Sommerfeld expansion to get C_V:

The energy and number densities are:

$$u = \int_{-\infty}^{+\infty} \varepsilon\, g(\varepsilon) f(\varepsilon)\, d\varepsilon$$

$$n = \int_{-\infty}^{+\infty} g(\varepsilon) f(\varepsilon)\, d\varepsilon \quad \text{where} \quad g(\varepsilon) = \frac{2}{(2\pi)^3} \frac{4\pi k^2}{k/m} = \frac{1}{\pi^2} mk = \frac{m}{\pi^2}\sqrt{2m\varepsilon}$$

$$\text{units: } [g] = \frac{1}{\text{energy}} \frac{1}{\text{length}^3}$$

$$\hbar^2/m \approx 7.63\, \text{eV} \cdot \text{Å}^2$$

$$\Rightarrow g(\varepsilon) = \frac{\sqrt{2}}{\pi^2} \left(\frac{m}{\hbar^2}\right)^{3/2} \sqrt{\varepsilon}$$

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

Both of these integrals are of the form $\int \underbrace{H(\varepsilon) f(\varepsilon)\, d\varepsilon}_{du}$. If we integrate by parts this becomes:

$$\int_{-\infty}^{+\infty} K(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon + K(\varepsilon) f(\varepsilon)\Big|_{-\infty}^{+\infty} = \int_{-\infty}^{+\infty} K(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon, \text{ where } K(\varepsilon) = \int_{-\infty}^{\varepsilon} H(\varepsilon')\, d\varepsilon'.$$

$$\text{Now, } -\frac{\partial f}{\partial \varepsilon} = \frac{\beta e^{\beta(\varepsilon-\mu)}}{[e^{\beta(\varepsilon-\mu)} + 1]^2} = \frac{\beta}{[e^{\beta(\varepsilon-\mu)/2} + e^{-\beta(\varepsilon-\mu)/2}]^2} \text{ looks like a}$$

delta function and satisfies $\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) = f(-\infty) - f(+\infty) = 1 \Rightarrow$ it is

reasonable to expand K about μ:

$$\int H(\varepsilon) f(\varepsilon)\, d\varepsilon = \int \left(\sum_{n=0}^{\infty} \frac{(\varepsilon-\mu)^{2n}}{(2n)!} \frac{d^{2n} K(\varepsilon)}{d\varepsilon^{2n}}\Big|_{\mu} \right)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon$$

$$= \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \sum_{n=1}^{\infty} (k_B T)^{2n} \frac{d^{2n-1} H(\mu)}{d\varepsilon^{2n-1}} \int_{-\infty}^{+\infty} \frac{x^{2n}}{2n!} \, -\frac{d}{dx} \frac{1}{1+e^x}\, dx$$

$$\int \frac{x^{2n}}{2n!} \frac{d}{dx}\left(\frac{1}{1+e^x}\right) dx = \int \frac{x^{2n-1}}{(2n-1)!} \frac{1}{1+e^x} dx \quad ; \ 2n! = \Gamma(2n+1)$$

$$= 2\int_0^\infty \frac{x^{2n-1}}{(2n-1)!} \left[e^{-x} - e^{-2x} + e^{-3x} - e^{-4x} + \cdots\right] dx$$

$$= 2\sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{k^{2n}} \int_0^\infty \frac{x^{2n-1}}{(2n-1)!} e^{-x} dx$$

$$= 2\left[1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \cdots\right]$$

$$= 2\left[1 + \frac{1}{2^{2n}} + \frac{1}{3^{2n}} + \frac{1}{4^{2n}} + \cdots\right] - 4\left[\frac{1}{2^{2n}} + \frac{1}{4^{2n}} + \frac{1}{6^{2n}} + \cdots\right]$$

$$= 2\,\zeta(2n) - 2^{-2(n-1)}\zeta(2n) \quad , \text{where } \zeta(2n) = \left[1 + 2^{-2n} + 3^{-2n} + \cdots\right]$$

Riemann zeta function

Know: $\zeta(2) = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \cdots = \frac{\pi^2}{6}$

