VIII. Single-particle density of states

- Gases: particles are not localized
  ⇒ need to handle indistinguishability of particles
- Non-interacting / independent particles
  ⇒ we can consider single particle states

Filling N particles into single-particle states:

Dilute / High T	Otherwise
• "classical gas"	• quantum gas
• but still need to handle indistinguishability, usually by a factor of $\frac{1}{N!}$ in evaluating Z	• rules for single-particle state occupancy, need to consider fermions or bosons
• Maxwell-Boltzmann distribution for occupying single-particle states	• f_{FD} or f_{BE} for occupying single-particle states

Recall:

$$n_i = g_i\left(\frac{1}{e^{(\varepsilon_i-\mu)/kT}\pm 1}\right) \qquad \begin{cases} \text{"+" FD} \\ \text{"−" BE} \end{cases}$$

$$n_i = g_i\left(\frac{N e^{-\beta\varepsilon_i}}{\sum_i g_i e^{-\beta\varepsilon_i}}\right) \qquad \text{"classical limit"}$$

All three expressions have the same mathematical form.

$$\underset{\substack{\uparrow \\ \text{\# particles in a group} \\ \text{of single-particle} \\ \text{states of energy } \varepsilon_i \\ \text{(in equilibrium)}}}{n_i} = g_i \underbrace{\left(\begin{matrix}\text{"distribution} \\ \text{function"}\end{matrix}\right)}_{\substack{\uparrow \\ \text{\# particles in a single-particle} \\ \text{state of energy } \varepsilon_i\text{, when} \\ \text{system is in equilibrium}}}$$

g_i = # single-particle states in a group, all with energy ε_i
↑
still discrete in nature

Aim: Here, we will study the continuum limit of g_i for gases,

i.e., $g(\varepsilon)\,d\varepsilon \equiv$ # single-particle states in the energy interval ε to $\varepsilon + d\varepsilon$

$g(\varepsilon)$ = "density of (single-particle) states in energy"

<u>The point is:</u>

- We know (Ch. VII)

$$n_i = g_i\left(\frac{1}{e^{\beta(\varepsilon_i-\mu)}\pm 1}\right) \qquad \begin{array}{l} + \text{ Fermions} \\ - \text{ Bosons} \end{array}$$

$$n_i = g_i\left(\frac{N e^{-\beta\varepsilon_i}}{Z}\right) \qquad \begin{array}{c} \text{Classical} \\ \text{[Maxwell-Boltzmann]} \end{array}$$

(···) give # particles in <u>a single-particle state</u> of energy ε_i

- <u>Questions:</u>

{ Are there single-particle states at energy ε_i?
{ How many single-particle states are there at energy ε_i?

The information is embedded in g_i or $g(\varepsilon)d\varepsilon$

[e.g. if $g(\varepsilon)=0$ for some energy, there are no single-particle states to be filled in! This is the case in the band-gap of a semiconductor]

{ Finding $g(\varepsilon)d\varepsilon$ is <u>NOT</u> a statistical physics problem.
{ It is a QM (or classical physics) problem.

But we need it to move on!

<u>What if we know $g(\varepsilon)d\varepsilon$?</u>

$$N = \sum_{\text{levels } i} n_i = \sum_{\text{levels } i} g_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}\pm 1}$$

$$= \sum_{\text{states } i} \frac{1}{e^{\beta(\varepsilon_i-\mu)}\pm 1}$$

$$\therefore \quad \boxed{N = \int \underbrace{g(\varepsilon)}_{} \underbrace{\frac{1}{e^{\beta(\varepsilon-\mu)}\pm 1}}_{\text{fermions/bosons per state}} d\varepsilon} \qquad (1)$$

reflects details of system: 3D/2D/1D?
type of particles?

$$E = \sum_{\text{levels } i} \varepsilon_i n_i = \sum_{\text{levels } i} g_i \varepsilon_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}\pm 1}$$

$$= \sum_{\text{states } i} \frac{\varepsilon_i}{e^{\beta(\varepsilon_i-\mu)}\pm 1}$$

$$\therefore \quad \boxed{E = \int g(\varepsilon)\cdot\varepsilon\cdot\frac{1}{e^{\beta(\varepsilon-\mu)}\pm 1}\, d\varepsilon} \qquad (2)$$

Eqs. (1) and (2) are the key starting equations for studying Ideal Fermi Gas (+ sign) and Ideal Bose Gas (− sign). Eq. (1) serves to give $\mu(T)$.

At the end,

- in additional to $g(\varepsilon)d\varepsilon$,
- we will know how to handle

$$\underset{\text{"levels } i\text{"} \to \text{cells } i}{\sum} g_i (\cdots)$$

$$= \sum_{\text{single-particle states } i} (\cdots) \equiv \sum_{\text{s.p. states } i} (\cdots)$$

A. Particle-in-a-(big) box: Counting states in k-space

(a) 1D big box (standing wave solutions)

These are single-particle states

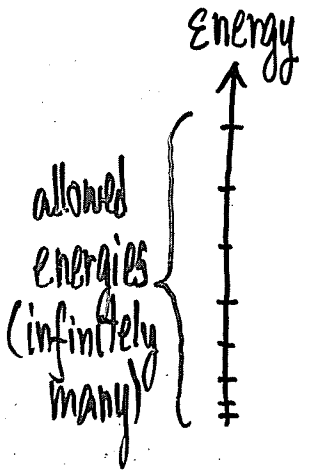
$$\psi_{n_x}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_x \pi x}{L}\right) = \sqrt{\frac{2}{L}} \sin(k_{x,n_x} x) \quad \text{energy eigenstates}$$

$$\varepsilon_{n_x} = \frac{n_x^2 \pi^2 \hbar^2}{2mL^2} = \frac{\hbar^2 k_{x,n_x}^2}{2m} \quad \text{energy eigenvalues}$$

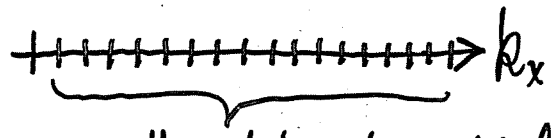
$n_x = 1, 2, 3, \cdots$

The point is:

- The box makes allowed k_x discrete (quantized), and allowed energy ε_{n_x} discrete (quantized).



