

Sommerfeld expansion - Summary

want to do integrals of the form

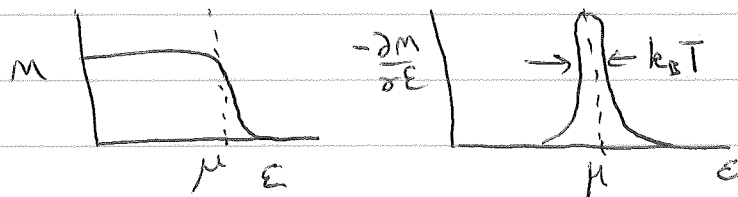
$$\Phi = \int_0^{\infty} d\varepsilon \frac{\phi(\varepsilon)}{z^{-1} e^{\beta\varepsilon} + 1} = \int_0^{\infty} d\varepsilon \phi(\varepsilon) n(\varepsilon) \quad \text{with } n(\varepsilon) = \frac{1}{z^{-1} e^{\beta\varepsilon} + 1}$$

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

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

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

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



so integral is only non zero within region of width $k_B T$ around $\mu \approx \varepsilon_F = k_B T_B$ 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 this expansion integrate to some thing non zero. Since the integral 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 $\phi(x) = \frac{1}{\Gamma(n)} x^{n-1}$

$$\text{Define } \xi = \beta \mu = \ln z$$

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

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

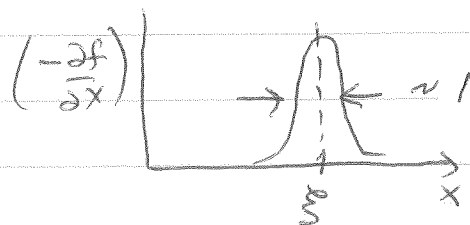
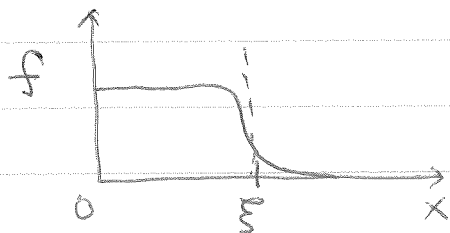
$$\Phi = \int_0^{\infty} dx \left(\frac{\partial \psi}{\partial x} \right) f(x) \quad \text{integrate by parts}$$

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

$$= \int_0^{\infty} dx \psi(x) \left(-\frac{\partial f}{\partial x} \right) \quad \text{since } \psi(0) = 0 \text{ and } f(\infty) = 0$$

1st term vanishes

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



$$\xi \sim \frac{\epsilon_F}{k_B T} \quad \text{large}$$

expand $\psi(x)$ about $x = \xi$

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

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

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

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

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

is symmetric about $y = 0$.

\Rightarrow all the integrals for n odd vanish!

To sum over only n even terms, let $n = 2n$.

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

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

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

For $n \geq 1$ one can show

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

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

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

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

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

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

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

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

This gives a power series in temperature.

To see this, transform back to the energy variable

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

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

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

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

we get

$$m(\epsilon) \equiv \frac{1}{z^{-1} e^{\beta \epsilon} + 1}$$

$$\Phi = \int_0^{\infty} d\epsilon \phi(\epsilon) m(\epsilon)$$

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

Example

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

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

Now as $T \rightarrow 0$, $\mu \rightarrow \epsilon_F$ 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 hand side is $\mathcal{O}(k_B T)^2$ is small, we can approximate ~~the right hand side~~ as it as

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

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

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

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

Shows that chemical potential μ decreases from ϵ_F by $\mathcal{O}(k_B T)^2$ at low T

For free electrons where $g(\epsilon) = C\sqrt{\epsilon}$
 $g'(\epsilon) = \frac{1}{2}C\frac{1}{\sqrt{\epsilon}}$

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

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

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

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

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

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

ground state energy density $\approx (\mu - \epsilon_F) g(\epsilon_F) \epsilon_F$ as before
 replace $\mu \approx \epsilon_F$ as before

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

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

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

specific heat per volume

$$c_v \equiv \frac{C_v}{V} = \frac{1}{V} \left(\frac{dU}{dT} \right) = \left(\frac{dU}{dT} \right) / V$$

$$c_v = \frac{\pi^2}{3} k_B^2 T g(E_F)$$

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

$$n = \int_0^{E_F} dE g(E) = \frac{2}{3} C E_F^{3/2} \Rightarrow C = \frac{3}{2} \frac{n}{E_F^{3/2}}$$

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

$$c_v = \frac{\pi^2}{2} \left(\frac{k_B T}{E_F} \right) n k_B$$

or total specific heat $C_v = V c_v$ $nV = N$

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

\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 .

electronic specific heat per volume

$$C_V^{\text{elec}} = \frac{\pi^2}{2} \left(\frac{k_B T}{E_F} \right) \frac{N k_B}{V} \left(1 + o \left(\frac{k_B T}{E_F} \right)^2 \right)$$

compare to classical result $C_V^{\text{classical}} = \frac{N k_B}{V}$

The correct result for degenerate fermi gas is a factor

$$\frac{\pi^2}{2} \left(\frac{k_B T}{E_F} \right) = \frac{\pi^2}{2} \left(\frac{T}{T_F} \right) \text{ smaller than classical result by factor } \sim \frac{10^2}{10^4} = 10^{-2} \text{ at room temperature}$$

also, classical C_V is indep of T , whereas fermi gas result is $\propto T$.

At low T , the ionic contribution to C_V is

$$C_V^{\text{ion}} = \frac{12\pi^4}{5} \left(\frac{T}{\Theta_D} \right)^3 \frac{N k_B}{V}$$

$$\frac{C_V^{\text{elec}}}{C_V^{\text{ion}}} = \frac{\pi^2}{2} \left(\frac{k_B T}{E_F} \right) \frac{5}{12\pi^4} \left(\frac{\Theta_D}{T} \right)^3 \approx \frac{5}{24\pi^2} \left(\frac{\Theta_D}{T_F} \right) \left(\frac{\Theta_D}{T} \right)^2$$

$$\approx 1 \text{ when } T^* = \sqrt{\frac{5}{24\pi^2} \left(\frac{\Theta_D}{T_F} \right)} \Theta_D \approx 0.15 \left(\frac{\Theta_D}{T_F} \right)^{1/2} \Theta_D$$

for metals, $T_F \sim 10^4 \text{ } ^\circ\text{K}$, $\Theta_D \sim 10^2 \text{ } ^\circ\text{K}$

$$T^* = 0.15 \sqrt{10^{-2}} \Theta_D \approx 0.015 \Theta_D$$

So ionic contrib to C_V dominates over electronic contrib until $T \lesssim 0.01 \Theta_D$ i.e. at $0(1) \text{ } ^\circ\text{K}$. The electronic contrib dominates at lower temperatures.