Unit 3-9: The Degenerate Fermi Gas, the Sommerfeld Model for Electrons in a Conductor

In the previous section we discussed the limit of $z \ll 1$, where quantum effects are small and we are approaching the classical limit. Now we will look at the opposite case where quantum effects are dominant. We will start with a gas of fermions.

Since $z \ll 1$ corresponds to the limit of low density / high temperature, now we consider the gas of fermions in the high density / low temperature limit. This is known as the *degenerate* limit. We will consider first the case of $T \to 0$.

Recall first that, for non-relativisitc, non-interacting, indistinguishable particles, the density of single particle states per unit energy, per unit volume, is,

$$g(\epsilon) = \frac{2g_s}{\sqrt{\pi}\lambda^3} \frac{1}{k_BT} \sqrt{\frac{\epsilon}{k_BT}} \qquad \text{where } \lambda = \left(\frac{h^2}{2\pi m k_BT}\right)^{1/2} \text{ is the thermal wavelength.} \qquad (3.9.1)$$
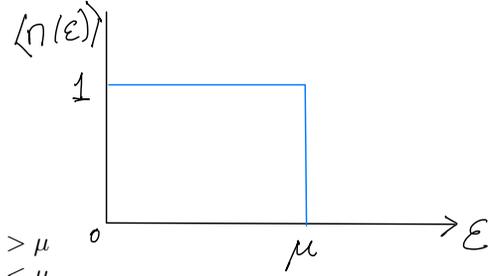
The T=0 Fermi gas

The ground state and the Fermi energy:

Here,

$$\langle n(\epsilon) \rangle = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \qquad (3.9.2)$$

As $T \to 0$ ($\beta \to \infty$), then

$$e^{\beta(\epsilon-\mu)} \to \begin{cases} \infty & \text{for } \epsilon > \mu \\ 0 & \text{for } \epsilon < \mu \end{cases} \quad \Rightarrow \quad \langle n(\epsilon) \rangle \to \begin{cases} 0 & \text{for } \epsilon > \mu \\ 1 & \text{for } \epsilon < \mu \end{cases}$$

$$(3.9.3)$$

Thus all states with $\epsilon < \mu$ are filled, and all states with $\epsilon > \mu$ are empty. This is the $T = 0$ ground state of the Fermi gas. We therefore see that $\mu(T = 0)$ is the energy of the highest single particle energy level that is occupied in the ground state. One calls this energy the *Fermi energy*, $\epsilon_F \equiv \mu(T = 0)$.

This simple nature of the $T = 0$ ground state of the Fermi gas, where all states below ϵ_F are filled and all states above ϵ_F are empty, makes it easy to compute many properties of the ground state. When computing an average of some observable $X(\epsilon)$ over the occupied states, we simply need to integrate,

$$\int_0^\infty d\epsilon\, g(\epsilon)\, \langle n(\epsilon) \rangle X(\epsilon) = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\, X(\epsilon) \qquad (3.9.4)$$

At $T = 0$ the total number of particles is,

$$N = g_s \sum_{\substack{\mathbf{k} \\ \text{such that} \\ \frac{\hbar^2 k^2}{2m} \le \epsilon_F}} [1] \qquad \text{count the occupied states} \qquad (3.9.5)$$

The particle density is then,

$$n = \frac{N}{V} = \frac{g_s}{V} \sum_{\substack{\mathbf{k} \\ \text{such that} \\ \frac{\hbar^2 k^2}{2m} \le \epsilon_F}} [1] = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon) = \frac{2g_s}{\sqrt{\pi}\lambda^3} \frac{1}{k_BT} \int_0^{\epsilon_F} d\epsilon \sqrt{\frac{\epsilon}{k_BT}} = \frac{2g_s}{\sqrt{\pi}\lambda^3} \frac{2}{3} \left(\frac{\epsilon_F}{k_BT}\right)^{3/2} \qquad (3.9.6)$$

So

$$\epsilon_F = k_B T \left[\frac{3}{4} \frac{\sqrt{\pi} n \lambda^3}{g_s} \right]^{2/3} = k_B T \lambda^2 \left[\frac{3}{4} \frac{\sqrt{\pi} n}{g_s} \right]^{2/3} = k_B T \frac{h^2}{2\pi m k_B T} \left[\frac{3}{4} \frac{\sqrt{\pi} n}{g_s} \right]^{2/3} = \frac{4\pi \hbar^2}{2m} \left[\frac{3}{4} \frac{\sqrt{\pi} n}{g_s} \right]^{2/3} \quad (3.9.7)$$

$$= \frac{\hbar^2}{2m} \left[(4\pi)^{3/2} \frac{3}{4} \frac{\sqrt{\pi} n}{g_s} \right]^{2/3} = \frac{\hbar^2}{2m} \left[\frac{6\pi^2 n}{g_s} \right]^{2/3} \quad (3.9.8)$$

so,

$$\boxed{\epsilon_F = \frac{\hbar^2}{2m} \left[\frac{6\pi^2 n}{g_s} \right]^{2/3} \equiv \frac{\hbar^2 k_F^2}{2m}} \qquad \text{is the Fermi energy} \quad (3.9.9)$$

where

$$k_F = \left[\frac{6\pi^2 n}{g_s} \right]^{1/3} \qquad \text{is the Fermi wavenumber} \quad (3.9.10)$$

The Fermi wavenumber is the wavenumber of the most energetic particle in the ground state.