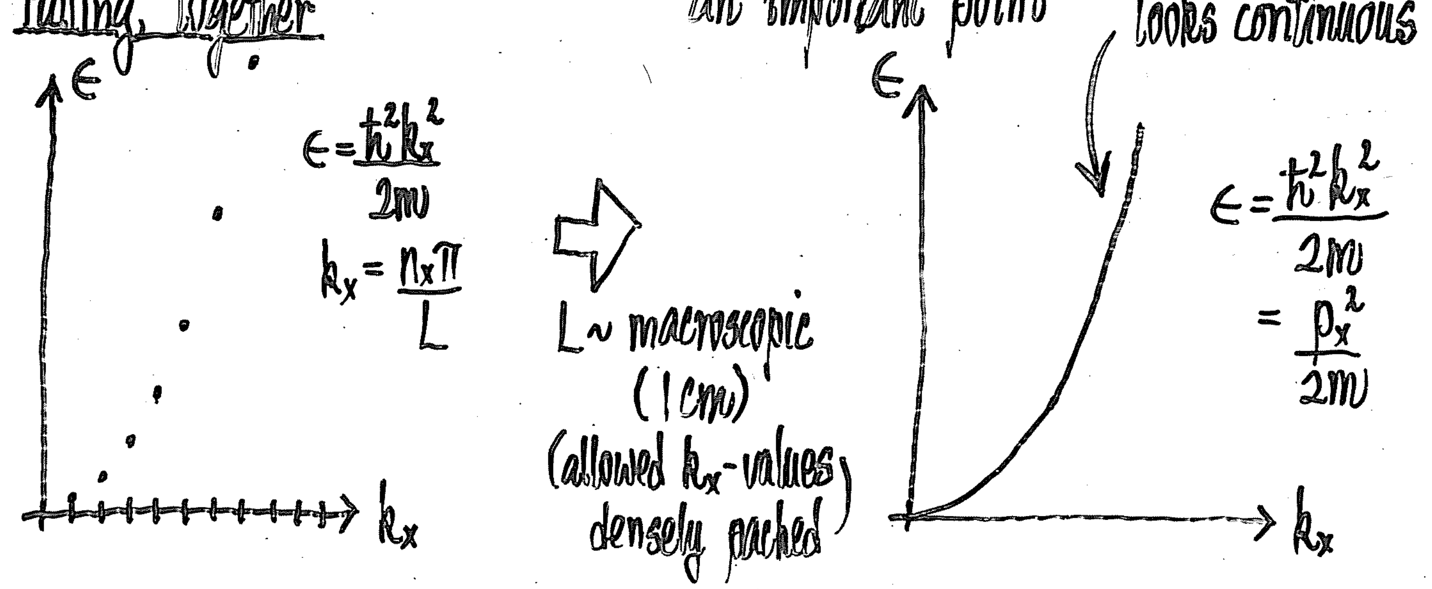
$$\boxed{k_{x,n_x} = n_x \frac{\pi}{L}}$$



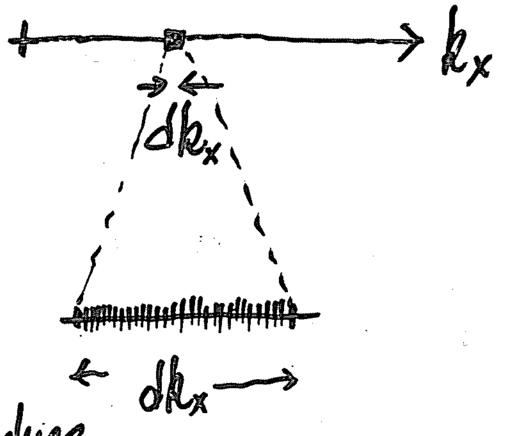
- allowed k_x-values (infinitely many)
- evenly spaced in k_x-axis (k-space)

↑ an important point

Putting together



- Each allowed k_x-value (thus a single-particle state) "occupies" $\frac{\pi}{L}$ of the k-space (k_x-axis) [Key result]
- <u>How many allowed k-values</u> are there in a "length element" dk_x in k-space?



allowed k-values

$$= \frac{dk_x}{\left(\frac{\pi}{L}\right)} = \left(\frac{L}{\pi}\right) dk_x$$

= # allowed n_x-values

- Apart from a possible spin-degeneracy factor G_s, this is the number of single-particle states in dk_x
  ($G_s = (2s+1) = 2$ for spin-half ($s = \frac{1}{2}$) particles)

<u>Application</u>:

- We often encounter $\sum_{\substack{\text{single-particle}\\\text{states}}}$ in evaluating quantities, e.g., z.
- $\sum_{\substack{\text{single-particle}\\\text{states}}} (\cdots) = \sum_{n_x=1}^{\infty} (\cdots)$
- Can <u>replace</u> $\sum_{n_x=1}^{\infty} F(k_x)$ <u>by</u> $\underbrace{\frac{L}{\pi}}\int_0^\infty \underbrace{dk_x}\, F(k_x)$

come together when k_x is treated <u>continuously</u>.

