Sommerfeld expansion - Summary

want to do integrals of the form

$$\Phi = \int_0^\infty d\varepsilon \, \frac{\phi(\varepsilon)}{z^{-1} e^{\beta\varepsilon}+1} = \int_0^\infty d\varepsilon \, \phi(\varepsilon)\, n(\varepsilon) \quad \text{with } n(\varepsilon) = \frac{1}{z^{-1}e^{\beta}+1}$$

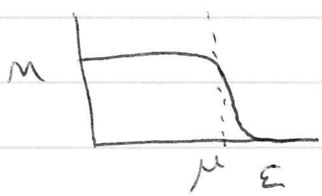
the fermi occupation function

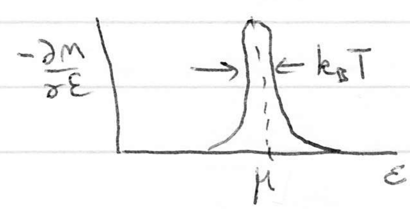
integrate by parts with $\psi(\varepsilon) = \int_0^\varepsilon d\varepsilon' \, \phi(\varepsilon')$ so that $\frac{d\psi}{d\varepsilon} = \phi$

$$\Phi = \Big[\psi(\varepsilon)\, n(\varepsilon)\Big]_0^\infty + \int_0^\infty d\varepsilon \, \psi(\varepsilon)\left(-\frac{\partial n}{\partial \varepsilon}\right)$$

vanishes since $\psi(0)=0$ by definition of ψ, and $n(\varepsilon\to\infty)=0$

$$\Phi = \int_0^\infty d\varepsilon \, \psi(\varepsilon)\left(-\frac{\partial n}{\partial \varepsilon}\right)$$





so integrand is only non zero within region of width $k_B T$ around $\mu \approx \varepsilon_F = k_B T_F$ and $k_B T / k_B T_F \ll 1$

at low temperature.

So expand $\psi(\varepsilon)$ about $\varepsilon = \mu$ in a Taylor series. Because $-\frac{\partial n}{\partial \varepsilon}$ is even function of $\varepsilon - \mu$, only even powers in the expansion integrate to some thing non zero. Since the integrand is only non zero for $|\varepsilon - \mu| \sim k_B T$, the result is a power series in $\left(\frac{T}{T_F}\right)^{2n}$. This is the Sommerfeld expansion

Sommerfeld Expansion

transform variables to $x = \beta\epsilon$.

Then we want to do integrals of the form

$$\Phi \equiv \int_0^\infty dx \, \frac{\phi(x)}{z^{-1} e^{x} + 1}$$

$\phi(x)$ is any function of x.

For example, to get the "standard" function $f_n(z)$, we use $\phi(x) = \frac{1}{\Gamma(n)} x^{n-1}$

Define $\xi = \beta\mu = \ln z$

$$\Phi = \int_0^\infty dx \, \frac{\phi(x)}{e^{x-\xi} + 1}$$

Define $\psi(x) \equiv \int_0^x \phi(x')\,dx'$, $f(x) \equiv \frac{1}{[e^{x-\xi} + 1]}$ fermi function

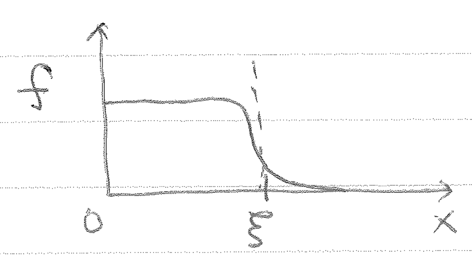
$$\Phi = \int_0^\infty dx \left(\frac{\partial \psi}{\partial x}\right) f(x) \quad \text{integrate by parts}$$

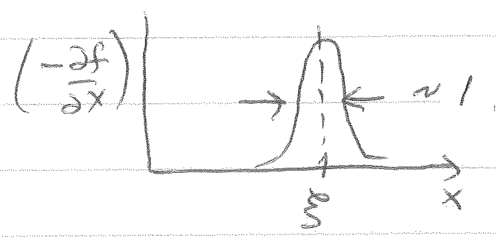
$$= \psi(x) f(x) \Big|_0^\infty + \int_0^\infty dx \, \psi(x) \left(-\frac{\partial f}{\partial x}\right)$$

$$= \int_0^\infty dx \, \psi(x) \left(-\frac{\partial f}{\partial x}\right)$$

since $\psi(0) = 0$ and $f(\infty) = 0$
1st term vanishes

Now we use the fact that at low T, $\left(-\frac{\partial f}{\partial x}\right)$ is strongly peaked about $x = \xi$





