \frac{1}{2}\mu_B B D(\epsilon_F)$$



Similarly, $N_- = \frac{1}{2}\int_{+\mu B}^{\epsilon_F} d\epsilon\, f(\epsilon)\, D(\epsilon - \mu B) = \frac{1}{2}\int_0^{\epsilon_F} d\epsilon\, f(\epsilon)\, D(\epsilon) - \frac{1}{2}\mu_B B D(\epsilon_F)$

There are some extra electrons in spin up direction due to B.

$$M = \mu(N_+ - N_-) \simeq \mu^2 D(\epsilon_F) B \qquad D(\epsilon_F) = \frac{3N}{2\epsilon_F} = \frac{3N}{2k_B T_F}$$

$$\chi = \frac{\partial M}{\partial H} = \mu^2 D(\epsilon_F) = \frac{3N}{2k_B T_F}\mu^2 B$$

In reality, there ~~a~~ is another contribution to susceptibility. contribution. Spatial motion of electrons is affected by magnetic field - causes a diamagnetic moment equal to $-1/3$ of paramagnetic moment

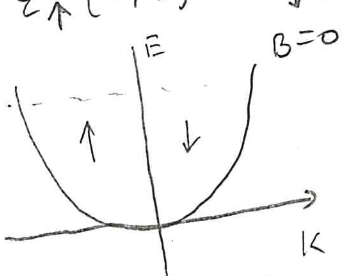
$$M = \left(\frac{3}{2} - \frac{1}{3}\cdot\frac{3}{2}\right)\frac{N\mu_B^2}{k_B T_F}$$

$$= \frac{N\mu_B^2}{k_B T_F}$$

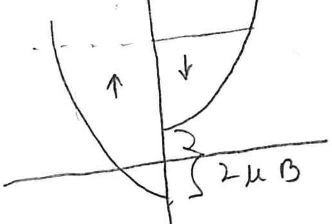
Motivation for using split-band diagram

Note at $B=0$, moments pointing in $\pm z$ direction have same energy $\epsilon_\uparrow(k) = \epsilon_\downarrow(k) = \frac{\hbar^2 k^2}{2m}$. when a magnetic field is applied, the total energy changes due to Zeeman contribution, But, more importantly, with opposite signs for $\uparrow$ and $\downarrow$ moments. Assume $\vec{B} = B\hat{z}$ $\varepsilon_\uparrow(k,B) = \frac{\hbar^2k^2}{2m} - \mu B$ and $\varepsilon_\downarrow(k,B) = \frac{\hbar^2k^2}{2m} + \mu B$. Therefore energy of every spin with moments parallel to the direction of B is reduced by $-\mu B$, and energy of every spin with moments antiparallel to B is raised by $+\mu B$

$$\varepsilon_\uparrow(k,B) - \varepsilon_\downarrow(k,B) = 2\mu B.$$



$\varepsilon_\uparrow = \varepsilon_\downarrow = \hbar^2k^2/2m$



$\varepsilon_\uparrow = \frac{\hbar^2k^2}{2m} - \mu B$

$\varepsilon_\downarrow = \frac{\hbar^2k^2}{2m} + \mu B$

The split-band, therefore, merely reflects that energy of $\uparrow$ moments have reduce by $-\mu B$ for all electrons irrespective of k value, and energy of all $\downarrow$ moments have increased by $+\mu B$. This picture carries over to the case of Ferromagnets.

Total energy of free-electron gas

It is instructive and useful to work out Pauli Paramagnetism from energy minimization point of view, ie, the groundstate energy is always a mininum. Let us quickly review the energy of a free electron gas at $B=0$ and $T=0$

For discrete energy eigenvalues ε_i with n_i states, the total energy is $\quad E = \sum_i n_i \varepsilon_i$

In the continuous case, $\quad n \to \int_0^{\varepsilon_F} f(\epsilon) D(\epsilon)\, d\epsilon$

$$\Rightarrow \varepsilon = \int_0^{\epsilon_F} f(\epsilon) D(\epsilon)\, \epsilon\, d\epsilon$$

Recall, $D(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}$ and $\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$

$$\Rightarrow \varepsilon_F^{3/2} = \left(\frac{\hbar^2}{2m}\right)^{3/2}\left(\frac{3\pi^2 N}{V}\right)$$

