

FINAL REVIEW

QUANTUM STATISTICAL MECHANICS

Let us consider a system of many particles, each of which could have energy E_s (s indicates the energy level, each of which has degeneracy g_s).

Let us also assume that the system has total energy E , and a total number of particles N . Then, the average number of particles in each state, with energy E_s is:

$$P_s = \frac{m_s}{g_s} \left\{ \begin{array}{l} \leftarrow \text{\# particles with} \\ \text{energy } E_s \\ \leftarrow \text{degeneracy of} \\ \text{energy level } s \end{array} \right. = e^{-\frac{(E_s - \mu)}{k_B T}} \quad \begin{array}{l} \text{MAXWELL-BOLTZMANN} \\ \text{DISTINGUISHABLE PARTICLES} \end{array}$$
$$= \frac{1}{e^{\frac{(E_s - \mu)}{k_B T}} - 1} \quad \begin{array}{l} \text{BOSE-EINSTEIN} \\ \text{IDENTICAL BOSONS} \end{array}$$
$$= \frac{1}{e^{\frac{(E_s - \mu)}{k_B T}} + 1} \quad \begin{array}{l} \text{FERMI-DIRAC} \\ \text{IDENTICAL FERMIONS} \end{array}$$

μ = chemical potential; it is a function of T

Typical constraints:

$$N = \sum_s m_s$$

$$E = \sum_s E_s \cdot m_s$$

In some of our problems, we remove the first constraint ($N = \sum m_s$) and thus obtain that $\mu(T) = 0$. Also, our concern becomes finding what g_s is, for the system at hand. Here are some examples:

- 1) 3D photons in a box: in the k -space, each state occupies a volume $\frac{\pi^3}{V}$. An octant shell at radius K occupies the volume $\frac{1}{8} 4\pi K^2 dK$.

Since the energy of a single photon is $\hbar c K$, that shell is the locus

of all states with the same energy. Hence, its volume divided by the volume of a single state gives the degeneracy of the energy state with energy $\hbar\omega$
 (note: we assume V large enough that the states become dense in the k -space, and I can replace the discrete E_s with the continuous $E_k = \hbar\omega(k)$).

Finally:

$$g_s \xrightarrow{\substack{\text{discrete} \\ \downarrow}} \xrightarrow{\substack{\text{continuous} \\ \downarrow}} g(k)dk = \frac{1}{8} \frac{4\pi k^2 dk}{\pi^3/V} \cdot \underset{\substack{\text{POLARIZATION of photons} \\ \downarrow}}{2} = \frac{V k^2}{\pi^2} dk$$

what is the probability of having a photon with energy E_k ? Bosons \rightarrow B-E:

$$p(E_k) = g(k) \cdot \frac{1}{e^{E_k/k_B T} - 1}$$

\leftarrow from here we can work in terms of $\omega = ck$
 (remember the piece $g(\omega)d\omega = g(k)dk \Rightarrow$ need a factor $c : \frac{d\omega}{dk} = c$)

not really a probability but proportional to

2) 3D phonons in a crystal: again, we move to k -space:

$$g(k)dk = \underbrace{\frac{1}{8} 4\pi k^2 dk}_{\text{shell volume}} \cdot \underbrace{\frac{1}{\pi^3/V}}_{\substack{\downarrow \\ \text{volume of} \\ \text{1 state}}} \cdot \underbrace{3}_{\substack{\uparrow \\ \text{POLARIZATIONS of} \\ \text{phonons}}}$$

this time, there is a max value of k that can be achieved.

$$g(k)dk = g(\omega)d\omega \Rightarrow g(\omega) = g(k(\omega)) \frac{dk}{d\omega} = \frac{3}{2} V \frac{\omega^2}{\pi^2 v^3}$$

(dispersion relation: $\omega = v \cdot k$)

$$U = \text{total energy in phonons} = \int_0^{\omega_{\max}} g(\omega) \cdot \frac{1}{e^{\hbar\omega/k_B T} - 1} \cdot \hbar\omega d\omega$$

\uparrow density of states
 \uparrow B-E probability distribution
 \uparrow energy of 1 state

Since there exists a ω_{\max} , I have a finite number of possible states. Let us call this $3N$ (not to be confused with a number of phonons: since we set $\mu=0$, the number of phonons is not constrained).

$$3N = \int_0^{W_{max}} g(W) dW : \text{provides relation between } W, W_{max}, N.$$

3) 3D Fermi gas of electrons: \rightarrow in this case, $\mu \neq 0$: the number of electrons is fixed, while photons and phonons can be created and destroyed

$$g(k) dk = \frac{1}{8} 4\pi k^2 dk \cdot \frac{1}{\pi^3/V} \cdot 2$$

$T=0$
 all electrons occupy, in ground state, the lowest possible energies, but cannot use same state twice. In k-space, they occupy an octant of radius E_F

$$N = \text{number of electrons} = \int_0^{k_F} g(k) \cdot \frac{1}{e^{(E_k - \mu)/k_B T} + 1} dk$$

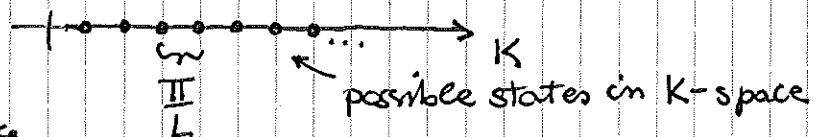
$$E_F = \frac{\hbar^2 k_F^2}{2m} \quad \text{Fermi energy}$$

$$E = \text{total energy} = \int_0^{k_F} g(k) \cdot \frac{1}{e^{(E_k - \mu)/k_B T} + 1} \cdot \frac{\hbar^2 k^2}{2m} dk$$

Equations for N and E allow me to find formulae for k_F and $\mu(T)$ as a function of n (= density of electrons, N/V), T and E .

