Stoner model & Stoner criterion

In Stoner's ferromagnets, the magnetic moment is provided by the spin of the itinerant electrons. Well known examples of elementary materials showing this type of ferromagnetism are iron (Fe), cobalt (Co) and nickel (Ni). In most cases, ferromagnetism appears as a continuous 2^{nd} order phase transition, at the material-dependent critical temperature T_c, called the Curie temp.

We consider now the Stoner model of electrons with repulsive contact interaction:

$$\hat{H} = \sum_{k,s} \varepsilon_k \hat{a}_k^+ \hat{a}_k + \overbrace{U \int d^3r \, \hat{\rho}_\uparrow(r) \hat{\rho}_\downarrow(r)}^{\text{contact interaction}}$$

where $\hat{\rho}_s(r)$ is the electron density $\hat{\Psi}_s^+(r)\hat{\Psi}_s(r)$ and $U > 0$. Note that because of the Pauli principle, the contact interaction involves only electrons with different spins.

We now introduce a <u>mean field approximation</u> by writing

$$\hat{\rho}_s(r) = n_s + [\hat{\rho}_s(r) - n_s]$$

where $n_s = \langle \hat{\rho}_s(r) \rangle$ and we assume that the deviation from the mean value is small:

$$\underbrace{\langle (\hat{\rho}_s(r) - n_s)^2 \rangle}_{\sim \text{ fluctuation}} \ll n_s^2$$

Recalling $\hat{\Psi}_s^{(+)}(r) = \frac{1}{\sqrt{V}} \sum_k \varphi_k^{(*)}(r)\, \hat{a}_{k,s}^{(+)}$ and neglecting terms proportional to $(\hat{\rho}_s(r) - n_s)^2$ we get the m.f. Hamiltonian:

$$\hat{\mathcal{H}} \cong \sum_{k,s} \varepsilon_k \hat{a}_{k,s}^{+} \hat{a}_{k,s} + U \int d^3r \left[\hat{\rho}_\uparrow(r) n_\downarrow + \hat{\rho}_\downarrow(r) n_\uparrow - n_\uparrow n_\downarrow \right]$$

$$\overset{(*)}{=} \sum_{k,s} \left(\varepsilon_k + U n_{\bar{s}} \right) \hat{a}_{k,s}^{+} \hat{a}_{k,s} - U \cdot V\, n_\uparrow n_\downarrow \qquad (\ddagger)$$

where $\bar{s}$ denotes the spin opposed to s. Note how the coupling to particles with different spins induces an energy shift in this model, via the spin dependent exchange interaction. The many body problem has been reduced to an <u>effective one-particle problem</u>!

(*) For example:

$$\int d^3r\, \hat{\rho}_\uparrow(r)\, n_\downarrow = n_\downarrow \int d^3r\, \frac{1}{V} \overbrace{\sum_k \varphi_k(r)\, \hat{a}_{k,\uparrow}^{+}}^{\Psi_\uparrow^{+}(r)} \times \underbrace{\sum_{k'} \varphi_{k'}(r)\, \hat{a}_{k',\uparrow}}_{\Psi_\uparrow(r)}$$

$$= n_\downarrow \sum_k \hat{a}_{k,\uparrow}^{+} \hat{a}_k$$

using <u>orthonormality</u> of the basis functions:

$$\frac{1}{V} \int d^3r\, \varphi_k^{*}(r)\, \varphi_{k'}(r) = \underline{\delta_{kk'}}$$

We now look at the density of one spin species. For example we have:

$$\boxed{f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}}$$

$$n_\uparrow = \langle \hat{\Psi}^+_\uparrow \hat{\Psi}_\uparrow \rangle = \frac{1}{V} \sum_k \langle \hat{a}^+_k \hat{a}_k \rangle$$

$$= \frac{1}{V} \sum_k f(\underbrace{\varepsilon_k + U n_\downarrow}) \longrightarrow \text{shifted energy levels.}$$

where f is the Fermi-Dirac distribution and we used the form (7) of the Hamiltonian. We can write further

$$= \int d\varepsilon \, \underbrace{\frac{1}{V} \sum_k{}' \delta(\varepsilon - \varepsilon_k - U n_\downarrow)}_{\equiv \frac{1}{2} N(\varepsilon - U n_\downarrow), \text{ density of states.}} f(\varepsilon)$$

This and the corresponding equation for $n_\downarrow$ are the consistency equations for this approximation.

The total spin and the total magnetization can be written as

$$n_0 = n_\uparrow + n_\downarrow \qquad\qquad m = n_\uparrow - n_\downarrow$$

such that

$$n_0 = \frac{1}{2} \int d\varepsilon \left\{ N(\varepsilon - U n_\downarrow) + N(\varepsilon - U n_\uparrow) \right\} f(\varepsilon)$$

$$= \frac{1}{2} \sum_s \int d\varepsilon \; N\left(\varepsilon - \frac{U n_0}{2} - s \frac{U m}{2}\right) f(\varepsilon)$$

and analogously

$$m = \frac{1}{2}\int d\varepsilon \left\{ N(\varepsilon - U n_\downarrow) - N(\varepsilon - U n_\uparrow) \right\} f(\varepsilon)$$

$$= \frac{1}{2}\sum_s{}' \, s \int d\varepsilon \, N\!\left(\varepsilon - \frac{U n_0}{2} - s\,\frac{U m}{2}\right) f(\varepsilon)$$

where $s=+1$ for $\uparrow$ and $s=-1$ for $\downarrow$. These two equations can not be solved analytically and are generally treated numerically.

