Non-interacting Identical Fermions ('Fermi Gas')

Zero Temperature:

We first study non-interacting non-relativistic fermions in three spatial dimensions at $T=0$. The single particle levels are given by $\varepsilon_{\vec{p}} = \dfrac{\vec{p}^{\,2}}{2m}$. Recall that in the grand canonical ensemble, the average occupation of these levels is given by,

$$\langle \hat{n}_{\vec{p}} \rangle = n_{\vec{p}} = \frac{1}{e^{\beta\left(\frac{p^2}{2m}-\mu\right)}+1}$$

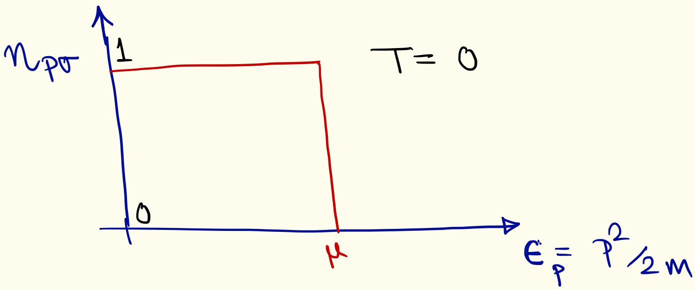
Nominally, fermions also carry a half odd-integer spin e.g. electron spin is $1/2$. Thus for electrons one can write,

$$n_{\vec{p}\sigma} = \frac{1}{e^{\beta\left(\frac{p^2}{2m}-\mu\right)}+1} \qquad \sigma = 1/2, -1/2$$

($\equiv S^z$ component of spin)

Let's look at the fermi function closely to understand this system. At zero temperature,

$$\beta \to \infty \Rightarrow n_{\vec{p}\sigma} \to \theta(\mu - \varepsilon_{\vec{p}})$$



This means that all levels with energy $\epsilon_p < \mu$ are filled. One can determine μ in terms of the total number of fermions N.

factor of two due to spin

$$N = 2 \sum_{\vec{p}} \theta(\mu - \varepsilon_{\vec{p}})$$

$$= 2 \frac{V}{(2\pi)^3} \int d^3k \; \theta\left(\mu - \frac{\hbar^2 k^2}{2m}\right)$$

$$= 2V \frac{4\pi k_F^3}{3 \times (2\pi)^3} \quad \text{where } k_F = \sqrt{\frac{2m\mu}{\hbar^2}}$$

$$= \frac{k_F^3 V}{3\pi^2} = \frac{1}{3\pi^2}\left[\frac{2m\mu}{\hbar^2}\right]^{3/2} V$$

Total energy E at $T=0$:

$$E = 2 \sum_{\vec{p}} \frac{\hbar^2 k^2}{2m} \, \theta\left(\mu - \frac{\hbar^2 k^2}{2m}\right)$$

$$= 2 \frac{V}{(2\pi)^3} \int_0^{k_F} \frac{\hbar^2}{2m} k^2 \, 4\pi k^2 \, dk$$

$$= \frac{2 V}{8\pi^3} \frac{\hbar^2}{2m} \times 4\pi \frac{k_F^5}{5}$$

$$= \left[\frac{\hbar^2 k_F^2}{2m}\right] \frac{1}{\pi^2} \frac{k_F^3}{5} V$$

Using $\frac{k_F^3 V}{3\pi^2} = N$ from above, one obtains,

$$\frac{E}{N} = \frac{3}{5}\left[\frac{\hbar^2 k_F^2}{2m}\right] = \frac{3}{5} \varepsilon_F$$

where $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$
$= \mu(T=0)$
is called "Fermi Energy".

Basic check:

Recall $dE = -P\,dV + \mu\, dN$ at $T=0$

$$\Rightarrow \mu = \left.\frac{dE}{dN}\right|_V$$

From above, $E = \frac{3}{5} N \varepsilon_F = \frac{3}{5} N \frac{\hbar^2}{2m}\left[\frac{3\pi^2 N}{V}\right]^{2/3}$

$$= \frac{3}{5}\left[\frac{3\pi^2}{V}\right]^{2/3} \frac{\hbar^2}{2m} N^{5/3}$$

$$\Rightarrow \frac{dE}{dN} = \frac{3}{5}\left[\frac{3\pi^2}{V}\right]^{2/3} \frac{\hbar^2}{2m} \frac{5}{3} N^{2/3}$$

$$= \frac{\hbar^2 k_F^2}{2m} = \mu \text{ , as expected !}$$

Now, let's look at pressure,

$$P = -\left.\frac{dE}{dV}\right|_N$$

$$= \frac{3}{5}(3\pi^2)^{2/3} \frac{\hbar^2}{2m} N^{5/3} \times \frac{2}{3} V^{-5/3}$$

$$= \frac{2}{3}\frac{E}{V}$$

Thus, a fermi gas has a non-zero pressure even at the zero temperature. This is completely different than a classical ideal gas where $P = \rho T = 0$ at $T = 0$.