From the above we have,

$$\epsilon_F \sim n^{2/3} \qquad \text{and} \qquad k_F \sim n^{1/3} \quad (3.9.11)$$

Since $n \sim 1/\ell^3$, with ℓ the average spacing between particles, then we see that $k_F \sim 1/\ell$.

It is often convenient to express the density of states in terms of ϵ_F. From Eq. (3.9.1) we have,

$$g(\epsilon) = C\sqrt{\epsilon} \qquad \text{where } C \text{ is independent of } \epsilon \qquad \Rightarrow \qquad g(\epsilon_F) = C\sqrt{\epsilon_F} \quad (3.9.12)$$

So

$$n = \frac{N}{V} = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon) = \int_0^{\epsilon_F} d\epsilon\, C\sqrt{\epsilon} = \frac{2}{3} C \epsilon_F^{3/2} \qquad \Rightarrow \qquad C = \frac{3}{2} \frac{n}{\epsilon_F^{3/2}} \quad (3.9.13)$$

and so,

$$g(\epsilon_F) = C\sqrt{\epsilon_F} = \frac{3}{2} \frac{n}{\epsilon_F^{3/2}} \epsilon_F^{1/2} \Rightarrow \boxed{g(\epsilon_F) = \frac{3}{2} \frac{n}{\epsilon_F}} \quad (3.9.14)$$

The density of states at the Fermi energy $g(\epsilon_F)$, which we will see is an important parameter for describing many properties of the degenerate Fermi gas, is roughly the particle density n divided by the Fermi energy ϵ_F.

Finally,

$$g(\epsilon) = g(\epsilon_F)\frac{g(\epsilon)}{g(\epsilon_F)} = g(\epsilon_F)\frac{C\sqrt{\epsilon}}{C\sqrt{\epsilon_F}} \Rightarrow \boxed{g(\epsilon) = \frac{3}{2} \frac{n}{\epsilon_F} \sqrt{\frac{\epsilon}{\epsilon_F}}} \quad (3.9.15)$$

Ground state energy:

The total energy density of the Fermi gas at $T = 0$ is given by,

$$\frac{E}{V} = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\, \epsilon \quad (3.9.16)$$

Use $g(\epsilon) = C\sqrt{\epsilon}$, with $C = \dfrac{3}{2}\dfrac{n}{\epsilon_F^{3/2}}$,

$$\frac{E}{V} = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\,\epsilon = C\int_0^{\epsilon_F} d\epsilon\, \epsilon^{3/2} = \frac{2}{5}C\,\epsilon_F^{5/2} = \frac{3}{5}n\epsilon_F \qquad (3.9.17)$$

We can now write for the energy *per particle*

$$\frac{E}{N} = \frac{E}{V}\frac{V}{N} = \frac{3}{5}n\,\epsilon_F\,\frac{1}{n} \quad\Rightarrow\quad \boxed{\frac{E}{N} = \frac{3}{5}\epsilon_F} \qquad (3.9.18)$$

We can now compute the pressure in the ground state,

$$p = -\left(\frac{\partial A}{\partial V}\right)_{T,N} = -\left(\frac{\partial E}{\partial V}\right)_{T,N} \quad \text{at } T=0 \text{ where } A = E - TS = E \qquad (3.9.19)$$

so

$$p = -\frac{3}{5}N\left(\frac{\partial \epsilon_F}{\partial V}\right)_{T,N} \qquad (3.9.20)$$

Using $\epsilon_F \sim n^{2/3} = (N/V)^{2/3}$ we have,

$$p = -\frac{3}{5}N\left(-\frac{2}{3}\right)\frac{\epsilon_F}{V} = \frac{2}{5}n\,\epsilon_F \qquad (3.9.21)$$

In contrast to the classical ideal gas where $p = Nk_BT/V = 0$ at $T = 0$, the pressure of the Fermi gas at $T = 0$ is finite. This is a consequence of the Pauli exclusion principle. Unlike the classical idea gas, where all particles go into the single particle ground state at $T = 0$, in the Fermi gas no two particles can go into the same single particle state. Hence the particles must fill up all single particle states up to ϵ_F, and so have finite energy E, and so pressure p, even in the ground state.

