SOLUTIONS - Tutorials N°2

PROBLEM 2

I - Free electron gas - DOS 3D

- In 3D : $\phi(E)$ = number of quantum states characterized by an energy < E.

$$\phi(E) = \frac{4/3\,\pi\left(2mE/\hbar^2\right)^{3/2}}{\left(\frac{2\pi}{L}\right)^3} \times 2$$

since 2 electrons can fit in a quantum state.

$$\phi(E) = \frac{\pi^2 V}{3} \times \left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

$$\phi(E) = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{V\pi^2}{3} E^{3/2}$$

Then $g(E) = DOS = \frac{d\phi(E)}{dE} = \frac{V\pi^2}{2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$

$$\boxed{g(E) = A\sqrt{E}} \quad (1)$$

- Internal Energy U : $U = \int_0^{+\infty} g(E)\, f(E)\, E\, dE$

at T=0K $\quad U_0 = \int_0^{E_F} g(E)\, E\, dE$

$$U_0 = A\int_0^{E_F} E^{3/2}\, dE = \frac{2}{5} A E_F^{5/2}$$

- Fermi Energy:

$E_F \Rightarrow$ normalization of the DOS.

$$N = \int_0^{E_F} g(E)\,dE = \int_0^{E_F} A E^{1/2}\,dE = \frac{2A}{3} E_F^{3/2}$$

So $E_F = \left(\frac{3N}{2A}\right)^{2/3}$ (2)

We can then express the internal energy at 0K:

$$U_0 = \frac{2}{5} A E_F^{5/2} = \frac{2}{5} \times \frac{3N}{2} E_F$$

$$\boxed{U_0 = \frac{3}{5} N E_F} \quad (3)$$

II. 3D gas at low T

$g(E)$ is considered as constant around E_F, when $T \ll \Theta_F$

- Chemical potential μ:

$\mu \Rightarrow$ normalization when $T \neq 0K$

$$N = \int_0^{+\infty} g(E) f(E)\,dE = \int_0^{+\infty} \frac{A E^{1/2}\,dE}{e^{\beta(E-\mu)}+1}$$

Applying Sommerfeld formula:

$$N = \int_0^{\mu} A E^{1/2}\,dE + \frac{\pi^2}{6\beta^2}\left(\frac{1}{2} A E_F^{-1/2}\right)$$

$\boxed{3}$ Assuming that N is constant whatever the value of T.
(N = number of electrons in the solid).

$$N = \int_0^{E_F} g(E)\,dE = \int_0^{E_F} AE^{1/2}\,dE = \int_0^{\mu} AE^{1/2}dE + \frac{\pi^2}{12\beta^2} AE_F^{-1/2}$$

$$\Leftrightarrow \int_{E_F}^{\mu} \underbrace{AE^{1/2}}_{\substack{g(E)\simeq \text{cte} \\ \text{around } E_F}} dE + \frac{\pi^2}{12\beta^2} AE_F^{-1/2} = 0$$

$$\Leftrightarrow AE_F^{1/2}(\mu - E_F) = -\frac{\pi^2}{12\beta^2} AE_F^{-1/2}$$

$$\Leftrightarrow \mu - E_F = -\frac{\pi^2}{12\beta^2} \times E_F^{-1}$$

$$\Leftrightarrow \boxed{\mu = E_F - \frac{\pi^2}{12\beta^2} E_F^{-1}} \quad (4)$$

One can verify that $\mu = E_F$ at $T = 0K$

- Internal Energy at $T \neq 0K$

$$U = \int_0^{+\infty} E\,g(E)\,f(E)\,dE = \int_0^{+\infty} \frac{AE^{3/2}dE}{e^{\beta(E-\mu)}+1} \simeq \int_0^{\mu} AE^{3/2}dE + \frac{\pi^2}{6\beta^2} \times \frac{3}{2} AE_F^{1/2}$$

$$U = \underbrace{\int_0^{E_F} AE^{3/2}dE}_{=U_0} + \underbrace{\int_{E_F}^{\mu} AE^{3/2}dE}_{=AE_F^{3/2}(\mu - E_F) \text{ when } T \text{ is low } (T \ll \theta_F)} + \frac{\pi^2}{4\beta^2} AE_F^{1/2}$$

$$U = U_0 + AE_F^{3/2}(\mu - E_F) + \frac{\pi^2}{4\beta^2} AE_F^{1/2}$$

with $A = \frac{3}{2} N E_F^{-3/2}$ (see equation (2))

$$U = U_0 + \frac{3}{2}N(\mu - E_F) + \frac{\pi^2}{4\beta^2} \times \frac{3}{2} N E_F^{-1}$$

with $\mu - E_F = -\frac{\pi^2}{12\beta^2} E_F^{-1}$

(see equation (4))

$$U = U_0 - \frac{\pi^2}{8\beta^2} N E_F^{-1} + \frac{3\pi^2}{8\beta^2} N E_F^{-1}$$

Then $\boxed{U = U_0 + \frac{\pi^2}{4\beta^2} N E_F^{-1}}$ (5)

- Specific heat => electronic contribution

$$C_{el} = \frac{dU}{dT} = \frac{d}{dT}\left[U_0 + \frac{\pi^2}{4} N k_B^2 T^2 / E_F\right]$$

$$C_{el} = \frac{\pi^2}{2} N k_B^2 T / k_B \Theta_F$$

$$\boxed{C_{el} = \frac{\pi^2}{2} N k_B \left(\frac{T}{\Theta_F}\right)}$$

Same contribution as 2D case.