The non-zero pressure is responsible for the stability of white dwarf stars. Pressure balances against gravity. We will study this later.

The above relation between pressure and energy is actually more general and holds at any temperature T (prove!).

Some numbers:

In metals, ε_F can be estimated using the fact that $\frac{V}{N} \sim a^3$ where a is the radius of the atom. For example, for sodium, $a \approx 4 \times 10^{-10}$ m. Mass $m = m_{electron} \approx 10^{-30}$ kg. Thus,

$$\varepsilon_F = \frac{\hbar^2}{2m} \left[\frac{3\pi^2 N}{V} \right]^{2/3}$$

$$\simeq 10^4 \text{ K}.$$

This is much larger than the room temperature.

Thus, ordinary metals are highly quantum objects at room temperature i.e. one needs quantum mechanics to understand even their basic properties e.g. conduction, reflection, heat capacity etc.

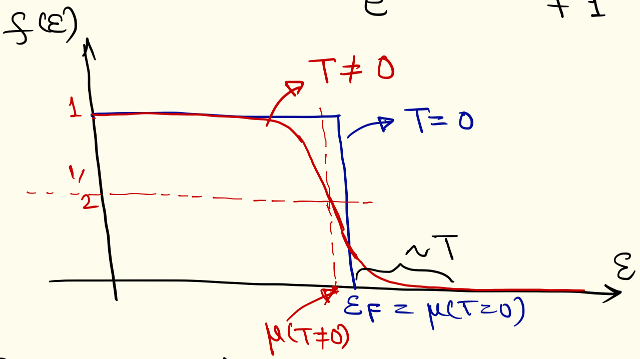
Metals at low but Non-zero temperature :

The important thing to note is that at $T \neq 0$, $\mu \neq \varepsilon_F$. Infact, μ will depend on temperature T so that the number of particles N does not change.

Let's first do an approximate calculation and after that, we will return to an exact one.

Recall that the Fermi-Dirac distribution, which tells the average occupation of a level at energy ε is:

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



$f(\varepsilon) = \frac{1}{2}$ at $\varepsilon = \mu$, <u>always</u>.

At low temperatures, μ will deviate from ε_F only slightly and $f(\varepsilon)$ will deviate from its $T=0$ value $(=\Theta(\mu-\varepsilon_F))$ only for $|\varepsilon-\mu| \sim T \ll \mu$.

Thus, one expects,

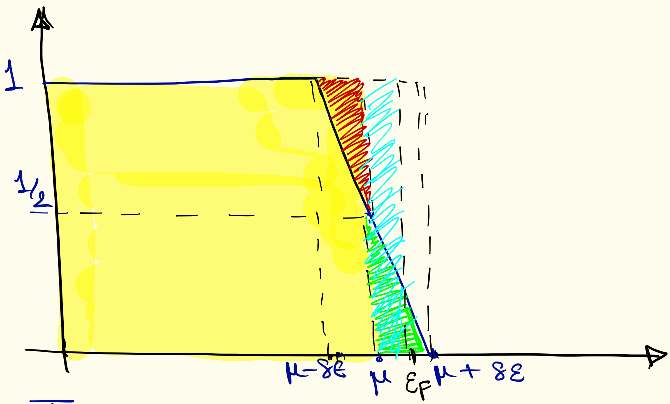
$$\frac{E(T\neq 0) - E(T=0)}{N} \propto \frac{T}{\epsilon_F} \times T = \frac{T^2}{\epsilon_F}$$

fraction of particles where $f(\varepsilon)$ differs from its $T=0$ value

energy carried by those particles.

Let's convert this intuition into an actual, approximate calculation:

At $T\neq 0$, we approximate $f(\varepsilon)$ by a ramp:



$\delta\varepsilon \propto T$

we will take $\delta\varepsilon = 3T$.

