XII. Ideal Fermi Gas and Ideal Bose Gas

▪ General Formulation based on $Q(T,V,\mu)$

Key Points

- $Q(T,V,\mu)$ can be evaluated exactly for non-interacting fermions/bosons
- From $Q(T,V,\mu)$, the Fermi-Dirac and Bose-Einstein distributions can be re-derived.
- Equations for studying Ideal Fermi Gas and Ideal Bose Gas are set up.

Background:

$$Q(T,V,\mu) = \sum_{N=0}^{\infty} \sum_{\substack{\text{all } N\text{-particle} \\ \text{states } i}} e^{\beta\mu N} e^{-\beta E_i(N)}$$

$$\Omega = -kT \ln Q$$

$$\langle N \rangle = kT \frac{\partial \ln Q}{\partial \mu} = \frac{1}{\beta}\left(\frac{\partial \ln Q}{\partial \mu}\right)_{T,V}$$

$$\langle E \rangle = \mu\langle N \rangle - \left(\frac{\partial \ln Q}{\partial \beta}\right)_{\mu,V}$$

$$\Omega = -pV$$

$$pV = kT \ln Q$$

General Equations

A. Grand Partition Function for Non-interacting Fermions and Bosons

Let's evaluate $Q(T,V,\mu)$ for non-interacting fermions/bosons

- Understanding $Q(T,V,\mu)$ (physical sense)

$$Q(T,V,\mu) = \sum_{N=0}^{\infty} \sum_{\substack{\text{all } N\text{-particle} \\ \text{states } i}} e^{\beta\mu \underbrace{N}_{\substack{\#\text{ particles} \\ \text{for the state} \\ \text{being summed}}}} e^{-\beta \underbrace{E_i(N)}_{\substack{\text{energy of the} \\ \text{state being} \\ \text{summed}}}} \quad (1)$$

equivalent to summing over ALL states (all values of N and all possible energies)

- Non-interacting particles
  - (particle-in-a-box) single-particle states
  - Label and line-up single-particle states

state labels:	1	2	3	⋯	i	⋯	
single-particle energies:	$\varepsilon_1 \leq$	$\varepsilon_2 \leq$	$\varepsilon_3 \leq$	$\cdots \leq$	ε_i	⋯	
Occupation numbers (# particle in s.p. state):	$n_1,$	$n_2,$	$n_3,$	$\cdots,$	$n_i,$	⋯	

- A string of occupation numbers

$$\{n_1, n_2, \cdots, n_i, \cdots\} \qquad (*)$$

n_1: # particles in state 1 of ε_1; n_i: # particles in state i of ε_i

corresponds to a state in the sums $\sum_{N=0}^{\infty} \sum_{\substack{\text{all } N\text{-particle} \\ \text{states } i}}$

For the state (*), it has

$$\left.\begin{aligned} N &= \sum_i n_i \quad \text{particles} \\ \text{and} \quad E(\{n_i\}) &= \sum_i n_i \varepsilon_i \quad \text{energy} \end{aligned}\right\} (2)$$

- $\displaystyle\sum_{N=0}^{\infty} \sum_{\substack{\text{all } N\text{-particle} \\ \text{states } i}} \Leftrightarrow \sum_{\substack{\text{all strings} \\ \{n_i\}}}$

- Fermions: $n_i = 0, 1$ (Pauli Exclusion Principle)

  Bosons: $n_i = 0, 1, 2, \cdots$

- $$\sum_{N=0} \sum_{\substack{\text{all } N\text{-particle} \\ \text{states } i}} \Leftrightarrow \sum_{\substack{\text{All states} \\ \text{of any } N \\ \text{and any energy}}} \begin{cases} \Leftrightarrow \left(\displaystyle\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \sum_{n_i=0}^{1} \cdots \right) & \text{fermions} \\ \quad [\text{sum over all strings}] & \\ \Leftrightarrow \left(\displaystyle\sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \sum_{n_i=0}^{\infty} \cdots \right) & \text{bosons} \end{cases} \quad (3)$$

(a) Fermions

Putting Eq.(3) and Eq.(2) into Eq.(1)

$$Q_F = \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \sum_{n_i=0}^{1} \cdots e^{\beta\mu \sum_i n_i - \beta \sum_i n_i \varepsilon_i}$$