$\zeta(4) = 1 + \frac{1}{2^4} + \frac{1}{3^4} + \cdots = \frac{\pi^4}{90} \quad \Rightarrow$

The original integral is :

$n=1: \ (2-1)\frac{\pi^2}{6} = \frac{\pi^2}{6}$

$n=2: \ \left(2 - \frac{1}{4}\right)\frac{\pi^4}{90} = \frac{7\pi^4}{4\cdot 90} = \frac{7\pi^4}{360} \quad \Rightarrow$

$$\boxed{\int_{-\infty}^{+\infty} H(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \frac{7\pi^4}{360}(k_B T)^4 H'''(\mu) + \cdots}$$

We can now apply this to compute c_V for free electrons:

$$n = \int_{-\infty}^{\mu} g(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 g'(\mu) + O(T^4)$$

We wish to solve this for $\mu(T)$. Since T only occurs in even powers, μ must be an even function of T. Also, using $n = \int_{-\infty}^{\varepsilon_F} g(\varepsilon)\,d\varepsilon \Rightarrow$

$$0 = \int_{\varepsilon_F}^{\mu} g(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 g'(\mu) + O(T^4)$$

$$= \sum_{n=0}^{\infty} \frac{(\mu-\varepsilon_F)^{n+1}}{(n+1)!} g^{(n)}(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 \left[g'(\varepsilon_F) + (\mu-\varepsilon_F) g''(\varepsilon_F) + \cdots \right] + O(T^4)$$

Since $\mu(T=0) = \varepsilon_F$, $(\mu - \varepsilon_F) = O(T^2)$. Keeping only $O(T^2)$ terms:

$$0 = (\mu-\varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 g'(\varepsilon_F) + O(T^4) \Rightarrow$$

$$\mu = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{1}{2\varepsilon_F} \Rightarrow$$

$$\boxed{\mu = \varepsilon_F \left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right] = \varepsilon_F \left[1 - 0.8225\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]}$$

$$u = \int_0^{\varepsilon_F} \varepsilon g(\varepsilon)\,d\varepsilon + \int_{\varepsilon_F}^{\mu} \varepsilon g(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \left[\mu g'(\mu) + g(\mu) \right] + O(T^4)$$

Again keeping terms to $O(T^2)$ only $\Rightarrow$

$$u = u_0 - \cancel{\frac{\pi^2}{12}(k_B T)^2 g(\varepsilon_F)} + \frac{\pi^2}{6}(k_B T)^2 \left[\cancel{\varepsilon_F g'(\varepsilon_F)} + g(\varepsilon_F) \right] + O(T^4)$$

$$= u_0 + \frac{\pi^2}{6}(k_B T)^2 g(\varepsilon_F) + O(T^4)$$

$$\Rightarrow \boxed{c_V = \frac{\pi^2}{3} k_B^2 T g(\varepsilon_F) + O(T^3) = \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B} \quad ; g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F}$$

3.29

4.935

Remarks:

(i) We can compare this to the Debye specific heat at low temperatures:

$$5\left(\frac{T}{T_F}\right) n' k_B \sim 200\left(\frac{T}{\Theta_D}\right)^3 n k_B$$

$$\Rightarrow \frac{Z}{40}\left(\frac{T}{T_F}\right) \sim \left(\frac{T}{\Theta_D}\right)^3$$

For copper, $Z = 1$, $T_F \sim 80{,}000^\circ K$, $\Theta_D \sim 300^\circ K$ $\Rightarrow$

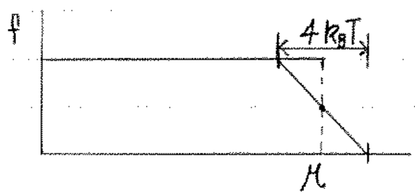
$$\frac{1}{40}\left(\frac{T}{80{,}000}\right) \sim \left(\frac{T}{300}\right)^3$$

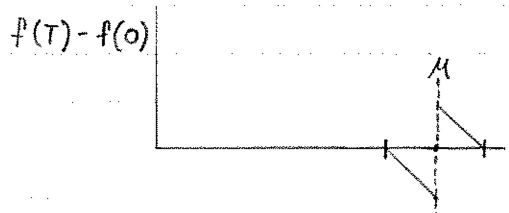
$$\frac{T}{3{,}200{,}000} \sim \frac{T^3}{27{,}000{,}000}$$

$$T \sim T^3/9 \;\rightarrow\; T \sim 3^\circ K.$$

If we do this by dimensional arguements (w/out 40^{-1}), we get $T \sim T^3/360 \rightarrow T \sim 18^\circ K$, which is off by 6.

