Solid State Theory
Solution 13

Problem 13.1 Susceptibility from the atomic and conduction electrons

In Lecture 24, we found that the Landau diamagnetic susceptibility and the Pauli paramagnetic susceptibly of the conduction electrons are given by

$$\chi_{Landau} = -\frac{1}{3}\chi_{Pauli} = -\frac{1}{3}\mu_B^2 N(\epsilon_F), \tag{1}$$

where $\mu_B = \frac{e\hbar}{2mc}$ (Bohr magneton) is the magnetic dipole of a bound electron with angular momentum $\hbar$. $N(\epsilon_F)$ is the density of states at the fermi energy. The total magnetic susceptibility of the conduction electrons is then

$$\chi_{c.e.} = \chi_{Landau} + \chi_{Pauli} = \frac{2}{3}\mu_B^2 N(\epsilon_F) \tag{2}$$

Moreover, the density of states at the fermi surface of a 3D isotropic system written in terms of the electron density n_c of conduction electrons and the fermi energy ϵ_F as

$$N(\epsilon_F) = \frac{3}{2}\frac{n_v}{\epsilon_F}, \tag{3}$$

where n_v is the density of the valence electrons. Therefore,

$$\chi_{c.e.} = \frac{\mu_B^2}{\epsilon_F} n_c. \tag{4}$$

On the other, hand, we found that the Langevin susceptibility of the core electrons is

$$\chi_{Langevin} = -\frac{e^2}{6mc^2} n_c \langle r^2 \rangle, \tag{5}$$

where n_c is the density of the core electrons. Using the definition of the Bohr magneton, we can re-write this equation as

$$\chi_{Langevin} = -\mu_B^2 \frac{2m}{3\hbar^2} n_v \langle r^2 \rangle \tag{6}$$

$$= -\frac{1}{3}\frac{\mu_B^2}{\epsilon_F} n_v \langle k_f^2 r^2 \rangle \tag{7}$$

Comparing the two expressions and noting that $n_v/n_c = Z_v/Z_c$, we obtain

$$\frac{\chi_{Langevin}}{\chi_{c.e.}} = -\frac{1}{3}\frac{Z_c}{Z_v}\langle (k_f r)^2 \rangle \tag{8}$$

Note that the total magnetic susceptibility is then given by

$$\chi_{Langevin} + \chi_{c.e.} = \chi_{c.e.}\left(1 - \frac{1}{3}\frac{Z_c}{Z_v}\langle (k_f r)^2 \rangle\right). \tag{9}$$

Therefore, an electron system is more likely to be diamagnetic as it has more closed shell electrons (i.e. as we go down the periodic table). A famous example is copper.

Problem 13.2 de Haas-van Alphen effect

The de Haas - van Alphen effect is observable under high magnetic field satisfying

$$T \leq \mu_B B \ll \mu, \tag{10}$$

where μ is the chemical potential and μ_B is the Bohr magneton. Writing the free energy by means of the Poisson formula

$$\frac{1}{2}F(0) + \sum_{n=1}^{\infty} F(n) = \int_0^{\infty} F(x)dx + 2\,\mathcal{R}\sum_{k=1}^{\infty}\int_0^{\infty} F(x)e^{2\pi ikx}dx, \tag{11}$$

where $\mathcal{R}$ stands for the real part. To obtain Eq. 11, we multiplied the Poisson equation

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{k=-\infty}^{\infty} e^{2\pi ikx}, \tag{12}$$

by the free energy $F(x)$ and integrated from 0 to ∞ on both sides. Thus, we obtain

$$F = F_0(\mu) + \frac{TmV}{\pi^2\hbar^3}\mathcal{R}\sum_{k=1}^{\infty} I_k, \tag{13}$$

with

$$I_k = -2\mu_B B\int_{-\infty}^{\infty}\int_0^{\infty} \ln\left[1 + \exp\left(\frac{\mu}{T} - \frac{p_z^2}{2mT} - \frac{2x\mu_B B}{T}\right)\right] e^{2\pi ikx}dxdp_z, \tag{14}$$

and $F_0(\mu)$ is the thermodynamic potential in the absence of the field. The factor $2\mu_B BmV/(\pi^2\hbar^3)$ is related to the number of states for the interval dp_z. Using the substitution

