# THERMAL & STATISTICAL PHYSICS
# SSP3133

# QUANTUM STATISTICS

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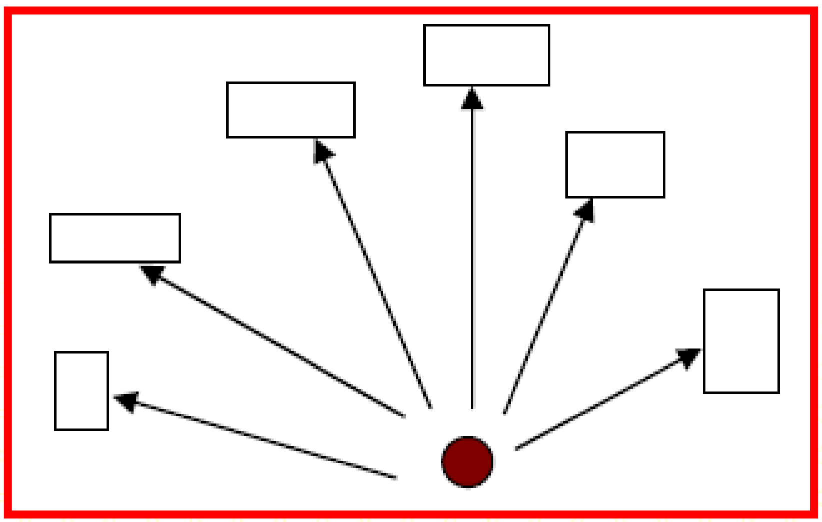
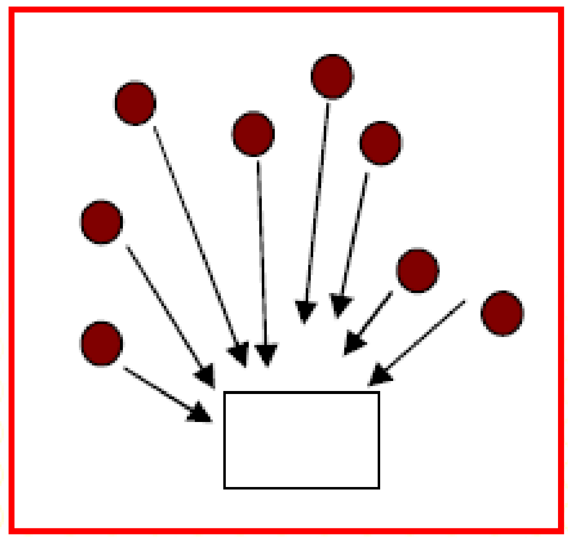
Acknowledgement : PROFESSOR DR RAMLI ABU HASSAN

# Classical & quantum statistics

<u>Classical statistics</u>: focus on individual paticle, which could occupy any of several possible quantum states

<u>Quantum statistics:</u> focus on individual quantum state, which could be occupied by various particles

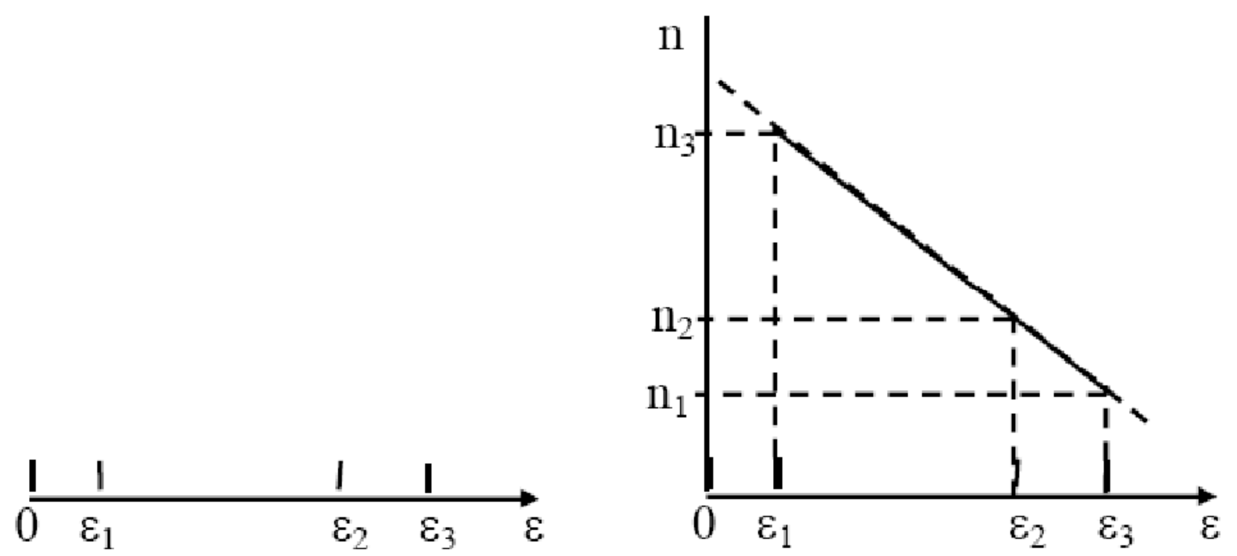




**Statistics of systems obeying quantum physics:** the statistical description of systems of particles that are subject to the laws of quantum physics rather than classical physics

Problems in QM

i. Finding the spectrum of the accessible states
ii. Finding the average number of particles occupying each state



# the occupation number: n

Note: consider the system to a certain quantum state s.

if $\varepsilon_s$ : the energy of single particle in this state

the probability that there are n particles in this state

Where

$$P_s = Ce^{-n\beta(\varepsilon_s - \mu)}$$

$$C = \left( \sum_n e^{-n\beta(\varepsilon_s - \mu)} \right)^{-1}$$

The average number of particles occupying the state

$$\bar{n} = \sum_n Pn = \left[\sum_n e^{-n\beta(\varepsilon_S - \mu)}\right]^{-1} \sum_n e^{-n\beta(\varepsilon_S - \mu)} n$$

let $x = \beta(\varepsilon_S - \mu)$

$$\bar{n} = \frac{\sum_n e^{-nx} n}{\sum_n e^{-nx}} = \frac{-\frac{\partial}{\partial x}\sum_n e^{-nx}}{\sum_n e^{-nx}} = -\frac{\partial}{\partial x}\ln\left(\sum_n e^{-nx}\right) \quad (*)$$

TWO types of particles:

# FERMIONS & BOSONS

FERMIONS: Only one particle may occupy a given state

BOSONS: no restriction on the number of particles that may occupy a given state

Note:

## 2 particles in 3 energy states

i) MB distribution – 9 possible configurations

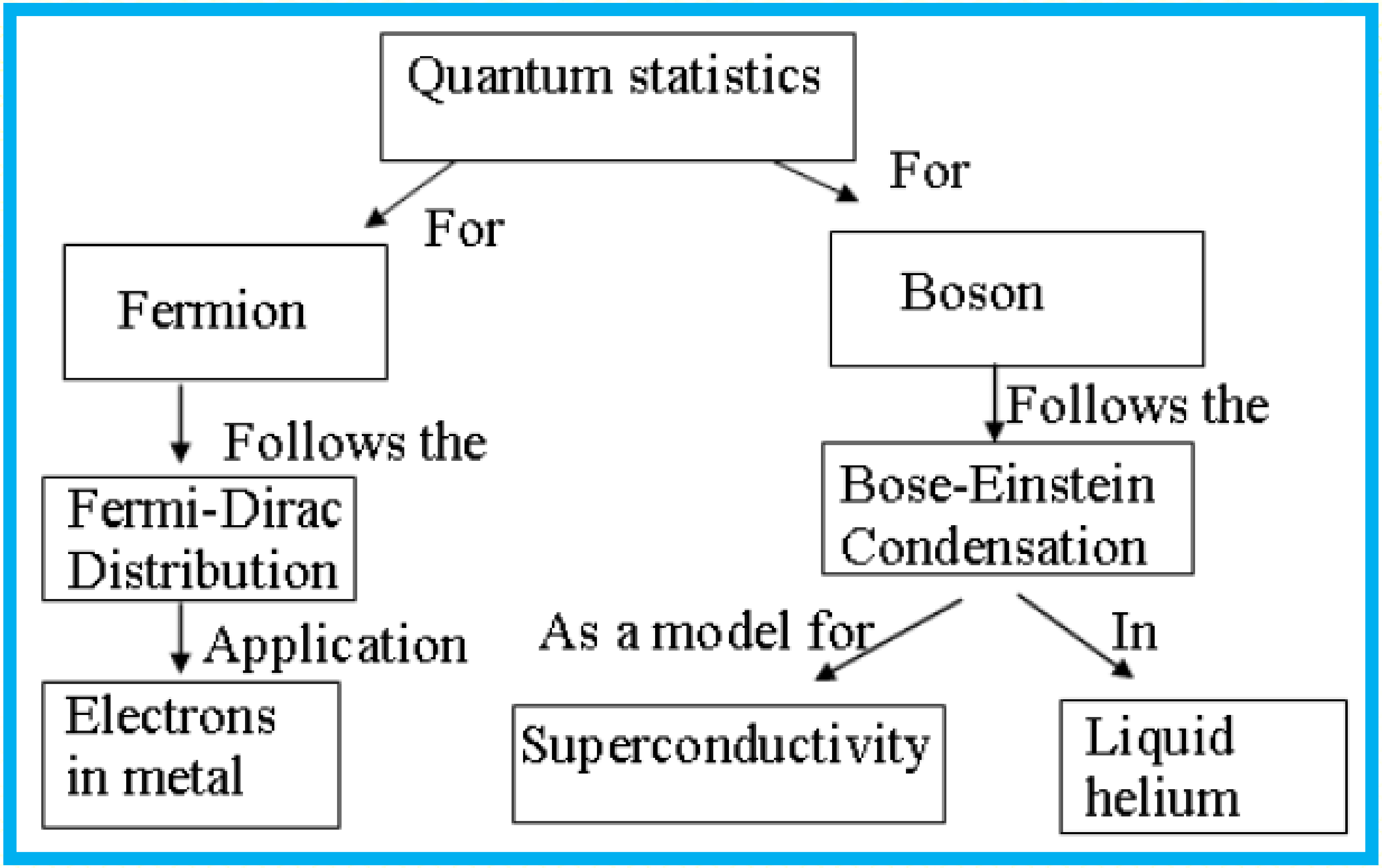
| Configuration | State 1 | State 2 | State 3 |
|---|---|---|---|
| 1 | AB | - | - |
| 2 | - | AB | - |
| 3 | - | - | AB |
| 4 | A | B | - |
| 5 | B | A | - |
| 6 | A | - | B |
| 7 | B | - | A |
| 8 | - | A | B |
| 9 | - | B | A |

ii) BE distribution – 6 possible configurations

| Configuration | State 1 | State 2 | State 3 |
|---|---|---|---|
| 1 | AA | - | - |
| 2 | - | AA | - |
| 3 | - | - | AA |
| 4 | A | A | - |
| 5 | A | | A |
| 6 | | A | A |

iii) FD distribution – 3 possible configurations

| Configuration | State 1 | State 2 | State 3 |
|---|---|---|---|
| 1 | A | A | |
| 2 | A | – | A |
| 3 | - | A | A |