The Fermi Gas at Finite Temperature

At finite temperature we have,

$$\langle n(\epsilon)\rangle = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \qquad (3.9.22)$$

As shown in the sketch, the region where this finite temperature $\langle n\rangle$ differs from the $T = 0$ ground state is a region of width $\sim k_BT$ about the chemical potential μ.

So the $T = 0$ approximation is good when $k_BT \ll \mu$. Using $\mu \approx \mu(0) = \epsilon_F$ we have for this condition,
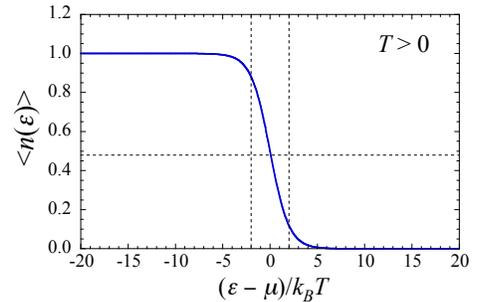
$$k_BT \ll \epsilon_F \quad\Rightarrow\quad k_BT \ll \frac{\hbar^2}{2m}\left[\frac{6\pi^2\,n}{g_s}\right]^{2/3} \quad\Rightarrow\quad \frac{2\pi m k_BT}{h^2} = \frac{1}{\lambda^2} \ll \frac{1}{4\pi}\left[\frac{6\pi^2 n}{g_s}\right]^{2/3} \qquad (3.9.23)$$

$$\Rightarrow\quad \lambda^2 \gg 4\pi\left[\frac{g_s}{6\pi^2 n}\right]^{2/3} \quad\Rightarrow\quad n\lambda^3 \gg (4\pi)^{3/2}\frac{g_s}{6\pi^2} = \frac{4}{3\sqrt{\pi}}g_s \sim O(1) \qquad (3.9.24)$$

In contrast to the classical limit, which we showed was $z \approx n\lambda^2 \ll 1$, the limit of the degenerate Fermi gas is $n\lambda^3 \gg 1$. This is the low T, high density, limit.

One defines the *Fermi Temperature*,

$$T_F \equiv \epsilon_F/k_B \qquad (3.9.25)$$

as the temperature scale of the Fermi energy. The degenerate limit is when $k_B T \ll \epsilon_F = k_B T_F$, or when $T \ll T_F$.

For conduction electrons in a metal – a prime example of a degenerate Fermi gas – one typically has $T_F \approx 10,000\,\text{K}$. So electrons in a metal at room temperature and below are always in the degenerate limit. Originally, in the 1890's Drude used a classical ideal gas, with a Maxwell velocity distribution, to describe the conduction electors in a metal. This led to some successes, but also some glaring conflicts with experiments. It was then Sommerfeld who in 1927, after the development of quantum mechanics, realized that the conduction electrons should be regarded as a degenerate Fermi gas. This is now known as the *Sommerfeld model* for conduction electrons in a metal.

To compute averages of quantities $X(\epsilon)$ in the Fermi gas at finite temperature, we need to do integrals of the form,

$$\int_0^\infty d\epsilon\, g(\epsilon)\, \langle n(\epsilon) \rangle\, X(\epsilon) = \int_0^\infty d\epsilon\, \frac{g(\epsilon)\, X(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} \tag{3.9.26}$$

A systematic method to evaluate such integrals as an expansion about the ground state in powers of $k_B T / \epsilon_F$ is known as the *Sommerfeld expansion*, and is presented in an Appendix to this section of notes. Here we will use more "hand waving" arguments to discuss how various properties of the degenerate Fermi gas will depend on T.

Chemical potential at finite T:

We have discussed that the chemical potential μ at $T = 0$ is just the Fermi energy ϵ_F. How does the chemical potential vary as T increases from zero? Does μ increase? decrease? stay the same?

In a physical conductor, the density of conduction electrons n must stay fixed as T varies (we assume that any thermal expansion of the lattice constant is negligible). Therefore μ must vary with T so that,

$$n = \int_0^\infty d\epsilon\, g(\epsilon)\, \langle n(\epsilon) \rangle = \int_0^\infty d\epsilon\, \frac{g(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} \qquad \text{stays constant.} \tag{3.9.27}$$

Suppose as T increased that μ stayed constant at $\mu = \epsilon_F$ Consider the sketch below.
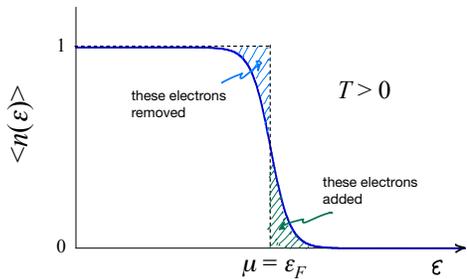
At finite T, some number of electrons get excited from below ϵ_F to above ϵ_F. The electrons that get removed from below ϵ_F are represented by the shaded area in the sketch below $\mu = \epsilon_F$. The electrons that get added above ϵ_F are represented by the shaded area in the sketch above $\mu = \epsilon_F$. Because $\partial \langle n \rangle / \partial \epsilon$ is symmetric about $\epsilon = \mu$, these two shaded areas in the sketch must be equal.