(Q_F: fermions)

$$= \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \sum_{n_i=0}^{1} \cdots e^{-\beta(\varepsilon_1-\mu)n_1} e^{-\beta(\varepsilon_2-\mu)n_2} \cdots e^{-\beta(\varepsilon_i-\mu)n_i} \cdots$$

$$= \underbrace{\left(\sum_{n_1=0}^{1} e^{-\beta(\varepsilon_1-\mu)n_1}\right)}_{\substack{\text{related to} \\ \text{s.p. state \#1}}} \underbrace{\left(\sum_{n_2=0}^{1} e^{-\beta(\varepsilon_2-\mu)n_2}\right)}_{\substack{\text{related to} \\ \text{s.p. state \#2}}} \cdots \underbrace{\left(\sum_{n_i=0}^{1} e^{-\beta(\varepsilon_i-\mu)n_i}\right)}_{\substack{\text{related to} \\ \text{s.p. state \#}i}} \cdots$$

$$= \prod_{i} \left(\sum_{n_i=0}^{1} e^{-\beta(\varepsilon_i-\mu)n_i} \right)$$

($\prod_i$: over s.p. states)

- factorized according to single-particle states
- $n_i = 0, 1$ (fermions)

$$= \prod_i \left(1 + e^{-\beta(\varepsilon_i-\mu)}\right)$$

$$\therefore \boxed{Q_F = \prod_i \left(1 + e^{-\beta(\varepsilon_i-\mu)}\right) \quad \text{(fermions)}} \quad \text{(Exact)} \quad (4)$$

($\prod_i$: product over all single-particle states)

(c.f. Z is hard to evaluate for fermions)

$Q_i^{(\text{fermions})} \equiv 1 + e^{-\beta(\varepsilon_i-\mu)}$ is called the grand partition function of the i^{th} single-particle state for fermions

(b) Bosons

$$Q_B = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_i=0}^{\infty}\cdots e^{\beta\mu\sum_i n_i} e^{-\beta\sum_i \varepsilon_i n_i}$$

Bosons

$$= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_i=0}^{\infty}\cdots e^{-\beta(\varepsilon_1-\mu)n_1} e^{-\beta(\varepsilon_2-\mu)n_2}\cdots e^{-\beta(\varepsilon_i-\mu)n_i}\cdots$$

$$= \left(\sum_{n_1=0}^{\infty} e^{-\beta(\varepsilon_1-\mu)n_1}\right)\left(\sum_{n_2=0}^{\infty} e^{-\beta(\varepsilon_2-\mu)n_2}\right)\cdots\left(\sum_{n_i=0}^{\infty} e^{-\beta(\varepsilon_i-\mu)n_i}\right)\cdots$$

$$= \prod_i \left(\sum_{n_i=0}^{\infty} e^{-\beta(\varepsilon_i-\mu)n_i}\right)$$

- factorized according to single-particle states
- $n_i = 0, 1, 2, \cdots$ (bosons)

$$= \prod_i \frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$$= \prod_i \left(1-e^{-\beta(\varepsilon_i-\mu)}\right)^{-1}$$

$$\therefore \boxed{Q_B = \prod_i \frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}} = \prod_i\left(1-e^{-\beta(\varepsilon_i-\mu)}\right)^{-1} \text{ (bosons)}} \quad \text{(Exact)} \quad (5)$$

product over all single-particle states

(c.f. Z is hard to evaluate for bosons)

$Q_i^{(bosons)} \equiv \left(1-e^{-\beta(\varepsilon_i-\mu)}\right)^{-1}$ is called the grand partition function of the i^{th} single-particle state for bosons

Summary

$$\boxed{Q_{\substack{F\\B}} = \prod_i \left(1 \pm e^{-\beta(\varepsilon_i-\mu)}\right)^{\pm 1}}$$

writing Eq. (4) and Eq. (5) together

$+$: fermions
$-$: bosons

And everything follows.

Next, we will work out a set of equations for non-interacting fermions (Sec. B) and bosons (Sec. C).