$\xi \gtrsim 1$

$\xi \sim \frac{\epsilon_F}{k_B T}$ large expand $\psi(x)$ about $x = \xi$

$$\psi(x) = \sum_{n=0}^{\infty} \left.\frac{d^n\psi}{dx^n}\right|_{x=\xi} \frac{(x-\xi)^n}{n!}$$

$$\Rightarrow \quad \Phi = \sum_{n=0}^{\infty} \left.\frac{d^n\psi}{dx^n}\right|_{x=\xi} \int_0^{\infty} dx \, \frac{(x-\xi)^n}{n!} \left(-\frac{\partial f}{\partial x}\right)$$

since $\left(-\frac{\partial f}{\partial x}\right)$ is zero except for a region of order 1 about $x = \xi \gg 1$, we can replace the lower limit of the integral by $-\infty$ without any noticeable change

Then we can make a change of variables $y = x - \xi$ and the integrals become

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

Now $$-\frac{\partial f}{\partial y} = \frac{e^y}{(e^y+1)^2} = \frac{e^y}{e^{2y} + 2e^y + 1} = \frac{1}{e^y + 2 + e^{-y}}$$

is symmetric about $y = 0$.

$\Rightarrow$ all the integrals for n odd vanish!

To sum over only n even terms, let $n \to 2n$

$$\Phi = \sum_{n=0}^{\infty} \frac{d^{2n}\psi}{dx^{2n}}\Big|_{x=\xi} \int_{-\infty}^{\infty} dy \, \frac{y^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial y}\right)$$

let $a_n \equiv \int_{-\infty}^{\infty} dy \, \frac{y^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial y}\right)$, $a_0 = \int_{-\infty}^{\infty} dy \left(-\frac{\partial f}{\partial y}\right) = 1$

The a_n are just numbers that be computed.
They contain no system parameters whatsoever

For $n \geq 1$ one can show

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

$$= \left(2 - \frac{1}{2^{2(n-1)}}\right) \zeta(2n)$$

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

In particular $a_1 = \frac{\pi^2}{6}$, $a_2 = \frac{7\pi^4}{360}$

$$\Phi = \sum_{n=0}^{\infty} a_n \frac{d^{2n}\psi}{dx^{2n}}\Big|_{x=\xi} = \psi(\xi) + \sum_{n=1}^{\infty} a_n \frac{d^{2n}\psi}{dx^{2n}}\Big|_{x=\xi}$$

use $\frac{d\psi}{dx} = \phi$ to finally get $\qquad \psi(x) = \int_0^x dx' \, \phi(x')$

$$\Phi = \int_0^{\xi} dx \, \phi(x) + \sum_{n=1}^{\infty} a_n \frac{d^{2n-1}\phi}{dx^{2n-1}}\Big|_{x=\xi}$$

$$= \int_0^{\xi} dx \, \phi(x) + \frac{\pi^2}{6} \frac{d\phi}{dx}\Big|_{x=\xi} + \frac{7\pi^4}{360} \frac{d^3\phi}{dx^3}\Big|_{x=\xi} + \cdots$$

This gives a power series in temperature.

To see this, transform ~~back~~ to the energy variable

$x = \beta\epsilon$, $\epsilon = k_B T x$

$$\Phi \equiv \int_0^\infty d\epsilon \frac{\phi(\epsilon)}{z^{-1}e^{\beta\epsilon}+1} = k_B T \left\{ \int_0^\infty dx \frac{\phi(k_B T x)}{z^{-1}e^{x}+1} \right\}$$

using $k_B T \int_0^{\xi = \mu/k_B T} dx \, \phi(k_B T x) = \int_0^\mu d\epsilon \, \phi(\epsilon)$

and $\frac{d\phi}{dx} = \frac{d\phi}{d\epsilon}\frac{d\epsilon}{dx} = \frac{d\phi}{d\epsilon} k_B T$

we get

$$n(\varepsilon) \equiv \frac{1}{z^{-1}e^{\beta\varepsilon}+1}$$

$$\Phi = \int_0^\infty d\epsilon \, \phi(\epsilon) \, n(\epsilon)$$

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

Example

① density $n = \frac{N}{V} = \int_0^\infty d\epsilon \, g(\epsilon) \, n(\epsilon) \Rightarrow \phi(\epsilon) \equiv g(\epsilon)$