Because n must stay fixed, the number of electrons removed below ϵ_F should equal the number of electrons added above ϵ_F.

The number of electrons per unit volume that get removed from below ϵ_F is then just the density of states $g(\epsilon_F - k_B T)$ just below ϵ_F, multiplied by the relevant energy width $\Delta\epsilon \approx k_B T$, or $\approx g(\epsilon_F - k_B T)k_B T$. The number of electrons per unit volume that get added above ϵ_F is similarly $\approx g(\epsilon_F + k_B T)k_B T$. But since $g(\epsilon) \sim \sqrt{\epsilon}$ is an *increasing* function of ϵ, there are more energy states within $k_B T$ above ϵ_F than there are energy states within $k_B T$ below ϵ_F, i.e. $g(\epsilon_F + k_B T)k_B T > g(\epsilon_F - k_B T)k_B T$. Thus keeping $\mu = \epsilon_F$ fixed would result in increasing the number of electrons in the system. This cannot be!

The only way we can keep the density of electrons n constant is for the chemical potential μ to *decrease* as T increases. From the Sommerfeld expansion one finds,

$$\mu(T) = \epsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{g'(\epsilon_F)}{g(\epsilon_F)} \qquad \text{where } g' = dg/d\epsilon. \tag{3.9.28}$$

For free non-relativistic electrons in a box we had $g(\epsilon) = C\sqrt{\epsilon}$, so $g'/g = 1/2\epsilon$, and we then have for the relative shift in the chemical potential,

$$\frac{[\epsilon_F - \mu(T)]}{\epsilon_F} = \frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_F}\right)^2 \sim \left(\frac{T}{T_F}\right)^2 \ll 1 \tag{3.9.29}$$

Contribution to specific heat at constant volume C_V due to conduction electrons:

When we increase the temperature to T, the electrons within $k_B T$ below ϵ_F will absorb thermal energy and get excited to within $k_B T$ above ϵ_F. Such electrons increase their energy by an amount $\sim k_B T$. Since $g(\epsilon_F)$ is the number of electrons per unit volume per unit energy at ϵ_F, and $k_B T$ is the energy interval over which such electrons can get excited, then the total number of excited electrons per unit volume is roughly $g(\epsilon_F)(k_B T)$. Hence the increase in energy per unit volume is roughly,
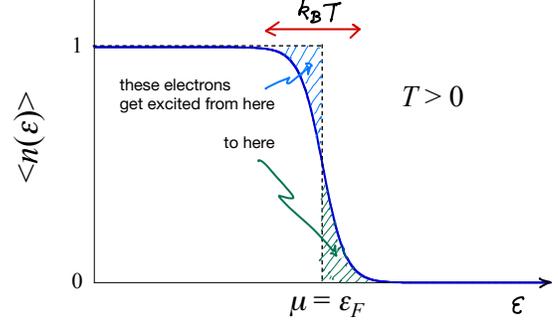
$$\Delta u \;=\; [\text{number of electrons excited}] \times [\text{energy absorbed by each excited electron}] \tag{3.9.30}$$

$$\approx\; [g(\epsilon_F)k_B T] \times [k_B T] \;=\; g(\epsilon_F)(k_B T)^2 \tag{3.9.31}$$

The specific heat per unit volume, at constant volume, is then,

$$c_V \;=\; \frac{C_V}{V} \;=\; \left(\frac{\partial \Delta u}{\partial T}\right)_{V,N} \approx\; 2g(\epsilon_F)k_B^2 T \qquad \text{since } g(\epsilon_F) \text{ depends on } N \text{ and } V, \text{ but } not\ T \tag{3.9.32}$$

For *free electrons* with $g(\epsilon_F) = \dfrac{3}{2}\dfrac{n}{\epsilon_F}$ we have,

$$c_V \;\approx\; \frac{3n}{\epsilon_F} k_B^2 T \;=\; 3nk_B\left(\frac{T}{T_F}\right) \tag{3.9.33}$$

The Sommerfeld expansion, taking into account also the shift in $\mu(T)$ at finite T, gives for free electrons the more precise result,

$$c_V \;=\; \frac{\pi^2}{2}nk_B\left(\frac{T}{T_F}\right) \tag{3.9.34}$$

We can compare this to what we have for a classical ideal gas, $c_V = (3/2)nk_B$, a constant at all temperature. Thus, while a classical gas gives a constant c_V, the degenerate Fermi gas gives a c_V that decreases linearly as temperature decreases $\sim T/T_F$. At room temperature $T \sim 100\,\text{K}$ (it is a cold room, we are in Rochester), then the c_V of the degenerate Fermi gas is smaller than that of the classical gas by a factor $\sim (T/T_F) \sim 10^2/10^4 \sim 10^{-2}$.

