

H1

# PH107 Formulas - Endsem

H6

*Joyfully crafted by Jujhaar Singh :)*

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Planck's Law

LM-3: Compton Effect

LM-4: Heat Capacity and Quantum Theory

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H2

## LM-2: Black Body Radiation

H3 Rayleigh-Jean's Law

$$U(\nu)d\nu = \frac{8\pi\nu^2}{c^3} k_B T d\nu$$

H3 Planck's Law

$$U(\nu)d\nu = \frac{8\pi\nu^2}{c^3} \cdot \frac{h\nu}{e^{h\nu/k_B T} - 1} d\nu = \frac{8\pi\nu^2}{c^3} k_B T \cdot \frac{h\nu/k_B T}{e^{h\nu/k_B T} - 1} d\nu$$

$$QC = \frac{h\nu/k_B T}{e^{h\nu/k_B T} - 1}, \text{ and thus we obtain:}$$

$$U(\nu)d\nu = \frac{8\pi\nu^2}{c^3} k_B T d\nu \cdot QC(\text{quantum correction})$$

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## LM-3: Compton Effect

$$\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos \theta)$$

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## LM-4: Heat Capacity and Quantum Theory

H3 Heat Capacity of Gases

$$c_v = \frac{f}{2} R$$

Where  $f$  is the number of degrees of freedom of the molecules of the gas

Energy available per molecule at room temperature is given by

$$E/\text{molecule} \approx 25\text{meV}$$

H3 Dulong-Petit's Law: Classical Theory for heat capacity of solids

for a single atom moving in one direction  $\langle E \rangle = k_B T$

for a single atom moving in all 3 directions  $\langle E \rangle = 3k_B T$

$$E = 3Nk_B T = 3RT$$

$$c_v = \frac{dE}{dT} = 3R$$

### H3 Einstein's Quantum Mechanical Theory for heat capacity of Solids

$$E_n = \left( n + \frac{1}{2} \right) \cdot h\nu_E$$

for one direction:

$$E = \frac{h\nu}{e^{h\nu/k_B T} - 1}$$

and for that same atom oscillating in all 3 directions, we have:

$$E = \frac{3h\nu}{e^{h\nu/k_B T} - 1}$$

$$E = N \cdot \frac{3h\nu}{e^{h\nu/k_B T} - 1} = 3Nk_B T \cdot \frac{h\nu/k_B T}{e^{h\nu/k_B T} - 1} = 3RT \cdot \frac{h\nu/k_B T}{e^{h\nu/k_B T} - 1}$$

We define  $\theta_E = h\nu/k_B$  as the Einstein temperature of the solid and thus get

$$E = 3RT \cdot \frac{\theta_E/T}{e^{\theta_E/T} - 1}$$

In all the equations stated above,  $\nu = \nu_E$ , which is known as the Einstein frequency of the solid.

### H3 Debye Model

A few new assumptions made by Debye

$$\nu_{max} = \nu_D$$

$$\lambda_{min} = \lambda_D$$

$$\lambda_D = 2d \text{ where } d \text{ is distance between atoms}$$

At low temperatures

$$c_v \propto T^3$$

## H2 LM-5: Wave Particle duality and de Broglie's hypothesis

### H3 de Broglie Hypothesis

$$\lambda_D = \frac{h}{p}$$

### H3 Bragg's Law

$$(\text{path difference})\Delta\lambda = 2d \sin \theta$$

Where  $\theta$  is the angle of the incident rays with the surface of the lattice.

### H3 Davisson-Germer Experiment

We generally look at only first order phenomena, ie  $\Delta\lambda = \lambda$ , and find that for the angle b/w the electron gun and detector being  $\phi$  and applying Bragg's Law, we get

$$\lambda = 2d \sin \theta = 2d \cos \phi/2$$

## H2 LM-6: Wave Packets, Group Velocity and Phase Velocity

Here are some basic and useful formulas to keep in mind from here on

$$p = \hbar k = \frac{h}{\lambda}$$

$$\text{for particles: } E = \frac{p^2}{2m} = \frac{1}{2}mv^2$$

$$\text{for photons: } E = \hbar\omega = h\nu$$

### H3 Group and Phase Velocity

$$v_p = \frac{\omega}{k} = \nu\lambda$$

$$v_g = \frac{d\omega}{dk}$$

For photons, we also define

$$v_p = \frac{\omega}{k} = \frac{E}{p}$$

$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$$

### H3 Dispersive and non-dispersive mediums

Whenever  $v_g \neq v_p$  we say that the medium is dispersive:

