Roadmap (Ch. XIII)

We have: for Non-interacting fermions

$$\langle N\rangle = \sum_r \frac{1}{e^{\beta(\varepsilon_r-\mu)}+1} = \sum_r f_{FD}(\varepsilon_r) = \sum_r \langle n_r\rangle$$

$$\langle E\rangle = \sum_r \varepsilon_r f_{FD}(\varepsilon_r) = \sum_r \frac{\varepsilon_r}{e^{\beta(\varepsilon_r-\mu)}+1}$$

$$pV = -\Omega = kT \sum_r \ln\left[1+e^{-\beta(\varepsilon_r-\mu)}\right]$$

Valid for non-interacting fermions

- good for any spatial dimensions
- good for any form of $\varepsilon(k)$

relate to how we turn $\sum_r (\cdots)$ into $\int \underbrace{g(\varepsilon)}_{\text{density of states}} (\cdots)\, d\varepsilon$

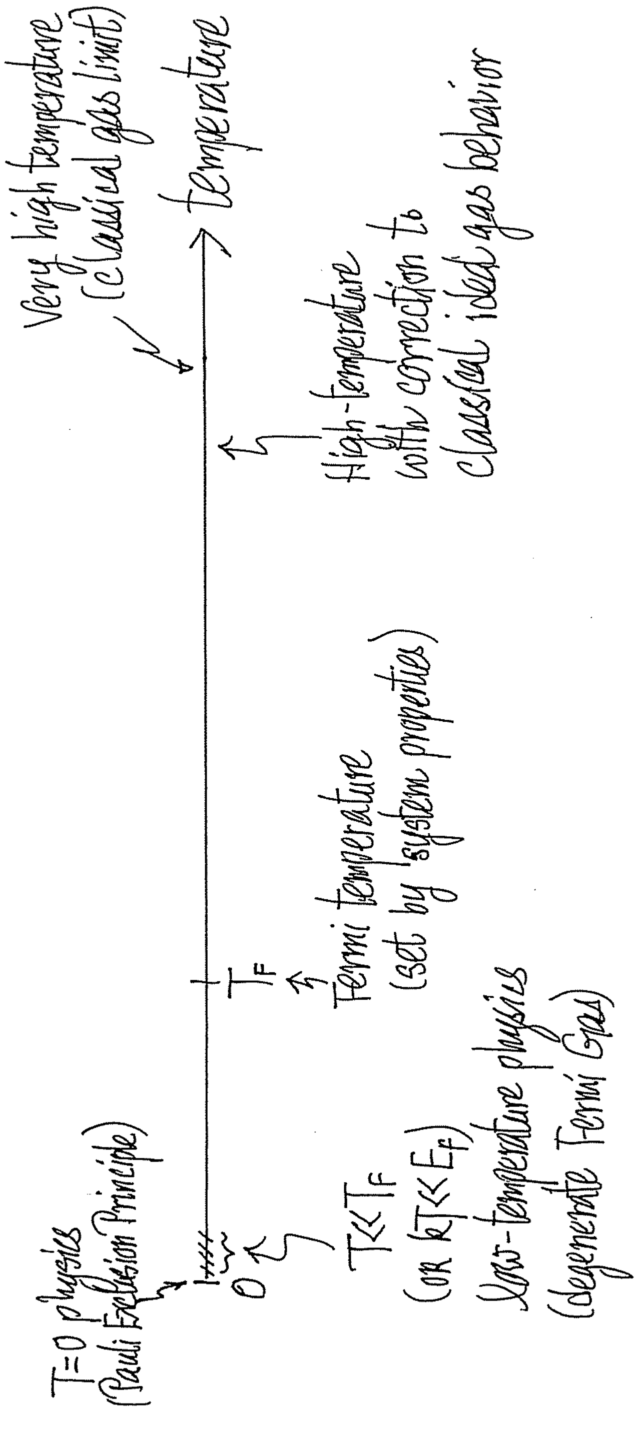
Next, we will apply the formulas to study a 3D non-relativistic Ideal Fermi Gas, where

$$g(\varepsilon) = 2 \cdot \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$$

spin degeneracy

$G_s = 2\cdot\left(\frac{1}{2}\right)+1$

We will study...



XIII. Ideal Fermi Gas

Sample system: A non-interacting gas of fermions inside a large 3D box of volume V.

[Variations: 3D, 2D, 1D
Confining potential: Box, other than a box
Dispersion relation: Non-relativistic $\varepsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$
OR relativistic]

Background knowledge⁺: Q_F, $\Omega = -kT \ln Q_F$,
Fermi-Dirac distribution, U, S, $\langle N \rangle$, etc.

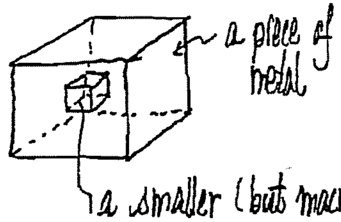
Turning $\underset{\text{single-particle states}}{\sum} (\cdots)$ into $\int d\varepsilon\, \underbrace{g(\varepsilon)}_{\text{Density of states}} (\cdots)$

Real systems:

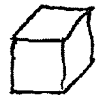
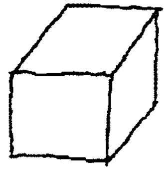
- "gas" of electrons in a metal (small mass of electron $\Rightarrow \lambda_{th} \sim \left(\frac{V}{N}\right)^{1/3}$ is usually the case)
- ^{3}He liquid
- neutrons in neutron stars/white dwarf stars

⁺See Ch. XII. The concept of single-particle density of states $g(\varepsilon)$ was discussed in Ch. VIII.

- Consider non-relativistic fermions: $\epsilon = \frac{\hbar^2 k^2}{2m}$ in a 3D box



← Formally, N may fluctuate.
But $\langle N \rangle$ is highly representative of the number of particles
$\Rightarrow$ Can treat $\langle N \rangle$ as (a fixed) N in thermodynamics

More, the number density $\frac{\langle N \rangle}{V}$ in  ($\sim 10^{22}$–10^{23} cm^{-3}) is the same as that in  and 

The point is: It doesn't matter if we talk about $\langle N \rangle$ or simply take N as fixed, for macroscopic systems. $\langle N \rangle / V$ is a property of the material.
[Except when you go to nanosized pieces or clusters]

i.e. $\frac{\langle N \rangle}{V}$ is a property of the material, independent of T.

A. Equations for $\langle N\rangle$, U, Ω

Recall: 3D free particle $\left(\varepsilon = \frac{\hbar^2 k^2}{2m}\right)$ DOS

$$D(k)dk = \frac{V}{\pi^3}\,\frac{4\pi k^2}{8}\,dk \qquad (k\text{-space})$$

$\Downarrow$ change $k \to \varepsilon$ (dispersion relation)

$$g(\varepsilon)\,d\varepsilon = G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}\;d\varepsilon \qquad (\text{see p. VII-⑪})$$

spin-degeneracy factor [electrons, $s=\frac{1}{2} \Rightarrow G_s = 2$]

Important: comes from 3D free particles

$$g(\varepsilon) = A\sqrt{\varepsilon} \quad \text{with } A = G_s \cdot \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$$

Electrons are fermions $\Rightarrow$ Fermi-Dirac distribution

$$\langle N\rangle = \sum_r \frac{1}{e^{\beta(\varepsilon_r-\mu)}+1}$$

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

turn sum over single-particle states into an integral

$$\Rightarrow \boxed{\langle N\rangle = \frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon} \qquad (1)$$

Notes on (1)

- As discussed, we can treat $\langle N\rangle$ just as a fixed N or note that $\frac{\langle N\rangle}{V}$ = electron number density

$$= \frac{G_s}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \qquad (*)$$

a property of material†

[i.e., a number for Na, another number for Cu, etc.]

  - For a given metal, Eq. (*) tells us how the chemical potential μ shifts (usually only slightly) with temperature, i.e., $\mu(T)$.