B. Fermi-Dirac Distribution and Equations for Ideal Fermi Gas

$$Q_F = \prod_i \left(1 + e^{-\beta(\varepsilon_i - \mu)}\right) \qquad \text{(F1)}$$

product over single-particle states i

(a) Grand potential and Equation of state

$$\Omega = -kT \ln Q_F = -kT \sum_i \ln\left[1 + e^{-\beta(\varepsilon_i - \mu)}\right] \qquad \text{(F2)}$$

But $\Omega = -pV$,

$$\therefore \boxed{pV = kT \sum_i \ln\left[1 + e^{-\beta(\varepsilon_i - \mu)}\right]} \qquad \text{(F3)}$$

pV: gives equation of state

$\sum_i$: sum over s.p. states (this can be handled by $\sum_i (\cdots) \to \int g(\varepsilon)(\cdots)\, d\varepsilon$)

$g(\varepsilon)$: density of states

(b) Fermi-Dirac distribution re-derived

$\langle N \rangle$ = mean number of particles ← same as N in thermodynamics

$$= -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \sum_i \frac{e^{-\beta(\varepsilon_i - \mu)}}{1 + e^{-\beta(\varepsilon_i - \mu)}}$$

$$= \underbrace{\sum_i}_{\text{sum over s.p. states}} \underbrace{\frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}}_{\#\text{ fermions in a s.p. state of energy } \varepsilon_i} = \sum_i \underbrace{f_{FD}(\varepsilon_i)}_{\text{Fermi-Dirac distribution}} = \sum_i \langle n_i \rangle \qquad \text{(F4)}$$

$$\therefore f_{FD}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu)} + 1} \qquad \text{(F5)}$$

is re-derived based on $Q_F(T, V, \mu)$

- It carries the same meaning as discussed in Ch. VII, i.e. number of fermions per single-particle state of energy ε.

Recall: In Ch. VII, the Fermi-Dirac distribution was found to be the most probable distribution.
We used two Lagrange multipliers

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

We did not identify the multipliers α (or μ) and β in Ch. VII.

Here, we derived $f_{FD}(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1} = \dfrac{1}{e^{\frac{(\varepsilon-\mu)}{kT}}+1}$

by grand canonical ensemble.

In grand canonical ensemble, we have temperature T and chemical potential μ from the beginning of the formalism.

$\therefore$ The Lagrange multipliers are identified!

$\langle N\rangle = \langle N\rangle(T,\mu,V)$ is an equation for $\mu(T)$ †

$$\langle N\rangle = \sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1} = \int_0^\infty g(\varepsilon)\frac{1}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \qquad \text{(F4)}$$

For real material particles, e.g. atoms, molecules, electrons, etc., $\langle N\rangle$ is very sharp and plays the role of N in thermodynamics.

> For material particles,
>
> $\langle N\rangle$ should NOT depend on temperature T

- Look at the equation above, LHS is a constant, and RHS has β and μ.

> $\therefore$ for a temperature T, one has to adjust μ so that the integral gives $\langle N\rangle$
>
> $\Rightarrow$ it is an equation‡ for $\mu(T)$.

This is what one would expect, as $e^{-\beta\mu} = e^{\alpha}$, where α is the Lagrangian multiplier introduced (see Ch. VII) to take care of the constraint of a fixed number of particles.

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† The discussion here also holds for Bosons.

‡ Recall that, e.g. in 3D $g(\varepsilon) \propto V$. So it is really the fermion number density $\frac{\langle N\rangle}{V}$ that determines $\mu(T)$.

(c) Mean Energy $\langle E \rangle$

- Physical Meaning

$$\langle E \rangle = \sum_i \varepsilon_i \, f_{FD}(\varepsilon_i) \qquad (F6)$$

energy of s.p. state i

particles in a state of energy ε_i

total energy

sum over s.p. states

$$= \int_0^\infty g(\varepsilon)\, \varepsilon \, f_{FD}(\varepsilon) d\varepsilon = \int_0^\infty g(\varepsilon) \frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \qquad (F6)$$

- Or plug formula

$$\langle E \rangle = \mu \langle N \rangle - \left(\frac{\partial \ln Q}{\partial \beta}\right)_{\mu, V}$$

$$= \mu \langle N \rangle - \frac{\partial}{\partial \beta} \sum_i \ln\left(1 + e^{-\beta(\varepsilon_i - \mu)}\right)$$

$$= \mu \langle N \rangle + \sum_i \frac{(\varepsilon_i - \mu)\, e^{-\beta(\varepsilon_i-\mu)}}{1 + e^{-\beta(\varepsilon_i - \mu)}}$$

$$= \mu \langle N \rangle - \mu \underbrace{\sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}} + \sum_i \varepsilon_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}$$

$$= \mu \langle N \rangle - \mu \langle N \rangle + \sum_i \varepsilon_i f_{FD}(\varepsilon_i)$$

$$= \sum_i \varepsilon_i f_{FD}(\varepsilon_i) \quad \text{(as expected)} \qquad (F6)$$

- After obtaining $\mu(T)$ from Eq. (F4), Eq. (F6) gives $E(T)$ and thus the heat capacity.