- if  $v_p > v_g \implies$  *normal dispersion*
- if  $v_g > v_p \implies$  *anomalous dispersion*

When we have the condition  $v_p = v_g$  we say that medium is non dispersive.

## H2 LM-7: Fourier Transform and Heisenberg's Uncertainty Principle

### H3 Heisenberg's Uncertainty Principle

1. In terms of momentum and position

$$\Delta p_k \cdot \Delta k \geq \frac{\hbar}{2} \text{ where } k \in \{x, y, z\}$$

2. In terms of energy and time

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

## H2 LM-8: The Schrödinger Equation and its properties

### H3 Schrödinger Equation

- Time Dependent Schrödinger Equation(TDSE)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

- Time Independent Schrödinger Equation(TISE)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U\Psi = E\Psi$$

Normalisation of a wave function

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$$



### H3 Observables and Operators

Observable	Symbol	Operator
Position	$\hat{x}$	$x$
Momentum	$\hat{p}$	$-i\hbar \frac{\partial}{\partial x}$
Potential Energy	$\hat{U}$	$U(x)$
Kinetic Energy	$\hat{K}$	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
Total Energy	$\hat{E}$	$i\hbar \frac{\partial}{\partial t}$

For a normalised wave function:

$$\langle o \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{O} \Psi dx$$
$$\langle o^2 \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{O}^2 \Psi dx$$

### H3 Eigen functions and values

$$\hat{O}\Psi = e\Psi$$

- $\Psi$  is an Eigen function of the operator  $\hat{O}$
- $e$  is the Eigen value

## H2

### LM-9: Free Particle

We take the potential to be 0 and the energy of the particle to be some value  $E$ .

Now, we can solve the Schrodinger equation in the following way:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

Solving this, we get simply,

$$\Psi = A \sin kx + B \cos kx$$

H2

## LM-10: Particle in a Box

### H3 The equation

The form of the potential energy for a particle in a box is

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{else} \end{cases}$$

The Schrodinger equation for a particle in a box is as follows

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

**Solutions:**

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$
$$k = \frac{n\pi}{L} = \frac{\sqrt{2mE_n}}{\hbar}$$
$$n = 1, 2, 3, \dots$$

Expression for **energy**:

$$E_n = \frac{\hbar^2 k^2}{2m} = n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 \frac{h^2}{8mL^2}$$

The minimum energy which the system has in its ground state is called the **Zero Point Energy**.

### H3 Orthonormality

Whenever  $n \neq m$ :

$$\langle \Psi_m | \Psi_n \rangle = 0$$

### H3 Adding time dependence

The time dependent solution of the above general equation can be found by multiplying a factor of  $\exp(-iE_n t/\hbar)$

$$\Psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \exp(-iE_n t/\hbar)$$

To find  $E_n$  the formula mentioned before can be used.

### H3 Probability of observing a particular wave function on measurement

The probability is proportional to the square of its coefficient

$$P(n) = |c_n|^2$$

### H3 Finding the coefficient of a particular state in an arbitrary solution

- Take the function  $\Psi$  at  $t = 0$
- Now take the conjugate of the function  $\Psi_n(x)$ , which will be  $\Psi_n^*$
- Now simply find the following integral (assuming normalization)

$$C_n = \langle \Psi_n(x) | \Psi(x, 0) \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x) \Psi(x, 0) dx$$

### H3 Finding Energy of the general solution

$$\langle \hat{H} \rangle = \sum_{i=1}^n c_i^2 E_i$$

## H2 LM-11: Particle in Finite Potential Box

In this case we consider the potential to look like:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ V_0 & \text{else} \end{cases}$$

### H3 Solutions of TISE for regions of constant potential

If  $E < V_0$

$$\Psi = A \exp(\alpha x) + B \exp(-\alpha x)$$
$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

If  $E > V_0$

$$\Psi = A \exp(ikx) + B \exp(-ikx) = A' \sin kx + B' \cos kx$$
$$k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

### H3 Solution of TISE for Particle in a finite box

$\Psi_1, \Psi_2, \Psi_3$  correspond to the regions  $(-\infty, 0), (0, L)$  and  $(L, \infty)$  respectively.