Previously we discussed the contribution to the specific heat of a solid due to vibrations of the ionic lattice (phonons). The Debye model gave, at low temperatures $T \ll \Theta_D$,

$$c_V^{\text{ions}} \;=\; \frac{12\pi^4}{5}nk_B\left(\frac{T}{\Theta_D}\right)^3 \;\sim\; T^3 \tag{3.9.35}$$

Here we found that the contribution to the specific heat of a metal due to conduction electrons is,

$$c_V^{\text{elec}} \;=\; \frac{\pi^2}{2}nk_B\left(\frac{T}{T_F}\right) \;\sim\; T \tag{3.9.36}$$

The total specific heat of a metal is the sum of these two contributions, $c_V^{\text{metal}} = c_V^{\text{elec}} + c_V^{\text{ion}}$.

Since $c_V^{\text{elec}} \sim (T/T_F)$, with $T_F \sim 10{,}000\,\text{K}$, while $c_V^{\text{ions}} \sim (T/\Theta_D)^3$, with $\Theta_D \sim 100\,\text{K}$, then c_V^{ions} will be the dominant contribution near room temperature. However, since $c_V^{\text{ions}} \sim T^3$ while $c_V^{\text{elec}} \sim T$, then it must be the case that, at sufficiently small T, c_V^{elec} will become dominant. This crossover will happen at a T^* such that,

$$1 = \frac{c_V^{\text{elec}}}{c_V^{\text{ions}}} = \frac{\pi^2}{2}nk_B\left(\frac{T^*}{T_F}\right)\frac{5}{12\pi^4 nk_B}\left(\frac{\Theta_D}{T^*}\right)^3 = \frac{5}{24\pi^2}\left(\frac{\Theta_D}{T_F}\right)\left(\frac{\Theta_D}{T^*}\right)^2 \tag{3.9.37}$$

$$\Rightarrow \quad T^* = \sqrt{\frac{5}{24\pi^2}\left(\frac{\Theta_D}{T_F}\right)}\;\Theta_D \;\simeq\; 0.15\left(\frac{\Theta_D}{T_F}\right)^{1/2}\Theta_D \tag{3.9.38}$$

With $T_F \sim 10^4\,\mathrm{K}$ and $\Theta_D \sim 10^2\,\mathrm{K}$, we get $T^* \sim 0.05\,\Theta_D \sim O(1)\,K$. So one has to go to very low temperatures in order to see the contribution to the specific heat from the conduction electrons!

Appendix: The Sommerfeld Expansion

We wish to evaluate integrals of the form,

$$\Phi = \int_0^\infty d\epsilon\, g(\epsilon)\, \langle n(\epsilon)\rangle\, X(\epsilon) = \int_0^\infty d\epsilon\, \frac{g(\epsilon)\, X(\epsilon)}{\mathrm{e}^{\beta(\epsilon-\mu)}+1} = \int_0^\infty d\epsilon\, \frac{\phi(\epsilon)}{\mathrm{e}^{\beta(\epsilon-\mu)}+1} \qquad \text{where } \phi(\epsilon) = g(\epsilon)X(\epsilon). \qquad (3.9.39)$$

So for example, to compute the density n we would use $\phi(\epsilon) = g(\epsilon)$; to compute the energy E/V we would use $\phi(\epsilon) = g(\epsilon)\epsilon$.

To simplify the algebra, let us take $x = \beta\epsilon$ and $\xi = \beta\mu$, and consider the integral,

$$\tilde{\Phi} = \beta\Phi = \int_0^\infty dx\, \frac{\tilde{\phi}(x)}{\mathrm{e}^{x-\xi}+1} \qquad \text{where } \tilde{\phi}(x) \equiv \phi(x/\beta). \qquad (3.9.40)$$

Note the "standard function" $f_n(z)$ is obtained by using $\tilde{\phi}(x) = x^{n-1}/\Gamma(n)$ and $z = \mathrm{e}^\xi$.