(d) Key concepts on Ideal Fermi Gas

How does $f_{FD}(\varepsilon)$ or $n_{FD}(\varepsilon)$ look like?

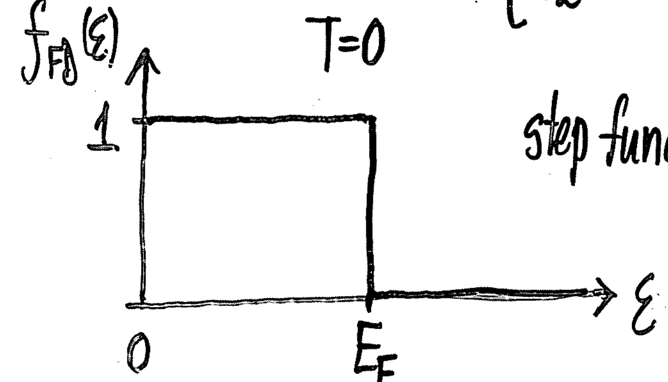
$$\boxed{f_{FD}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}}$$

(i) $T \to 0$ limit, let $\mu(T=0) \equiv E_F$ = Fermi energy†

[Note: μ in general is temperature-dependent]

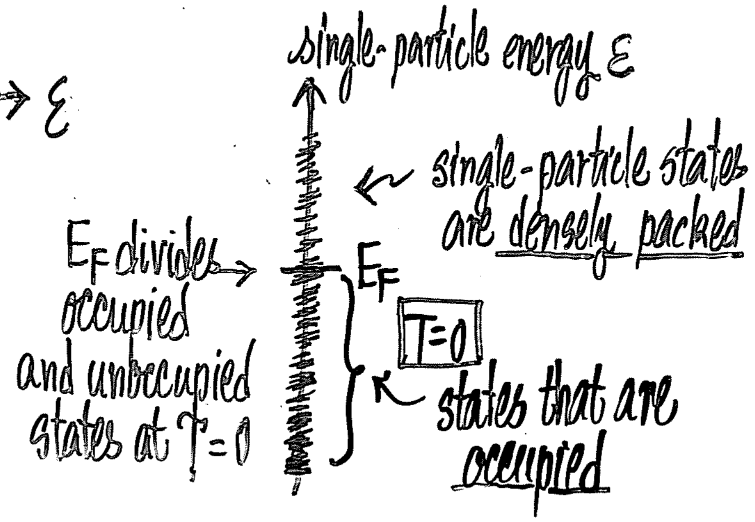
$$\lim_{T\to 0} f_{FD}(\varepsilon) = \lim_{T \to 0} \frac{1}{e^{(\varepsilon - \varepsilon_F)/kT} + 1}$$

$$= \begin{cases} 1 & \text{if } \epsilon < E_F \\ 0 & \text{if } \epsilon > E_F \\ 1/2 & \text{if } \epsilon = E_F \end{cases} \qquad (T=0)$$



$\boxed{\mu(T=0) \text{ is called } E_F}$

step function or θ-function $\theta(E_F - \epsilon)$



† For metals, in which the conduction electrons form a Fermi Gas, E_F/k is typically $\sim 10^4$ K, i.e. $E_F \sim$ a few eV.

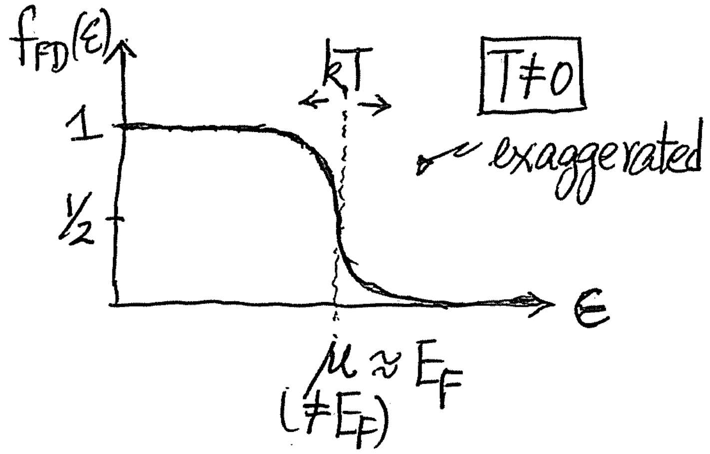
∴ Due to Pauli Exclusion Principle, $\underbrace{\mu(T=0)}_{E_F}$ is rather high (positive)