$$\epsilon \to \frac{p_z^2}{2m} - 2x\mu_B B,$$

we arrive at

$$I_k = -\int_{-\infty}^{\infty}\int_0^{\infty} \ln\left[1 + \exp\left(\frac{\mu-\epsilon}{T}\right)\right] \exp\left(\frac{\pi ik\epsilon}{\mu_B B}\right) \exp\left(-i\frac{\pi kp_z^2}{2m\mu_B B}\right) d\epsilon dp_z, \tag{15}$$

where the lower limit for the $d\epsilon$ integral is taken to be 0 because the most significant contribution to the integral is from ϵ near μ. For the dp_z integral the most important values are $p_z^2/2m \approx \mu_B B$. Now evaluating the gaussian p_z integral by means of

$$\int_{-\infty}^{\infty} e^{-i\alpha p^2}dp = e^{-i\pi/4}\sqrt{\frac{\pi}{\alpha}} \tag{16}$$

we have

$$I_k = -e^{-i\pi/4}\sqrt{\frac{2m\mu_B B}{k}}\int_0^{\infty} \ln[1 + e^{(\mu-\epsilon)/T}] \exp\left(i\frac{\pi k\epsilon}{\mu_B B}\right) d\epsilon. \tag{17}$$

Next, we integrate twice by parts using

$$\int udv + vdu = uv,$$

with

$$u \to \ln[1 + e^{(\mu-\epsilon)/T}],$$

and

$$dv \to \exp\left(i\frac{\pi k\epsilon}{\mu_B B}\right).$$

Substituting $\eta \to (\epsilon - \mu)/T$ to obtain

$$I_k = \frac{\sqrt{2m}}{T\pi^2}\left(\frac{\mu_B B}{k}\right)^{5/2} \exp\left(\frac{i\pi k\mu}{\mu_B B} - \frac{i\pi}{4}\right)\int_{-\infty}^{\infty} \frac{e^\eta}{(1+e^\eta)^2} \exp\left(\frac{i\pi kT}{\mu_B B}\eta\right) d\eta, \tag{18}$$

where we replaced the lower limit of the integral from $-\mu/T$ to infinity by the assumption $\mu \gg T$. The η integration can be carried out with the help of the identity

$$\int_{-\infty}^{\infty} \frac{e^\eta}{(1+e^\eta)^2} \exp\left(i\alpha\eta\right) d\eta = \frac{\pi\alpha}{\sinh\left(\pi\alpha\right)}. \tag{19}$$

The above identity is obtained by the substitution $u = 1/(e^\eta + 1)$ and noticing that the resulting expression can be written using beta functions

$$\int_0^1 (1-u)^{i\alpha} u^{-i\alpha} = \Gamma(1+i\alpha)\Gamma(1-i\alpha)/\Gamma(2) = \frac{i\pi\alpha}{i\sinh\pi\alpha} \tag{20}$$

And we finally obtain the formula for the part of free energy which oscillates with the magnetic field

$$\tilde{F} = \frac{\sqrt{2}(m\mu_B B)^{3/2} TV}{\pi^2\hbar^3} \sum_{k=1}^{\infty} \frac{\cos\left(\frac{\pi\mu k}{\mu_B B} - \frac{1}{4}\pi\right)}{k^{3/2}\sinh\left(\frac{\pi^2 kT}{\mu_B B}\right)}. \tag{21}$$

To obtain the magnetisation we only integrate the most rapidly varying parts of $\tilde{\Omega}$, which are the cosines in the numerators

$$\tilde{M} = -\frac{\sqrt{2\mu_B}(m)^{3/2}\mu TV}{\pi\hbar^3\sqrt{B}} \sum_{k=1}^{\infty} \frac{\sin\left(\frac{\pi\mu k}{\mu_B B} - \frac{1}{4}\pi\right)}{k^{1/2}\sinh\left(\frac{\pi^2 kT}{\mu_B B}.\right)}. \tag{22}$$

As we saw in the lecture, the frequency of this function is at a given magnetic field is independent of temperature. However, also notice that the amplitude is exponentially small for $\mu_b B \ll T$.