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

Now as $T \to 0$, $\mu \to \epsilon_F$ the fermi energy

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

But ϵ_F was determined by $n = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)$

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

since left had side is $O(kT)^2$ is small, we can approx ~~the right had side as~~ it as

$$\int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon) \approx (\mu - \epsilon_F)\, g(\epsilon_F)$$

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

so $\mu - \epsilon_F \sim O(k_B T)^2$ is small, so to lowest order can evaluate $\frac{dg}{d\epsilon}$ on right had side at $\epsilon = \epsilon_F$ instead of $\epsilon = \mu$

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

Shows that chemical potential μ decreases from ϵ_F by $O(kT)^2$ at low T

For free electrons where $g(\epsilon) = C\sqrt{\epsilon}$

$$g'(\epsilon) = \tfrac{1}{2} C \frac{1}{\sqrt{\epsilon}}$$

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

$$\boxed{\mu(T) \simeq \epsilon_F\left(1 - \frac{1}{3}\left(\frac{\pi k_B T}{2\epsilon_F}\right)^2\right) = \epsilon_F\left(1 - \frac{1}{3}\left(\frac{\pi}{2}\frac{T}{T_F}\right)^2\right)}$$

Correction is small for metals at room temp as $T_F \sim 10{,}000\,°K$

② energy $\dfrac{E}{V} = \displaystyle\int_0^\infty d\epsilon\, g(\epsilon)\,\epsilon\, n(\epsilon) \Rightarrow \phi(\epsilon) = g(\epsilon)\,\epsilon$

$$u = \frac{E}{V} = \int_0^\mu d\epsilon\, g(\epsilon)\,\epsilon + \frac{\pi^2}{6}(k_B T)^2\left[g(\mu) + \mu g'(\mu)\right]$$

$$= \underbrace{\int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\,\epsilon}_{=u(0)} + \underbrace{\int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon)\,\epsilon}_{\simeq(\mu-\epsilon_F)g(\epsilon_F)\epsilon_F} + \frac{\pi^2(k_B T)^2}{6}\left[g(\mu) + \mu g'(\mu)\right]$$

ground state energy density

as before

replace $\mu \approx \epsilon_F$ as before

$$u(T) = u(0) + (\mu - \epsilon_F)\,g(\epsilon_F)\,\epsilon_F + \frac{\pi^2(k_B T)^2}{6}\left[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\right]$$

$$= u(0) + \left[-\frac{\pi^2}{6}(k_B T)^2\frac{g'(\epsilon_F)}{g(\epsilon_F)}\right] g(\epsilon_F)\,\epsilon_F + \frac{\pi^2(k_B T)^2}{6}\left[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\right]$$

$$\boxed{u(T) = u(0) + \frac{\pi^2(k_B T)^2}{6}\, g(\epsilon_F)}$$

specific heat per volume

$$c_V = \frac{C_V}{V} = \frac{1}{V}\left(\frac{dE}{dT}\right)_V = \left(\frac{du}{dT}\right)_V$$

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

for free electrons we can write $g(\epsilon) = C\sqrt{\epsilon}$

$$n = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon) = \frac{2}{3} C \epsilon^{3/2} \Rightarrow C = \frac{3}{2}\frac{n}{\epsilon^{3/2}}$$

$$\Rightarrow g(\epsilon_F) = \frac{3}{2}\frac{n}{\epsilon_F^{3/2}} \cdot \epsilon_F^{1/2} = \frac{3}{2}\frac{n}{\epsilon_F}$$ density of states at fermi energy

$$\boxed{c_V = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) n k_B}$$

or total specific heat $C_V = V c_V$ $\qquad nV = N$

$$C_V = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) N k_B$$

$\Rightarrow$ specific heat due to fermi gas of electrons in a conductor is $C_V \sim T$ at low temperatures

We already saw that specific heat due to ionic vibrations (phonons) in a solid went like $C_V \sim T^3$ at low temperatures (Debye model)

$\Rightarrow$ electronic contribution to C_V dominates at sufficiently low T.