⇒ $T=0$ physics sets a high energy scale for fermi systems

(ii) At finite temperature

Note: Typically, temperature of interest T is much smaller than E_F/k ($T=0$ property)
($kT \ll E_F$ OR $T \ll E_F/k \equiv T_F$)

- $f_{FD}(\varepsilon)$ smears out over a width of $\sim kT$ around E_F



tail at high ε falls off exponentially

- Due to Pauli Exclusion Principle, states with energy deep below E_F are not affected, since thermal energy $\sim kT$ is not enough to excite the fermions in these states to unoccupied states above E_F.
- Most important piece of physics in understanding metal physics & neutron stars physics. It comes from quantum mechanics (QM) and the necessity of considering quantum nature of particles ($\lambda_{th} > d$) in these systems.

(iii) Very high temperature

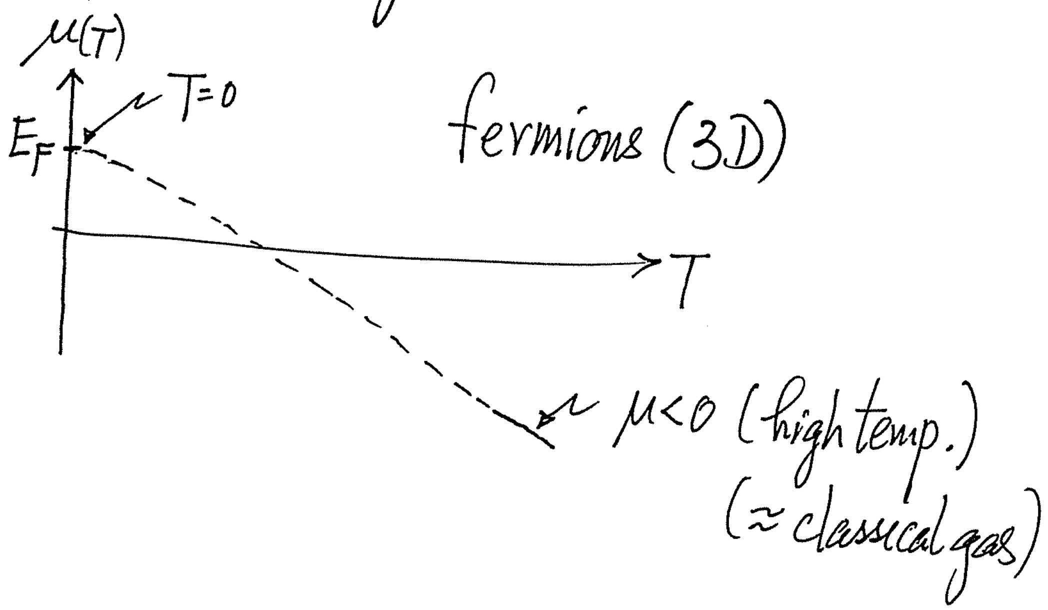
Fermi Gas $\approx$ classical gas

$$\left[\text{as } \left(\frac{V}{N}\right)^{1/3} > \frac{h}{\sqrt{2\pi mkT}}\right] \quad \text{quantum effect diminishes}$$

For classical gas, $\mu < 0$

recall: $\mu = -kT \ln\left[\frac{V}{N}\cdot\left(\frac{\sqrt{2\pi mkT}}{h}\right)^3\right]$ for classical gas (3D)

(iv) Put information together



(e) A useful relation for Entropy: S in terms of $f_{FD}(\varepsilon)$ (Optional)

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

$$1 - f_{FD}(\varepsilon) = e^{\beta(\varepsilon-\mu)} \cdot \underbrace{\frac{1}{e^{\beta(\varepsilon-\mu)}+1}}_{f_{FD}(\varepsilon)}$$

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

OR $\boxed{\beta(\varepsilon-\mu) = \ln(1-f_{FD}(\varepsilon)) - \ln(f_{FD}(\varepsilon))}$