However, for low temperatures T and small magnetization $m \ll n_0$ we can obtain an approximate solution using the following trick. We can expand μ for small T and m as

$$\mu(m,T) = \varepsilon_F + \overbrace{\Delta\mu(m,T)}^{\text{small}}$$

where we absorb the constant energy shift $-\frac{U n_0}{2}$ in the definition of ε_F. This also applies to the above equations for n_0 and m. For m small we write (*)

$$n_0 \cong \int d\varepsilon \, f(\varepsilon) \left[N(\varepsilon) + \frac{1}{2}\left(\frac{U m}{2}\right)^2 N''(\varepsilon) \right] + O(m^3)$$
$$- \Delta\mu \, f'(\varepsilon) N(\varepsilon)$$

where the first order of the Taylor expansion cancels among the two spins. (f denotes $f|_{\Delta\mu = 0}$)

Let us now introduce the Sommerfeld expansion: Consider the integral

$$f|_{\Delta\mu=0} = \frac{1}{e^{\beta(\varepsilon-\varepsilon_F)}+1}$$

$$\int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon)\, N(\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon \frac{N(\varepsilon)}{e^{\beta(\varepsilon-\varepsilon_F)}+1}$$

$$\overset{x=\beta(\varepsilon-\varepsilon_F)}{=} \frac{1}{\beta}\int_{-\infty}^{\infty} dx \frac{N(\varepsilon_F+\frac{x}{\beta})}{e^{x}+1}$$

Now divide the Integration range in two parts above and below $x=0$, and look at the "lower" part:

$$\frac{1}{\beta}\int_{-\infty}^{0} dx \frac{N(\varepsilon_F+\frac{x}{\beta})}{e^{x}+1} = \frac{1}{\beta}\int_{-\infty}^{0} dx\, N(\varepsilon_F+\frac{x}{\beta}) - \frac{1}{\beta}\int_{-\infty}^{0} dx \frac{N(\varepsilon_F+\frac{x}{\beta})}{e^{-x}+1}$$

Use: $\frac{1}{e^{x}+1} = 1 - \frac{1}{e^{-x}+1}$

$$= \int_{-\infty}^{\varepsilon_F} d\varepsilon\, N(\varepsilon) - \frac{1}{\beta}\int_{0}^{\infty} dx \frac{N(\varepsilon_F-\frac{x}{\beta})}{e^{x}+1}$$

Recombining, we obtain

$$\int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon) N(\varepsilon) = \int_{-\infty}^{\varepsilon_F} d\varepsilon\, N(\varepsilon) + \underbrace{\frac{1}{\beta}\int_{0}^{\infty} dx \frac{N(\varepsilon_F+\frac{x}{\beta}) - N(\varepsilon_F-\frac{x}{\beta})}{e^{x}+1}}$$

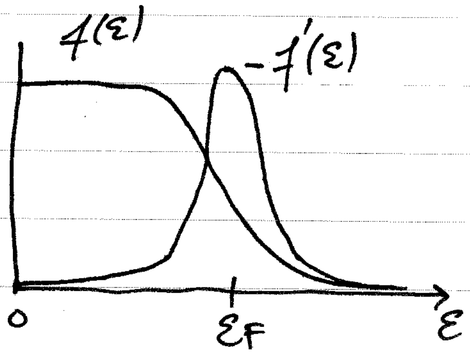
using the definition of the derivative $\longrightarrow \frac{1}{\beta}\int_{0}^{\infty} dx \frac{2N'(\varepsilon_F)\,\frac{x}{\beta}}{e^{x}+1}$ as $\beta\to\infty$

such that, using $\int_0^\infty dx \frac{x}{e^x+1} = \frac{\pi^2}{12}$, we obtain the Sommerfeld expansion:

$$\boxed{\int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon)\, N(\varepsilon) \cong \int_{-\infty}^{\varepsilon_F} d\varepsilon\, N(\varepsilon) + \frac{\pi^2}{6}\,\frac{N'(\varepsilon_F)}{\beta^2}} \quad \text{as } \beta\to\infty$$

Going back to our expansion for n_0, eq. (*), we see that the first term is given by the above equation. The second terms can be computed using partial integration and the fact that

$$\int_0^\infty d\varepsilon\, \overbrace{f'(\varepsilon)}^{\to -\delta(\varepsilon-\varepsilon_F) \text{ as } \beta\to\infty}\, g(\varepsilon) \cong -g(\varepsilon_F)$$