The total number of fermions

$$N \approx \int_0^{\mu(T)} D(\varepsilon)\, d\varepsilon \qquad (= \text{Area of yellow rectangle})$$

$$- D\left(\mu - \frac{\delta\varepsilon}{2}\right)\frac{\delta\varepsilon}{4} \qquad (= \text{Area of red triangle})$$

$$+ D\left(\mu + \frac{\delta\varepsilon}{2}\right)\frac{\delta\varepsilon}{4} \qquad (= \text{Area of green triangle})$$

where $D(\varepsilon)$ is the density of states.

Reminder: $N = \frac{V}{8\pi^3} 4\pi \int \frac{k^2\, dk}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} + 1}$

Change of variables: $\frac{\hbar^2 k^2}{2m} = \varepsilon$

$$N = \frac{V}{2\pi^2} \int \frac{\frac{m}{\hbar^2}\left[\frac{2m\varepsilon}{\hbar^2}\right]^{1/2} d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}$$

$$= \int \frac{D(\varepsilon)\, d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} \Rightarrow D(\varepsilon) \propto \sqrt{\varepsilon}.$$

Also. at $T=0$:

$$N(T=0) = \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon$$

Subtracting,

$$N(T) - N(T=0) \simeq \int_{\varepsilon_F}^{\mu} D(\varepsilon)\, d\varepsilon + \frac{1}{4}(\delta\varepsilon)^2 D'(\varepsilon_F)$$

$$\simeq (\mu - \varepsilon_F) D(\varepsilon_F) + \frac{1}{4}(\delta\varepsilon)^2 D'(\varepsilon_F)$$

Since number of particles is fixed, $\Rightarrow$

$$\mu \approx \varepsilon_F - \frac{1}{4}\frac{D'(\varepsilon_F)}{D(\varepsilon_F)}(\delta\varepsilon)^2$$

Since $D(\varepsilon) \propto \sqrt{\varepsilon} \Rightarrow \dfrac{D'(\varepsilon_F)}{D(\varepsilon_F)} = \dfrac{1}{2\varepsilon_F}$

If we take $\delta\varepsilon \approx 3T$,

$$\Rightarrow \boxed{\mu(T) \approx \varepsilon_F - \frac{9}{8}\frac{T^2}{\varepsilon_F}}$$

The exact answer (we will calculate it soon) is $\mu(T) = \varepsilon_F - \dfrac{\pi^2}{12}\dfrac{T^2}{\varepsilon_F}$, so not too different.

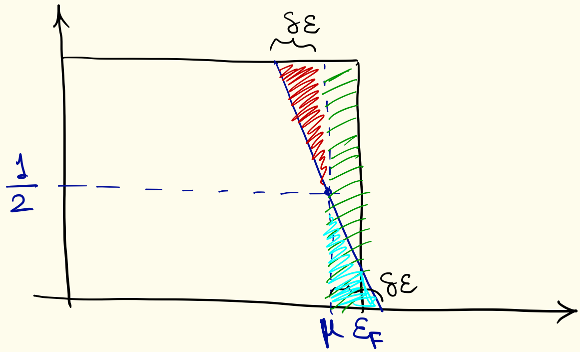
Since $\frac{T}{T_F}$ at room temperature is of the order of 10^{-2} $\Rightarrow$ $\left|\frac{\mu - \varepsilon_F}{\varepsilon_F}\right| \sim 10^{-4}$

at the room temperature $\Rightarrow$ rather small.

Why is the sign negative?

Why is the dependence quadratic in T?

Let's calculate the change in total energy within this 'ramp' approximation:



$$E(T) - E(T=0) \approx -(\varepsilon_F - \mu)\, D(\varepsilon_F)\, \varepsilon_F$$

(= contribution from green shaded area)

$$+ \frac{1}{4}\left(\mu + \frac{\delta\varepsilon}{2}\right) D\left(\mu + \frac{\delta\varepsilon}{2}\right) \delta\varepsilon$$ (= Blue Δ)

$$- \frac{1}{4}\left(\mu - \frac{\delta\varepsilon}{2}\right) D\left(\mu - \frac{\delta\varepsilon}{2}\right) \delta\varepsilon$$ (= red Δ)

$$= -\frac{(\delta\varepsilon)^2 D(\varepsilon_F)}{8} + \frac{1}{4}(\delta\varepsilon)^2 \left[\varepsilon D(\varepsilon)\right]' \Big|_{\varepsilon=\varepsilon_F}$$

$$= -\frac{(\delta\varepsilon)^2 D(\varepsilon_F)}{8} + \frac{1}{4}(\delta\varepsilon)^2 D'(\varepsilon_F)\,\varepsilon_F + \frac{1}{4}(\delta\varepsilon)^2 D(\varepsilon_F)$$