Quantum statistics
For
For
Fermion
Boson
Follows the
Follows the
Fermi-Dirac Distribution
Bose-Einstein Condensation
Application
As a model for
In
Electrons in metal
Superconductivity
Liquid helium

# Bose - Einstein statistics

-Indian physicist Satyendra Bose derived the quantum statistics of photons by assuming them as indistinguishable particles.

-Albert Einstein applied it to atoms.

-Note: **atoms:** the particle number is conserved (if they are trapped in a box or a magnetic field)

**Photons** can randomly be emitted and absorbed (e.g. from the walls of a box).

B-ED - Class of statistics that applies to elementary particles called **bosons**, which include the photon, pion, and the W and Z particles.

Particles behaving according to the B-E distribution are called **bosons**--- having spin values 0, 1, 2,..etc.

Q-statistics --- Bose-Einstein statistics

For B-E stat.

$$\sum_{n} e^{-nx} = \frac{1}{1-e^{-x}} \qquad \text{FOR } X>0$$

From (*)

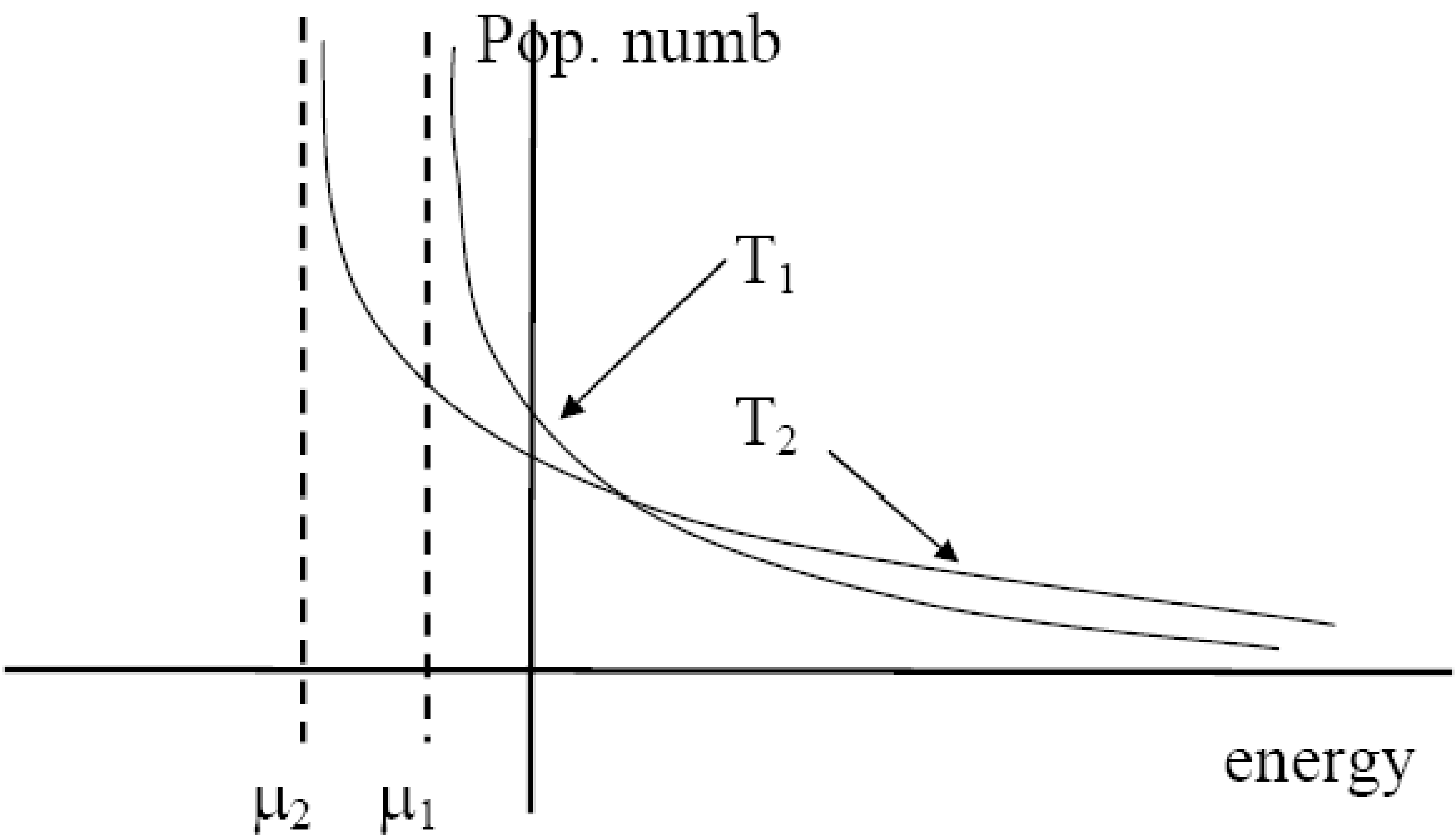
$$\bar{n}_{bosons} = -\frac{\partial}{\partial x}\ln\left(1-e^{-x}\right)^{-1} = \frac{\partial}{\partial x}\ln\left(1-e^{-x}\right)$$

$$= \frac{e^{-x}}{1-e^{-x}} = \frac{1}{e^{x}-1}$$

But $x = \beta(\varepsilon_S - \mu) > 0$

$$\bar{n} = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$

Note: at $\varepsilon = \mu$, the population number would be infinite



At low temperatures, an unlimited number of bosons can be in the same energy state, a phenomenon called condensation.

$$f(E) = \frac{1}{Ae^{E/kT} - 1}$$

f(E): the probability a particle will have energy E

A : for photon equals to one

$e^{E/kT}$: the exponential dependence on energy and temperature

-1: the quantum difference which arises from the fact the particles are indintinguishable

$$f(E) = \frac{1}{e^{\frac{E-\mu}{kT}} - 1}$$

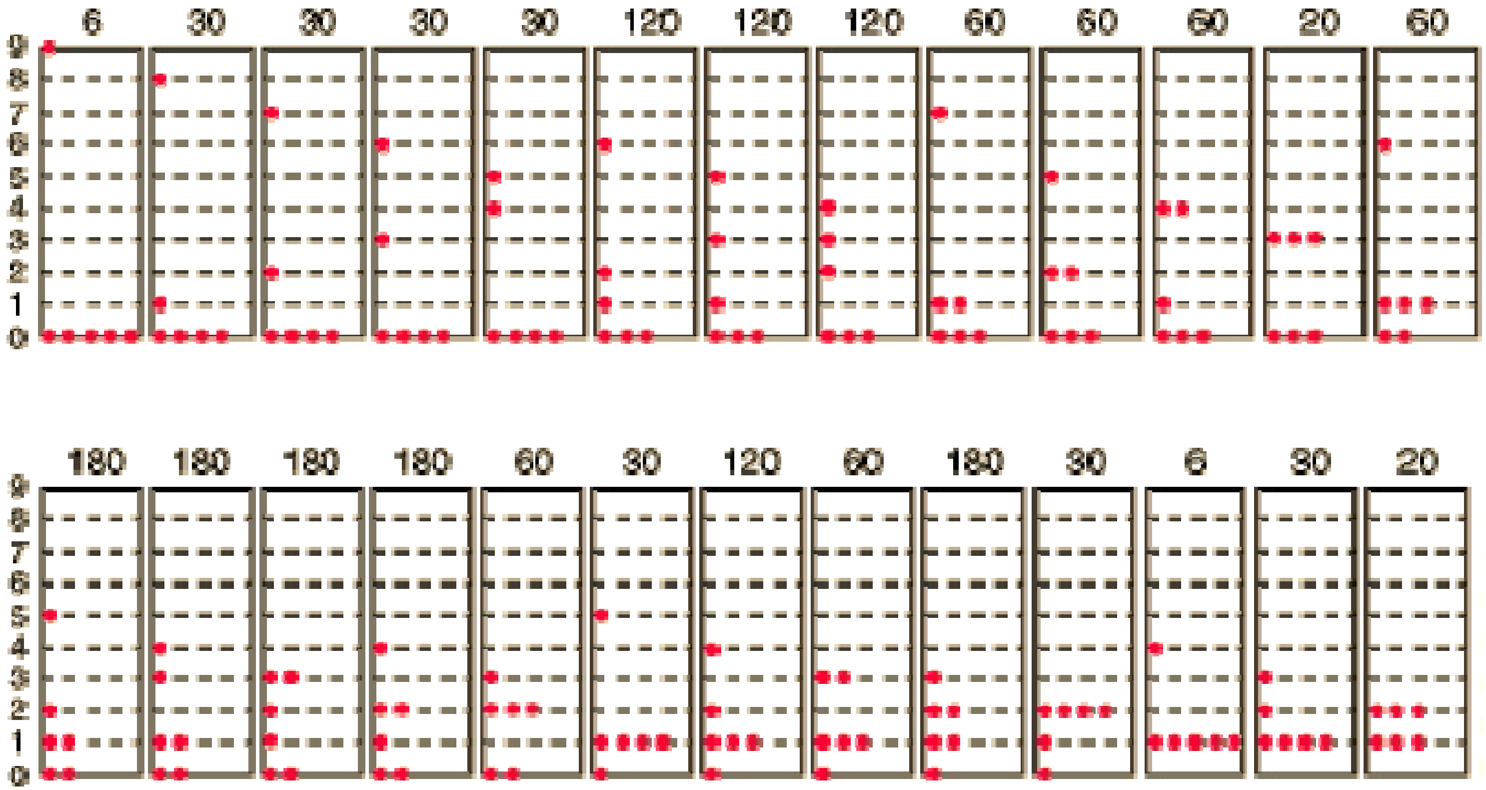
where:

$E$ is the energy
$k_B$ is Boltzmann's constant
$T$ is absolute temperature
μ is the chemical potential

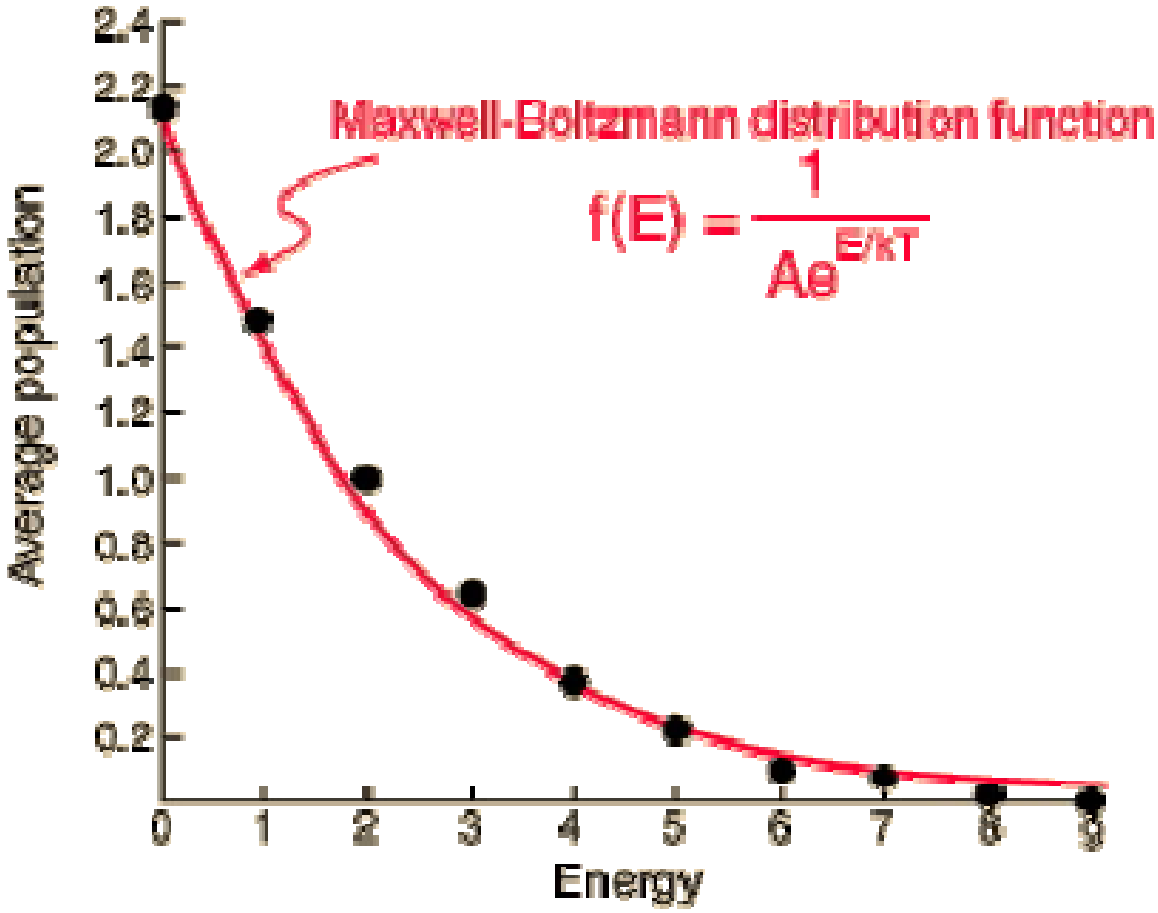
Example

How many ways can you distribute 9 units of energy among 6 identical, distinguishable / indistinguishable bosons?

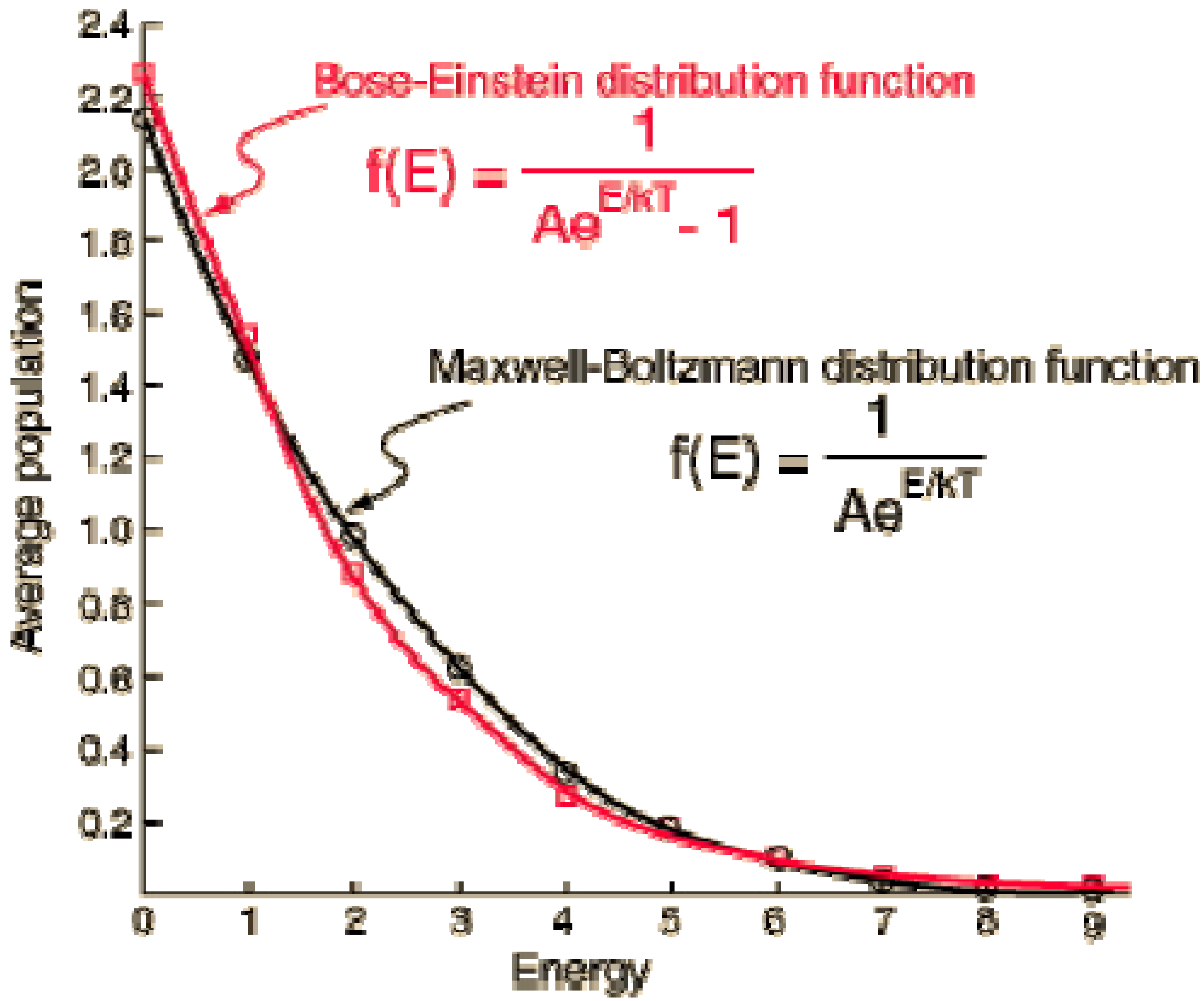
Note: for M-B stat



| Energy level | Average number |
|---|---|
| 0 | 2.143 |
| 1 | 1.484 |
| 2 | 0.989 |
| 3 | 0.629 |
| 4 | 0.378 |
| 5 | 0.210 |
| 6 | 0.105 |
| 7 | 0.045 |
| 8 | 0.015 |
| 9 | 0.003 |



| Energy level | Average number Maxwell - Boltzmann | Average number Bose-Einstein |
|---|---|---|
| 0 | 2.143 | 2.269 |
| 1 | 1.484 | 1.538 |
| 2 | 0.989 | 0.885 |
| 3 | 0.629 | 0.538 |
| 4 | 0.378 | 0.269 |
| 5 | 0.210 | 0.192 |
| 6 | 0.105 | 0.115 |
| 7 | 0.045 | 0.077 |
| 8 | 0.015 | 0.038 |
| 9 | 0.003 | 0.038 |



# Fermi-Dirac statistics

- Class of statistics that applies to particles called fermions.
- Fermions have half-integral values of the quantum mechanical property called spin and that two fermions cannot exist in the same state.
- Protons, neutrons, electrons, and many other elementary particles are fermions.