Entropy S

$$S = -\frac{\partial\Omega}{\partial T} = k\beta^2\frac{\partial\Omega}{\partial\beta} = -k\beta^2\frac{\partial}{\partial\beta}\left(\frac{\ln Q}{\beta}\right) = k\ln Q - \beta k\frac{\partial \ln Q}{\partial\beta}$$

$$\Rightarrow \frac{S}{k} = \ln Q - \beta\frac{\partial\ln Q}{\partial\beta}$$

$$= \sum_i \ln\left(1 + e^{-\beta(\varepsilon_i-\mu)}\right) + \beta\sum_i(\varepsilon_i-\mu)\, f_{FD}(\varepsilon_i)$$

$$= \sum_i \ln\left(\frac{1}{1-f_{FD}(\varepsilon_i)}\right) + \sum_i f_{FD}(\varepsilon_i)\left[\ln(1-f_{FD}(\varepsilon_i)) - \ln(f_{FD}(\varepsilon_i))\right]$$

$$\Rightarrow \boxed{\frac{S}{k} = -\sum_i\Big((1-f_{FD}(\varepsilon_i))\ln(1-f_{FD}(\varepsilon_i)) + f_{FD}(\varepsilon_i)\ln(f_{FD}(\varepsilon_i))\Big)}$$

Note: All the results so far are general in the sense that no explicit reference is made on the single-particle dispersion relation and thus the density of states.

Summary: Fermions

$$Q_F(T,\mu,V) = \prod_i \left(1 + e^{-\beta(\varepsilon_i-\mu)}\right)$$

$$\langle N\rangle = \sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}$$ which is an equation for $\mu(T)$

$$\langle n_i\rangle \equiv f_{FD}(\varepsilon_i) = \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}$$

$$\langle E\rangle = \sum_i \varepsilon_i f_{FD}(\varepsilon_i) = \sum_i \frac{\varepsilon_i}{e^{\beta(\varepsilon_i-\mu)}+1}$$ an equation for $E(T)$

$$pV = kT\sum_i \ln\left[1+e^{-\beta(\varepsilon_i-\mu)}\right]$$ an equation of state

$$S = -k\sum_i \Big((1-f_{FD}(\varepsilon_i))\ln(1-f_{FD}(\varepsilon_i)) + f_{FD}(\varepsilon_i)\ln(f_{FD}(\varepsilon_i)) \Big)$$

- These are general for a system with non-interacting fermions.

- If we are given more information about the system, (what are the particles? 1D/2D/3D? $\varepsilon(\vec{k})$?) then $\sum_i(\cdots)$ (over all single particle states) can be treated as $\int g(\varepsilon)(\cdots)\,d\varepsilon$. ($g(\varepsilon)$: DOS (see Ch. VIII))

C. Bose-Einstein Distribution and Equations for Ideal Bose Gas

$$Q_B = \prod_i \frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}} \qquad \text{(B1)}$$

product over single-particle states i

(a) Grand potential and Equation of state

$$\Omega = -kT\ln Q_B = kT\sum_i \ln\left[1-e^{-\beta(\varepsilon_i-\mu)}\right] \qquad \text{(B2)}$$

But $\Omega = -pV$,

$$\therefore\ \boxed{pV = -kT\sum_i \ln\left[1-e^{-\beta(\varepsilon_i-\mu)}\right]} \qquad \text{(B3)}$$

gives equation of state

(b) Bose-Einstein Distribution re-derived

$\langle N\rangle$ = mean number of particles ← same as N in thermodynamics

$$= -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V} = \sum_i \frac{e^{-\beta(\varepsilon_i-\mu)}}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$$= \underbrace{\sum_i}_{\text{sum over s.p. states}} \underbrace{\frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}}_{\#\text{ bosons in a s.p. state of energy } \varepsilon_i} = \sum_i \underbrace{f_{BE}(\varepsilon_i)}_{\text{Bose-Einstein distribution}} = \sum_i \langle n_i\rangle \qquad \text{(B4)}$$

$\therefore\ f_{BE}(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}-1}$ (B5)

is re-derived based on $Q_B(T,V,\mu)$

It carries the same meaning as discussed in Ch. VII, i.e. <u>number of bosons per single-particle state</u> of energy ε.

- As such, $f_{BE}(\varepsilon) \geq 0$ for all single-particle states.
  [This has important consequence]
- The derivation here also justifies the Lagrange Multipliers $\beta = \frac{1}{kT}$ and $\alpha = -\mu\beta$.
- Eq. (B4):

$$\langle N\rangle = \sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1} \qquad \text{(B4)}$$

is an equation for determining $\mu(T)$ for systems consisting of real bosonic particles.