<u>Key Physics concepts</u>

(a) <u>Fitting of Waves to a box</u>

- $\underbrace{\text{Wavelengths} \leftrightarrow k\text{-values} \leftrightarrow \varepsilon_{n_x}}$

are selected by "<u>fitting waves to a box</u>"

∴ Results (each allowed k_x-value (a s.p. state) occupies $\left(\frac{\pi}{L}\right)$ of k-space) <u>are general</u>!

<u>Meaning</u>: Fitting <u>EM waves</u> (photon problems)
Fitting <u>elastic waves</u> in a solid (phonon problems)
etc.

(b) <u>Many ways</u> to execute "sum over s.p. states"

$$\begin{tikzcd}
\sum\limits_{\text{all s.p. states}} (\cdots) \arrow[r] \arrow[dr] \arrow[ddr] & \sum\limits_{\text{over } n_x=1,2,\cdots} (\cdots) & \\
 & \sum\limits_{\text{over all } k_x\text{-values}} (\cdots) \arrow[r] & \int_0^\infty (\cdots) \frac{L}{\pi} dk_x \\
 & \sum\limits_{\substack{\text{over energy of}\\\text{each state one-by-one}}} (\cdots) \arrow[r] & \int_0^\infty (\cdots)\, g(\varepsilon)\, d\varepsilon
\end{tikzcd}$$

(1D example)
↑
concept is general

$\frac{L}{\pi} \equiv$ "Density of states in k-space"

(this is a constant because the allowed k_x values are uniformly distributed)

$$\boxed{\text{Q: How about 2D big-box and 3D big-box?}}$$

Also, how about changing $\int dk_x$ to $\int d\varepsilon$?

1D: $\frac{L}{\pi}\int_0^\infty dk_x\, F(k_x)$

$$\downarrow$$

$$\int_0^\infty d\varepsilon\, \underbrace{g_{1D}(\varepsilon)}\, F(\varepsilon)$$

but $\varepsilon(k_x) = \frac{\hbar^2 k_x^2}{2m}$

for free particles (dispersion relation)

density of (single-particle) states in energy (1D) or simply density of states (DOS)

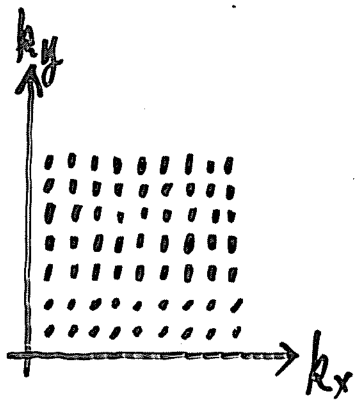
(b) 2D big box

$$\psi_{n_x,n_y}(x,y) = \sqrt{\frac{4}{L^2}}\,\sin\Big(\underbrace{\frac{n_x\pi}{L}}_{k_x}x\Big)\,\sin\Big(\underbrace{\frac{n_y\pi}{L}}_{k_y}y\Big)\,; \quad n_x = 1,2,3,\dots \quad n_y = 1,2,3,\dots$$

$$\epsilon(k_x,k_y) = \frac{\pi^2\hbar^2(n_x^2+n_y^2)}{2mL^2} = \frac{\hbar^2(k_x^2+k_y^2)}{2m} = \frac{\hbar^2k^2}{2m}$$

$\vec{k} = (k_x, k_y)$

Allowed k-values are:



- regular array in k-space (k_x-k_y plane)

- Each allowed $\vec{k}$-value occupies $\left(\frac{\pi}{L}\right)^2$ of $\vec{k}$-space [Key result]
- How many allowed $\vec{k}$-values are there in an "area element" d^2k or $dk_x dk_y$ in $\vec{k}$-space?

$$\#\text{ allowed } \vec{k}\text{-values} = \frac{d^2k}{\left(\frac{\pi}{L}\right)^2} = \underbrace{\left(\frac{L}{\pi}\right)^2}\, d^2k = \left(\frac{L}{\pi}\right)^2 dk_x dk_y$$

[Note: L^2 = Area A of system]

2D Density of states in k-space

2D:

$$\sum_{\substack{\text{single-particle}\\ \text{states}}} F = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty} F \to \left(\frac{L}{\pi}\right)^2 \int_0^\infty dk_x \int_0^\infty dk_y\, F(k_x,k_y) \quad \text{(2D)}$$

$$= \left(\frac{L}{\pi}\right)^2 \int \frac{d^2k}{4}\, F(\vec{k}) \qquad \underbrace{\int d^2k\,(\dots)}_{\text{over full } \vec{k}\text{-space}}$$

(which can be carried out in any convenient coordinates)

- "$\frac{1}{4}$": since $\int_0^\infty dk_x \int_0^\infty dk_y$ only over 1st quadrant
- assumes $F(\vec{k}) = F(|\vec{k}|)$, which is often the case.