The Fermi-Dirac function f(E) gives the probability that an electron (for example) has energy E at temperature T given by:

$$f(E) = \frac{1}{e^{\frac{E-E_f}{kT}} + 1}$$

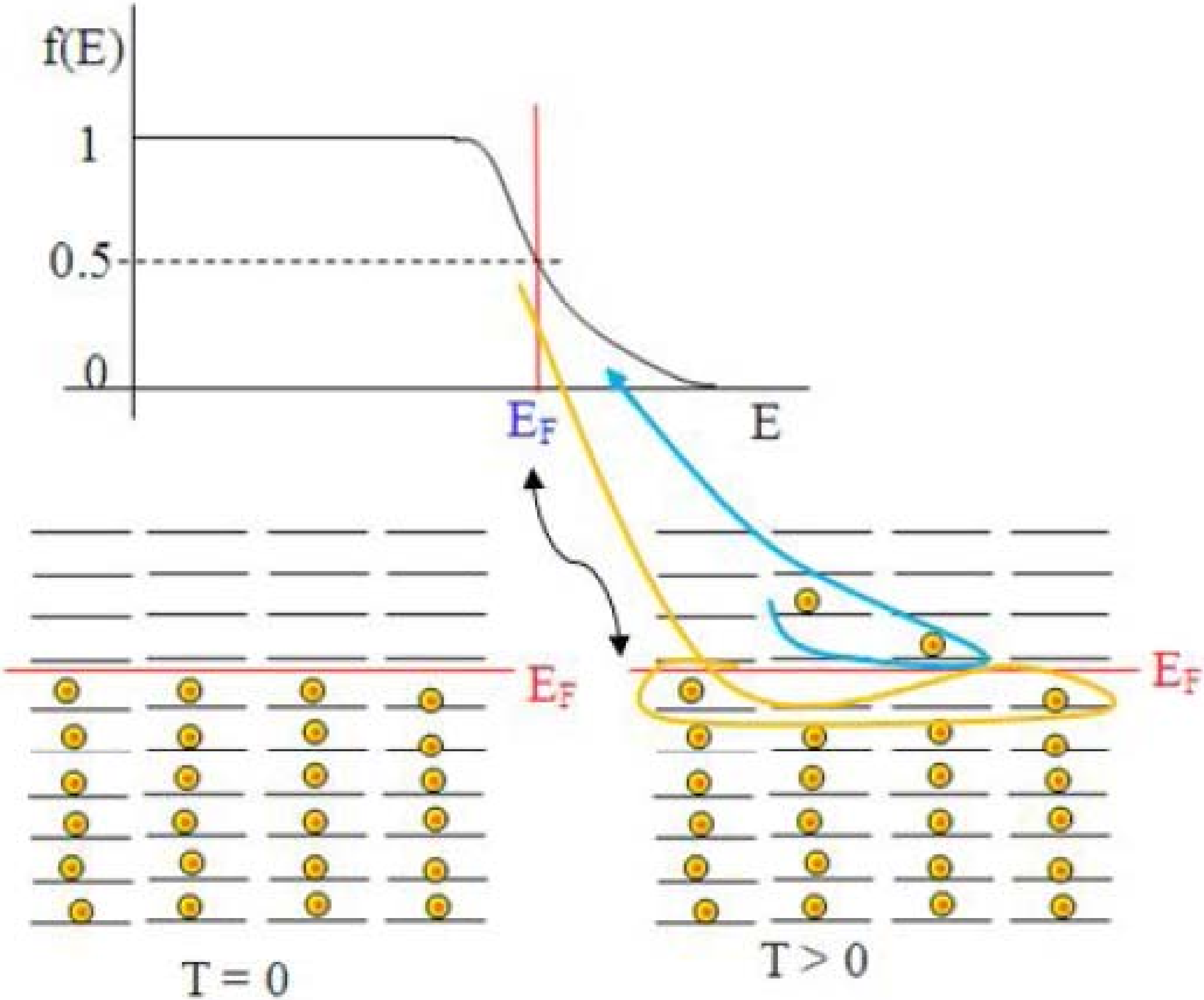
Where $E_f$ is the Fermi energy.

The **Fermi energy** ($E_f$) of a system of non-interacting fermions is the smallest possible increase in the ground state energy when exactly one particle is added to the system

Is equivalent to the chemical potential ($E_f = \mu$) of the system in its ground state at T=0 K.

The **Fermi level** is the top of the collection of electron energy levels at absolute zero temperature.

The Fermi energy or Fermi level, $E_f$ is defined as *the energy at which the probability of occupation of the electron state is 1/2*.



f(E)
1
0.5
0
$E_F$
E
$E_F$
$E_F$
T = 0
T > 0

# The Fermi-Dirac Distribution

$$f(E) = \frac{1}{e^{\frac{E-E_f}{kT}} + 1}$$

At 0K fermions will fill up all available energy states below a level $E_F$ with one particle.

At higher temperature some are elevated to levels above $E_F$

Term + 1: the quantum difference which arises from the fact that the particles are indistinguishable

Fermions are particles with half-integer spin.

By the Pauli Exclusion Principle, only one fermions can occupy a given state at a time.

That means that the occupation number for state s can be only $n_s = 0$ or $n_s = 1$

-conservation of particle number. $\sum_s n_s = N$

Note: $$\sum_{n=0}^{1} e^{-nx} = 1 + e^{-x}$$ n can be 1 or 0

$$Z = \sum_{n_1=0}^{1} e^{-\beta n_1(\varepsilon_1-\mu)} \sum_{n_2=0}^{1} e^{-\beta n_2(\varepsilon_2-\mu)} \ldots\ldots\ldots\ldots$$

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

The mean number of particles in state s

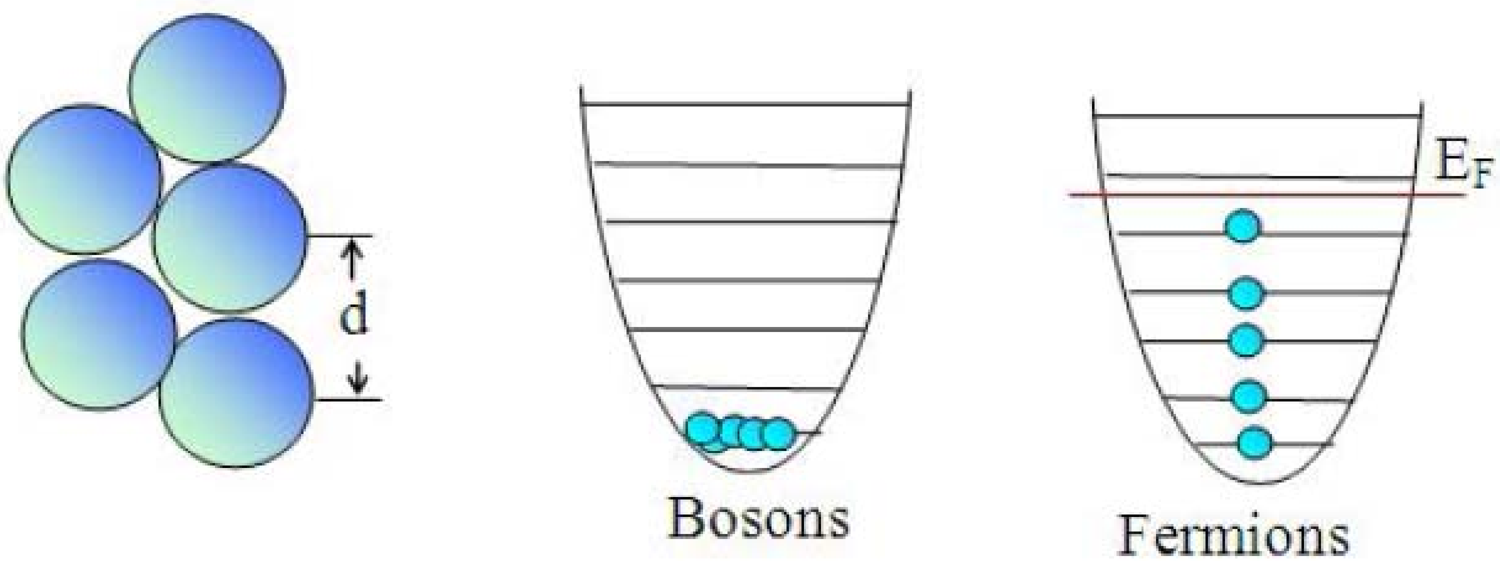
$$\overline{n}_s = -\frac{1}{\beta}\frac{\partial \ln Z}{\partial \varepsilon_s}$$

$$= -\frac{1}{\beta}\frac{\partial}{\partial \varepsilon_s}\left[\ln(1 + e^{-\beta(\varepsilon_s-\mu)} + \ldots\right]$$

$$= \frac{e^{-\beta(\varepsilon_s-\mu)}}{1+e^{-\beta(\varepsilon_s-\mu)}}$$

And finally $$\bar{n}_s = \frac{1}{e^{\beta(\varepsilon_s - \mu)} + 1}$$

This is known as the Fermi-Dirac Distribution also called Fermi function




at T = 0, Bosons: the energy is $\mu$ Fermions: the highest energy is $E_F$

# Fermi-Dirac distribution / Fermi Function

The Fermi function f(E) gives the probability that a given available electron energy state will be occupied at a given temperature.

