Magnetism in materials

Week 07

1. In first approximation, the Pauli paramagnetic susceptibility is temperature-independent and is given by

$$\chi_{P0} = \frac{3n\mu_0\mu_B^2}{2k_BT_F} \tag{1}$$

where n is the electron density and T_F the Fermi temperature. Show that for a metal at $T \ll T_F$ the first temperature-dependent correction to the Pauli magnetic susceptibility is

$$\chi_P = \chi_{P0}\left(1 - \frac{\pi^2 T^2}{12T_F^2}\right) \tag{2}$$

and estimate the size of this correction for a typical metal at room temperature.

Hint Use the low temperature Sommerfeld expansion

$$\int_{-\infty}^{\infty} \frac{H(E)}{\exp\left(\frac{E-\mu}{k_BT}\right)+1}dE = \int_{-\infty}^{\mu} H(E)dE + \frac{\pi^2}{6}(k_BT)^2H'(\mu) + O([k_BT]^4) \tag{3}$$

and the fact that for small T the chemical potential is related to the Fermi energy by

$$\mu \approx E_F\left(1 - \frac{\pi^2 T^2}{12T_F^2}\right) \tag{4}$$

solution

$$\chi_P = \mu_0\mu_B^2 \int_0^{+\infty} g'(E)f(E)dE$$

with $g(E)$ the electron density of states, and f(E) the Fermi-Dirac distribution, so using the Sommerfeld expansion

$$\int_0^{+\infty} g'(E)f(E)dE \approx \int_0^{\mu} g'(E)dE + \frac{\pi^2}{6}(k_BT)^2 g''(\mu) \tag{5}$$

$$\approx \int_0^{E_F} g'(E)dE + (\mu - E_F)g'(E_F) + \frac{\pi^2}{6}(k_BT)^2 g''(E_F) \tag{6}$$

note that we can substitute E_F to μ in the argument of g'' since this is already multiplied by a factor $(k_BT)^2$ so it is a correction of higher order. Assuming a free electron band

$$g(E) = \frac{3n}{2E_F^{3/2}}\sqrt{E} \tag{7}$$

$$g'(E) = \frac{3n}{4E_F^{3/2}}E^{-1/2} \tag{8}$$

$$g''(E) = -\frac{3n}{8E_F^{3/2}}E^{-3/2} \tag{9}$$

The first integral gives

$$\int_0^{E_F} g'(E)dE = g(E)|_0^{E_F} = g(E_F) \tag{10}$$

so

$$\chi_P \approx \mu_0\mu_B^2[g(E_F) + (\mu - E_F)g'(E_F) + \frac{\pi^2}{6}(k_BT)^2 g''(E_F)] \tag{11}$$

$$= \mu_0\mu_B^2\left[\frac{3n}{2E_F} + \left(-E_F\frac{\pi^2(k_BT)^2}{12(k_BT_F)^2}\right)\frac{3n}{4E_F^2} + \frac{\pi^2}{6}(k_BT)^2\left(-\frac{3n}{8E_F^3}\right)\right] \tag{12}$$

$$= \frac{3\mu_0\mu_B^2 n}{2E_F}\left[1 - \frac{\pi^2(k_BT)^2}{24(k_BT_F)^2} - \frac{\pi^2(k_BT)^2}{24(k_BT_F)^2}\right] \tag{13}$$

$$= \frac{3\mu_0\mu_B^2 n}{2E_F}\left[1 - \frac{\pi^2(k_BT)^2}{12(k_BT_F)^2}\right] \tag{14}$$

For typical metals the Fermi temperature is in the order of 10^5 K, so at room temperature $(T/T_F)^2 \approx 10^{-5}$

2. When the temperature increases the chemical potential has to decrease to conserve the total number of electrons, so it becomes more relevant the contribution from the high energy tale $(E-\mu) \gg k_BT$ where the Fermi-Dirac distribution is well approximated by $f(E) \approx e^{-(E-\mu)/k_BT}$. Show that in this regime the chemical potential can be approximated as

$$\mu = k_BT\left[\frac{3}{2}\ln\left(\frac{T_F}{T}\right) + \ln\left(\frac{4}{3\sqrt{\pi}}\right)\right] \tag{15}$$

Show that in this regime the Pauli susceptibility is well approximated by

$$\chi_P = \frac{n\mu_0\mu_b^2}{k_BT} \tag{16}$$

Hint Impose that the total number of electrons is conserved.
Use the integral $\int_0^\infty \sqrt{x}e^{-x}dx = \frac{\sqrt{\pi}}{2}$