- Eq. (1) indicates that we should learn how to do integrals of the form:

$$\int_0^\infty \frac{f(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \quad \text{where } f(\varepsilon) \text{ is some function of } \varepsilon$$

which is related to

$$\int_0^\infty \frac{z^{x-1}}{e^{z}+1}\,dz \qquad (\text{see Appendix})$$

---

† For metals, $\langle N\rangle/V \sim 10^{22}/\text{cm}^3$ typically. For neutron stars, $\langle N\rangle/V$ is much larger.

$$U = \text{Mean energy of the Fermi gas}$$
$$= \sum_r \varepsilon_r \frac{1}{e^{\beta(\varepsilon_r-\mu)}+1}$$
$$= \int_0^\infty g(\varepsilon)\cdot\varepsilon\cdot\frac{1}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \leftarrow \text{(general)}$$

$$\boxed{U = \frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon} \quad (2)$$

← 3D free fermions in a box of volume V

$$\Omega = \text{Grand Potential} = -\frac{1}{\beta}\ln Q$$
$$= -\frac{1}{\beta}\sum_r \ln\left(1+e^{-\beta(\varepsilon_r-\mu)}\right)$$
$$= -\frac{1}{\beta}\int_0^\infty g(\varepsilon)\ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)d\varepsilon \leftarrow \text{(general)}$$

$$\Rightarrow \boxed{\Omega = -\frac{1}{\beta}\frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\underbrace{\int_0^\infty \varepsilon^{1/2}\ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)d\varepsilon}_{\text{do this integral by parts}}} \quad (3)$$

$$= -\frac{1}{\beta}\frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)\left(\frac{d}{d\varepsilon}\varepsilon^{3/2}\right)d\varepsilon\cdot\left(\frac{2}{3}\right)$$

note how this factor comes about!

$$\therefore \Omega = +\frac{2}{3}\frac{1}{\beta}\frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \varepsilon^{3/2}\left(\frac{d}{d\varepsilon}\ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)\right)d\varepsilon$$

[note: the "surface term" vanishes]

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

(Note: factors of β cancelled)

$$= -\frac{2}{3}U$$

But $pV = -\Omega$

$$\therefore \boxed{pV = \frac{2}{3}U} \quad (4)$$

for a fermi gas (3D non-relativistic)

- Trace where that $\frac{2}{3}$ comes from
- Follow the derivation and see if $pV = \frac{2}{3}U$ holds in a Bose gas
- compare result with photon gas

Summary: For given $\langle N\rangle/V$,
- Eq. (1) gives $\mu(T)$
- Using $\mu(T)$ in Eqs. (2) and (3) gives $U(T)$ and the equation of state for a Fermi Gas.

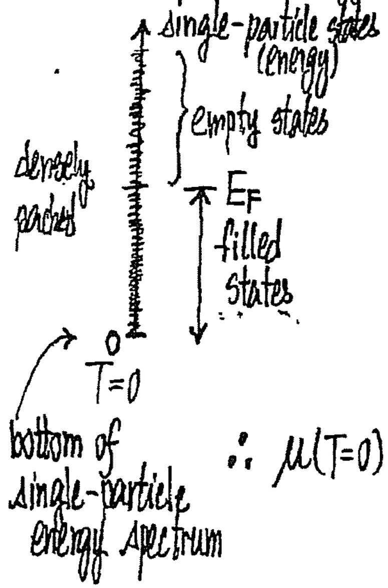
B. T=0 case

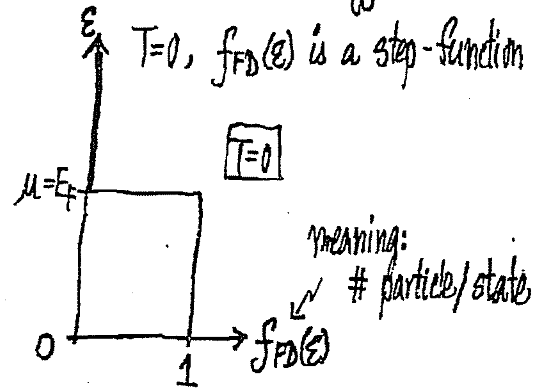
- This is referred to as the completely degenerate Fermi gas.
- Physically, for fermions, each single-particle state can be occupied by at most one particle.

$T=0 \Rightarrow$ ground state of the gas

$\Rightarrow$ fill particles into single-particle states in such a way that the energy is minimum

$\Rightarrow$ fill single-particle states up to some energy called E_F, the Fermi energy.





$\therefore \mu(T=0) \equiv E_F$

The point is: For fermi gas, even at T=0, the problem itself sets an energy scale E_F and hence a temperature scale $T_F = E_F/k$. With this scale, then we can decide whether the temperature (actual temp.) we are interested in (e.g. $T \approx 300\,K$ for a piece of metal) refers to low temperature ($T \ll T_F$) or high temperature.

At $T=0$, $$\frac{1}{e^{\beta(\varepsilon-\mu)}+1} \rightarrow \begin{cases} 1 & \varepsilon < \mu(T=0) = E_F \\ 0 & \varepsilon > \mu(T=0) = E_F \end{cases}$$

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

becomes, at $T=0$

$$\boxed{\langle N \rangle = \int_0^{E_F} g(\varepsilon)\,d\varepsilon} \quad (5)$$ (Note: upper limit is E_F)

Eq. (5) determines E_F for a given gas ($\langle N \rangle / V$).

$$\langle N\rangle = G_s\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{E_F}\epsilon^{1/2}\,d\epsilon$$

$$= \frac{2}{3}G_s\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E_F^{3/2} \qquad (*) \qquad \frac{\langle N\rangle}{V}\sim E_F^{3/2}$$

$$= \frac{2}{3}\underbrace{G_s\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E_F^{1/2}}_{g(E_F)\,=\,\text{DOS at the Fermi energy.}}\cdot E_F$$

$$= \frac{2}{3}\,g(E_F)\cdot E_F$$

From (*), $E_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2}{G_s}\frac{\langle N\rangle}{V}\right)^{2/3}$

$$= \frac{\hbar^2}{2m}\left(3\pi^2\frac{\langle N\rangle}{V}\right)^{2/3} \qquad [G_s = 2 \text{ for electrons}]$$

$$\Rightarrow \boxed{E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}} \quad (6)$$

$n \equiv \frac{\langle N\rangle}{V}$ = conduction electron number density $\sim 10^{22}\,\text{cm}^{-3}$ (metals)

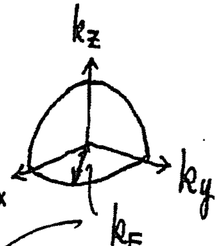
$E_F \propto n^{2/3}$

higher density $\Rightarrow$ higher E_F

Writing $E_F = \frac{\hbar^2}{2m}k_F^2$; k_F = <u>Fermi wave vector</u>

$\Rightarrow k_F = \left(\frac{6\pi^2}{G_s}\frac{\langle N\rangle}{V}\right)^{1/3} \propto n^{1/3}$

gives the extent of occupied states in k-space



states with $|k| < k_F$ are occupied

<u>Define Fermi Temperature T_F</u>

$$\boxed{T_F = \frac{E_F}{k}}$$

- For metals, $n \sim 10^{22}\,\text{cm}^{-3}$, $E_F \sim$ a few eV, $T_F \sim 10^4$ K
- E_F sets an energy scale and T_F is the accompanying temperature scale.
- At room temperature, $T \ll T_F$. Thus, in studying the physics of metals at room temperature (or lower temp.), we really need to take into account the details of the Fermi-Dirac distribution, i.e., the fact that electrons are fermions.

<u>U at T=0</u> :

$$U = \sum_r \varepsilon_r \frac{1}{e^{\beta(\varepsilon_r-\mu)}+1} = \langle E\rangle$$

At T=0, $U = \int_0^{E_F}\epsilon\, g(\epsilon)\, d\epsilon = G_s\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{E_F}\epsilon^{3/2}d\epsilon$

$$= \frac{2}{5}G_s\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E_F^{5/2} \qquad (**)$$

$$= \frac{2}{5}G_s\frac{V}{4\pi^2}\left(\frac{\hbar^2}{2m}\right)\left(\frac{6\pi^2}{G_s}\frac{\langle N\rangle}{V}\right)^{5/3}$$

- It is more interesting to look at the energy per particle (the energy here is mean kinetic energy)

$$\langle N\rangle = \frac{2}{3}\frac{G_s V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{3/2} \qquad \text{(see (*))}$$

From (**), $U = \frac{2}{5} G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{3/2}\cdot E_F$

$$= \frac{2}{5}\cdot\frac{3}{2}\langle N\rangle \cdot E_F$$

$$\Rightarrow \boxed{U = \frac{3}{5}\langle N\rangle E_F} \qquad (7)$$

$$\Rightarrow \boxed{\frac{U}{\langle N\rangle} = \frac{3}{5}E_F}$$

This is a T=0 K result. Due to the fact that they are fermions, they are forced to occupy higher single-particle states. This results in a high energy per particle (the fact $g(\epsilon)\sim\sqrt{\epsilon}$ implying more states at higher energies also contributes).