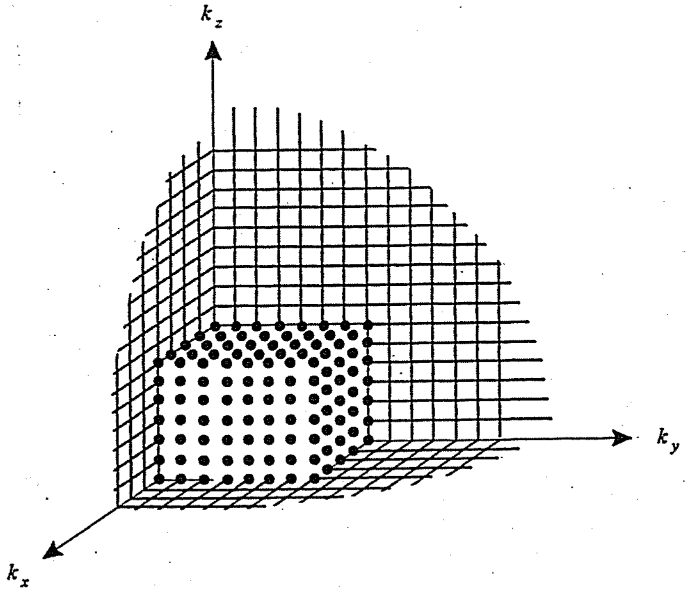
(c) 3D big box (usual case for gases)

- The translational motion is characterized by†

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{V}}\, \sin\Big(\underbrace{\frac{n_x\pi}{L}}_{k_x}x\Big)\, \sin\Big(\underbrace{\frac{n_y\pi}{L}}_{k_y}y\Big)\, \sin\Big(\underbrace{\frac{n_z\pi}{L}}_{k_z}z\Big)$$

$$\epsilon(\vec{k}) = \epsilon(k_x,k_y,k_z) = \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2+n_y^2+n_z^2\right)$$

$$n_x = 1,2,3,\dots;\quad n_y = 1,2,3,\dots;\quad n_z = 1,2,3,\dots$$



- Allowed $\vec{k}$-values form a regular array in $\vec{k}$-space

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† Actually, we should use travelling wave solutions plus periodic B.C.. But the resulting DOS $g(E)$ turns out to be the same.

- Each allowed $\vec{k}$-value occupies $\left(\frac{\pi}{L}\right)^3$ of $\vec{k}$-space [Key result]
- How many allowed $\vec{k}$-values are there in a "volume element" d^3k or $dk_x\,dk_y\,dk_z$ in $\vec{k}$-space?

$$\#\text{ allowed } \vec{k}\text{-values} = \frac{d^3k}{\left(\frac{\pi}{L}\right)^3} = \left(\frac{L}{\pi}\right)^3 d^3k$$

$$= \frac{V}{\pi^3}\,d^3k = \underbrace{\frac{V}{\pi^3}}\,dk_x\,dk_y\,dk_z \qquad (3D)$$

3D Density of states in $\vec{k}$-space

3D:

$$\sum_{\substack{\text{single-particle}\\ \text{states}}} F = \sum_{n_x=1}^{\infty}\sum_{n_z=1}^{\infty}\sum_{n_y=1}^{\infty} F \rightarrow \frac{V}{\pi^3}\int_0^{\infty} dk_x \int_0^{\infty} dk_y \int_0^{\infty} dk_z\, F(\vec{k})$$

$$= \frac{V}{\pi^3}\int \frac{d^3k}{8}\, F(\vec{k}) \qquad \left[\text{now over } \underline{\text{all}}\ \vec{k}\text{-space}\right]$$

- "$\frac{1}{8}$" since $\int_0^{\infty} dk_x \int_0^{\infty} dk_y \int_0^{\infty} dk_z$ over $\frac{1}{8}$ of whole $\vec{k}$-space
- assume the integrand depends only on $|\vec{k}|$. This is the case if $F(\vec{k})$ depends on $\vec{k}$ through the energy, i.e., $F(\vec{k}) = F(\epsilon(\vec{k}))$.

- Thus, including a spin-degeneracy factor G_s:

(assume $F(\vec{k}) = F(\epsilon(\vec{k}))$ and is spin-independent)

$$\sum_{\substack{\text{single-particle}\\ \text{states}}} F(\epsilon(\vec{k})) = \sum_{\substack{\text{spin}\\ \text{states}}} \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} F(\varepsilon(\vec{k}))$$

$\varepsilon(k)$ where $k = |\vec{k}|$

$$\rightarrow G_s \frac{V}{\pi^3} \int_0^{\infty} dk_x \int_0^{\infty} dk_y \int_0^{\infty} dk_z \, F(\underset{\underset{\varepsilon(k)}{\parallel}}{\varepsilon(\vec{k})})$$

$$= G_s \frac{V}{\pi^3} \int \frac{d^3k}{8} F(\varepsilon(k))$$

spherical coordinates

$$= G_s \frac{V}{(2\pi)^3} \int d^3k \, F(\varepsilon(k))$$

[see remark] ← important remark

$$= G_s \frac{V}{(2\pi)^3} \int_0^{k} 4\pi k^2 dk \, F(\varepsilon(k))$$

$$\boxed{\begin{array}{l} \therefore \text{ We have the result that (3D)} \\ \displaystyle\sum_{\substack{\text{single-particle}\\ \text{states}}} F(k) = \sum_{\substack{\text{spin}\\ \text{states}}} \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} F(k) = G_s \frac{V}{(2\pi)^3} \int_0^{\infty} 4\pi k^2 F(k) dk \end{array}}$$

This is the <u>main result</u>.

Remark: Although we obtain the result within the context of fitting solutions to the Schrödinger Eq. to the boundary conditions of an infinite well, the result is also valid for matching <u>other waves</u> in a cavity.