We are considering  $E < V_0$ .

$$\Psi_1 = A \exp(\alpha x) + B \exp(-\alpha x)$$

$$\Psi_2 = C \sin kx + D \cos kx$$

$$\Psi_3 = G \exp(\alpha x) + H \exp(-\alpha x)$$

The boundary conditions:

$$\Psi_1(0) = \Psi_2(0)$$

$$\Psi_3(0) = \Psi_2(0)$$

$$\Psi_1'(0) = \Psi_2'(0)$$

$$\Psi_3'(0) = \Psi_2'(0)$$

$$\Psi_1(-\infty) = 0$$

$$\Psi_3(\infty) = 0$$

Some direct simplifications we get by the last two conditions are:  $B = 0$  and  $G = 0$

### H3 Energy states for particle in a finite potential box

We won't really be finding the coefficients from the above equations, but rather a relation between the coefficients to get us a way to relate to the total energy of a stationary state.

First note that:

Define  $k_0^2 := \frac{2mV_0}{\hbar^2}$ , then,

$$\alpha^2 = k_0^2 - k^2$$

$$\implies \frac{\alpha}{k} = \sqrt{\frac{k_0^2}{k^2} - 1}$$

$$\text{and } \frac{k_0^2}{k^2} = \frac{V_0}{E}$$

$$\implies \frac{\alpha}{k} = f'(E) = \sqrt{\frac{V_0}{E} - 1}$$

$$= f(k) = \sqrt{\frac{(k_0 L/2)^2}{(kL/2)^2} - 1}$$

Now, also notice that by solving the equations in the previous section, we can obtain the following equation:

$$\frac{\alpha \cos kL - k \sin kL}{\alpha \sin kL + k \cos kL} = -\frac{\alpha}{k}$$

$$\frac{\alpha/k - \tan kL}{1 + \alpha/k \tan kL} = -\frac{\alpha}{k}$$

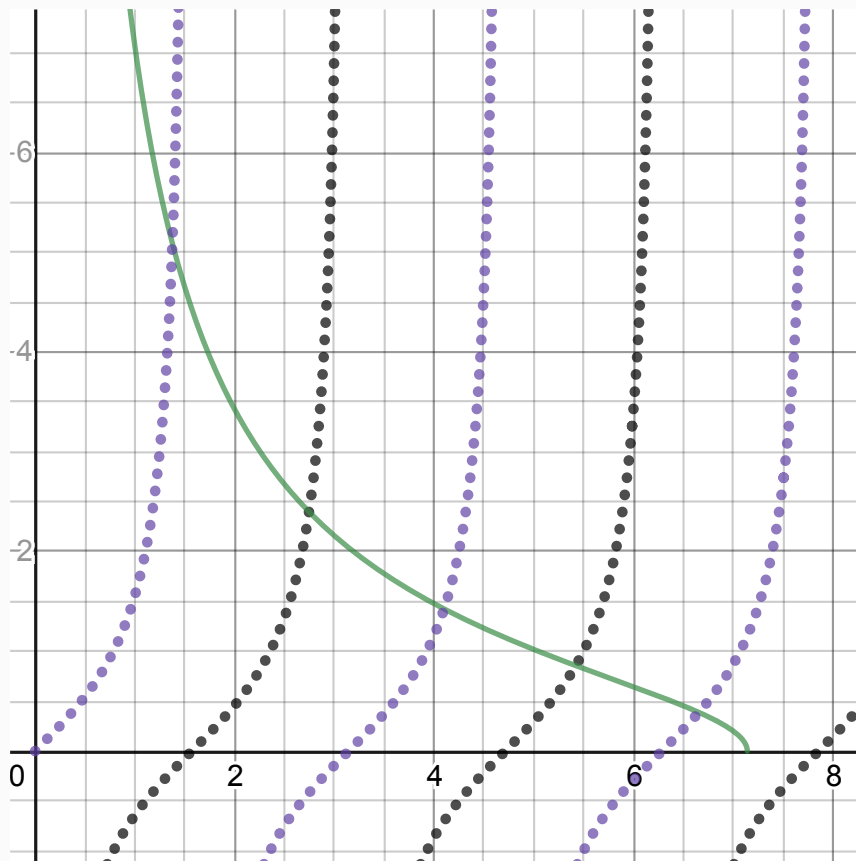
Solving the above equation, we can obtain:

$$\tan kL/2 = \alpha/k$$

OR

$$-\cot kL/2 = \alpha/k$$

Now using the above equation, we can solve for values of energy graphically. We will plot the graph taking  $kL/2$  on the x axis and the value of each of the RHS and LHS functions on the y axis. The intersections of the graphs will give us the solutions.



Each purple line(graph of  $\tan x$ ) in the above graph meets the x axis at  $x = n\pi$  and each of the black lines(graph of  $-\cot x$ ) meets the x axis at  $x = (2n + 1)\pi/2$  where  $n$  is an integer. The green line is the graph of the function  $f(k)$  as defined above.

### H3 Penetration length

$$\delta_n = \frac{1}{\alpha_n}$$

### H3 Approximation to infinite potential box

It can be approximated to an infinite potential box of length  $L + 2\delta_n$ . This approximation may be used to attain approximate values of energy.

## H2 LM-12: Step Potential, Scattering and Tunneling

### H3 Basic Step potential

The potential in this case is of the form

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

The solution to the TISE will look like

for  $E > V_0$

$$\Psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\Psi_2 = Ce^{ik_2x} + De^{-ik_2x}$$

for  $E < V_0$

$$\Psi_1 = Ae^{ikx} + Be^{-ikx}$$

$$\Psi_2 = De^{\alpha x} + Ce^{-\alpha x}$$

Where  $\alpha, k, k_1$  and  $k_2$  take their regular values based on the potential in their region and the total energy.

$\Psi_1$  and  $\Psi_2$  correspond to the first and second region respectively.

Consider the case  $E > V_0$ .

It is elementary to see that  $D = 0$ . The rest of the coefficients can be found by applying boundary conditions:

$$\Psi_1 = A \left[ e^{ik_1x} + \left( \frac{k_1 - k_2}{k_1 + k_2} \right) e^{-ik_1x} \right]$$
$$\Psi_2 = A \left[ \left( \frac{2k_1}{k_1 + k_2} \right) e^{ik_2x} \right]$$

### H4 Transmission and Reflection coefficients

Transmission and reflection coefficients add up to 1

$$T + R = 1$$

For the case where  $E > V_0$

$$R = \frac{k_1}{k_1} \left| \frac{B}{A} \right|^2 = \frac{k_1}{k_1} \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

$$T = \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2 = \frac{k_2}{k_1} \left| \frac{2k_1}{k_1 + k_2} \right|^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

For the case where  $E < V_0$

Now, we will simply replace  $k_1$  with  $k$  and  $k_2$  with  $i\alpha$ , giving us:

$$R = \frac{k}{k} \left| \frac{k - i\alpha}{k + i\alpha} \right|^2 = 1$$

#### H4 Penetration length

We define penetration length for the case where  $E < V_0$  as:

$$\delta = \frac{1}{\alpha}$$

### H3 Step potential of finite width and Tunneling

The potential is of the form

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < L \\ 0 & x > L \end{cases}$$

#### H4 Form of solutions

$$\Psi_1 = Ae^{ikx} + Be^{-ikx}$$

for  $E > V_0$

$$\Psi_2 = Ce^{ik'x} + De^{-ik'x}$$

for  $E < V_0$

$$\Psi_2 = De^{\alpha x} + Ce^{-\alpha x}$$

$$\Psi_3 = Fe^{ikx} + Ge^{-ikx}$$

Where  $\alpha$ ,  $k$  and  $k'$  take their regular values based on the potential in their region and the total energy.