Define,

$$\psi(x) = \int_0^x dx'\, \tilde{\phi}(x') \qquad \text{and} \qquad f(x) = \frac{1}{\mathrm{e}^{x-\xi}+1} \quad \text{is the Fermi function} \qquad (3.9.41)$$

then,

$$\tilde{\Phi} = \int_0^\infty dx\, \left(\frac{\partial\psi}{\partial x}\right) f(x) \qquad \text{integrate by parts} \qquad (3.9.42)$$

$$= \psi(x)f(x)\Big|_0^\infty + \int_0^\infty dx\, \psi(x)\left(-\frac{df}{dx}\right) \qquad (3.9.43)$$

$$= \int_0^\infty dx\, \psi(x)\left(-\frac{df}{dx}\right) \qquad \text{boundary term vanishes since } \psi(0) = 0 \text{ and } f(\infty) = 0 \qquad (3.9.44)$$

Now we use the fact that, at low T, $(-df/dx)$ is strongly peaked about $x = \xi$, so the only place the integrand is not negligible is near $x = \xi$.

So we expand $\psi(x)$ about $x = \xi$,

$$\psi(x) = \sum_{n=0}^\infty \frac{d^n\psi}{dx^n}\bigg|_{x=\xi} \frac{(x-\xi)^n}{n!} \qquad (3.9.45)$$
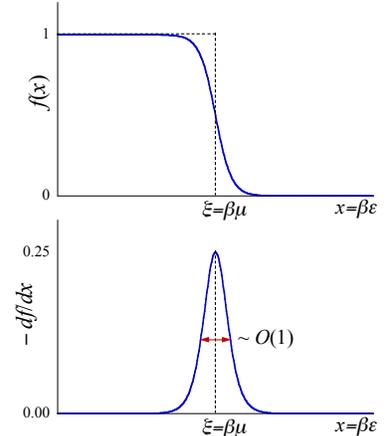
and then,

$$\tilde{\Phi} = \sum_{n=0}^\infty \frac{d^n\psi}{dx^n}\bigg|_{x=\xi} \int_0^\infty dx\, \frac{(x-\xi)^n}{n!}\left(-\frac{df}{dx}\right) \qquad (3.9.46)$$

Now since $(-df/dx) \approx 0$ except for a region of order $O(1)$ about $x = \xi \gg 1$ (since $\xi = \mu/k_B T \approx \epsilon_F/k_B T = T_F/T$), we can replace the lower limit of the integral by $-\infty$ without any noticeable change in its value.

Then, making a change of variables to $y = x - \xi$, the integrals in the above sum become,

$$\int_{-\infty}^\infty dy\, \frac{y^n}{n!}\left(-\frac{df}{dy}\right) \qquad \text{where } f(y) = \frac{1}{\mathrm{e}^y+1} \qquad (3.9.47)$$

Now

$$\left(-\frac{df}{dy}\right) = \frac{e^y}{(e^y+1)^2} = \frac{e^y}{e^{2y}+2e^y+1} = \frac{1}{e^y+2+e^{-y}} \tag{3.9.48}$$

is symmetric about $y = 0$, so the integrals for all odd values of n vanish by symmetry!

Since the sum is now over only n even, we let $n \to 2n$ and sum on all integer n,

$$\tilde{\Phi} = \sum_{n=0}^{\infty} \left.\frac{d^{2n}\psi}{dx^{2n}}\right|_{x=\xi} \int_{-\infty}^{\infty} dy\, \frac{y^{2n}}{(2n)!} \left(-\frac{df}{dy}\right) \tag{3.9.49}$$

Define constants,

$$a_n \equiv \int_{-\infty}^{\infty} dy\, \frac{y^{2n}}{(2n)!} \left(-\frac{df}{dy}\right), \qquad a_0 = \int_{-\infty}^{\infty} dy \left(-\frac{df}{dy}\right) = 1 \tag{3.9.50}$$

The a_n are just *numbers* that can be computed, they contain no parameters of the system at all. For $n \geq 1$ one can show that,

$$a_n = 2\left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \frac{1}{5^{2n}} - \cdots\right) = \left(2 - \frac{1}{2^{2(n-1)}}\right)\zeta(2n) \tag{3.9.51}$$

where,

$$\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \cdots \qquad \text{is the Riemann zeta function} \tag{3.9.52}$$

In particular,

$$a_1 = \frac{\pi^2}{6}, \qquad a_2 = \frac{7\pi^4}{360} \tag{3.9.53}$$

So with the constants a_n we can write,

$$\tilde{\Phi} = \sum_{n=0}^{\infty} a_n \left.\frac{d^{2n}\psi}{dx^{2n}}\right|_{x=\xi} = \psi(\xi) + \sum_{n=1}^{\infty} a_n \left.\frac{d^{2n}\psi}{dx^{2n}}\right|_{x=\xi} \tag{3.9.54}$$