The same result is obtained by:

- How many states are there with wave number less than $k = |\vec{k}|$?

$$\frac{1}{8}\left(\frac{4\pi}{3}k^3\right) \cdot \frac{1}{\left(\frac{\pi}{L}\right)^3} = \frac{V}{6\pi^2} k^3$$

Up to a spin degeneracy factor

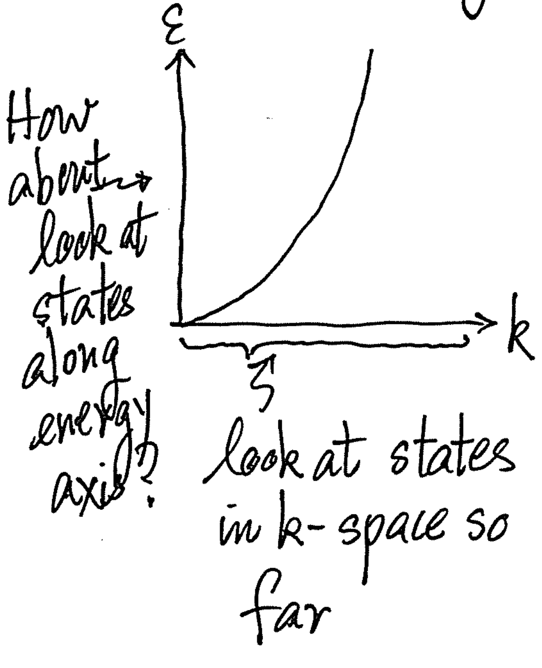
- How many states are there with wavenumber between k to $k+dk$?

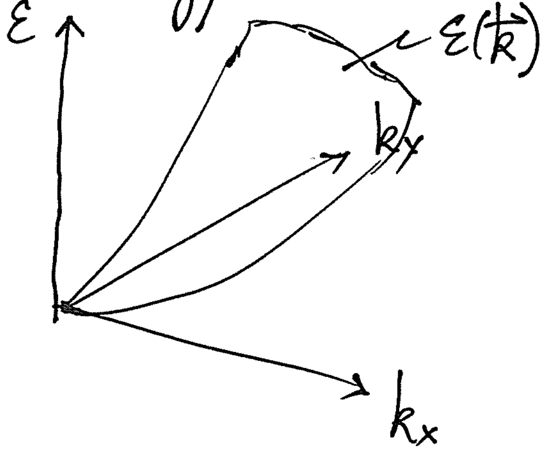
$$\frac{V}{6\pi^2}(k+dk)^3 - \frac{V}{6\pi^2}k^3 = \frac{V}{2\pi^2} k^2 dk$$

$$= \frac{V}{(2\pi)^2} \cdot 4\pi k^2 dk$$

Up to here, look at s.p. states in k-space.

How about going into the energy axis?





B. Density of states (DOS) in energy: $g(\epsilon)$

- Very often, the integrand involves the single-particle energy $F(\mathcal{E})$.

  $\therefore$ Want to turn $\int d^3k$ into $\int d\mathcal{E}$

- To do this, we need to know the relation between $\mathcal{E}$ and k, i.e., $\underbrace{\mathcal{E}(k)}$.

  This relation is generally called the dispersion relation[†].

- For particle-in-a-box, we have

$$\mathcal{E}(\vec{k}) = \mathcal{E}(k) = \frac{\hbar^2 k^2}{2m} \quad \text{(free particle)}$$

$$\Rightarrow k = \sqrt{\frac{2m}{\hbar^2}\mathcal{E}}$$

Also,

$$d\mathcal{E} = \frac{\hbar^2 k\,dk}{m}$$

$$k\,dk = \frac{m}{\hbar^2}\,d\mathcal{E}$$

$$\Rightarrow k^2 dk = \frac{m}{\hbar^2}\sqrt{\frac{2m}{\hbar^2}}\sqrt{\mathcal{E}}\,d\mathcal{E}$$

[†] For problems concerning other types of waves, $\omega(\vec{k})$ is the dispersion relation. E.g. for photons $\omega = ck$ or $\mathcal{E} = c\hbar k$

Thus, (apart from a spin-degeneracy factor G_s)

$$\frac{V}{(2\pi)^3}\int_0^\infty 4\pi k^2 dk\, F(\mathcal{E}(k)) = \frac{V}{(2\pi)^3}\int_0^\infty 4\pi \frac{m}{\hbar^2}\sqrt{\frac{2m}{\hbar^2}}\sqrt{\mathcal{E}}\,F(\mathcal{E})d\mathcal{E}$$

$$= \int_0^\infty \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\mathcal{E}}}\; F(\mathcal{E})\,d\mathcal{E}$$

$$= \int_0^\infty g(\mathcal{E})\; F(\mathcal{E})\,d\mathcal{E}$$

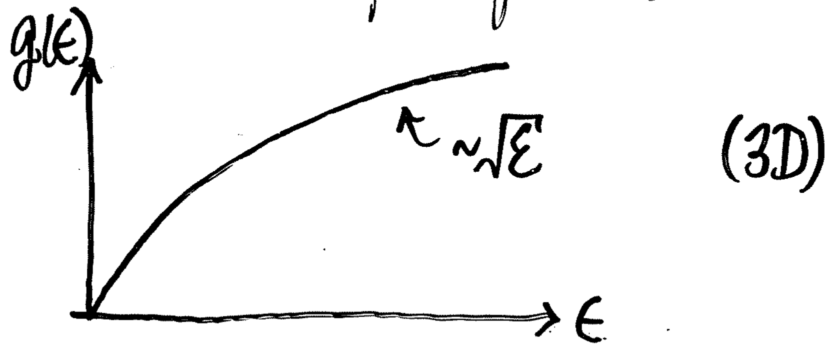
where

$$\boxed{g(\mathcal{E}) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\mathcal{E}} \;\propto\; \mathcal{E}^{1/2} \text{ is the 3D density of states in energy for free particles}}$$

Main result[†]

← apart from a factor G_s

(for electrons (spin-half), there is a factor of $G_s = 2$)



Q: How does $g(\epsilon)$ depend on ϵ in 2D, 1D?