Interesting note: $\mu(0) = E_F$ (yes, it's OK)
 ($\phi(E) = 0$ if $E > E_F$, and $= 1$ if $E < E_F$, when $T=0$, hence $\mu(0) = E_F$)

4) 1D Fermi gas of electrons:



$$g(k) dk = 2 \frac{dk}{\pi/L}$$

\uparrow spin-up or spin-downs
 \leftarrow infinitesimal length in k-space
 \leftarrow 1D volume occupied by one state

T=0 CASE:

$$N = \text{number of electrons on wire} = \frac{2L}{\pi} \cdot k_F = \int_0^{k_F} \frac{2L}{\pi} dk$$

$$k_F = \frac{\pi n}{2} \quad \text{linear density of electrons}$$

$$E_F = \text{Fermi energy} = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{8m}$$

linear density of electrons, do not confuse with particles in quantum well...

WKB APPROXIMATION

The really fast summary of WKB techniques:

1) $E > V(x)$:

$$\psi(x) \approx \frac{C_+}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int^x p(x') dx'} + \frac{C_-}{\sqrt{p(x)}} e^{-\frac{i}{\hbar} \int^x p(x') dx'}$$

$$\approx \frac{1}{\sqrt{p(x)}} \left\{ C_s \sin\left(\frac{1}{\hbar} \int^x p(x') dx'\right) + C_c \cos\left(\frac{1}{\hbar} \int^x p(x') dx'\right) \right\}$$

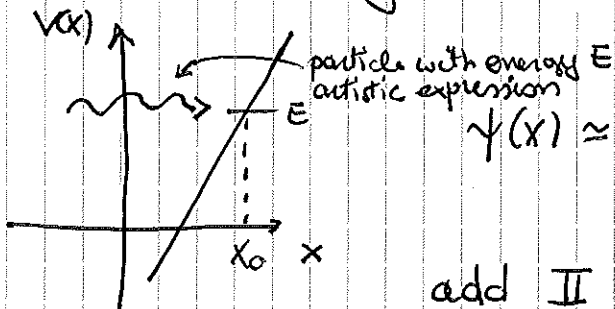
where $p(x) = \sqrt{2m(E - V(x))}$

2) $E < V(x)$:

$$\psi(x) \approx \frac{C_+}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar} \int^x |p(x')| dx'} + \frac{C_-}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar} \int^x |p(x')| dx'}$$

note: $|p(x)|$
 ↙ ↘
 modulus

3) connection formulae:

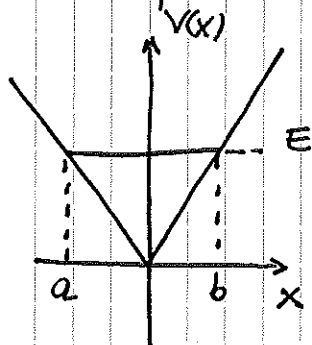


classical turning point

$$\psi(x) \approx \frac{1}{\sqrt{p(x)}} C_s \sin\left(\frac{1}{\hbar} \int_x^{x_0} p(x') dx' + \frac{\pi}{4}\right)$$

add $\frac{\pi}{4}$ for each soft wall (soft wall: $\frac{dV}{dx} \neq \infty$)

Example:

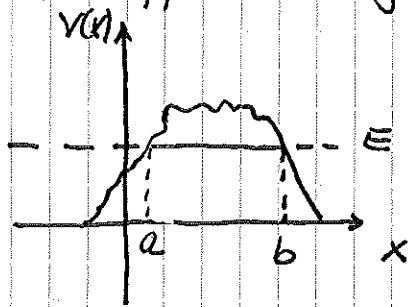


quantization condition:

$$\frac{1}{\hbar} \int_a^b \sqrt{2m(E - V(x))} dx + 2 \cdot \frac{\pi}{4} = n \cdot \pi$$

↑
two soft walls

4) Approximate formula for tunnelling



$$T = \text{tunnelling probability} = e^{-2\gamma}$$

$$\gamma = \frac{1}{\hbar} \int_a^b \sqrt{2m(E - V(x))} dx$$

← $E < V(x)$: need modulus

"lifetime formula":

$$\tau = \frac{2\pi}{v} e^{2\gamma}$$

where π is some scale of distance relevant in the problem (e.g., the nucleus radius in the Gamow's model of α decays) and v is some velocity scale relevant in the problem (e.g., $v = \sqrt{\frac{\hbar^2 T}{m}}$, if we are considering our particle as moving due to thermal motion)

NOTE: WKB works in semi-classical limit: wavelength associated with state with energy E is much smaller than the scale over which the potential $V(x)$ varies.

THE VARIATIONAL PRINCIPLE

$$E_{\text{ground state}} \leq \langle \psi | H | \psi \rangle \quad \forall \psi$$

one can obtain a better estimate of $E_{\text{ground state}}$ by making ψ a function of some parameter λ_i , then minimize $\langle \psi | H | \psi \rangle$ as a function of λ_i :

$$\frac{\partial \langle H \rangle}{\partial \lambda_i} = 0 \quad \text{for some } \tilde{\lambda}_i, \text{ then calculate } \langle H(\tilde{\lambda}_i) \rangle$$

IMPORTANT: $\psi(\lambda_i)$ must be normalized: $\langle \psi(\lambda_i) | \psi(\lambda_i) \rangle = 1$. The normalization coefficient may depend on λ_i !