Pressure at T=0

$$pV = \frac{2}{3}U$$

$$\Rightarrow p = \frac{2}{3}\frac{U}{V} = \frac{2}{3}\frac{1}{V}\cdot\frac{3}{5}\langle N\rangle E_F$$

$$= \frac{2}{5}\frac{\langle N\rangle}{V} E_F \leftarrow \sim\left(\frac{\langle N\rangle}{V}\right)^{2/3}$$

$$= \frac{2}{5}\left(\frac{\hbar^2}{2m}\right)\left(\frac{6\pi^2}{G_s}\right)^{2/3}\left(\frac{\langle N\rangle}{V}\right)^{5/3} \propto \left(\frac{\langle N\rangle}{V}\right)^{5/3} \qquad (8)$$

- This is T=0 K result in a Non-interacting fermi gas.
- This pressure comes solely from the Pauli Exclusion Principle, which keeps the fermions from "falling" all into the $\vec{k}=0$ single-particle state.

Classical Ideal gas, $p = \frac{NkT}{V} \xrightarrow[T\to 0K]{} 0$.

So, a Fermi gas behaves very differently from a classical ideal gas.

We know that, the classical gas behaviour breaks down at low temperatures when $\lambda_{th}\sim(V/N)^{1/3}$, then quantum effects set in. This fermionic pressure due to Pauli's principle is important in the evolution of a star!

C. "Low temperature" physics of a Fermi Gas

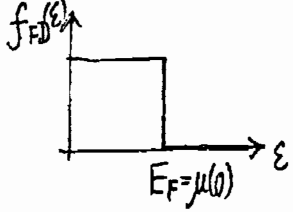
$$\underbrace{0 < kT \ll E_F}\,(= kT_F)$$

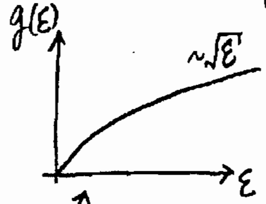
In this case, the Fermi gas is said to be degenerate.

Key physics idea

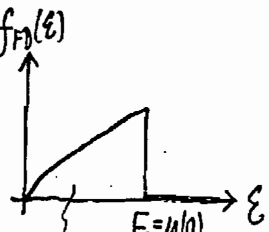
$kT \ll E_F \Rightarrow$ the physics is given by the small change in $f_{FD}(\varepsilon)$, when compared with $T=0$ case.

$\boxed{T=0}$



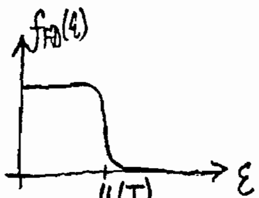


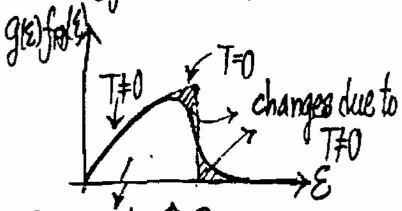
does NOT depend on temperature



Area under curve $= \int_0^{E_F} g(\varepsilon) f_{FD}(\varepsilon) = N$

$\boxed{T \neq 0 \ (T \ll T_F)}$





Area under  $= \int_0^{\infty} g(\varepsilon) f_{FD}(\varepsilon) = N$

(the same N)

$\therefore$ changes in physics at $T \neq 0$ are due to small changes in the electron occupations near E_F!

- For $T \ll T_F$ ($kT \ll E_F$), we have $\frac{kT}{E_F} \ll 1$.

$\therefore$ We expect $\frac{kT}{E_F}$ to serve as a small parameter.

That is to say, we expect:

$$U(T) = U(0)\,[1 + \underbrace{(\text{something})}_{\text{goes like } a\left(\frac{kT}{E_F}\right) + b\left(\frac{kT}{E_F}\right)^2 + \cdots \ (\text{tiny})}]$$

due to changes near E_F at finite T

$$\mu(T) = \underbrace{E_F}_{\mu(T=0)}\,[1 + \overbrace{(\text{something})}^{\text{tiny}}]$$

and we look for the lowest order correction†

- It is important to keep this in mind as we proceed, as the mathematics is a bit messy in deriving the results.

As we expect $\mu(T) \approx E_F$ (shift is tiny for $kT \ll E_F$), the results here are good when $0 < kT \ll \mu$.

---

† It is useful to recall that we do have exact expression for $U(T)$ and an exact equation to solve for $\mu(T)$, which are good for all temperatures (see Sec. A).

(a) A useful formula: A mathematical Aside

$$I = \int_0^\infty f(\varepsilon)\, f_{FD}(\varepsilon)\, d\varepsilon$$

f_{FD}: Fermi-Dirac distribution

$f(\varepsilon)$: some function of ε (e.g. $g(\varepsilon)$ to get $\langle N\rangle$, $\varepsilon g(\varepsilon)$ to get $\langle E\rangle$, etc.)

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

Very often, we only need results for $kT \ll \mu$ (or $\beta\mu \gg 1$).

$$\boxed{I = \int_0^\infty \frac{f(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1}\, d\varepsilon = \int_0^\mu f(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(kT)^2 f'(\mu) + \cdots^{*}} \quad (9)$$

- Key point: know how to apply (9)

- The physics behind the integral

Write: $f(\varepsilon) = \frac{d}{d\varepsilon}\left(\int_0^\varepsilon f(\varepsilon')\, d\varepsilon'\right)$

$$= \frac{d}{d\varepsilon} F(\varepsilon)$$

Define: $F(\varepsilon) = \int_0^\varepsilon f(\varepsilon')\, d\varepsilon'$

e.g. $\begin{cases} f(\varepsilon) = \varepsilon^{1/2} \quad (\sim \text{DOS}) \\ F(\varepsilon) = \frac{2}{3}\varepsilon^{3/2} \end{cases}$

Then,

$$I = \int_0^\infty f(\varepsilon)\, f_{FD}(\varepsilon)\, d\varepsilon$$

$$= \int_0^\infty f_{FD}(\varepsilon)\left[\frac{d}{d\varepsilon}F(\varepsilon)\right] d\varepsilon$$

(then integration by parts)

---

* The next term is $\frac{7\pi^4}{360}(kT)^4 f'''(\mu)$, but we won't need it here!

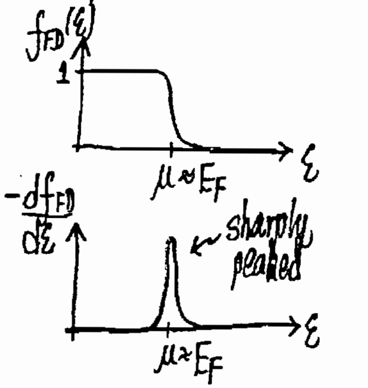
$$I = f_{FD}(\varepsilon)\, F(\varepsilon)\Big|_0^\infty - \int_0^\infty F(\varepsilon)\left[\frac{d}{d\varepsilon} f_{FD}(\varepsilon)\right] d\varepsilon$$

(usually this term vanishes. If not, keep it as $-F(0)$)

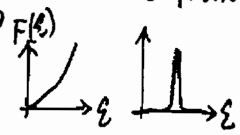
$$= -\int_0^\infty F(\varepsilon) \underbrace{\left[\frac{d}{d\varepsilon} f_{FD}(\varepsilon)\right]}_{\text{sharply peaked around } \epsilon \sim \mu \sim E_F} d\varepsilon$$

$\Downarrow$

contribution to I comes from $\epsilon \sim \mu$



(like a delta-function)

$$= \int_0^\infty$$  $$d\varepsilon$$

$\therefore$ only $F(\varepsilon)$ in the vicinity of $\varepsilon \sim \mu$ matters!