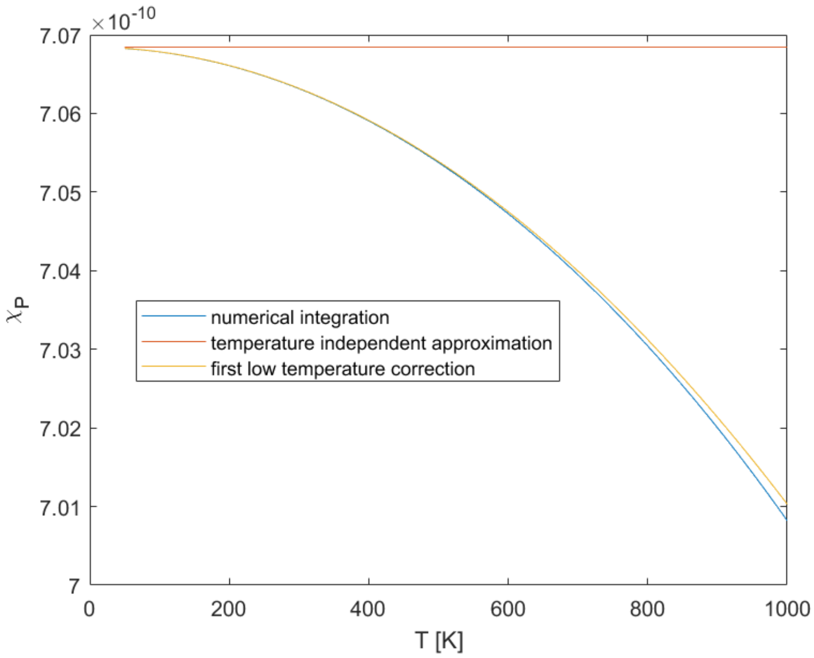

Figure 1: Pauli paramagnetic susceptibility at $T \ll T_F$ for a metal with $T_F = 10^4\,\mathrm{K}$. The blue curve is computed via numerical integration of the Fermi-Dirac distribution, the orange and yellow curves show respectively the temperature independent χ_{P0} and temperature dependent $\chi_{P0}\left(1 - \frac{\pi^2 T^2}{12 T_F^2}\right)$.

solution In the non-degenerate limit $f(E) \approx e^{-(E-\mu)/k_B T}$, imposing that the electron density is n for all T

$$n = \int_0^\infty f(E) g(E) dE = \int_0^\infty \frac{3n}{2E_F^{3/2}} \sqrt{E} \exp\left(-\frac{E-\mu}{k_B T}\right) \tag{17}$$

$$= \frac{3n}{2E_F^{3/2}} (k_B T)^{3/2} e^{-\mu/k_B T} \int_0^\infty \sqrt{x} e^{-x} dx \tag{18}$$

$$= \frac{3n\sqrt{\pi}}{4} \left(\frac{T}{T_F}\right)^{3/2} e^{-\mu/k_B T} \tag{19}$$

from which

$$\mu = k_B T \left[\frac{3}{2} \ln\left(\frac{T_F}{T}\right) + \ln\left(\frac{4}{3\sqrt{\pi}}\right)\right] \tag{20}$$

integrating by part the Pauli magnetization is

$$M \approx \mu_B^2 B \int_0^\infty g'(E) f(E) dE \tag{21}$$

$$= -\mu_B^2 B \int_0^\infty g(E) f'(E) dE \tag{22}$$

In the non-degenerate limit $f(E) \approx e^{-(E-\mu)/k_B T}$ so

$$f'(E) = -\frac{f(E)}{k_B T} \tag{23}$$

and

$$M = \frac{\mu_B^2 B}{k_B T} \int_0^\infty g(E) f(E) = \frac{\mu_B^2 B}{k_B T} n \tag{24}$$

and

$$\chi_P = \frac{M}{H} = \frac{\mu_B^2 \mu_0 n}{k_B T} \tag{25}$$

The susceptibility is then equivalent to the one of n localized moments (of magnitude μ_B) per unit volume.

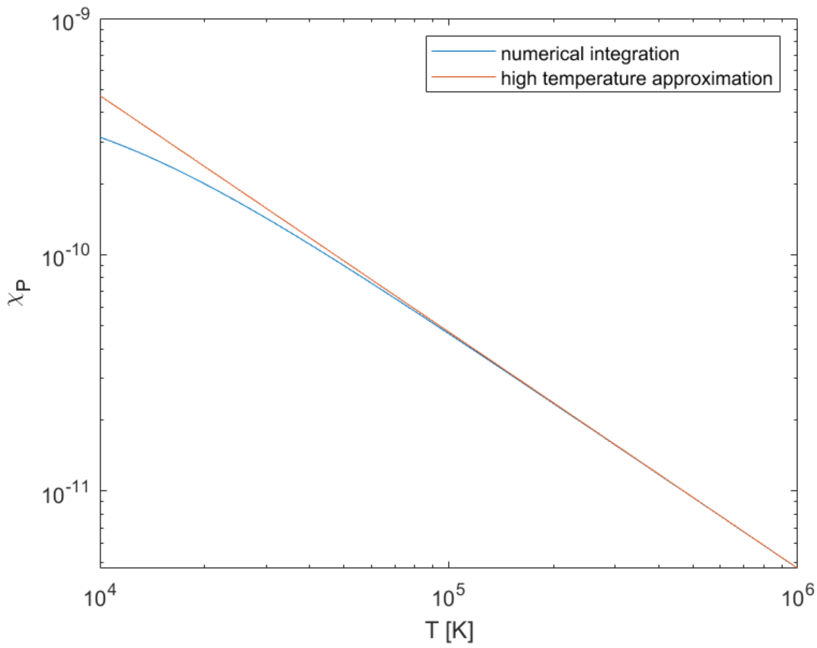

Figure 2: Pauli paramagnetic susceptibility at $T \geq T_F$ for a metal with $T_F = 10^4\,\mathrm{K}$. The blue curve is computed via numerical integration of the Fermi-Dirac distribution, the orange one shows $\chi_P = \frac{n\mu_0\mu_b^2}{k_B T}$.