[†] Remark: We obtained the result using standing waves. One can obtain the same result using traveling wave solutions and periodic boundary condition.

- For 3D spin-half particles, e.g. electrons

$$\boxed{g(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}}$$ (Important result)

- Here is another standard procedure to obtain $g(\varepsilon)$.

Let $\boxed{n(<\varepsilon) \equiv \#\text{ single-particle states with energy } \underline{\text{less than } \varepsilon}}$

$$n(<\varepsilon) = \underset{\substack{\uparrow\\ \text{spin}\\ 2=2s+1}}{2} \cdot \underbrace{\frac{V}{(2\pi)^3}}_{\substack{\uparrow\\ \text{DOS in}\\ \vec{k}\text{-space}}} \cdot \underbrace{\frac{4\pi}{3}\left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2}}_{\nwarrow \text{ volume of a sphere in k-space of radius } \left(\frac{2m\varepsilon}{\hbar^2}\right)^{1/2}}$$

Then,

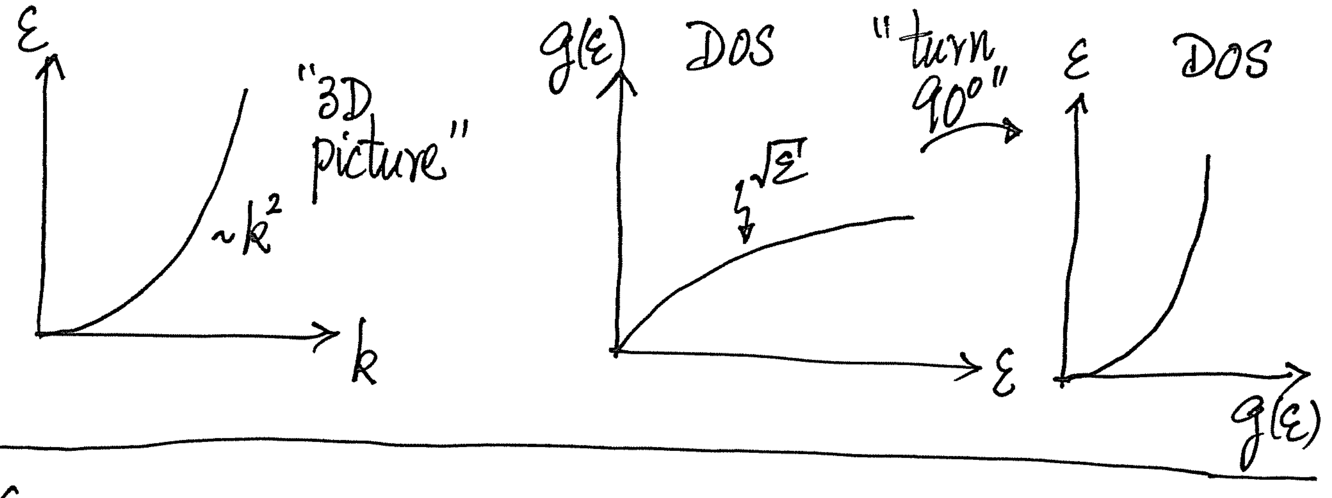
$$\boxed{g(\varepsilon) = \frac{dn(<\varepsilon)}{d\varepsilon}} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{1/2}$$ same result!

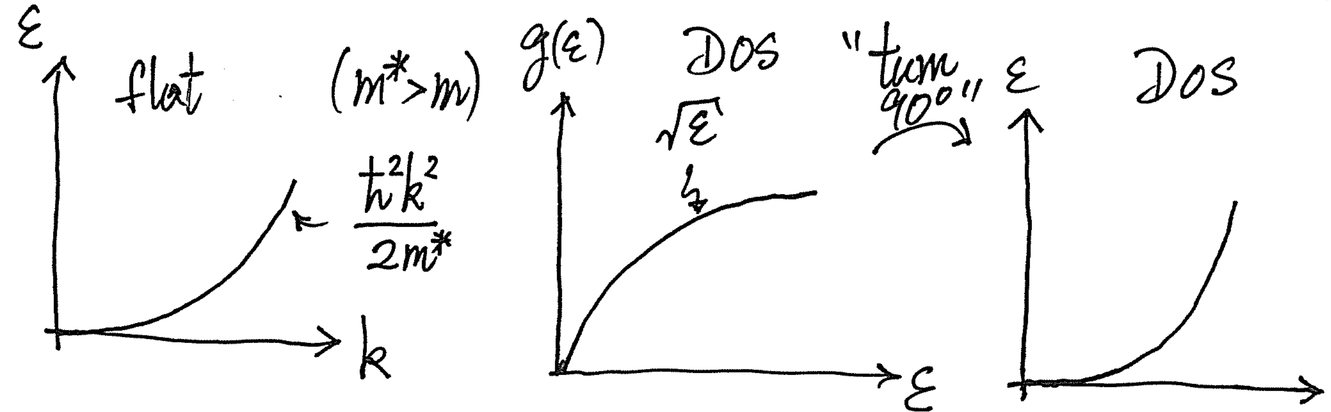
Things to remember...