(c) <u>Mean Energy $\langle E\rangle$</u>

- Physical Meaning

$$\langle E\rangle = \sum_i \varepsilon_i\, f_{BE}(\varepsilon_i) \qquad \text{(B6)}$$

total energy; sum over s.p. states; energy of s.p. state i; # particles in a state of energy ε_i

$$= \int_0^\infty g(\varepsilon)\,\varepsilon\, f_{BE}(\varepsilon)\,d\varepsilon = \int_0^\infty g(\varepsilon)\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon \qquad \text{(B6)}$$

- OR plug formula

$$\langle E\rangle = \mu\langle N\rangle - \left(\frac{\partial \ln Q}{\partial\beta}\right)_{\mu,V}$$

$$= \mu\langle N\rangle + \frac{\partial}{\partial\beta}\sum_i \ln\left[1 - e^{-\beta(\varepsilon_i-\mu)}\right]$$

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

$$= \sum_i \varepsilon_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$

$$= \sum_i \varepsilon_i\, f_{BE}(\varepsilon_i) \quad \text{(as expected)} \qquad \text{(B6)}$$

- After obtaining $\mu(T)$ from Eq. (B4), Eq. (B6) gives $E(T)$.

(d) Key Concepts on Ideal Bose Gas

$$f_{BE}(\varepsilon_i) = \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1} \quad (B5)$$ Bose-Einstein Distribution

physical meaning: # bosons in a single-particle state of energy ε_i

$\therefore$ $f_{BE}(\varepsilon_i)$ cannot be negative for all single-particle states

Notice that there is "-1" in Eq. (B5)

For $f_{BE}(\varepsilon_i) \geq 0$ for all s.p. states (any ε_i)

$\Rightarrow$ $\boxed{\mu < \varepsilon_i \text{ for all s.p. states } i}$

In particular, this has to be true for the lowest single-particle state (single-particle ground state) of energy $\varepsilon_1 = \varepsilon_{lowest}$, i.e.

$$\boxed{\mu < \varepsilon_{lowest}} \quad (B7) \quad \text{(Bosons)}$$

so that $f_{BE}(\varepsilon_i) \geq 0$ for all s.p. states

Meaning: μ may vary with temperature, but at most μ takes on a limiting value of

$\mu \to \varepsilon_{lowest}$ from below.

- For particle-in-a-big-box,

$$\varepsilon_{lowest} = \frac{\pi^2\hbar^2}{2mL^2} \sim \frac{\hbar^2}{mL^2} \quad \text{with } L \sim \underbrace{\text{mm-cm}}_{\text{macroscopic}}$$

$$\approx 0$$

$\therefore$ Practically, the physical requirement on μ becomes $\boxed{\mu < 0}$. (Bosons)

This must be true for all temperatures.

$\therefore$ $\boxed{\mu < 0 \text{ for all temperatures (Bosons)}}$

Very high temperature

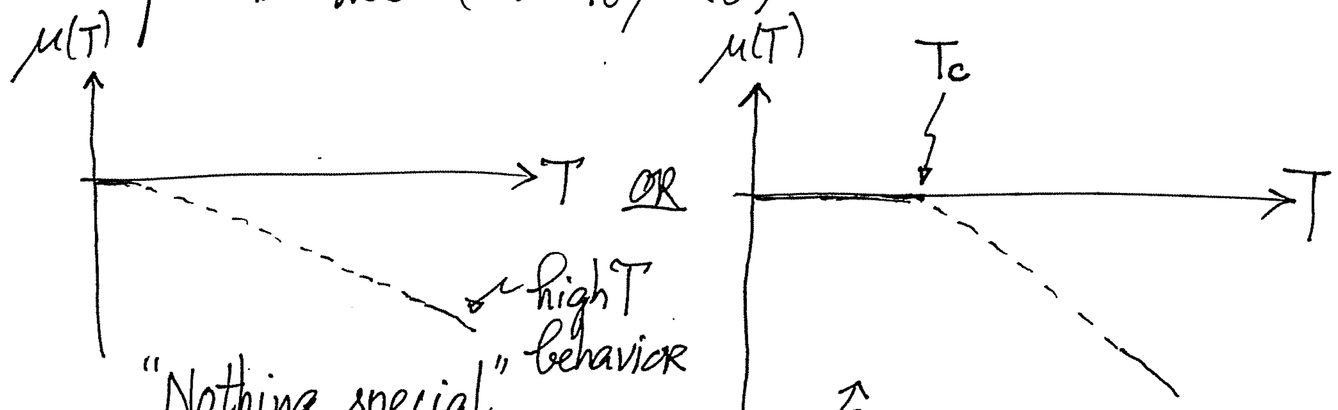
Bose gas $\approx$ $\underbrace{\text{classical gas}}$ (Quantum effect diminishes)

$$\mu = -kT \ln\left[\left(\frac{V}{N}\right)\left(\frac{\sqrt{2\pi mkT}}{h}\right)^3\right] \quad (3D)$$