Note: $\mu = \left(\frac{\partial E}{\partial N}\right)_{S,V} = -T\left(\frac{\partial S}{\partial N}\right)_{E,V}$ $\mu \equiv - kT\alpha$

The Fermi energy is defined as $E_F = - \alpha(T)kT$

$\alpha(T)$: the number of particles in a particular system at temperature $T$,

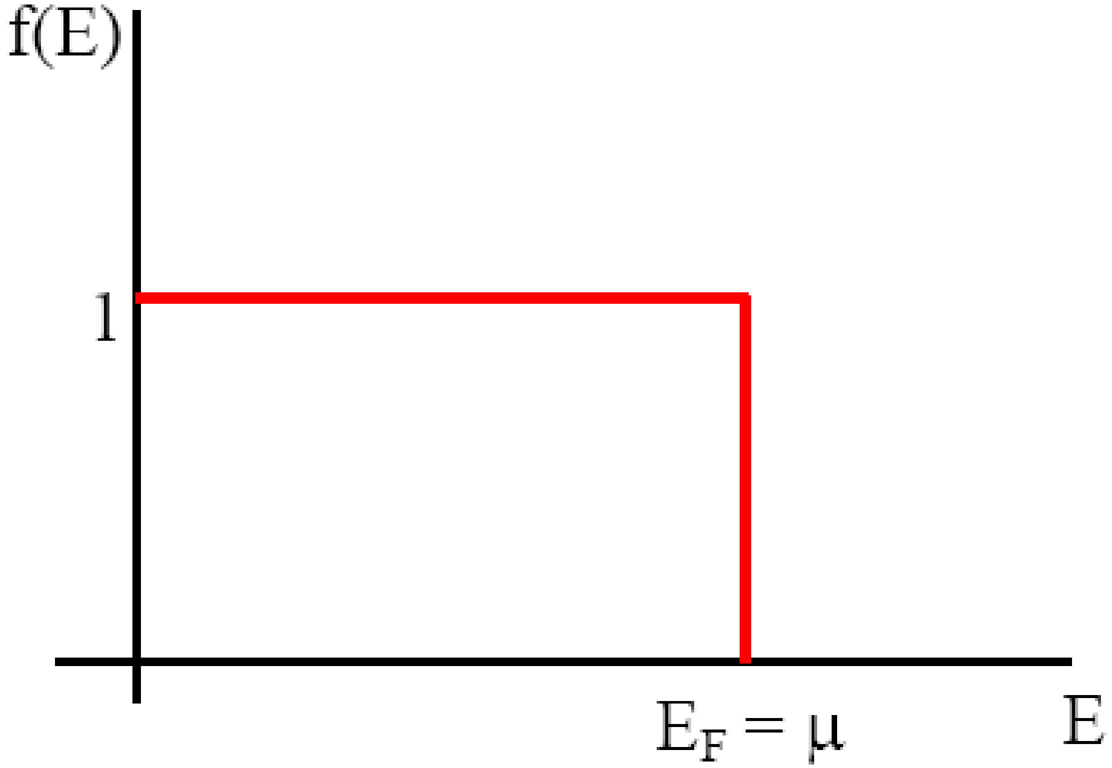
$$f(E) = \frac{1}{e^{\frac{E-E_f}{kT}} + 1}$$

At 0 K no electrons can be above the valence band, since none have energy above the Fermi level and there are no available energy states in the band gap.

At T = 0 K, $\beta = 1/kT = \infty$

If $E < E_f$ | Then f(E) = 1 | $e^{\frac{E-E_f}{kT}} = e^{-\infty} = 0$

If $E > E_f$ | Then f(E) = 0 | $e^{\frac{E-E_f}{kT}} = e^{\infty} = \infty$


f(E)
1
$E_F = \mu$
E

Increasing T

If $E = E_f$ then $f(E) = ½$

If E > EF , let say $E \geq E_F + 3kT$

Then $$e^{\frac{E-E_f}{kT}} = e^3 > 1$$

Approximation:

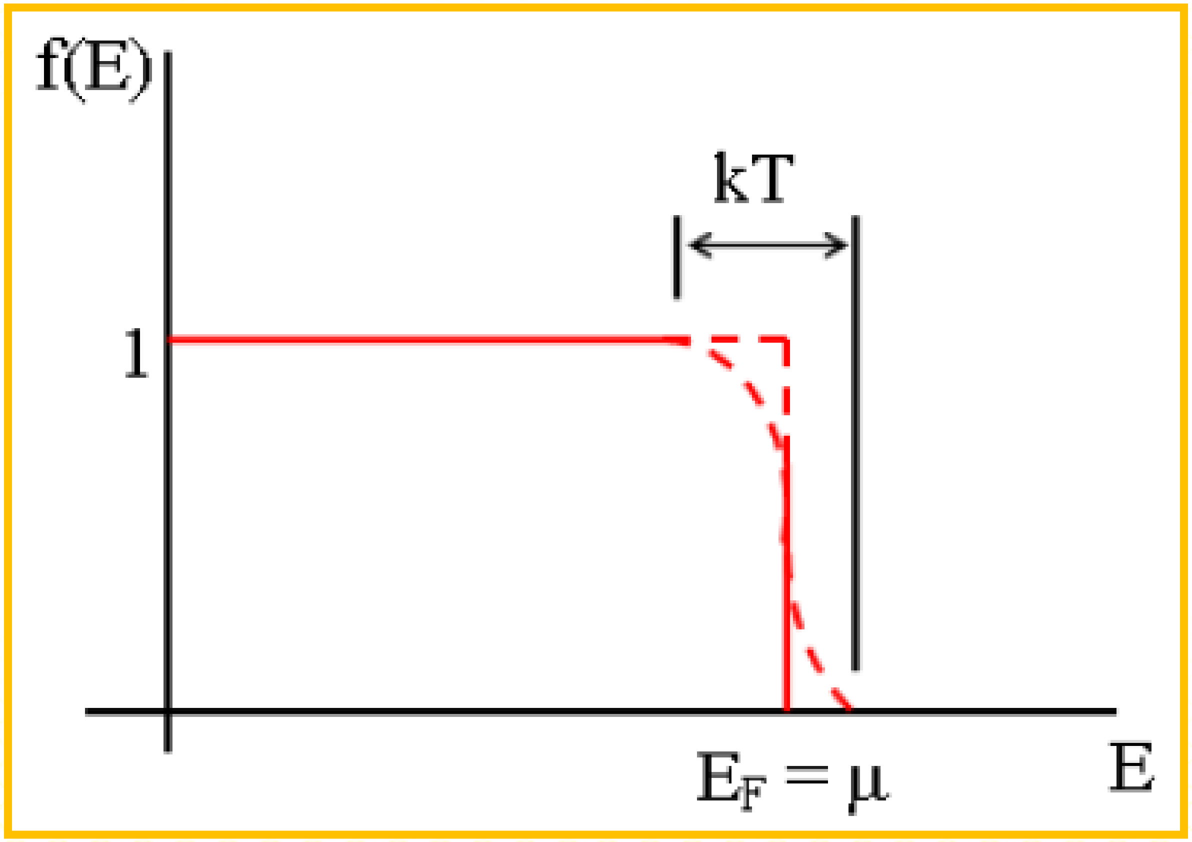
$$f(E) = e^{\frac{-(E-E_f)}{kT}}$$

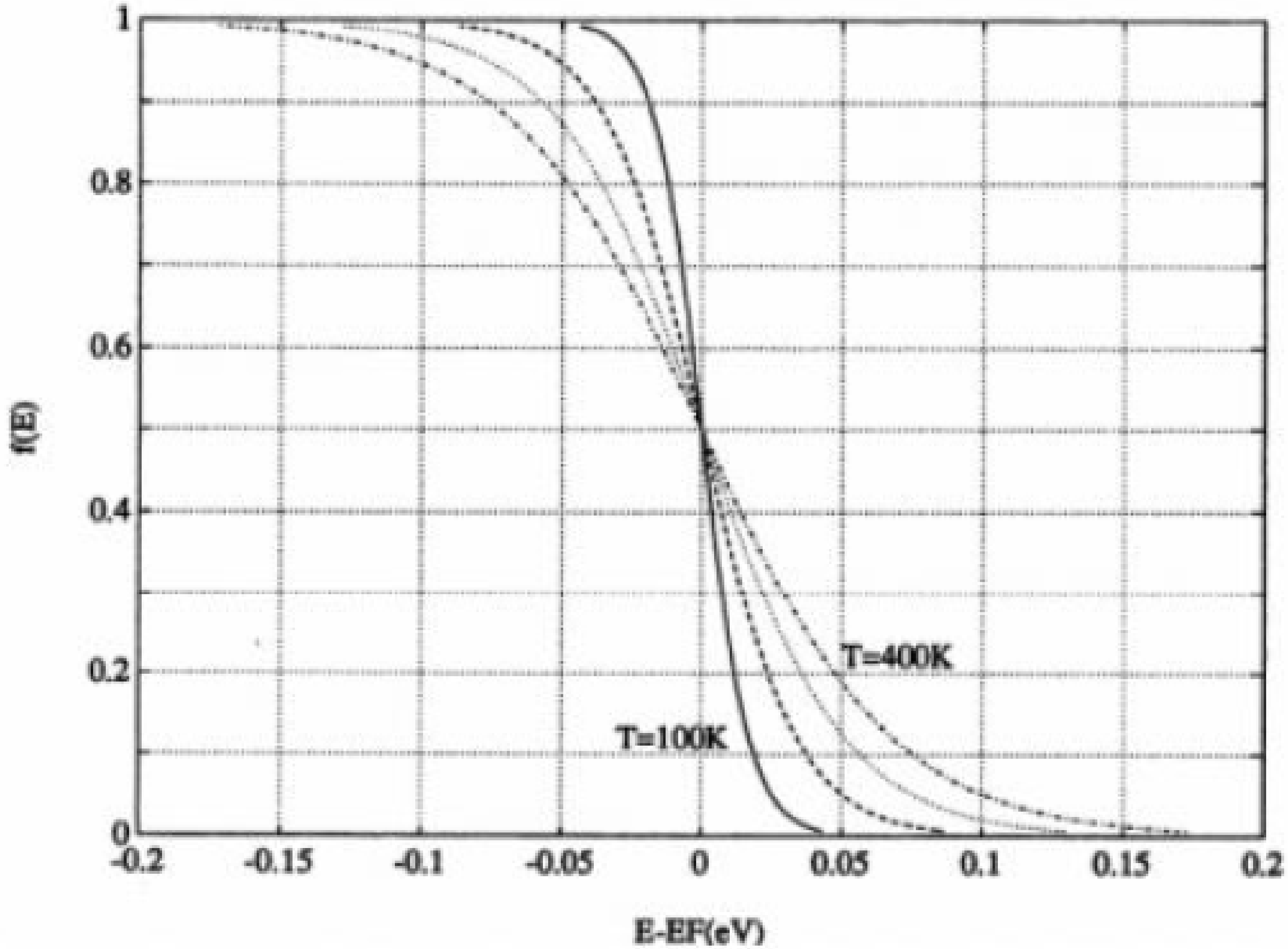
If $E < E_F$ let say $E \leq E_F - 3kT$

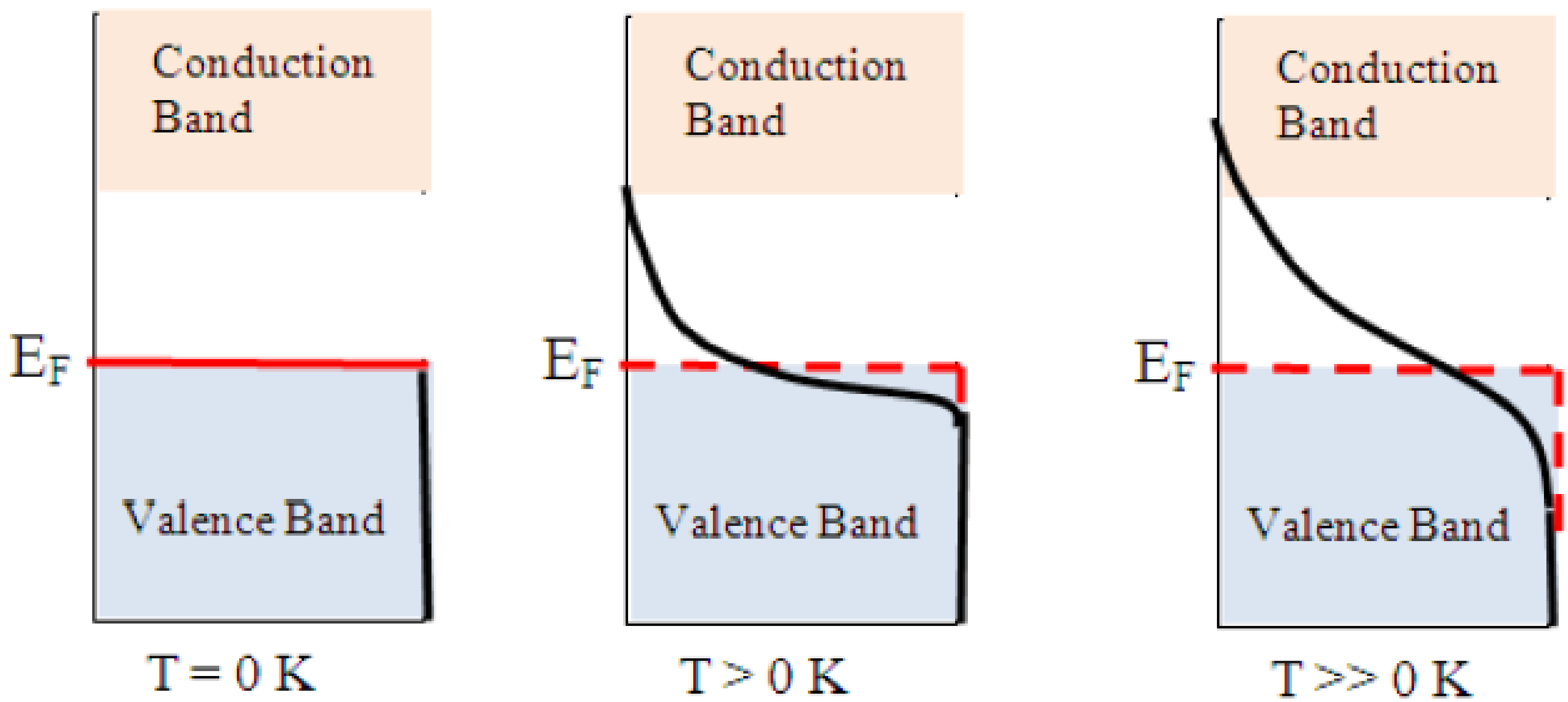
Then $$e^{\frac{E-E_f}{kT}} = e^{-3} << 1$$

Approximation:

$$f(E) = 1 - e^{\frac{(E - E_f)}{kT}}$$

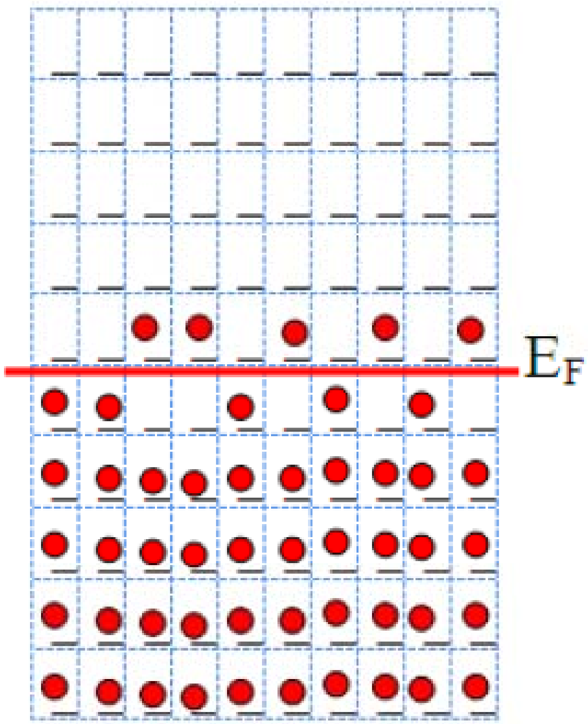


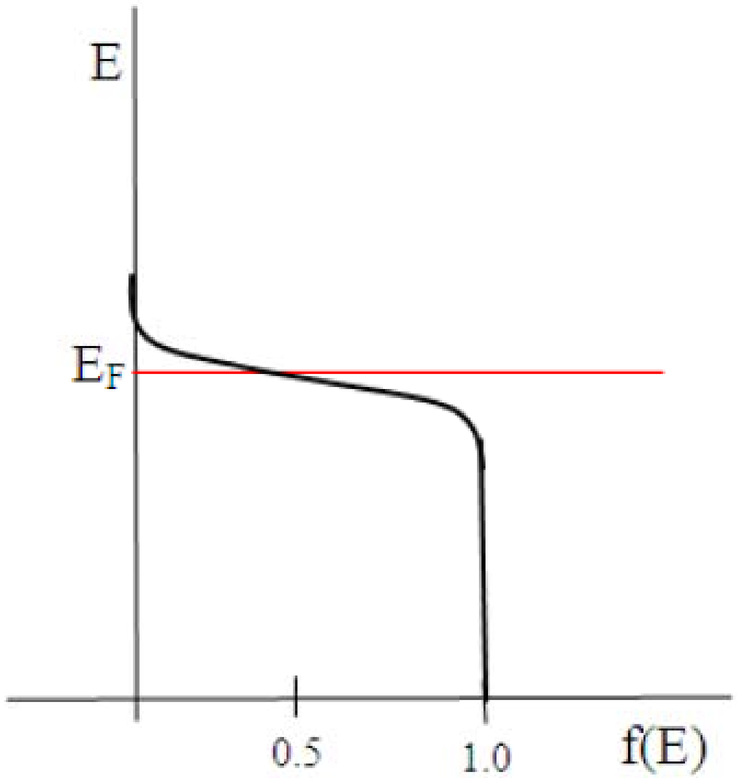

1
0.8
0.6
0.4
0.2
0
f(E)
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2
E-EF(eV)
T=400K
T=100K


Conduction Band
E_F
Valence Band
T = 0 K
Conduction Band
E_F
Valence Band
T > 0 K
Conduction Band
E_F
Valence Band
T >> 0 K

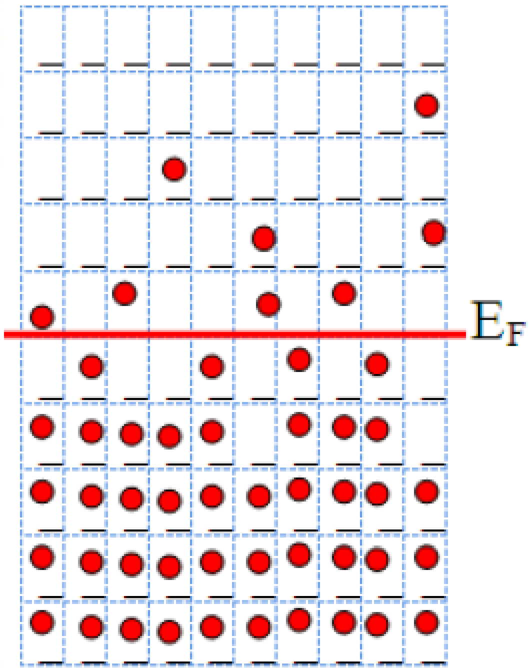
At high temperature, some electrons can reach the conduction band and contribute to electric current.