- Expand $F(\varepsilon)$ around μ:

$$F(\varepsilon) = F(\mu) + F'(\mu)(\varepsilon-\mu) + \frac{F''(\mu)}{2!}(\varepsilon-\mu)^2 + \cdots$$

then I becomes

$$I = F(\mu) - F'(\mu)\int_0^\infty (\varepsilon-\mu)\left(\frac{d}{d\varepsilon}f_{FD}\right) d\varepsilon - \frac{F''(\mu)}{2}\int_0^\infty (\varepsilon-\mu)^2\left(\frac{d}{d\varepsilon}f_{FD}\right) d\varepsilon + \cdots$$

$\therefore$ need to consider $-\int_0^\infty (\varepsilon-\mu)^r \left(\frac{df_{FD}}{d\varepsilon}\right) d\varepsilon \;\Big|\; r=1,2,3,\cdots$

$$= -\int_0^\infty (\varepsilon-\mu)^r \frac{d}{d\varepsilon}\left(\frac{1}{e^{\beta(\varepsilon-\mu)}+1}\right) d\varepsilon$$

$x = \frac{\varepsilon-\mu}{kT}$

exact $\rightsquigarrow$ $$= -\int_{-\frac{\mu}{kT}}^\infty (x\,kT)^r \frac{d}{dx}\left(\frac{1}{e^x+1}\right) dx$$

(note lower bound)

approximate $\rightsquigarrow$ $$\approx -\int_{-\infty}^\infty (kT)^r x^r \frac{d}{dx}\left(\frac{1}{e^x+1}\right) dx$$

$(kT \ll \mu)$

$$= (kT)^r \int_{-\infty}^\infty x^r \frac{e^x}{(e^x+1)^2} dx$$

$$= (kT)^r \int_{-\infty}^\infty x^r \underbrace{\frac{1}{(e^x+1)(e^{-x}+1)}}_{\text{even function about } x=0} dx$$

$$= \begin{cases} 0 & r \text{ is odd} \\ \neq 0 & r \text{ is even} \end{cases}$$

lowest non-vanishing term is:

$$-\int_0^\infty (\varepsilon-\mu)^2 \left(\frac{df_{FD}}{d\varepsilon}\right) d\varepsilon = (kT)^2 \int_{-\infty}^\infty \frac{x^2}{(e^x+1)(e^{-x}+1)} dx$$

$$= \frac{\pi^2}{3}(kT)^2$$

claimed the integral is $\frac{\pi^2}{3}$

$$\therefore I = F(\mu) + \frac{\pi^2}{6} F''(\mu)(kT)^2$$

Recall: $F(\varepsilon) \equiv \int_0^\varepsilon f(\varepsilon')\, d\varepsilon'$

$$\boxed{I = \int_0^\infty \frac{f(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \approx \int_0^\mu f(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(kT)^2 \underbrace{f'(\mu)}_{\left.\frac{df(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\mu}} + \cdots} \quad (9)$$

- This is echoing our previous discussion that the physics is dominated by what is happening near the Fermi energy, for $kT \ll \mu$. ("Fermi surface effect")

(b) <u>The shift of μ with temperature</u>: $\mu(T)$

$\mu(T=0) = E_F$

For a 3D Fermi gas: $\mu(T)$

$$\langle N \rangle = \int_0^\infty \underbrace{g(\varepsilon)}_{\text{DOS plays the role of } f(\varepsilon) \text{ in Eq.(9)}} \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \quad \text{(determines } \mu\text{)}$$

- But for a system, $\langle N \rangle$ or $\langle N \rangle / V$ (e.g. electron density in a metal) is the same for different T.

$\therefore$ $\langle N\rangle$ is given by the $T=0$ result in terms of E_F (or $\mu(T=0)$)

i.e., $\langle N\rangle = \frac{2}{3}\underbrace{\frac{G_{\text{s}} V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}}_{\mathcal{A}} E_F^{3/2}$ (see XIII-(9))

$= \frac{2}{3}\mathcal{A}E_F^{3/2}$

$G_s = (2S+1)$ spin degeneracy

Recall: $g(\mathcal{E}) = G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\mathcal{E}} = \mathcal{A}\,\mathcal{E}^{1/2}$

$g'(\mathcal{E}) = \frac{1}{2}\mathcal{A}\,\mathcal{E}^{-1/2}$

T=0 result

$$\therefore \langle N\rangle = \frac{2}{3}\mathcal{A}E_F^{3/2} = \int_0^{\mu} g(\mathcal{E})\,d\mathcal{E} + \frac{\pi^2}{6}(kT)^2 g'(\mu) \underbrace{+\cdots}_{\text{ignore}}$$

$T\neq 0$

$$= \mathcal{A}\left[\frac{2}{3}\mu^{3/2} + \frac{\pi^2}{12}(kT)^2\mu^{-1/2} + \cdots\right]$$

$$\Rightarrow E_F^{3/2} = \mu^{3/2} + \frac{\pi^2}{8}(kT)^2\mu^{-1/2} + \cdots$$

$[\mu(0)]^{3/2}$

$$= \mu^{3/2}\left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2 + \cdots\right]$$

Note: the small parameter $\left(\frac{kT}{\mu}\right)$ appears!

$$\therefore \mu(T) = E_F\left(1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2 + \cdots\right)^{-2/3}$$

$$\approx E_F\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{\mu}\right)^2 + \cdots\right)$$

note the sign (3D, non-relatistic, box)

Obtain $\mu(T)$ by successive approximation:

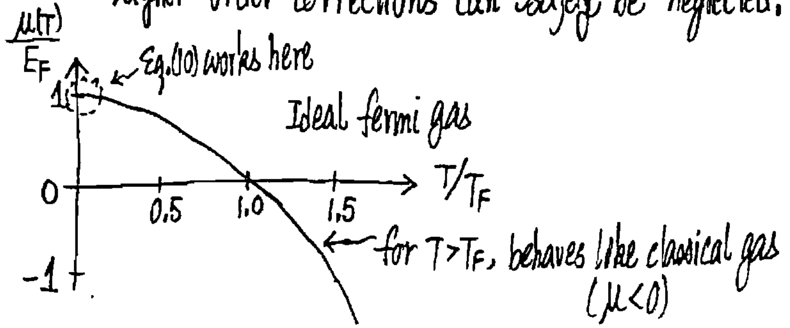
- to zeroth order in $\left(\frac{kT}{E_F}\right)$: $\mu^{(0)} \approx E_F = \mu(T=0)$
- lowest order correction:

$$\boxed{\mu(T) \approx E_F\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)} \qquad (10)$$

shifts downward!

the next correction term is $O\left(\frac{kT}{E_F}\right)^4$

- Now, it is obvious that "low temperature" means $kT \ll E_F$
- There is no $\left(\frac{kT}{E_F}\right)^1$, $\left(\frac{kT}{E_F}\right)^3$, etc correction.
- Thus, the leading order correction goes like $\left(\frac{kT}{E_F}\right)^2$. For $kT \ll E_F$, (e.g. $kT/E_F \sim 10^{-2}$ for metals at room temperature) $\mu(T)$ only shifts slightly, and higher order corrections can safely be neglected.

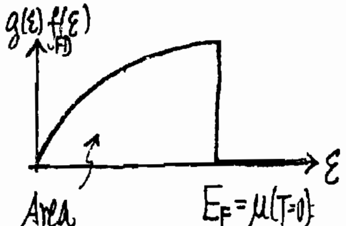


Why does $\mu(T)$ shift downwards: the physics?

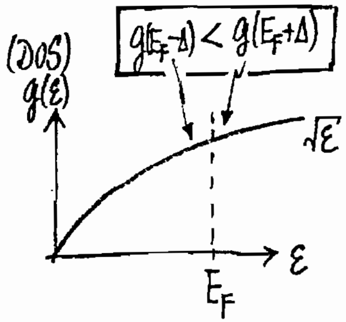
[3D box, non-relativistic]

$$\langle N\rangle = \int_0^\infty g(\varepsilon)\, f_{FD}(\varepsilon)\, d\varepsilon$$

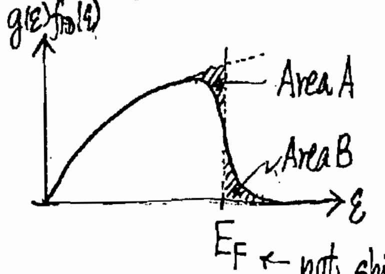
$\boxed{T=0}$



Area $= \langle N\rangle$ $=$ fixed



$\boxed{T\neq 0}$ What if (which is wrong) μ does not change?



Assume $\mu(T) = E_F$ ← wrong!

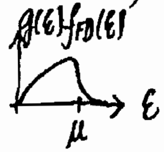
Area under curve $\neq \langle N\rangle$!

- Area A $<$ Area B because $g(\varepsilon \gtrsim E_F) > g(\varepsilon \lesssim E_F)$ and $f_{FD}(\varepsilon)$ is symmetrical about μ

\# missing particles with energy $< E_F$ due to thermal excitations $\neq$ \# particles with energy $> E_F$ due to thermal excitations

trouble!