Taking $f(\epsilon) = 1$ at $T=0$

$$\text{So, } E = \int_0^{\epsilon_F} \left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}\, d\epsilon = \left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\varepsilon_F} \varepsilon^{3/2}\, d\epsilon$$

$$\Rightarrow \varepsilon = \frac{2}{5}\left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{3/2}\, \epsilon_F$$

$$\Rightarrow \varepsilon = \frac{\cancel{2}}{5}\left(\frac{\cancel{V}}{\cancel{2\pi^2}}\right)\cancel{\left(\frac{2m}{\hbar^2}\right)^{3/2}}\cancel{\left(\frac{\hbar^2}{2m}\right)^{3/2}}\left(\frac{3\cancel{\pi^2}N}{\cancel{V}}\right)\varepsilon_F = \frac{3}{5} N \varepsilon_F$$

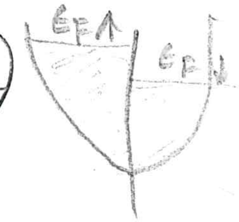
Or, $\boxed{\varepsilon = \frac{3}{5} N \epsilon_F}$

Total energy is greater than $\frac{1}{2} N\varepsilon_F$ due to parabolic bands

Since $N_\uparrow = N_\downarrow = \frac{N}{2}$ at $B=0$

$$\varepsilon_\uparrow = \frac{3}{5}\frac{N}{2}\varepsilon_F = \frac{3}{10} N\epsilon_F = \varepsilon_\downarrow = E_0$$ in the calculation performed next.

Pauli Paramagnetism (from total energy)



Lets say $N_\uparrow = \frac{N}{2}(1+\Delta)$; $N_\downarrow = \frac{N}{2}(1-\Delta)$

$N = N_\uparrow + N_\downarrow$ / $N_\uparrow - N_\downarrow = \Delta N$

$$\epsilon_\uparrow^{\to KE} = \frac{3}{5} N_\uparrow \epsilon_F = \frac{3}{5} N_\uparrow \frac{\hbar^2}{2m}\left(\frac{3\pi^2}{V} N_\uparrow\right)^{2/3}$$

$$\epsilon_\uparrow = \frac{3}{5}\left(\frac{\hbar^2}{2m}\right)\left(\frac{3\pi^2}{V}\right)^{2/3} N_\uparrow^{5/3} = \underbrace{\frac{3}{5}\frac{N}{2}\left(\frac{\hbar^2}{2m}\right)\left(\frac{3\pi^2 N}{2V}\right)^{2/3}}_{E_0}(1+\Delta)^{5/3}$$

$$= E_0 (1+\Delta)^{5/3} \qquad E_0 = \frac{3}{5}\frac{N}{2}\epsilon_F$$

$2/3$

$$\epsilon_\downarrow = E_0(1-\Delta)^{5/3}$$

Magnetic energy $= -\mu B(N_\uparrow - N_\downarrow) = -\mu B\left(\frac{N}{2} + \frac{N}{2}\Delta - \frac{N}{2} + \frac{N}{2}\Delta\right)$

$= -N\mu\Delta B$

Total energy $= \underbrace{\epsilon_\uparrow + \epsilon_\downarrow}_{\text{Total KE}} +$ Magnetic energy

$$= 1\, E_0\left[(1+\Delta)^{5/3} + (1-\Delta)^{5/3}\right] - N\Delta\mu B$$

we are minimizing this energy. $\Rightarrow \frac{dE}{d\Delta} = 0$

$$E_0\left[\frac{5}{3}(1+\Delta)^{2/3} - \frac{5}{3}(1-\Delta)^{2/3}\right] - N\mu B = 0$$

$$\Rightarrow E_0\left[5/3\left(1+\frac{2}{3}\Delta\right) - 5/3\left(1-\frac{2}{3}\Delta\right)\right] - N\mu B = 0$$

$$\Rightarrow E_0\left[\frac{10}{9}\Delta + \frac{10}{9}\Delta\right] - N\mu B = 0 \Rightarrow \Delta = \frac{9}{20}\frac{N\mu B}{E_0}$$

$$M = (N_\uparrow - N_\downarrow)\mu = \Delta N \mu = \frac{9}{20}\frac{N^2\mu^2 B}{E_0} = \frac{9^3}{20}\frac{N^2\mu^2 B}{\frac{3}{10}N\epsilon_F} = \frac{3}{2}N\mu^2 B$$

same result