Heat capacity of 3D electron gas
by Dr. Colton, Physics 581 (last updated: Fall 2020)

Electron gas: we'll assume quadratic dispersion, namely $E = \frac{\hbar^2 k^2}{2m}$.

(a) Density of states in 3D

$$\mathcal{D}(E) = \frac{1}{(2\pi/L)^3} \cdot 4\pi k^2 \cdot \frac{1}{dE/dk} \cdot 2 \text{ (factor of 2 from spin degeneracy)}$$

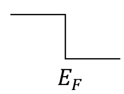
use $E = \frac{\hbar^2 k^2}{2m} \rightarrow k = \frac{1}{\hbar}\sqrt{2mE}$; then $\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar^2}{m} \cdot \left(\frac{1}{\hbar}\sqrt{2mE}\right) = \frac{\hbar\sqrt{2E}}{\sqrt{m}}$

$$\mathcal{D}(E) = \frac{V}{8\pi^3} \cdot \left(4\pi\left(\frac{2mE}{\hbar^2}\right)\right) \cdot \left(\frac{1}{\frac{\hbar\sqrt{2E}}{\sqrt{m}}}\right) \tag{1}$$

$$\boxed{\mathcal{D}(E) = \frac{V}{2\pi^2} \cdot \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}}$$

(b) Fermi energy calculation

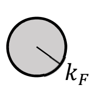
$$N = \int_0^{\omega_D} \mathcal{D}(E) f(E)\, dE$$

$f(E) =$  at 0 deg Kelvin

$$N = \int_0^{E_F} \mathcal{D}(E) dE$$
$$= \frac{V}{2\pi^2} \cdot (2m/\hbar^2)^{3/2} \cdot \underbrace{\int_0^{E_F} E^{1/2} dE}_{(E_F^{3/2})/(3/2)}$$

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

Alternate derivation: k-space sphere



$$number\ of\ states = volume \times \left(\frac{num.states}{volume}\right) \times 2 \tag{2}$$

$$N = \left(\frac{4}{3}\pi k_F^3\right) \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3} \cdot 2 = \frac{V}{3\pi^2} k_F^3 = \frac{V}{3\pi^2} \cdot \left(\frac{1}{\hbar}\sqrt{2mE_F}\right)^3$$

$$\boxed{E_F = \frac{\hbar^2}{2m} \cdot \left(3\pi^2 \frac{N}{V}\right)^{2/3}}$$

(c) Calculate $\mathcal{D}(E_F)$…Solve Eq. 2 for V and plug into Eq. 1

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

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

then $\mathcal{D}(E_F)$ becomes

$$\mathcal{D}(E_F) = \left(3\pi^2 N \left(\frac{\hbar^2}{2mE_F}\right)^{3/2}\right)\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{1/2}$$

$$\boxed{\mathcal{D}(E_F) = \frac{3}{2}\frac{N}{E_F}}$$

(d) Energy calculation:

$$U = \int_0^\infty \mathcal{D}(E)f(E)E\, dE$$

let $\mathcal{D}(E) \approx \mathcal{D}(E_F)$ Also, $f(E) = \frac{1}{e^{(E-\mu)/kT}+1}$ let $\mu \approx E_F$, a constant.

$$\boxed{U \approx \mathcal{D}(E_F)\int_0^\infty \frac{E}{e^{(E-E_F)/kT}+1}\, dE}$$

(e) Heat capacity calculation: $C_V = \frac{\partial U}{\partial T} \rightarrow$ take $\frac{\partial}{\partial T}$ inside the integral

$$\frac{\partial}{\partial T}\left(\frac{1}{e^{(E-E_F)/kT}+1}\right) = -\frac{1}{\left(e^{(E-E_F)/kT}+1\right)^2}\left(e^{(E-E_F)/kT}\right)\left(\frac{E-E_F}{k}\cdot\frac{-1}{T^2}\right)$$

$$C_V = \mathcal{D}(E_F)\frac{1}{kT^2}\int_0^\infty \frac{(E-E_F)\, E\, e^{(E-E_F)/kT}}{(e^{(E-E_F)/kT}+1)^2}\, dE$$

Let $x = \frac{E-E_F}{kT} \rightarrow E = kTx + E_f, dE = kTdx$

$$\boxed{C_V = \mathcal{D}(E_F)k\int_{-E_F/kT}^\infty \frac{xe^x}{(e^x+1)^2}(kTx+E_F)\, dx}$$

(f) Heat capacity, small T approximation: take integral from $-\infty$ to ∞, then the E_F part integrates to 0 since $\frac{xe^x}{(e^x+1)^2}$ is odd.

$$C_V = \mathcal{D}(E_F)k^2T \underbrace{\int_{-\infty}^\infty \frac{x^2e^x}{(e^x+1)^2}dx}_{\pi^2/3 \text{ from mathematica}}$$

$$C_V = \left(\frac{3}{2}\frac{N}{E_F}\right)k^2T\left(\frac{\pi^2}{3}\right)$$

$$\boxed{C_V = \frac{\pi^2}{2}\frac{k^2T}{E_F}N}$$ The contribution to the heat capacity from the electron gas!