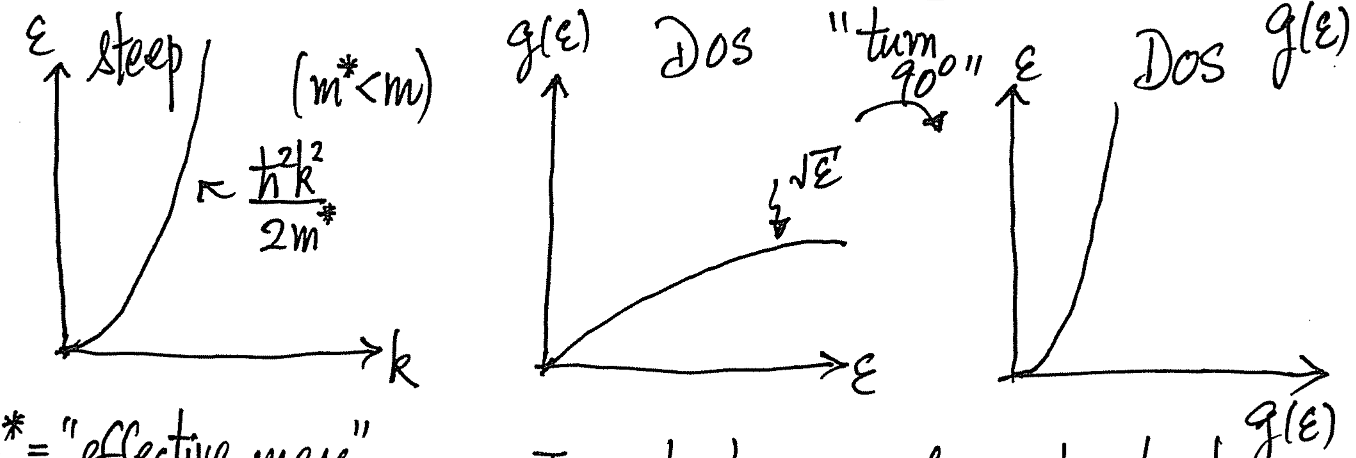
3D free-electron "band"

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$ (parabolic dispersion relation)

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







m^* = "effective mass"

Important sense for understanding semiconductor physics

C. Discussions

- As long as the particles are non-interacting, then we can talk about single-particle states and $g(\varepsilon)$. The method used here is applicable to other cases, i.e., when $\varepsilon(k)$ is not the free particle expression.
- With $g(\varepsilon)$ AND the distributions (FD, BE, MB), one can understand much physics of gases.

⌐ E.g., N free fermions ($s=\frac{1}{2}$) in volume V, system in equilibrium at temp. T

$$n_i = g_i f_{FD}$$

$$\sum_i n_i = N$$

$$N = \int_0^\infty 2\cdot g(\varepsilon)\, f_{FD}(\varepsilon)\, d\varepsilon$$

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

We will discuss the ideal fermi gas in a later chapter.

▪ this equation serves to fix μ (where μ is the chemical potential, but in our derivation it is a multipler for the constraint of a given N) for a given temp. T. ┘

E.g. Application to free-electron (Fermi) gas

$$N = \sum_{\text{cells } i} g_i f_{FD}(\varepsilon_i) = \sum_{\substack{\text{all s.p.}\\ \text{states } i}} \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1} \qquad ①$$

$$E = \sum_{\text{cells } i} \varepsilon_i g_i f_{FD}(\varepsilon_i) = \sum_{\substack{\text{all s.p.}\\ \text{states } i}} \frac{\varepsilon_i}{e^{\beta(\varepsilon_i-\mu)}+1} \qquad ②$$

Invoking $g(\varepsilon)$, a 3D free-electron gas is governed by

$$N = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\frac{(\varepsilon-\mu)}{kT}}+1}\, d\varepsilon \qquad (1')$$

[This determines $\mu(T)$]

$$E = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{e^{\frac{(\varepsilon-\mu)}{kT}}+1}\, d\varepsilon \qquad (2')$$

[With $\mu(T)$ from (1'), this gives $E(T)$ and other quantities, e.g. $C(T)$, follow.]

▪ Eqs. ① & ② are generally for any dimension

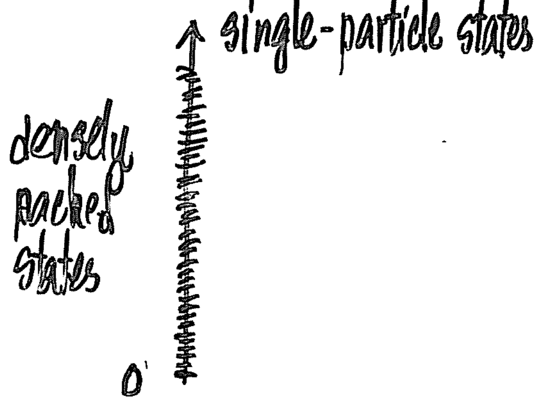
▪ Eqs. (1') & (2') are valid for $\underbrace{\text{3D}}$ particles with $\underbrace{\varepsilon = \frac{\hbar^2 k^2}{2m}}$.

← two conditions →

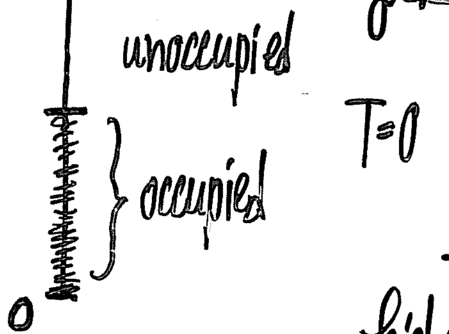
A word of warning - and interesting physics follows...

$$(*) \qquad N = V\mathcal{A}\int_0^\infty \sqrt{\varepsilon}\,\frac{1}{e^{\beta(\varepsilon-\mu)}\pm 1}\,d\varepsilon \qquad \text{fixes } \mu(T,V,N)$$

Note: Consider of integral near the lower bound $\int_0^\delta d\varepsilon$, $(\delta \approx 0)$ as a factor $\sqrt{\varepsilon}$ is in the integrand, the contribution to the whole integral for small ε is small.