In total we obtain:

$$n_0 \cong \int_0^{\varepsilon_F} d\varepsilon\, N(\varepsilon) + N(\varepsilon_F)\Delta\mu + \frac{\pi^2}{6}\frac{N'(\varepsilon_F)}{\beta^2} + \frac{1}{2}\left(\frac{Um}{2}\right)^2 N'(\varepsilon_F)$$

and analogously: (first and second orders vanish b/c of s prefactor)

$$m \cong \left(\frac{Um}{2}\right) \int d\varepsilon \Big\{ f(\varepsilon)\left(N'(\varepsilon) + \frac{1}{6} N'''(\varepsilon)\left(\frac{Um}{2}\right)^2\right) - \Delta\mu\, f'(\varepsilon) N'(\varepsilon) \Big\}$$

$$\cong \left(\frac{Um}{2}\right)\left[N(\varepsilon_F) + \frac{\pi^2}{6}\frac{N''(\varepsilon_F)}{\beta^2} + \frac{1}{6}\left(\frac{Um}{2}\right)^2 N''(\varepsilon_F) + \Delta\mu\, N'(\varepsilon_F)\right]$$

Now comes the trick: The first term in the expansion of n_0 is actually n_0 in the limit $\beta \to \infty$. Hence we find that (see remark next page)

$$\Delta\mu \cong -\frac{N'(\varepsilon_F)}{N(\varepsilon_F)}\left[\frac{\pi^2}{6\beta^2} + \frac{1}{2}\left(\frac{Um}{2}\right)^2\right]$$

inserting this in the expansion for m we obtain

$$m \cong N(\varepsilon_F)\left\{\left[1 - \frac{\pi^2}{6\beta^2} C_1\right]\left(\frac{Um}{2}\right) - \left(\frac{Um}{2}\right)^3 C_2\right]$$

with

$$C_1 = \left(\frac{N'(\varepsilon_F)}{N(\varepsilon_F)}\right)^2 - \frac{N''(\varepsilon_F)}{N(\varepsilon_F)}$$

and

$$C_2 = \frac{1}{2}\left(\frac{N'(\varepsilon_F)}{N(\varepsilon_F)}\right) - \frac{N''(\varepsilon_F)}{6\,N(\varepsilon_F)}.$$

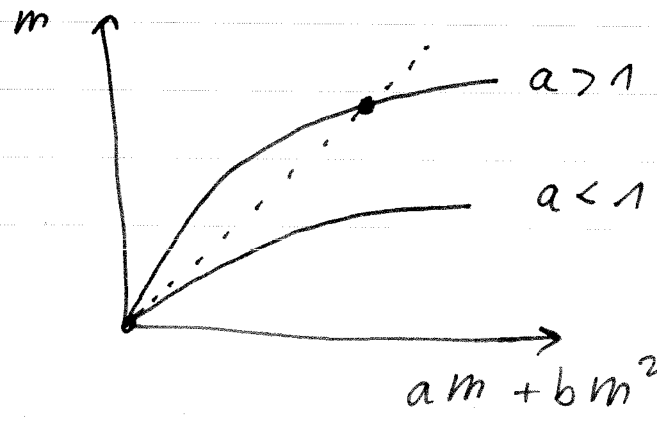
The structure of this equation is (assume $a, b > 0$)

$$m = am - bm^3$$

no ferromagn.

with solution

$$m = \begin{cases} 0 & a < 1 \\ \dfrac{a-1}{b}, & a > 1 \end{cases}$$



ferromagnetism

In our case we have:

$$a = N(\varepsilon_F)\left[1 - \frac{\pi^2}{6\beta^2} C_1\right]\left(\frac{U}{2}\right)$$

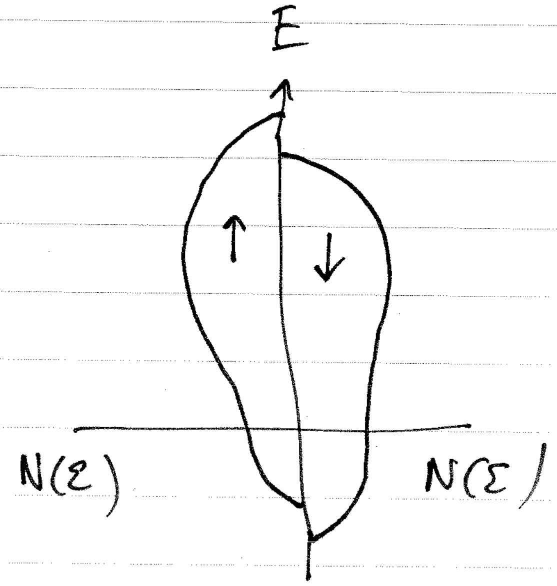
Hence we have ferromagnetism in the $T \to 0$ limit ($\beta \to \infty$) if $a > 1$, i.e.

$$\boxed{U N(\varepsilon_F) > 2}$$

which is the Stoner criterion.

Physical picture:

The Fermi sea of each spin is shifted by $\pm Um/2$, resulting in a finite magnetization



Remark: This is actually not that easy: you have to show that n_0 is actually $O(\Delta u^2)$.