Again, we get that  $G=0$ .

The rest of the coefficients can be found by applying the boundary conditions

#### H4 Reflection and Transmission coefficient

The reflection and transmission coefficients are defined as

$$R = \left| \frac{B}{A} \right|^2, T = \left| \frac{F}{A} \right|^2$$

We also have the relation:

$$T + R = 1$$

By solving for the coefficients, we arrive at the following formula for transmission coefficient

$$\begin{aligned} &\text{for } E < V_0 \\ &T = \left[ 1 + \frac{1}{4} \frac{V_0^2}{E(V_0 - E)} \sinh^2 \alpha L \right] \\ &\text{for } E > V_0 \\ &T = \left[ 1 + \frac{1}{4} \frac{V_0^2}{E(E - V_0)} \sin^2 k' L \right]^{-1} \end{aligned}$$

The maximum value ( $T_{max} = 1$ ) of T will be achieved when  $\sin k' L = 0$ , ie,  $k' L = n\pi$ . Only certain values of L will give this result. This effect is called **resonance**.

#### H4 Penetration length

We define penetration length for the case where  $E < V_0$  as:

$$\delta = \frac{1}{\alpha}$$

## H2 LM-14: Quantum Harmonic Oscillator

The potential function in the case of a QHO looks like

$$V(x) = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2$$

Ground state solution

$$\Psi(x) = Ae^{-Bx^2}$$

"A" can be found using the normalization condition, using which we get

$$A = \sqrt{B/\pi}^{1/4}$$

Higher solutions:



$n$	$E_n$	$\psi_n(x)$
0	$\frac{1}{2}\hbar\omega_0$	$\left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-\beta^2 x^2/2}$
1	$\frac{3}{2}\hbar\omega_0$	$\left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{2}} 2\beta x e^{-\beta^2 x^2/2}$
2	$\frac{5}{2}\hbar\omega_0$	$\left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{8}} (4\beta^2 x^2 - 2) e^{-\beta^2 x^2/2}$
3	$\frac{7}{2}\hbar\omega_0$	$\left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{48}} (8\beta^3 x^3 - 12\beta x) e^{-\beta^2 x^2/2}$
4	$\frac{9}{2}\hbar\omega_0$	$\left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{384}} (16\beta^4 x^4 - 48\beta^2 x^2 + 12) e^{-\beta^2 x^2/2}$

Energy values

$$E_n = \left(\frac{1}{2} + n\right) \hbar\omega$$

$$n = 0, 1, 2, \dots$$

## H2 LM-15: Application of Quantum Phenomena in higher dimensions

We simply assume the function to be a product of its "components"(not really) in the three directions

$$\Psi(x, y, z) = X(x)Y(y)Z(z)$$

Now, after putting this into the TISE, we can see that this can be treated independently in all three directions, the way we have been solving them in 1D.

Thus, each one of  $X, Y, Z$  is an independent solution of the 1D form and depends on a three independent parameters, say  $n_x, n_y, n_z$ .

$$E(n_x, n_y, n_z) = E_x(n_x) + E_y(n_y) + E_z(n_z)$$

## H2 LM-16: Fundamentals of Statistical Mechanics







### H3 Number of particles by energy

$$dN(E) = f(E)g(E)dE$$

is the number of particles between energies  $E$  and  $E + dE$ .

- $f(E)$  is called the **distribution function**
- $g(E)dE$  is called the **density of states**

### H3 Types of Particles

Property	Classical	Fermions	Bosons
Indistinguishable			
Follow Pauli's Exclusion Principle			
Spin	-	Half Integer	Integer
Wave function <sup>1</sup>	-	Anti-Symmetric	Symmetric

<sup>1</sup> The wave function row refers to symmetry of the wave function with respect to exchange of variables

## H2 LM-17: Density of States

In the quasi-continuous limit, we say that:

$$g_i \rightarrow g(E)dE$$

### H3 Density of states(in 3D) for particle in a box

$$g(\epsilon)d\epsilon = \frac{V}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\epsilon} d\epsilon$$

This expression is sometimes divided by volume to obtain density of states per unit volume.