Now use $\frac{d\psi}{dx} = \tilde{\phi}$ to get,

$$\tilde{\Phi} = \int_0^\xi dx\, \tilde{\phi}(x) + \sum_{n=1}^{\infty} a_n \left.\frac{d^{2n-1}\tilde{\phi}}{dx^{2n-1}}\right|_{x=\xi} = \int_0^\xi dx\, \tilde{\phi}(x) + \frac{\pi^2}{6}\left.\frac{d\tilde{\phi}}{dx}\right|_{x=\xi} + \frac{7\pi^4}{360}\left.\frac{d^3\tilde{\phi}}{dx^3}\right|_{x=\xi} + \cdots \tag{3.9.55}$$

When we convert from the variable x back to the variable ϵ, this gives an expansion as a power series in temperature. To see this, note $x = \epsilon/k_B T$ and transform back to the energy variable $\epsilon = k_B T x$,

$$\Phi = \int_0^\infty d\epsilon\, \frac{\phi(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} = \beta^{-1}\tilde{\Phi} = k_B T\, \tilde{\Phi} \tag{3.9.56}$$

Using,

$$k_B T \int_0^\xi dx\, \tilde{\phi}(x) = \int_0^\mu d\epsilon\, \phi(\epsilon) \qquad \text{and} \qquad \tilde{\phi}(x) = \phi(k_B T x) \quad \text{so} \quad \frac{d\tilde{\phi}}{dx} = \frac{d\phi}{d\epsilon}\frac{d\epsilon}{dx} = \frac{d\phi}{d\epsilon}k_B T \tag{3.9.57}$$

we get,

$$\Phi = \int_0^\infty d\epsilon\, \frac{\phi(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} = \int_0^\mu d\epsilon\, \phi(\epsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \left.\frac{d^{2n-1}\phi}{d\epsilon^{2n-1}}\right|_{\epsilon=\mu} \tag{3.9.58}$$

$$= \int_0^\mu d\epsilon\, \phi(\epsilon) + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{d\phi}{d\epsilon}\right|_{\epsilon=\mu} + \frac{7\pi^4}{360}(k_B T)^4 \left.\frac{d^3\phi}{d\epsilon^3}\right|_{\epsilon=\mu} + \cdots \tag{3.9.59}$$

This is the Sommerfeld expansion.

<u>Chemical potential:</u>

We can now apply the Sommerfeld expansion to compute how the chemical potential μ changes as T increases from zero.

We have for the density,

$$n = \frac{N}{V} = \int_0^\infty d\epsilon \, g(\epsilon) \langle n(\epsilon) \rangle = \int_0^\infty d\epsilon \, \frac{g(\epsilon)}{e^{\beta(\epsilon - \mu)} + 1} \qquad \Rightarrow \qquad \phi(\epsilon) = g(\epsilon) \tag{3.9.60}$$

$$n = \int_0^\mu d\epsilon \, g(\epsilon) + \frac{\pi^2}{6} (k_B T)^2 \left. \frac{dg}{d\epsilon} \right|_{\epsilon = \mu} + \cdots \tag{3.9.61}$$

$$= \int_0^{\epsilon_F} d\epsilon \, g(\epsilon) + \int_{\epsilon_F}^\mu d\epsilon \, g(\epsilon) + \frac{\pi^2}{6} (k_B T)^2 \left. \frac{dg}{d\epsilon} \right|_{\epsilon = \mu} + \cdots \tag{3.9.62}$$

Now we know that at $T = 0$, $n = \int_0^{\epsilon_F} d\epsilon \, g(\epsilon)$, and since n must stay constant as T varies, to lowest order we must have ,

$$\int_{\epsilon_F}^\mu d\epsilon \, g(\epsilon) = -\frac{\pi^2}{6} (k_B T)^2 \left. \frac{dg}{d\epsilon} \right|_{\epsilon = \mu} \tag{3.9.63}$$

Since the right hand side of the above equation is $\sim (k_B T)^2$ is small, so the left hand side must be small. And since we know $\mu \to \epsilon_F$ as $T \to 0$, we can therefore approximate,

$$\int_{\epsilon_F}^\mu d\epsilon \, g(\epsilon) \approx (\mu - \epsilon_F) g(\epsilon_F) \qquad \Rightarrow \qquad (\mu - \epsilon_F) \approx -\frac{\pi^2}{6} \frac{(k_B T)^2}{g(\epsilon_F)} \left. \frac{dg}{d\epsilon} \right|_{\epsilon = \mu} \tag{3.9.64}$$

So we see that $(\mu - \epsilon_F) \sim O(k_B T)^2$ is small, so to lowest order we can evaluate the derivative $dg/d\epsilon$ at $\epsilon = \epsilon_F$ rather than at $\epsilon = \mu$. We thus get

$$\boxed{\mu(T) = \epsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{g'(\epsilon_F)}{g(\epsilon_F)}} \qquad \text{where } g' = \frac{dg}{d\epsilon} \tag{3.9.65}$$

We thus see that the chemical potential μ decreases from ϵ_F by $O(k_B T)^2$ at low T.