(ii) We can get this result much more quickly by noting that $-\frac{\partial f(\mu)}{\partial \varepsilon} = \frac{1}{4k_BT}$ so that we can approximate f by:





odd fnt. of ε

$$u - u_0 = \int d\varepsilon\, \varepsilon g(\varepsilon)[f(T)-f(0)] \approx \int_{-2k_BT}^{2k_BT} d\varepsilon\, [\mu+\varepsilon][g(\mu)+g'(\mu)\varepsilon][f(T)-f(0)]$$

$$\approx [\mu g'(\mu) + g(\mu)]\, 2 \cdot \int_0^{2k_BT} d\varepsilon\, \varepsilon\left[\frac{1}{2} - \frac{\varepsilon}{4k_BT}\right]$$

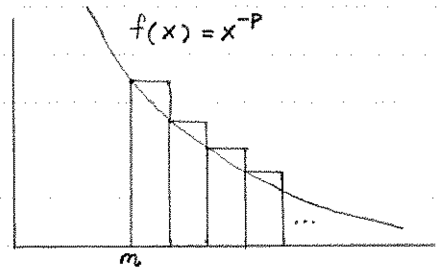
$$\approx \frac{3}{2} g(\varepsilon_F) \times 2\left[\frac{(2k_BT)^2}{4} - \frac{(2k_BT)^3}{12k_BT}\right] = g(\varepsilon_F)(k_BT)^2 \;\rightarrow\; c_V \sim 2 k_B^2 T g(\varepsilon_F)$$

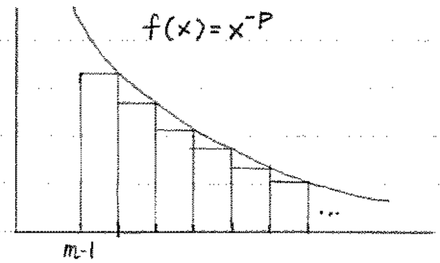
should be 3.29

Evaluation of the Riemann zeta function:

$$\zeta(p) = \sum_{k=1}^{m-1} \frac{1}{k^p} + \sum_{k=m}^{\infty} \frac{1}{k^p} \qquad ; p>1$$

The second term can be bounded by an integral:





$$\text{lower bound} = \int_m^\infty \frac{dx}{x^p} = \frac{m^{-p+1}}{p-1} \qquad \text{upper bound} = \int_{m-1}^\infty \frac{dx}{x^p} = \frac{(m-1)^{-p+1}}{p-1}$$

$$U.B. - L.B. = \frac{1}{p-1}\left\{\frac{1}{(m-1)^{p-1}} - \frac{1}{m^{p-1}}\right\} \approx \frac{1}{p-1}(p-1)\,m^{-p} = m^{-p}$$

Thus, approximate $\displaystyle \zeta(p) \approx \sum_{k=1}^{m-1} \frac{1}{k^p} + \frac{(m-\frac{1}{2})^{-p+1}}{p-1}$

$$\text{error} \approx \frac{1}{2} m^{-p}.$$

Example $\zeta(2) = \pi^2/6 = 1.645$. If $m=5$, then $\frac{1}{2}m^{-p} = 0.02$:

$$\zeta(2) \approx \left[1 + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + (4.5)^{-1}\right] \approx 1.646 \ \checkmark$$

$$\zeta(2.5) \approx \left[1 + \frac{1}{2^{2.5}} + \frac{1}{3^{2.5}} + \frac{1}{4^{2.5}} + \frac{(4.5)^{-1.5}}{1.5}\right] \approx 1.342 \pm 0.009$$