In case of fermions, we must multiply by a "degeneracy factor", which is 2 for the case of electrons.

H2

## LM-18: Classical distribution function

### H3 The dominant configuration

The configuration that has the highest probability of occurring out of all the others is called the **dominant configuration** or **equilibrium configuration**.

The constraints within which we maximize are:

$$\begin{aligned}\sum N_i &= N \\ \sum N_i E_i &= E\end{aligned}$$

where  $N_i$  is the number of particles in states having energy  $E_i$

### H3 Maxwell-Boltzmann statistics

Number of micro-states for a configuration with  $N_i$  classical particles in a state of energy  $E_i$  with degeneracy of  $g_i$ :

$$\frac{N!}{\prod N_i!} \prod g_i^{N_i}$$

### H4 Discrete energy states

Where  $g_i$  is the degeneracy of the states with energy  $E_i$  and  $N_i$  is the total number of particles in all energy states with energy  $E_i$

$$N_i = g_i A \exp(-E_i/kT)$$

where  $A = \frac{N}{\sum g_i \exp(-E_i/kT)}$

This can also be expressed in the form of probability as:

$$P_i = \frac{N_i}{N}$$

### H4 Quasi-continuous energy states

$$f_{MB}(\epsilon) = A \exp(-\epsilon/kT)$$

where  $A = \frac{N}{\int g(\epsilon) \exp(-\epsilon/kT) d\epsilon}$

The value of A is calculated using the expression for total number of particles.

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## LM-19: Quantum Distribution functions

### H3 Bose-Einstein statistics

Number of micro-states for a configuration with  $N_i$  **bosons** in a state of energy  $E_i$  with degeneracy of  $g_i$ :

$$\prod \frac{(N_i + g_i - 1)!}{N_i!(g_i - 1)!}$$

We maximize the above expression to find the dominant state and arrive at the condition for the Bose-Einstein statistics to obtain:

$$N_i = \frac{g_i}{A \exp(E_i/kT) - 1}$$

In the quasi-continuous approximation, we get:

$$f_{BE}(\epsilon) = \frac{1}{A \exp(\epsilon/kT) - 1}$$

The value of A is calculated using the expression for total number of particles.

### H3 Fermi-Dirac statistics

Number of micro-states for a configuration with  $N_i$  **fermions** in a state of energy  $E_i$  with degeneracy of  $g_i$ :

$$\prod \frac{g_i!}{N_i!(g_i - N_i)!}$$

We maximize the above expression to find the dominant state and arrive at the condition for the Fermi-Dirac statistics to obtain:

$$N_i = \frac{g_i}{\exp((E_i - E_F)/kT) + 1}$$

In the quasi-continuous approximation, we get:

$$f_{FD}(\epsilon) = \frac{1}{\exp((\epsilon - \epsilon_f)/kT) + 1}$$

In this equation, the constant that should have been there, has been replaced by the term  $\epsilon_F$  or the **Fermi Energy**.

**NOTE:** At  $T = 0K$ , the Fermi-Dirac function becomes 1 at all values of  $\epsilon$  that are less than  $\epsilon_F$  and 0 for all values that are larger

## H2

# Some more topics

## H3 Relativistic effects

When to consider it:

- $v$  is close to  $c$
- Energy/Kinetic Energy of electron is comparable to or larger than rest energy of electron ( $m_e c^2 = 511 \text{keV}$ )

What are the effects of considering relativity:

- $E_{total} = \sqrt{m_0^2 c^4 + p^2 c^2}$ , this includes the rest mass energy
- $KE = E_{total} - m_0 c^2$ , where  $E_{rest} = m_0 c^2$
- Now you may not use  $KE = p^2 / 2m$  and should use only the above definition

## H3 Dirac notation

Not needed in the exam, but I have used it in this document, so here it is (there is more to it than this, but for us, this is enough):

$$\langle A|B \rangle = \int A^* B dx$$
$$\langle A|\hat{O}B \rangle = \langle A|\hat{O}|B \rangle = \int A^* \hat{O}B dx$$