< 0 (by much)

- **Put together information on $\mu(T)$: (Bosons)**

Two possibilities (Recall $\mu < 0$)



$\boxed{\text{Some finite } T_c \text{ that } \mu \text{ approaches } 0}$

This is the case for 1D, 2D non-relativistic free Bosons

then something special happens at $T < T_c$

(Bose-Einstein Condensation)

This is the case for 3D non-relativistic free Bosons

(e) A useful relation and Entropy (Optional)

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

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

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

OR $\boxed{\beta(\varepsilon-\mu) = \ln(1+f_{BE}(\varepsilon)) - \ln(f_{BE}(\varepsilon))}$

Entropy S : S in terms of $f_{BE}(\varepsilon)$

$$S = -\frac{\partial\Omega}{\partial T} = +k\ln Q - \beta k \frac{\partial \ln Q}{\partial \beta}$$

$$\Rightarrow \frac{S}{k} = -\sum_i \ln\left(1-e^{-\beta(\varepsilon_i-\mu)}\right) + \beta\sum_i \frac{(\varepsilon_i-\mu)\, e^{-\beta(\varepsilon_i-\mu)}}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$$= \sum_i \ln(1+f_{BE}(\varepsilon_i)) + \sum_i f_{BE}(\varepsilon_i)\, \beta(\varepsilon_i-\mu)$$

$$= -\sum_i \Big(f_{BE}(\varepsilon_i)\ln f_{BE}(\varepsilon_i) - (1+f_{BE}(\varepsilon_i))\ln(1+f_{BE}(\varepsilon_i)) \Big)$$

Note: All the results so far are general in the sense that no explicit reference is made on the single-particle dispersion relation and thus the density of states.

Summary: Bosons

$$Q_B(T,\mu,V) = \prod_i \left(\frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}} \right)$$

- $\mu < \varepsilon_i$ for all single-particle states i, with μ approaches the lowest state from below as T drops

$$\langle N \rangle = \sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$ which is an equation for $\mu(T)$ for material bosons.

$$\langle n_i \rangle \equiv f_{BE}(\varepsilon_i) = \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$

$$\langle E \rangle = \sum_i \varepsilon_i f_{BE}(\varepsilon_i) = \sum_i \frac{\varepsilon_i}{e^{\beta(\varepsilon_i-\mu)}-1}$$

$$pV = -kT \sum_i \ln\left(1 - e^{-\beta(\varepsilon_i-\mu)}\right)$$

$$S = -k \sum_i \left(f_{BE}(\varepsilon_i) \ln f_{BE}(\varepsilon_i) - (1+f_{BE}(\varepsilon_i)) \ln(1+f_{BE}(\varepsilon_i)) \right)$$

- These are general for a system with non-interacting bosons.

- If we are given more information about the system, (what are the particles? 1D/2D/3D? $\varepsilon(\vec{k})$?) then $\sum_r (\cdots)$ can be turned into $\int g(\varepsilon)(\cdots)\, d\varepsilon$
  - $\sum_r$: sum over single-particle states
  - $g(\varepsilon)$: DOS

Students should be able to...

- Handle the summations over "N and all N-particle states" in $Q(T,V,\mu)$ and evaluate Q_F and Q_B for non-interacting fermions and bosons
- Apply standard formulas involving Q to obtain $\langle N \rangle$ and re-discover Fermi-Dirac and Bose-Einstein distributions and their physical meaning
- Apply formula or physical argument to obtain $\langle E \rangle$
- State behavior of μ in fermionic and bosonic systems
- State the restriction on μ in bosonic system
- Evaluate the entropy (optional)
- Establish sets of equations applicable to ideal Fermi Gas and ideal Bose Gas
- Identify where the effects of dimensionality, non-relativistic or relativistic, and dispersion relation enter the calculation.

Refs: Mandl: Sec. 11.2, Bowley & Sanchez: Sec. 9.7, 9.9, 10.1, 10.2, Yoshioka: Ch. 10, Pathria: Ch. 4, Sec. 7.1, Sec. 8.1