$\therefore$ μ must shift so as to give $\langle N\rangle$

- Shifting up or down?
  - The trouble stems from $g(\varepsilon) \sim \sqrt{\varepsilon}$ (increases with ε)
  - We need to shift μ so that the area under  is $\langle N\rangle$.
  - Since $g(\varepsilon)$ increases with ε, we need to suppress the occupancy of those states with $\varepsilon > E_F$

    $\Rightarrow$ μ should shift downward from E_F

(c) $U(T)$

$$U = \int_0^\infty \underbrace{g(\varepsilon)\cdot\varepsilon}_{\text{plays the role of } f(\varepsilon)} \cdot \frac{1}{e^{\beta(\varepsilon-\mu)}+1}\, d\varepsilon$$

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

using (9)

$$= A\left[\int_0^\mu \varepsilon^{3/2} d\varepsilon + \frac{\pi^2}{6}(kT)^2 \left(\frac{d}{d\varepsilon}\varepsilon^{3/2}\right)_{\varepsilon=\mu} + \cdots\right]$$

$$= A\left[\frac{2}{5}\mu^{5/2} + \frac{\pi^2}{6}(kT)^2 \frac{3}{2}\mu^{1/2} + \cdots\right]$$

$$= A\,\frac{2}{5}\mu^{5/2}\left[1 + \frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2 + \cdots\right]$$ ← but $\mu = \mu(T)$

$$U = \frac{3}{5}\cdot\underbrace{\frac{2}{3}\mathcal{A}E_F^{5/2}}_{\langle N\rangle E_F}\cdot\left(\frac{\mu}{E_F}\right)^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2+\cdots\right]$$

$$= \underbrace{\frac{3}{5}\langle N\rangle E_F}_{U(T=0)}\left\{\left(\frac{\mu}{E_F}\right)^{5/2}\left(1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2+\cdots\right)\right\}$$

$$\cong \frac{3}{5}\langle N\rangle E_F\left\{\left(1-\frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)^{5/2}\left(1+\frac{5\pi^2}{8}\left(\frac{kT}{E_F}\right)^2\right)\right\}$$

note

$$= \frac{3}{5}\langle N\rangle E_F\left(1-\frac{5}{24}\pi^2\left(\frac{kT}{E_F}\right)^2\right)\left(1+\frac{5\pi^2}{8}\left(\frac{kT}{E_F}\right)^2\right)$$

$$\approx \frac{3}{5}\langle N\rangle E_F\left(1+\frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2+\cdots\right)$$

$$= U(T=0) + \underbrace{\frac{\pi^2}{4}\langle N\rangle E_F\left(\frac{kT}{E_F}\right)^2}_{\text{change in } U \text{ due to } T\neq 0}+\cdots$$

$T=0$ value due to Pauli Exclusion Principle

Note: All the way, we intended to get a result which is good up to $\left(\frac{kT}{E_F}\right)^2$.

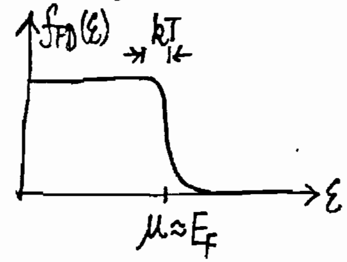
using $\langle N\rangle = \frac{2}{3}g(E_F)\cdot E_F$ (p. XIII-(9))

$$= U(T=0) + \frac{\pi^2}{4}\left(\frac{2}{3}g(E_F)E_F\right)E_F\left(\frac{kT}{E_F}\right)^2+\cdots$$

$$\Rightarrow \boxed{U = U(T=0) + \frac{\pi^2}{6}g(E_F)k^2T^2+\cdots} \qquad (11)$$

What is the physics? (Eq.(11)) A hand-waving argument

$T\neq 0$



- Compared with $T=0$ situation, only single-particle states in an interval $\sim kT$ near E_F are affected
- Number of particles excited (out of the Fermi sea) to states above E_F $\sim \underbrace{g(E_F)\cdot kT}_{\text{an estimate of the \# states occupied at } T=0 \text{ that would become unoccupied}}$ ($kT \ll E_F$ is used)
- Each excited particle gains an energy $\sim kT$

$$\therefore\; U \cong U(T=0) + \underbrace{\text{constant}}_{\text{our calculation shows that it is } \frac{\pi^2}{6}}\cdot g(E_F)k^2T^2 \quad \text{(qualitatively correct)}$$

A physical (measureable) consequence is that the electrons (fermions) contribute a heat capacity that goes linearly with T.

$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right)_{V,\langle N\rangle} = \frac{\pi^2}{3} k^2 g(E_F)\cdot \underbrace{T}_{\text{linear in } T} = \gamma T} \qquad (12)$$

can be measured

due to conduction electrons in a metal

linear in T (due to a gas of fermions)

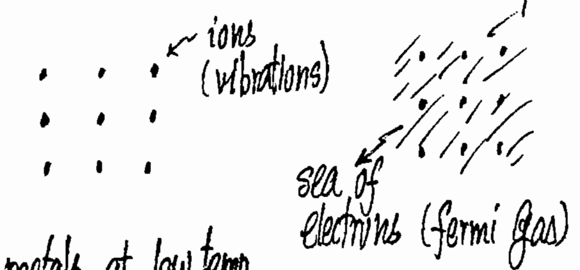
- C_V is a measurable quantity
- Take a metal as an example, there are several contributions to C_V.

<u>Recall</u>: Debye's model

↳ C_V of a solid due to <u>vibrations of ions</u> about equilibrium position

$\Rightarrow C_V^{(\text{lattice})} \sim T^3$ at low temperature

∴ <u>Metal</u>:



Expect for metals at low temp.,

$$C_V = \gamma T + \beta T^3$$

(stat. mech. of ideal fermi gas) ⇒ due to gas of electrons

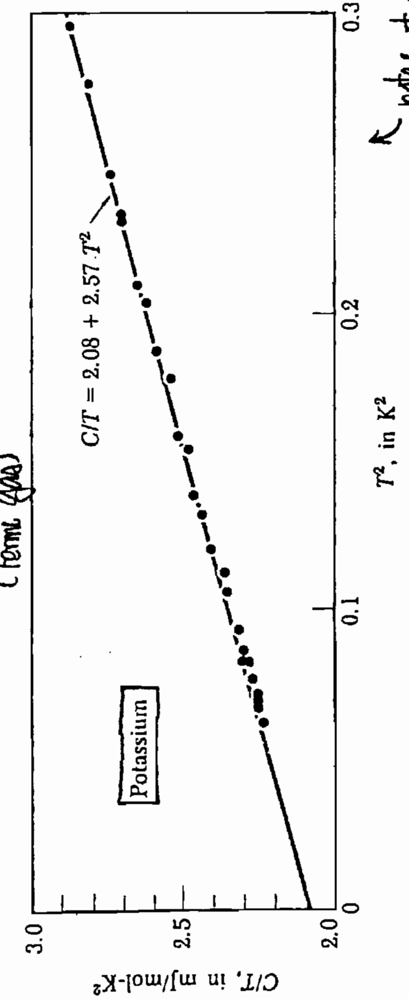
due to vibrations of ions ("phonons") ← (stat. mech. of quantum harmonic oscillators)

<u>Low-temp. data</u>

Heat capacity of metal

$$C = \underbrace{\gamma T}_{\substack{\text{electrons}\\ \text{contribution}\\ \text{(Fermi gas)}}} + \underbrace{\beta T^3}_{\substack{\text{from lattice vibration ("phonons")}\\ \text{(Bosons)}}} \Rightarrow \frac{C}{T} = \gamma + \beta T^2$$

$\Downarrow$ Plot $\frac{C}{T}$ vs T^2



Experimental heat capacity values for potassium, plotted as C/T versus T^2.

In Potassium, the "4s¹" electrons contribute to conduction and form a sea of electrons.

note: at very low temperature

- Both electronic and lattice vibrational contributions are observed.
- Can extract γ experimentally.
- Theoretically, $\gamma = \frac{\pi^2}{3} k^2 \overbrace{g(E_F)}^{G_S \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_F}}$. ∴ Measure $\gamma \Rightarrow$ information on $g(E_F)$

Remark:

- Classically, we expect $U = 3 \cdot \frac{1}{2}\langle N\rangle kT$ (free particles, equipartition theorem) (see figures)

and $C_V^{(classical)} = \frac{3}{2}\langle N\rangle k$ (independent of T)

Fermi gas: $C_V = \frac{\pi^2}{3} k\, g(E_F)\, T$

$$= \underbrace{\frac{\pi^2}{2}\langle N\rangle k}_{\sim C_V^{classical}} \left(\frac{kT}{E_F}\right)$$

$\rightarrow \sim 10^{-2}$ for electrons in metal

$\therefore$ $C_V^{classical}$ is large

$C_V^{classical}$ does not have T-dependence

both are inconsistent with exp'tal results.