For *free electrons*, where $g(\epsilon) = C\sqrt{\epsilon}$ and $g'(\epsilon) = \frac{1}{2} C \frac{1}{\sqrt{\epsilon}}$, the above becomes,

$$\mu(T) = \epsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{1}{2\epsilon_F} = \epsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\epsilon_F} \tag{3.9.66}$$

so we have,

$$\mu(T) = \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] = \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_F} \right)^2 \right] \tag{3.9.67}$$

So the relative shift in the chemical potential is,

$$\frac{\mu(T) - \mu(0)}{\epsilon_F} = -\frac{\pi^2}{12} \left(\frac{T}{T_F} \right)^2 \sim O\left(\frac{T}{T_F} \right)^2 \tag{3.9.68}$$

With $T_F \approx 10^4\,\mathrm{K}$ for a typical metal, we see that this shift in μ is very small at room temperatures and below.

Average energy:

We now use the Sommerfeld expansion to compute the average energy density at finite temperature.

$$u = \frac{E}{V} = \int_0^\infty d\epsilon\, g(\epsilon)\,\epsilon\, \langle n(\epsilon)\rangle = \int_0^\infty d\epsilon\, \frac{g(\epsilon)\epsilon}{e^{\beta(\epsilon-\mu)}+1} \qquad \Rightarrow \qquad \phi(\epsilon) = g(\epsilon)\epsilon, \quad \phi'(\epsilon) = g(\epsilon) + \epsilon g'(\epsilon) \tag{3.9.69}$$

So, to lowest order in the Sommerfeld expansion, we have,

$$u = \int_0^\mu d\epsilon\, g(\epsilon)\,\epsilon + \frac{\pi^2}{6}(k_B T)^2\Big[g(\mu) + \mu g'(\mu)\Big] \tag{3.9.70}$$

$$= \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\,\epsilon + \int_{\epsilon_F}^\mu d\epsilon\, g(\epsilon)\,\epsilon + \frac{\pi^2}{6}(k_B T)^2\Big[g(\mu) + \mu g'(\mu)\Big] \tag{3.9.71}$$

The first term is just u_0, the energy density in the ground state at $T = 0$. Because we know $|\mu - \epsilon_F| \sim (k_B T)^2$ is small, we can approximate the second term as $(\mu - \epsilon_F)g(\epsilon_F)\epsilon_F$, as we did in the calculation of $\mu(T)$. And similarly, since $|\mu - \epsilon_F|$ is small, we can evaluate the third term at $\mu = \epsilon_F$. So we now have to lowest order,

$$u(T) = u_0 + (\mu - \epsilon_F)g(\epsilon_F)\epsilon_F + \frac{\pi^2}{6}(k_B T)^2\Big[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\Big] \tag{3.9.72}$$

Now we use our result from Eq. (3.9.65) that $\mu - \epsilon_F = -\dfrac{\pi^2}{6}(k_B T)^2\dfrac{g'(\epsilon_F)}{g(\epsilon_F)}$ to get,

$$u(T) = u_0 + \left[-\frac{\pi^2}{6}(k_B T)^2\frac{g'(\epsilon_F)}{g(\epsilon_F)}\right]g(\epsilon_F)\epsilon_F + \frac{\pi^2}{6}(k_B T)^2\Big[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\Big] \tag{3.9.73}$$

and we finally have,

$$\boxed{u(T) = u_0 + \frac{\pi^2}{6}(k_B T)^2 g(\epsilon_F)} \tag{3.9.74}$$

Specific heat:

WIth the above $u(T)$, we can now compute the specific heat of the degenerate Fermi gas,

$$c_V = \frac{C_V}{V} = \frac{1}{V}\left(\frac{\partial E}{\partial T}\right)_{V,N} = \left(\frac{\partial u}{\partial T}\right)_{V,N} \tag{3.9.75}$$

$$\boxed{c_V = \frac{\pi^2}{3}k_B^2 T g(\epsilon_F)} \tag{3.9.76}$$

For *free electrons*, Eq. (3.9.14) gives $g(\epsilon_F) = \dfrac{3}{2}\dfrac{n}{\epsilon_F}$. Thus we get,

$$c_V = \frac{\pi^2}{3}k_B^2 T\left[\frac{3}{2}\frac{n}{\epsilon_F}\right] = \frac{\pi^2}{2}n k_B\left(\frac{k_B T}{\epsilon_F}\right) = \frac{\pi^2}{2}n k_B\left(\frac{T}{T_F}\right) \tag{3.9.77}$$