Since $D'(\varepsilon_F) = \dfrac{D(\varepsilon_F)}{2\varepsilon_F} \Rightarrow E(T) - E(0) = \dfrac{1}{4}(\delta\varepsilon)^2 D(\varepsilon_F)$

$$= \frac{9}{4} T^2 D(\varepsilon_F)$$

$$\Rightarrow \quad C_V = \frac{dE(T)}{dT} = \frac{9}{2} T \, D(\varepsilon_F)$$

The exact answer is $C_V = \dfrac{\pi^2}{3} T D(\varepsilon_F)$

Note that $C_V \sim T$ for the Fermi gas in all space dimensions (show this!).

Exact Calculation for the Specific Heat of the Fermi Gas

The total number of particles, N, is given by:

$$N = \sum_{\vec{p}\sigma} n_{\vec{p}\sigma}$$

$$= 2 \frac{V}{(2\pi)^3} \int \frac{4\pi k^2 \, dk}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} + 1}$$

$$= 4\pi \left[\frac{2m}{h^2}\right]^{3/2} V \int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}$$

$$\Rightarrow \varepsilon_F^{3/2} = \int_0^\infty \frac{\sqrt{\varepsilon}\, d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}$$

Similarly, the total energy E is:

$$E = \sum_{\vec{p}\sigma} n_{\vec{p}\sigma} \varepsilon_{\vec{p}\sigma} = \sum_{\vec{p}\sigma} n_{\vec{p}\sigma} \frac{p^2}{2m}$$

$$= 4\pi \left[\frac{2m}{h^2}\right]^{3/2} V \int_0^\infty \frac{\varepsilon^{3/2}\, d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}$$

Both of the above expressions are of the form

$$I = \int_0^\infty \frac{g(\varepsilon)\, d\varepsilon}{e^{(\varepsilon-\mu)\beta} + 1}$$

Since we are interested in the properties of the system only at temperatures $T \ll \varepsilon_F$, one can do a Taylor's expansion for the integral I. Let's see how it goes:
(see appendix A.13 of Garrod's book for similar discussion, although our discussion will be self-contained anyway).

First we note that at $T=0$ (i.e. $\beta=\infty$)

I becomes $I_0 = \int_0^\infty g(\varepsilon)\, \Theta\left(\frac{\mu-\varepsilon}{T}\right) d\varepsilon$

$$\left(= \int_0^\mu g(\varepsilon)\, d\varepsilon \right)$$

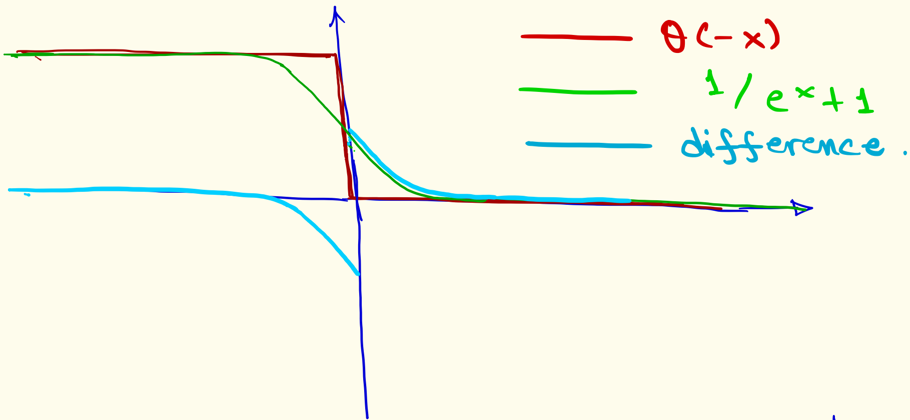
Let's consider the difference $\Delta I = I - I_0$.

$$\Delta I = \int_0^\infty \left[\frac{1}{e^{(\varepsilon-\mu)/T} + 1} - \Theta\left(\frac{\mu-\varepsilon}{T}\right) \right] g(\varepsilon)\, d\varepsilon$$

This is a bit messy. To make it look nicer, let's consider change of varibles to the dimensionless parameter $x = (\varepsilon - \mu)/T$.

$$\Delta I = T \int_{-\mu/T}^{\infty} \left[\frac{1}{e^{x}+1} - \theta(-x) \right] g(\mu + Tx) \, dx$$

The function $\frac{1}{e^{x}+1} - \theta(-x)$ looks like



Thus the difference approaches zero exponentially fast when $|x| \gg 1$. Since the lower limit of integration $= -\mu/T \ll 0$ at low temperatures (the regime of our interest), one can safely extend the limits of integration to $-\infty$. The error incurred under this approximation would be of the order of $e^{-\mu/T}$ which is <u>really</u> small e.g. when $\mu/T \approx 100$, then error $\approx e^{-100}$.