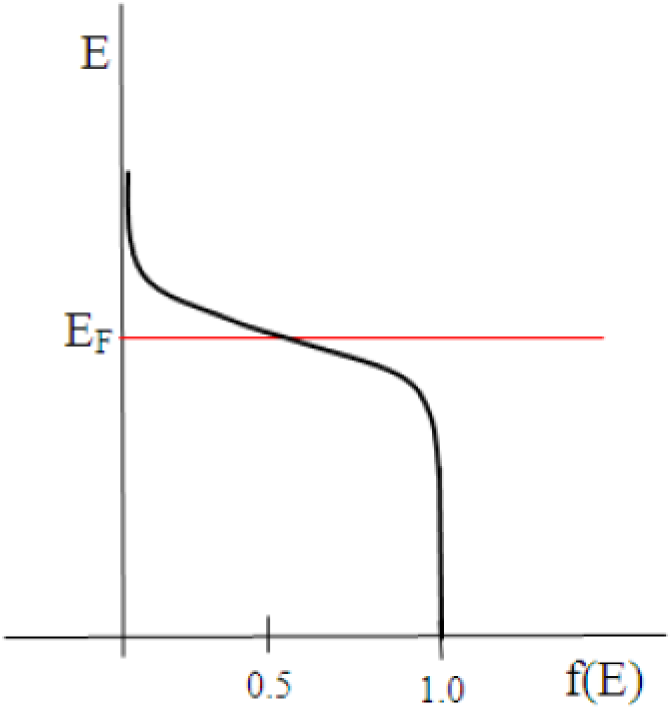
T ~300 K



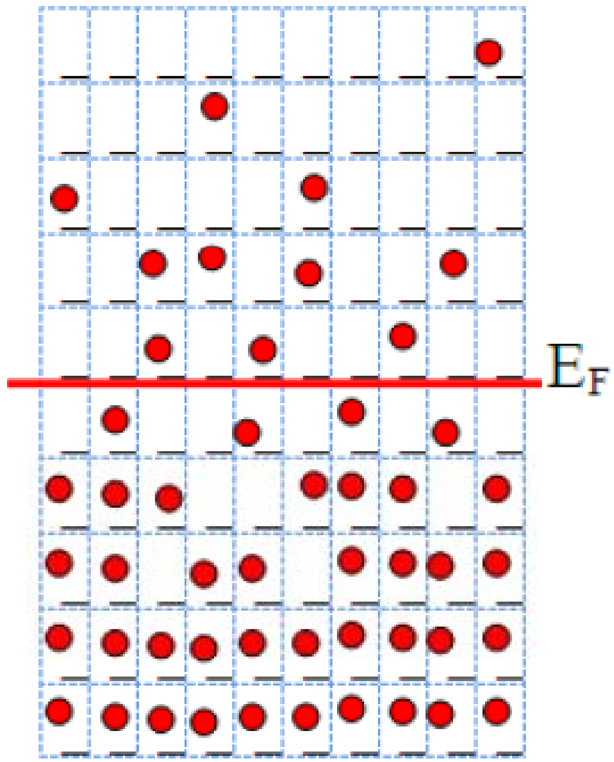



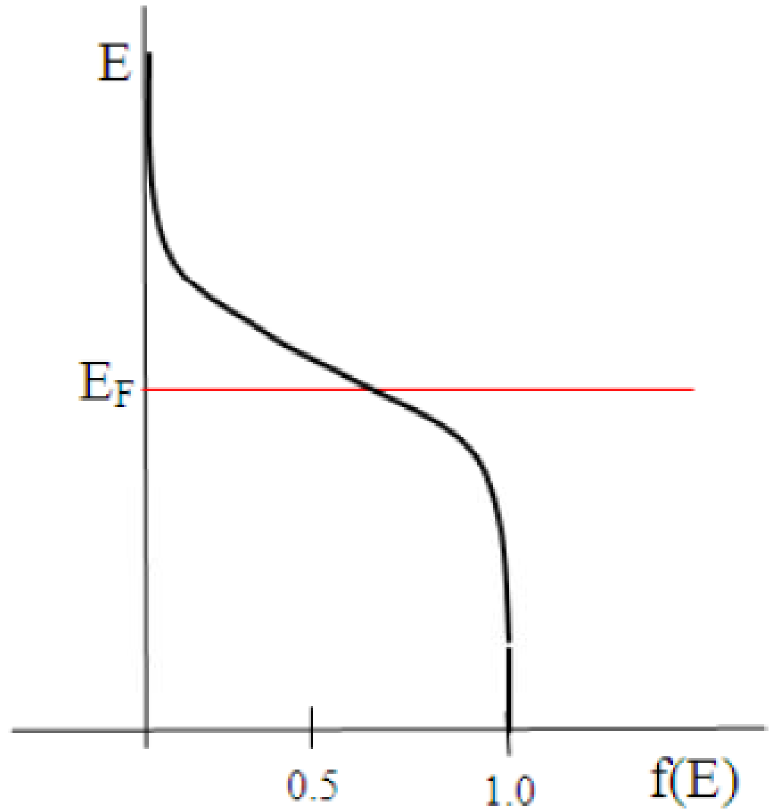
# T~ 800 K

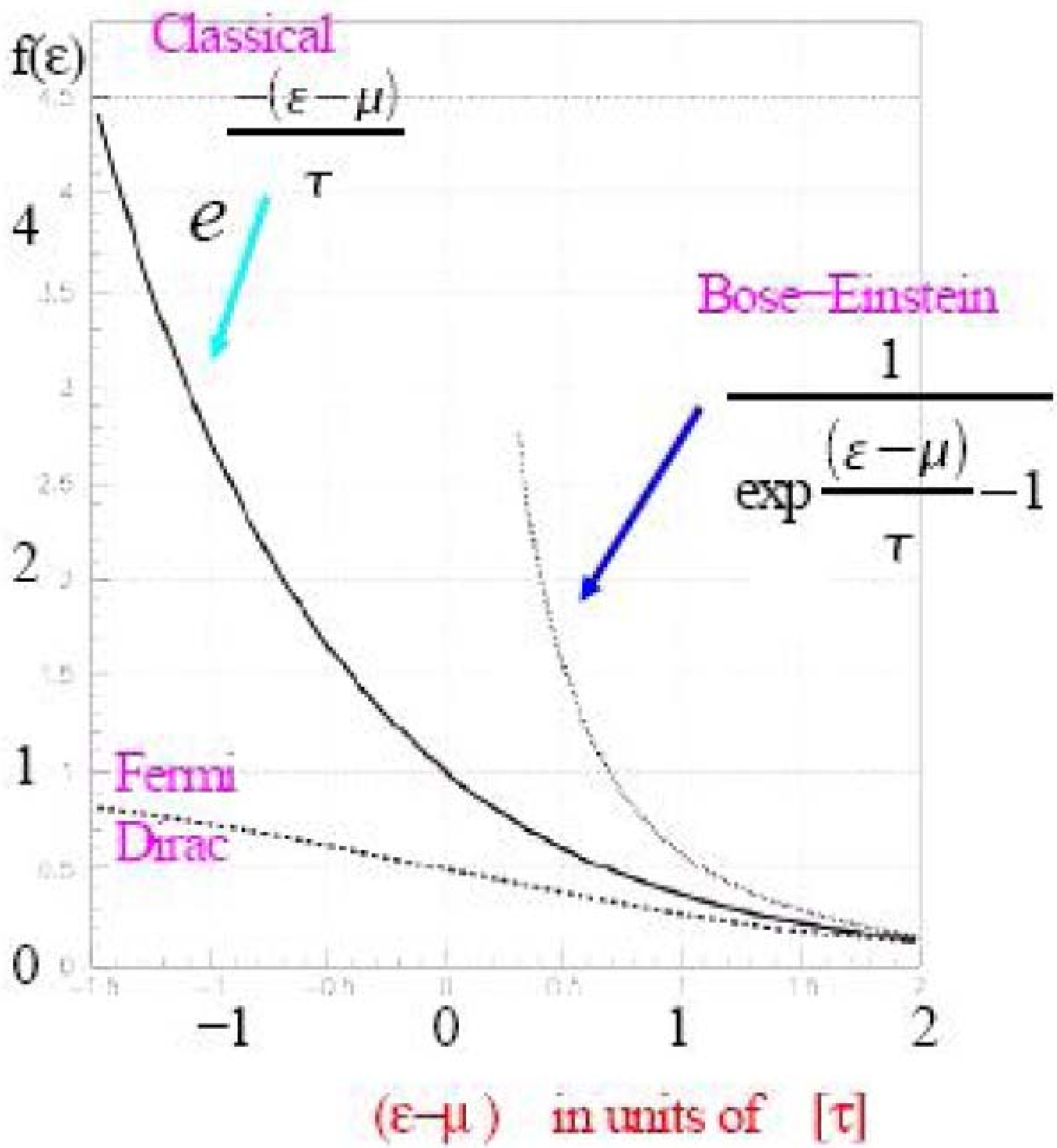


T~1300 K




f(ε)
Classical
$e^{\frac{-(\varepsilon-\mu)}{\tau}}$
Bose–Einstein
$\frac{1}{\exp\frac{(\varepsilon-\mu)}{\tau}-1}$
Fermi
Dirac
4
2
1
0
−1
0
1
2
(ε−μ) in units of [τ]

$$f(\varepsilon)_{BE} = \frac{1}{\exp\frac{(\varepsilon-\mu)}{\tau} - 1}$$

$$f(\varepsilon)_{FD} = \frac{1}{\exp\frac{(\varepsilon-\mu)}{\tau} + 1}$$

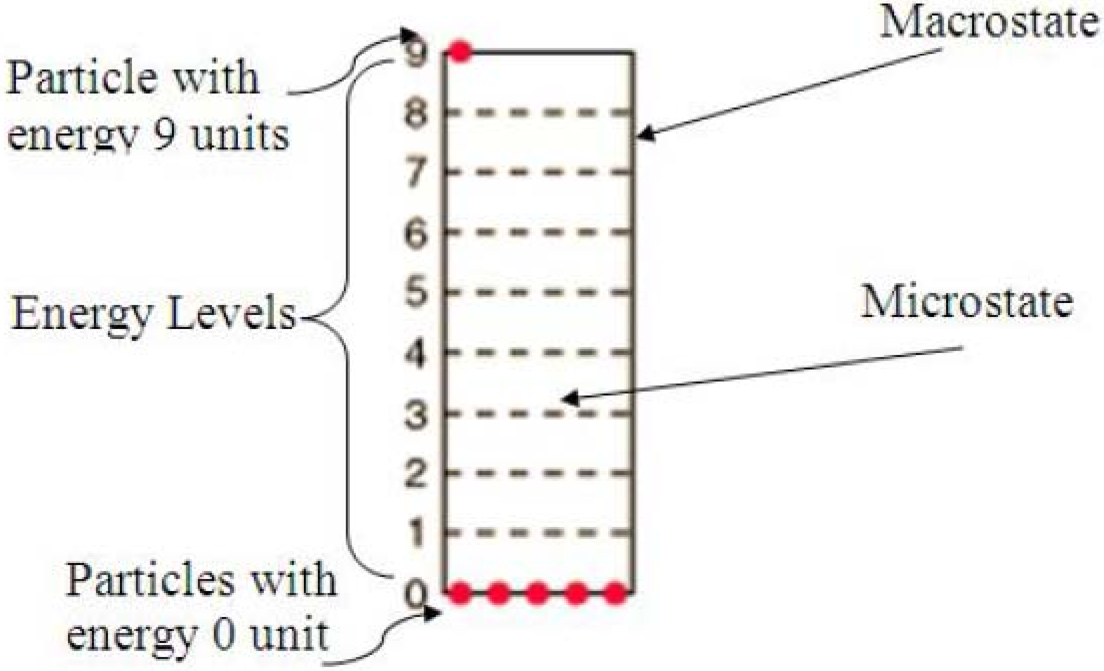
Large (ε - μ)/T BE & FD approach classical distribution, MB