Some numbers:

	$\langle N\rangle/V$	E_F	T_F	γ (free electron)
Sodium	$4.6\times10^{22}/cm^3$	4.7eV	5.5×10^4K	0.75 $mJ\cdot mol^{-1}\cdot deg^{-2}$
				[γ(exp't) = 1.63 $mJ\cdot mol^{-1}\cdot deg^{-2}$]
Copper	$8.5\times10^{22}/cm^3$	7eV	8.2×10^4K	0.5 $mJ\cdot mol^{-1}\cdot deg^{-2}$
				[γ(exp't) = 0.695 $mJ\cdot mol^{-1}\cdot deg^{-2}$]

Summary

(a) T=0 (completely degenerate case) [3D box, non-relativistic]

$$\langle N\rangle = \frac{2}{3}\mathcal{A} E_F^{3/2} = \frac{2}{3} g(E_F) E_F \qquad \Big| g(\varepsilon) = \mathcal{A}\varepsilon^{1/2}$$

$$E_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2}{G_S}\frac{\langle N\rangle}{V}\right)^{2/3} \propto \left(\frac{\langle N\rangle}{V}\right)^{2/3}$$

$$= \frac{\hbar^2}{2m}k_F^2 \quad ; \quad k_F = \left(\frac{6\pi^2}{G_S}\frac{\langle N\rangle}{V}\right)^{1/3} = \text{fermi wave vector}$$

$E_F = kT_F$; T_F = Fermi temperature

$$U = \frac{3}{5}\langle N\rangle E_F \quad ; \quad p = \frac{2}{5}\frac{\langle N\rangle}{V}E_F$$

[All these follow from the Pauli Exclusion Principle.]

(b) $T \neq 0$ ($kT \ll \mu$) (degenerate fermi gas) (low-temp.)

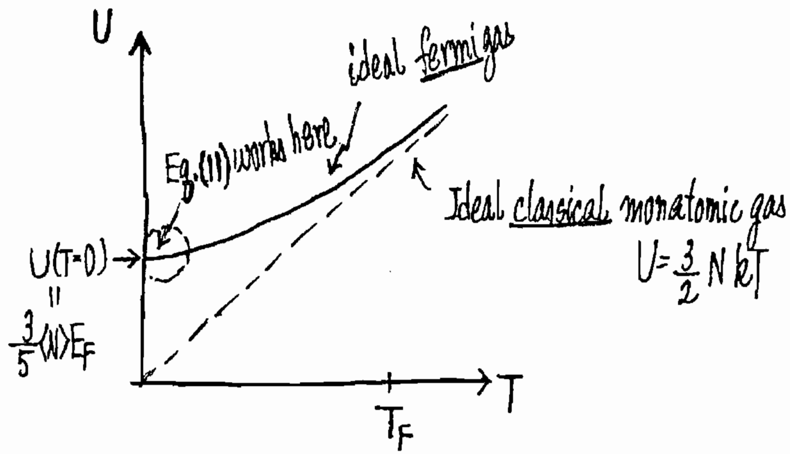
$$\mu(T) = E_F\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)$$

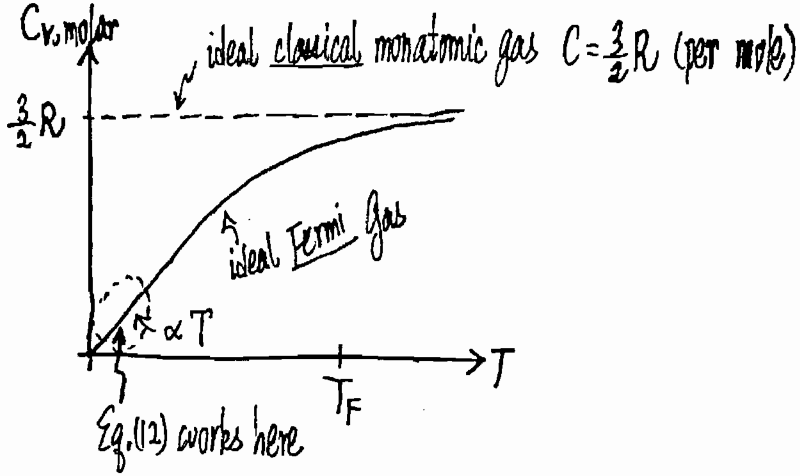
$$U = \frac{3}{5}\langle N\rangle E_F\left(1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)$$

$$C_V = \frac{\pi^2}{3} g(E_F) k^2 T = \frac{\pi^2}{2}\langle N\rangle k\left(\frac{kT}{E_F}\right) = \gamma T$$

$$p = \frac{2}{3}\frac{U}{V} = \frac{2}{5}\frac{\langle N\rangle}{V}E_F\left(1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)$$

[The key physics is: Only changes near E_F matter]





- To go beyond the low-temperature results (Eqs.(10), (11), (12)), we need to solve the general equations for $\mu(T)$ and $U(T)$, either by a better approximation or by numerical solutions.

D. Formal Equations for Ideal Fermi Gas

Aim: Re-write equations formally

$$pV = kT \ln Q_F = kT\, G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \varepsilon^{1/2} \ln(1+e^{\beta\mu}e^{-\beta\varepsilon})\, d\varepsilon$$

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

or simply

$$pV = \frac{2}{3} G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\varepsilon-\mu)}+1}\, d\varepsilon \qquad (D1)$$

$$\langle N\rangle = G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}+1}\, d\varepsilon \qquad (D2)$$

$G_s = 2s+1$ = spin degeneracy (spin-$\frac{1}{2}$ $\Rightarrow$ $s=\frac{1}{2}$ $\Rightarrow$ $G_s = 2$)

Define: $\xi \equiv e^{\beta\mu} = e^{\mu/kT}$ (also called z in some books)

- called absolute activity or fugacity
- since μ can shift and can take on negative values,

$$0 \le \xi < \infty \quad \text{(for fermions)}$$

high T, μ is negative (close to classical ideal gas)

low T limit (strongly degenerate ideal Fermi Gas)
(treated in Sec. B and C)

- Go back to Eq. (D1):

$$pV = G_s \frac{2}{3}\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{\xi^{-1}e^{\beta\varepsilon}+1}\, d\varepsilon$$

$$= G_s \frac{2}{3}\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{1}{\beta^{5/2}}\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^{x}+1}\, dx \qquad \left\{\begin{array}{l} x = \beta\varepsilon \\ d\varepsilon = \frac{dx}{\beta} \\ \varepsilon^{3/2} = \left(\frac{x}{\beta}\right)^{3/2}\end{array}\right.$$

$$= G_s \frac{2}{3}\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} kT\cdot(kT)^{3/2}\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^{x}+1}\, dx$$

$$\Rightarrow \frac{pV}{kT} = G_s \frac{2}{3}\frac{V}{4\pi^2}\left(\frac{2mkT}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^{x}+1}\, dx$$

$$= G_s \frac{2}{3}\frac{V}{4\pi^2}(2\sqrt{\pi})^3\left(\frac{\sqrt{2\pi mkT}}{h}\right)^3\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^{x}+1}\, dx$$

$$\boxed{\frac{pV}{kT} = G_s \frac{4}{3}\frac{V}{\sqrt{\pi}}\frac{1}{\lambda_{th}^3}\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^{x}+1}\, dx \qquad (D1')} \qquad \lambda_{th} = \frac{h}{\sqrt{2\pi mkT}}$$

- Similarly, Eq. (D2) becomes:

$$\langle N\rangle = G_s\cdot\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(kT)^{3/2}\int_0^\infty \frac{x^{1/2}}{\xi^{-1}e^{x}+1}\, dx$$

$$= G_s\cdot\frac{V}{4\pi^2}\cdot(2\sqrt{\pi})^3\left(\frac{\sqrt{2\pi mkT}}{h}\right)^3\int_0^\infty \frac{x^{1/2}}{\xi^{-1}e^{x}+1}\, dx$$

$$\Rightarrow \boxed{\langle N\rangle = G_s\cdot\frac{2}{\sqrt{\pi}}\frac{V}{\lambda_{th}^3}\int_0^\infty \frac{x^{1/2}}{\xi^{-1}e^{x}+1}\, dx \qquad (D2')}$$

Note that $\Gamma\left(\frac{5}{2}\right) = \frac{3}{2}\Gamma\left(\frac{3}{2}\right) = \frac{3}{2}\cdot\frac{1}{2}\Gamma\left(\frac{1}{2}\right) = \frac{3}{4}\sqrt{\pi}$

$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\Gamma\left(\frac{1}{2}\right) = \frac{\sqrt{\pi}}{2}$

Eqs. (D1') and (D2') can be rewritten as:

$$\frac{pV}{kT} = G_{Ts}\frac{V}{\lambda_{th}^3}\frac{1}{\Gamma\left(\frac{5}{2}\right)}\int_0^\infty \frac{x^{3/2}}{\xi^{-1}e^x+1}dx \qquad (D1'')$$

$$\langle N\rangle = G_{Ts}\frac{V}{\lambda_{th}^3}\frac{1}{\Gamma\left(\frac{3}{2}\right)}\int_0^\infty \frac{x^{1/2}\,dx}{\xi^{-1}e^x+1} \qquad (D2'')$$