Having made this approximation, one can now taylor expand:

$$\Delta I = T \int_{-\infty}^{\infty} \left[\frac{1}{e^x+1} - \theta(-x) \right] g(\mu + Tx)$$

$$= \sum_{n=0}^{\infty} T^{n+1} \left. \frac{d^n g(\varepsilon)}{d\varepsilon^n} \right|_{\varepsilon=\mu} \int_{-\infty}^{\infty} x^n \left[\frac{1}{e^x+1} - \theta(-x) \right]$$

The function $f = \frac{1}{e^x+1} - \theta(-x)$ is an odd f^n of x as may be obvious from the figure on the previous page. But lets check this explicitly:

If $x > 0$ $\quad f(x) = \frac{1}{e^x+1}$

$$f(-x) = \frac{1}{e^{-x}+1} - 1 = -\frac{1}{e^x+1} = -f(x)$$

Similarly, one can check $x < 0$.

$\Rightarrow \quad x^n \left[\frac{1}{e^x+1} - \theta(-x) \right]$ is an <u>even</u> f^n of x when n is <u>odd</u> and an <u>odd</u> f^n of x when n is <u>even</u>.

Since the limits of integration in ΔI are from $-\infty$ to $+\infty$, this implies that only odd values of n contribute.

$$\Delta I = \sum_{n \text{ odd}} T^{n+1} \left. \frac{d^n g(\varepsilon)}{d\varepsilon^n} \right|_{\varepsilon=\mu} \times 2 \times \underbrace{\int_0^\infty \frac{x^n \, dx}{e^x+1}}$$

$$= 2 \sum_{n \text{ odd}} T^{n+1} \left. \frac{d^n g(\varepsilon)}{d\varepsilon^n} \right| \underbrace{\left[1 - 2^{-n}\right] n! \, \zeta(n+1)}$$

How to do the integral $\displaystyle\int_0^\infty \frac{x^n}{e^x+1} dx$?

$$\int_0^\infty \frac{x^n}{e^x+1}\,dx = \int_0^\infty \frac{x^n\, e^{-x}}{1+e^{-x}}\,dx$$

$$= \sum_{m=0}^{\infty} \int_0^\infty x^n\, e^{-x}\, e^{-mx} (-)^m\, dx$$

$$= \sum_{m=1}^{\infty} \frac{1\; n!}{m^{n+1}} (-)^{m+1}$$

This looks a bit like Riemann-zeta fn but has the oscillating terms due to $(-)^m$.

Fret not!

Note that $\displaystyle\sum_{m=1}^{\infty} \frac{(-)^{m+1}}{m^{n+1}} - \zeta(n+1)$

$$= \sum_{m=1}^{\infty} \frac{(-)^{m+1}}{m^{n+1}} - \sum_{m=1}^{\infty} \frac{1}{m^{n+1}}$$

$$= -2\sum_{m=2,4,6,\ldots} \frac{1}{m^{n+1}} = -\frac{2}{2^{n+1}} \sum_{m=1}^{\infty} \frac{1}{m^{n+1}}$$

$$\Rightarrow \sum_{m=1}^{\infty} \frac{(-)^{m+1}}{m^{n+1}} = \zeta(n+1)\left[1-2^{-n}\right]$$

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

Using the known values of Riemann-zeta f^n for integers n, one thus find,

$$I = \int_0^{\mu} g(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6} g'(\mu) T^2 + \frac{7\pi^4}{360} g''(\mu) T^4 + \cdots$$

Let's apply the above formula to the problem at hand, namely specific heat of fermions at low temperatures.

$$N = 4\pi \left[\frac{2m}{h^2}\right]^{3/2} V \int_0^{\infty} \frac{\sqrt{\varepsilon}\, d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$$

$$= 4\pi \left[\frac{2m}{h^2}\right]^{3/2} V \left[\int_0^{\mu} \sqrt{\varepsilon}\, d\varepsilon + \frac{\pi^2}{6} \frac{1}{2\sqrt{\mu}} T^2 + \cdots \right]$$

$$\Rightarrow \underbrace{\frac{N}{4\pi V}\left[\frac{h^2}{2m}\right]^{3/2} \times \frac{3}{2}}_{\varepsilon_F^{3/2}} = \mu^{3/2} + \frac{\pi^2 T^2}{8\sqrt{\mu}}$$