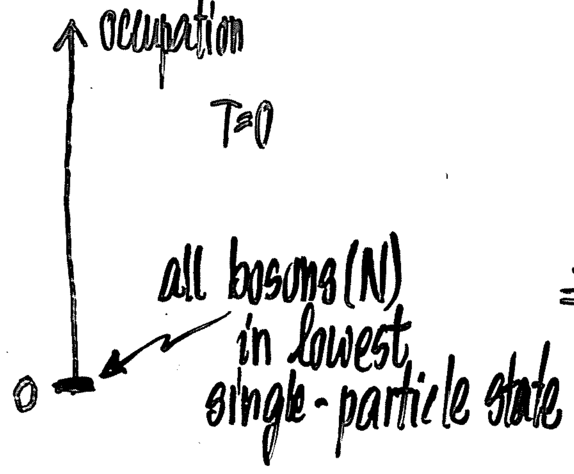
N non-interacting fermions (filling the states)



Due to Pauli Exclusion Principle, fermions have to fill up higher energy states

⇒ physics at $T \approx 0$ is NOT dominated by single-particle states of $\varepsilon \approx 0$
⇒ (*) OK

N-nonintering bosons



⇒ We need to be more careful about the occupation in the lowest ($\varepsilon = 0$) single-particle state
⇒ using (*) with care

[The physics that follows is the Bose-Einstein condensation]

Summary

Students should be able to:

- identify when one can consider single-particle states
- go from a discrete description to a continuum description
- state what $g(\varepsilon)\,d\varepsilon$ means
- argue how the allowed $\vec{k}$-values distribute in $\vec{k}$-space
- derive $g(\varepsilon)$ for given $\varepsilon(k)$ (and $\omega(k)$ for other waves)
- turn summation over states into integral over single-particle energies

Refs:

- Bowley/Sanchez: Sec. 5.8-5.9, Sec. 7.1-7.3
- Mandl: Appendix B
- Rosser: Appendix 3

Appendix : Periodic Boundary Condition

- We obtained

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

for 3D non-relativistic free particles (i.e. $\varepsilon = \frac{\hbar^2 k^2}{2m}$) based on particle-in-a-box solutions.

walls of box enforce $\psi = 0$ at walls (Standing Waves)

- In solid state physics, the preference is to use traveling waves (as you know electrons move around and conduct in metals).
- This appendix shows that imposing the periodic boundary condition (hence traveling waves) gives the same $g(\varepsilon)$.

Appendix : Periodic Boundary Condition

- The main result in Section A is

$$\sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty}(\cdots) \rightarrow \frac{V}{8\pi^3}\int d^3k\,(\cdots) \qquad (A1)$$

This is obtained by considering standing waves. The boundary condition is that the waves vanish at the walls of a box or cavity.

- Another popular boundary condition is the periodic boundary condition. It is often used in solid state physics. The idea is to stack up systems of L × L × L (already macroscopic) to cover the whole 3D space and thus to mimic an infinite system.

The periodic boundary condition requires:

$$\begin{aligned} \psi(x,y,z) &= \psi(x+L,y,z) \\ \psi(x,y,z) &= \psi(x,y+L,z) \\ \psi(x,y,z) &= \psi(x,y,z+L) \end{aligned} \qquad (A2)$$

Taking the Schrödinger equation $-\frac{\hbar^2}{2m}\nabla^2\psi = \varepsilon\psi$ as an example, we have

$$\psi(x,y,z) = A\, e^{i(k_x x + k_y y + k_z z)} \equiv A\, e^{i\vec{k}\cdot\vec{x}} \qquad (A3)$$

Here $\vec{k} = (k_x, k_y, k_z)$, with

$$k_x = \frac{2\pi}{L} n_x \quad , \quad n_x = 0, \pm 1, \pm 2, \ldots$$

$$k_y = \frac{2\pi}{L} n_y \quad , \quad n_y = 0, \pm 1, \pm 2, \ldots \qquad (A4)$$

$$k_z = \frac{2\pi}{L} n_z \quad , \quad n_z = 0, \pm 1, \pm 2, \ldots$$

after imposing the periodic boundary condition.

Note that the solutions (A3) are now *traveling waves*, and n_x, n_y, n_z (and hence k_x, k_y, k_z) can take on positive and negative values.

The single-particle energy eigenvalues are:

$$\epsilon = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) . \qquad (A5)$$

- Looking at (A4), the allowed $\vec{k}$-values are *uniformly distributed* in $\vec{k}$-space and the whole $\vec{k}$-space is allowed.

  Each allowed $\vec{k}$-point occupies a volume of $\left(\frac{2\pi}{L}\right)^3$ of $\vec{k}$-space.

- The number of allowed $\vec{k}$-values with wavevectors $\vec{k}$ lying in a volume d^3k around $\vec{k}$ is:

$$\left(\frac{L}{2\pi}\right)^3 d^3k = \frac{V}{\underbrace{(2\pi)^3}_{\text{density of states in } \vec{k}\text{-space}}} d^3k \qquad (A6)$$

Hence,

$$\underbrace{\sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty}}_{\text{sum over all single-particle states}} (\cdots) = \frac{V}{(2\pi)^3}\underbrace{\int}_{\text{over all } \vec{k}\text{-space}} d^3k \, (\cdots) \qquad (A7)$$

(apart from a spin-degeneracy factor g_s)

This is the same as Eq. (A1).

Remark:

It is good to see that the same final result emerges from different boundary conditions. For *macroscopic systems* that statistical mechanics deals with, it is the bulk properties that matter, but not the surface properties.