Defining:
$$\boxed{f_n(\xi) \equiv \frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x+1}dx}$$

we have

$$\frac{pV}{kT} = G_{Ts}\frac{V}{\lambda_{th}^3}f_{5/2}(\xi) \qquad (D1''')$$

and
$$\langle N\rangle = G_{Ts}\frac{V}{\lambda_{th}^3}f_{3/2}(\xi) \qquad (D2''')$$

- Exact
- Eq. (D2''') serves to give $\xi(T)$

$$\boxed{\frac{pV}{\langle N\rangle kT} = \frac{f_{5/2}(\xi)}{f_{3/2}(\xi)}} \quad (D3) \quad [\text{Exact}]$$

With $pV = \frac{2}{3}\langle E\rangle$, we have

$$\langle E\rangle = \frac{3}{2}pV = \frac{3}{2}\langle N\rangle kT\frac{f_{5/2}(\xi)}{f_{3/2}(\xi)} \qquad [\text{also exact}]$$

E. Close to Classical Ideal Gas Limit

- Eqs. (D1'''), (D2'''), (D3) are exact
- Most useful when we look at the limit that is close to the classical ideal gas (high temperature dilute). Why? In this case, μ is negative, [recall: classical gas $\mu = -kT\ln[\text{much bigger than } 1]$] we have $\xi \ll 1$ (close to zero).
  Keeping the first few terms of $f_n(\xi)$ in powers of ξ will be sufficient.

Remark:

$T=0$ or $kT \ll E_F$, Eqs. (D1''') and (D2''') are still exact but not too useful. We treated these cases in Secs. B and C.

Mathematical Aside

Inspecting (D1') and (D2'), we need to consider the integral

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

Remark: $n=5/2$ in Eq. (D1')
$n=3/2$ in Eq. (D2')

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

[Recall: $\xi \ll 1$ (high-Temp)]

$$= \int_0^\infty x^{n-1}\xi e^{-x}\sum_{j=0}^{\infty}(-1)^j\xi^j e^{-jx}\,dx$$

$$= \sum_{j=0}^{\infty}(-1)^j\xi^{j+1}\int_0^\infty x^{n-1}e^{-(j+1)x}dx$$

$$\left\{ \begin{array}{l} y=(j+1)x \\ \frac{dy}{(j+1)}=dx \\ x^{n-1}=\frac{y^{n-1}}{(j+1)^{n-1}} \end{array} \right.$$

$$= \sum_{j=0}^{\infty}\frac{(-1)^j\xi^{j+1}}{(j+1)^n}\underbrace{\int_0^\infty y^{n-1}e^{-y}dy}$$

$$= \sum_{k=1}^{\infty}(-1)^{k-1}\frac{\xi^k}{k^n}\cdot\Gamma(n)$$

$$= \underbrace{\left(\sum_{k=1}^{\infty}(-1)^{k+1}\frac{\xi^k}{k^n}\right)}\cdot\Gamma(n)$$

$$= f_n(\xi)\cdot\Gamma(n) \qquad \text{where } \boxed{f_n(\xi)\equiv\sum_{k=1}^{\infty}(-1)^{k+1}\frac{\xi^k}{k^n}} \;(\xi<1)$$

$$\therefore \boxed{\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x+1}dx = f_n(\xi)\cdot\Gamma(n)}$$

Key result

Example: Lowest-order correction to Ideal Gas Law

- Recall, Eq. (D2'') serves to fix $\mu(T)$ or $\xi(T)$

$$\langle N\rangle = G_s\frac{V}{\lambda_{th}^3}f_{3/2}(\xi)$$

For $\xi<1$, we have $f_n(\xi)=\sum_{k=1}^{\infty}(-1)^{k+1}\frac{\xi^k}{k^n}$

$$\therefore \langle N\rangle \approx G_s\frac{V}{\lambda_{th}^3}\left(\xi-\frac{\xi^2}{2^{3/2}}+\underbrace{\cdots}_{\text{ignore}}\right)$$

$$\Rightarrow \xi = \underbrace{\left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{G_s}\right)}_{\ll 1 \text{ (close to ideal gas limit)}} + \frac{\xi^2}{2^{3/2}} \quad \leftarrow \text{an equation for } \xi$$

$$\Rightarrow \xi \approx \left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{G_s}\right)+\frac{1}{2^{3/2}}\left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{G_s}\right)^2$$

there are higher order terms, if we keep more terms.

$$\text{Eq. (D3)} \Rightarrow \frac{pV}{\langle N\rangle kT} = \frac{f_{5/2}(z)}{f_{3/2}(z)} \quad \text{exact}$$

$$\approx \frac{z - \frac{z^2}{2^{5/2}}}{z - \frac{z^2}{2^{3/2}}}$$

$$\cong \left(1 - \frac{z}{2^{5/2}}\right)\left(1 + \frac{z}{2^{3/2}}\right)$$

$$\approx 1 + z\left(\frac{1}{2^{3/2}} - \frac{1}{2^{5/2}}\right) + \underbrace{\cdots}_{z^2,\ z^3,\ \text{etc.}}$$

$$= 1 + \frac{z}{4\sqrt{2}} + \cdots$$

$$= \underbrace{1}_{\text{ideal gas}} + \underbrace{\frac{1}{4\sqrt{2}}\left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{g_s}\right)}_{\text{lowest order correction due to fermionic nature of particles}} + \underbrace{\cdots}_{\text{higher order in } \left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{g_s}\right)}$$

lowest order correction due to fermionic nature of particles (c.f. $B_2(T)\frac{\langle N\rangle}{V}$)

c.f. positive term in $B_2(T)$ [repulsive]

- When $\left(\frac{\langle N\rangle}{V}\frac{\lambda_{th}^3}{g_s}\right) \ll 1$ or $\lambda_{th} \ll \left(\frac{V}{\langle N\rangle}\right)^{1/3}$

thermal de Broglie wavelength $\ll$ inter-particle separation

ideal fermi gas $\rightarrow$ classical ideal gas.

Ex: Work out the next correction term.

Other problems related to ideal Fermi Gas

- Stability of white dwarf stars
  where there is a degenerate electron gas inside the star (together with helium nuclei)
- Neutron stars
- Liquid ^{3}He
- Magnetic susceptibility due to free electrons in a metal

Students should be able to:

- identify when quantum nature should be considered
- derive how E_F depends on $\langle N\rangle/V$
- state the relationship between E_F, k_F, T_F
- contrast results with classical ideal gas
- argue what low temperature implies
- explain qualitatively and quantitatively the shift in μ at low temperatures

- explain qualitatively and quantitatively $U(T)$
- contrast the behaviour of $U(T)$ and $C_V(T)$ in an ideal gas with that in an ideal classical gas
- realize that there are several contributions to C_V
- realize that exp'ts can extract γ, hence $g(E_F)$
- state typical values of various quantities
- do typical integrals
- explore other applications through self-study
- correction to ideal gas law

Refs:

Rosser: Ch.12 (Sec.12.1-12.3)

Mandl: Sec. 11.5

Appendix A

In studying Fermi gas, we need to handle integrals of the form

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

where $f(\varepsilon)$ is some function of ε.

Very often, we only need results for $kT \ll \mu$ (or $\beta\mu \gg 1$).

Write $z = \beta(\varepsilon-\mu)$, then

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

$$= \frac{1}{\beta}\int_{-\beta\mu}^{\infty} \frac{f(\mu+zkT)}{e^z+1}\, dz$$

$$= \underbrace{\frac{1}{\beta}\int_{-\beta\mu}^{0} \frac{f(\mu+zkT)}{e^z+1}\, dz}_{\substack{\text{turn into two terms} \\ \text{write } z=-y \\ \text{and use } \frac{1}{e^{-y}+1} = 1-\frac{1}{e^y+1}}} + \frac{1}{\beta}\int_0^\infty \frac{f(\mu+zkT)}{e^z+1}\, dz$$

$$\therefore I = \frac{1}{\beta}\int_0^{\beta\mu} f(\underbrace{\mu-ykT}_{\varepsilon})\,dy - \frac{1}{\beta}\int_0^{\beta\mu}\frac{f(\mu-ykT)}{e^y+1}\,dy + \frac{1}{\beta}\int_0^\infty \frac{f(\mu+zkT)\,dz}{e^z+1}$$

$$= \int_0^\mu f(\varepsilon)\,d\varepsilon - \frac{1}{\beta}\int_0^{\beta\mu}\frac{f(\mu-zkT)\,dz}{e^z+1} + \frac{1}{\beta}\int_0^\infty \frac{f(\mu+zkT)}{e^z+1}\,dz$$

So far, it is <u>exact</u>!