Can replace μ by ε_F at this order.

$$\Rightarrow \quad \varepsilon_F^{3/2} = \mu^{3/2} + \frac{\pi^2 T^2}{8\sqrt{\varepsilon_F}}$$

$$\Rightarrow \quad \mu = \left[\varepsilon_F^{3/2} - \frac{\pi^2 T^2}{8\sqrt{\varepsilon_F}}\right]^{2/3}$$

$$= \varepsilon_F \left[1 - \frac{\pi^2 T^2}{8\,\varepsilon_F^2}\right]^{2/3}$$

$$\Rightarrow \quad \mu = \varepsilon_F - \frac{\pi^2 T^2}{12\,\varepsilon_F}$$

Recall that in the ramp approximation,

$$\mu = \varepsilon_F - \frac{1}{4}\frac{D'(\varepsilon_F)}{D(\varepsilon_F)}(\delta\varepsilon)^2$$

$$\approx \varepsilon_F - \frac{9}{8}\frac{T^2}{\varepsilon_F} \quad \text{if } \delta\varepsilon = 3T$$

a bit arbitrary.

Let's next calculate the total energy exactly:

$$E = 4\pi\left[\frac{2m}{h^2}\right]^{3/2} V \int_0^\infty \frac{\varepsilon^{3/2}\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$$

$$\Rightarrow \frac{1}{4\pi}\left(\frac{E}{V}\right)\left[\frac{h^2}{2m}\right]^{3/2} = \int_0^\mu \varepsilon^{3/2}\,d\varepsilon + \frac{\pi^2}{6}\times\frac{3}{2}\sqrt{\mu}\,T^2$$

$$= \frac{2}{5}\mu^{5/2} + \frac{\pi^2}{4}\mu^{1/2}T^2$$

$$= \frac{2}{5}\left[\varepsilon_F - \frac{\pi^2 T^2}{12\varepsilon_F}\right]^{5/2} + \frac{\pi^2}{4}\left[\varepsilon_F - \frac{\pi^2 T^2}{12\varepsilon_F}\right]^{1/2} T^2$$

$$= \frac{2}{5}\varepsilon_F^{5/2}\left[1 - \frac{\pi^2 T^2}{12\varepsilon_F^2}\times\frac{5}{2}\right]$$

$$+ \frac{\pi^2}{4}\varepsilon_F^{1/2}T^2\left[1 - \frac{\pi^2 T^2}{12\varepsilon_F}\times\frac{1}{2}\right]$$

$$= \frac{2}{5}\varepsilon_F^{5/2} + \varepsilon_F^{1/2}T^2\left[\frac{\pi^2}{4} - \frac{\pi^2}{12}\right]$$

Now note that

$$\frac{1}{4\pi}\left(\frac{\varepsilon}{V}\right)\left[\frac{h^2}{2m}\right]^{3/2} = \frac{\varepsilon}{N}\times\frac{2}{3}\varepsilon_F^{3/2}$$

$$\Rightarrow \frac{\varepsilon}{N} = \frac{2}{5}\varepsilon_F^{5/2}\times\frac{3}{2}\varepsilon_F^{-3/2}$$

$$+ \frac{T^2\pi^2}{6}\varepsilon_F^{1/2}\times\frac{3}{2}\varepsilon_F^{-3/2}$$

$$\Rightarrow \frac{E}{N} = \frac{3}{5}\varepsilon_F + \frac{\pi^2 T^2}{4\varepsilon_F}$$

$$\Rightarrow C_{V,N} = \left.\frac{dE}{dT}\right|_{V,N} = \frac{\pi^2}{2}\frac{TN}{\varepsilon_F}$$

Reformulation in terms of density of states:

$$D(\varepsilon_F) \sim \frac{V\, m^{3/2}\, \varepsilon_F^{1/2}}{h^3}$$

$$\sim \frac{N}{\varepsilon_F}$$

since $\frac{N}{V} \sim \frac{m^{3/2}\, \varepsilon_F^{3/2}}{h^3}$

$$\Rightarrow \quad c_{V,N} \sim T\, D(\varepsilon_F)$$

Putting exact pre-factors:

$$c_{V,N} = \frac{\pi^2}{3}\, T\, D(\varepsilon_F)$$