- Now, for $\mu \gg kT$, we replace the upper limit in the second integral $\int_0^{\beta\mu}(\ldots)dz$ by $\int_0^\infty(\ldots)dz$, so

$$I = \int_0^\mu f(\varepsilon)\,d\varepsilon + \underbrace{\frac{1}{\beta}\int_0^\infty \frac{f(\mu+zkT)-f(\mu-zkT)}{e^z+1}\,dz}$$

<u>Note</u>: Contribution from large z is negligible, because of the factor $1/e^z$.

For $\mu \gg kT$, (e.g. $\mu \sim 100\,kT$ for metals at room temp.) expand $f(\mu+zkT)$ and $f(\mu-zkT)$ about μ.

$$f(\mu+zkT) = f(\mu) + zkTf'(\mu) + \frac{(kT)^2}{2!}z^2f''(\mu) + \frac{(kT)^3}{3!}z^3f'''(\mu) + \cdots$$

$$f(\mu-zkT) = f(\mu) - zkTf'(\mu) + \frac{(kT)^2}{2!}z^2f''(\mu) - \frac{(kT)^3}{3!}z^3f'''(\mu) + \cdots$$

where $f'(\mu) = \left.\dfrac{df(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\mu}$, etc.

Key Point:

$$f(\mu+zkT) - f(\mu-zkT) = 2kTf'(\mu)z + \frac{2(kT)^3}{3!}f'''(\mu)z^3 + \cdots$$

$z^0, z^2, z^4, \cdots$ terms vanish!

Thus,

$$I \approx \underbrace{\int_0^{\mu} f(\varepsilon)\,d\varepsilon + 2(kT)^2 f'(\mu)\overbrace{\int_0^{\infty}\frac{z\,dz}{e^z+1}}^{\pi^2/12}}_{\text{usually retain first two terms}} + \frac{(kT)^3}{3}f'''(\mu)\underbrace{\int_0^{\infty}\frac{z^3\,dz}{e^z+1}}_{\text{note form of integral}}$$

Finally,

$$\boxed{\int_0^{\infty}\frac{f(\varepsilon)\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1} \approx \int_0^{\mu} f(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(kT)^2 f'(\mu) + \cdots \quad \text{for } kT \ll \mu}$$

This is the formula needed to calculate low-temperature properties of a Fermi Gas.

Appendix B

- We derived $\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x+1}dx = f_n(\xi)\Gamma(n)$

where $f_n(\xi) = \sum_{k=1}^{\infty}\frac{(-1)^{k+1}\xi^k}{k^n}$ for $\xi<1$

- How about $\int_0^\infty \frac{x^{n-1}}{e^x+1}dx$? ($\xi=1$ case)

$$\int_0^\infty \frac{x^{n-1}}{e^x+1}dx = f_n(1)\,\Gamma(n) \qquad \text{(B1)}$$

[$x=0$ will not cause trouble for $n>1$]

What is $f_n(1)$?

$$f_n(1) = \sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^n} = \underbrace{\sum_{k=0}^{\infty}\frac{1}{(2k+1)^n}}_{1,3,5\cdots\text{ terms}} - \underbrace{\sum_{k=1}^{\infty}\frac{1}{(2k)^n}}_{2,4,6\cdots\text{ terms}}$$

$$= \sum_{k=1}^{\infty}\frac{1}{k^n} - 2\sum_{k=1}^{\infty}\frac{1}{(2k)^n}$$

add in 2,4,6… terms, it has now 1,2,3,… terms

substract the added terms

$$= \left(1-2^{1-n}\right)\left(\sum_{k=1}^{\infty}\frac{1}{k^n}\right)$$

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

where $\zeta(n) \equiv \sum_{k=1}^{\infty}\frac{1}{k^n}$ is the Riemann zeta function

Key result

$$\therefore \boxed{\int_0^\infty \frac{x^{n-1}}{e^x+1}dx = \left(1-2^{1-n}\right)\zeta(n)\,\Gamma(n),\ n>1 \quad \text{(B2)}}$$

Riemann zeta function $\zeta(n) = \sum_{k=1}^{\infty}\frac{1}{k^n}$

Gamma function $\Gamma(n) = \int_0^\infty dy\, y^{n-1}e^{-y}$

E.g.: $\int_0^\infty \frac{x\,dx}{e^x+1} = \left(1-\frac{1}{2}\right)\Gamma(2)\zeta(2) = \frac{\pi^2}{12}$ (*)

- Eq. (B2) is the analogy of the Bose integral:

$$\int_0^\infty \frac{x^{n-1}}{e^x-1}dx = \zeta(n)\,\Gamma(n)\ ,\ n>1$$

Thus, the two integrals are related by a factor $(1-2^{1-n})$.

(*) $\Gamma(2) = 1$, $\zeta(2) = \frac{\pi^2}{6}$

This gives the "$\frac{\pi^2}{6}$" in the term $\frac{\pi^2}{6}(kT)^2\left(\frac{df}{d\varepsilon}\right)\Big|_{\varepsilon=\mu}$ in the Sommerfeld formula.

Appendix C: $\dfrac{1}{\Gamma(n)}\displaystyle\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x-1}dx$ for $0<\xi<1$

- Integrals $\displaystyle\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x-1}dx$ appear in discussion on the ideal Bose gas.

Why?

$$f_{BE}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}-1} = \frac{1}{e^{-\beta\mu}e^{\beta\varepsilon}-1} = \frac{1}{\xi^{-1}e^{\beta\varepsilon}-1}$$

For bosons, $\mu < 0$ ← lowest energy of single-particle states

$\therefore\ \underbrace{0<}_{\text{high-temp limit}}\ \xi \underbrace{< 1}_{\text{low-temp. limit}}$

$$\boxed{\text{Define: } g_n(\xi) \text{ as } \quad g_n(\xi) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x-1}dx \quad \text{or} \quad \int_0^\infty \frac{x^{n-1}}{\xi^{-1}e^x-1}dx = \Gamma(n)\cdot g_n(\xi)}$$

Consider

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

expand $\frac{1}{1-y}$

$$= \int_0^\infty dx\, x^{n-1}e^{-x}\xi\sum_{j=0}^\infty \xi^j e^{-jx}$$

$$= \sum_{j=0}^\infty \xi^{j+1}\int_0^\infty dx\, x^{n-1}e^{-(j+1)x}$$

$y=(j+1)x$

$$= \sum_{j=0}^\infty \frac{\xi^{j+1}}{(j+1)^n}\int_0^\infty dy\, y^{n-1}e^{-y}$$

$$= \underbrace{\sum_{k=1}^\infty \frac{\xi^k}{k^n}}\cdot\Gamma(n)$$

$$= g_n(\xi)\cdot\Gamma(n)$$

$$\therefore\ \boxed{g_n(\xi) = \sum_{k=1}^\infty \frac{\xi^k}{k^n}}$$

e.g. $\displaystyle\underbrace{\frac{2}{\sqrt{\pi}}}_{\frac{1}{\Gamma(\frac{3}{2})}}\int_0^\infty \frac{x^{1/2}dx}{\xi^{-1}e^x-1} = g_{3/2}(\xi)$

$\displaystyle\underbrace{\frac{4}{3\sqrt{\pi}}}_{\frac{1}{\Gamma(\frac{5}{2})}}\int_0^\infty \frac{x^{3/2}dx}{\xi^{-1}e^x-1} = g_{5/2}(\xi)$

- Limiting case of $\xi=1$ (useful in Bose-Einstein Condensation)

$$g_n(1) = \sum_{k=1}^\infty \frac{1}{k^n} = \zeta(n) \quad \text{Riemann zeta function}$$

$$\int_0^\infty \frac{x^{n-1}}{e^x-1}dx = \Gamma(n)\,\zeta(n)$$

This integral appears in:

- Debye model of solid (oscillators)
- ideal Bose Gas
- photon gas
- ⋮

Remark:

Riemann zeta function:

$$\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$$

- it converges for $n > 1$

n	$\zeta(n)$	
1	∞	
$\frac{3}{2}$	≈ 2.612	useful in 3D Ideal Bose Gas
2	$\frac{\pi^2}{6} \cong 1.645$	
$\frac{5}{2}$	≈ 1.341	
3	≈ 1.20206	use in photon gas
4	$\frac{\pi^4}{90} \approx 1.0823$	
5	≈ 1.0369	
6	$\frac{\pi^6}{945} \approx 1.017$