$$f(\varepsilon)_{classic} = e^{-\frac{(\varepsilon-\mu)}{\tau}}$$

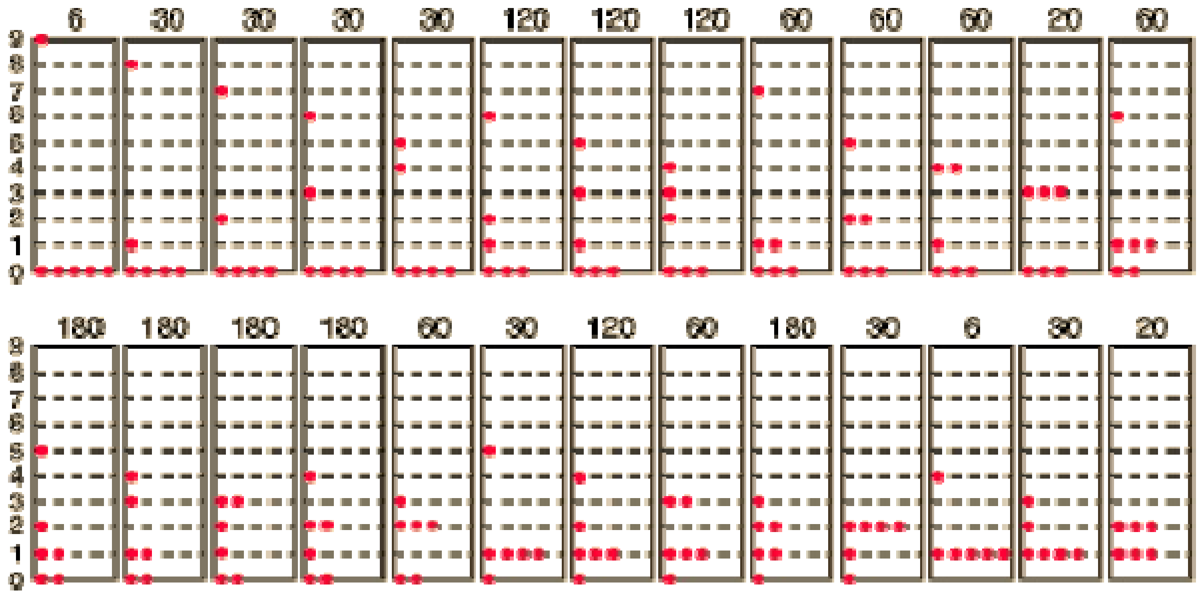
# Example

The distribution of 9 units of energy among 6 identical particles

Note:



# 1. MBD (each particle is presumed to be distinguishable)




-The total number of different states for distinguishable particles is 2002 = 6+30+30+..........

$$No.\ of\ \ microstates = \frac{N!}{n_1!n_2!n_3!....}$$

N: total number of particles

$n_i$: number of particles in level i

The first macrostates there are 6 microstates

$$\frac{6!}{5!1!} = 6$$

The second macrostates there are 30 microstates

$$\frac{6!}{4!1!1!} = 30 \qquad \text{Note: } 0! = 1$$

The number of microstates for ε units of energy among N equally probable states

$$\Omega(N,\varepsilon) = \frac{(\varepsilon + N - 1)!}{\varepsilon!(N-1)!}$$

For this case becomes

$$\Omega(N,\varepsilon) = \frac{(9+6-1)!}{9!(6-1)!} = \frac{14.13.12.11.10}{5.4.3.2.1} = 2002$$

To find average particles per energy level

For each macrostate, the number of particles in a given energy level is multiplied by the number of microstates.

The sum of those products is divided by the total number of microstates

$$n_j = \sum_i n_{ij} P_i$$

$n_{ij}$ = number of particles of energy $E_j$ in microstate i

$P_i$ = number of microstates in macrostate I divided by the total number of microstates

$n_j$ = average number of particles in energy level j the average number of particles in energy level 0

$$n_0 = 5x\frac{6}{2002} + 4x\frac{30}{2002} + 4x\frac{30}{2002} + 4x\frac{30}{2002} + \ldots\ldots$$

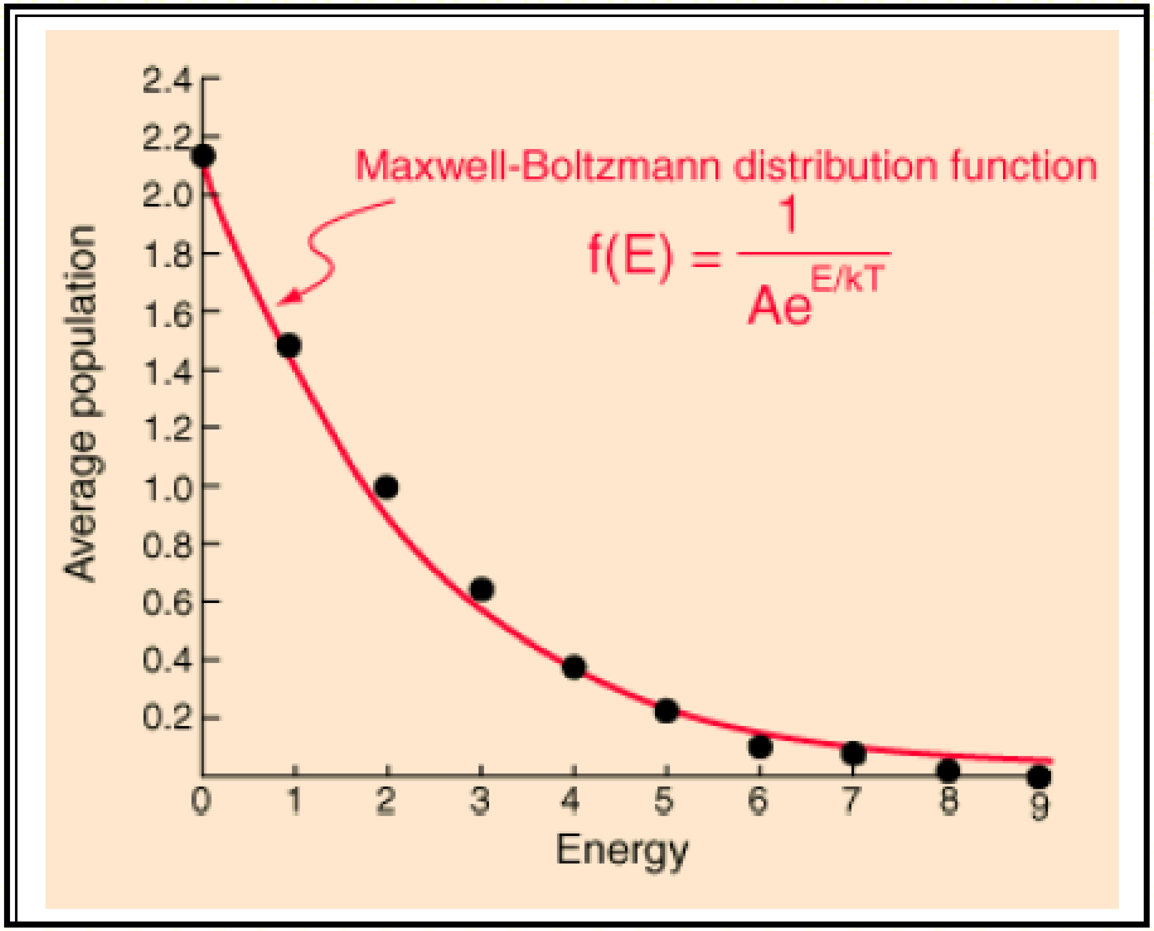
$$= \frac{1}{2002}\{5x6 + 4(4x30) + 3(3x120) + 3(3x60) + (3x20) + (2x60)$$

$$+ 4(2x180) + (2x60) + (1x30) + (1x120) + (1x60) + (1x180) + (1x30)\}$$

$n_0 = 2.143$

continue to calculate $n_1$, $n_2$,$n_3$,……..$n_9$

| Energy level | Average number |
|---|---|
| 0 | 2.143 |
| 1 | 1.484 |
| 2 | 0.989 |
| 3 | 0.629 |
| 4 | 0.378 |
| 5 | 0.210 |
| 6 | 0.105 |
| 7 | 0.045 |
| 8 | 0.015 |
| 9 | 0.003 |



## 2. BED *(identical, indistinguishable bosons)*

there are 26 microstates arising from 26 macrostates

The average occupancy is the sum of the numbers of particles in a given energy state over all the 26 distributions divided by 26.

For average particles in energy level 0,

$$n_0 = (5+4+4+\ldots\ldots)/26 = 59/26 = 2.269$$

continue ….

$n_1$ = ….., $n_2$= …. …..

# 3. FDD (fermions must obey the Pauli exclusion principle).

if the particles are electrons,

- a maximum of two particles can occupy each spatial state since there are two spin states each.
- 26 possible configurations for distinguishable particles are reduced to the 5 states which have no more than two particles in each state.

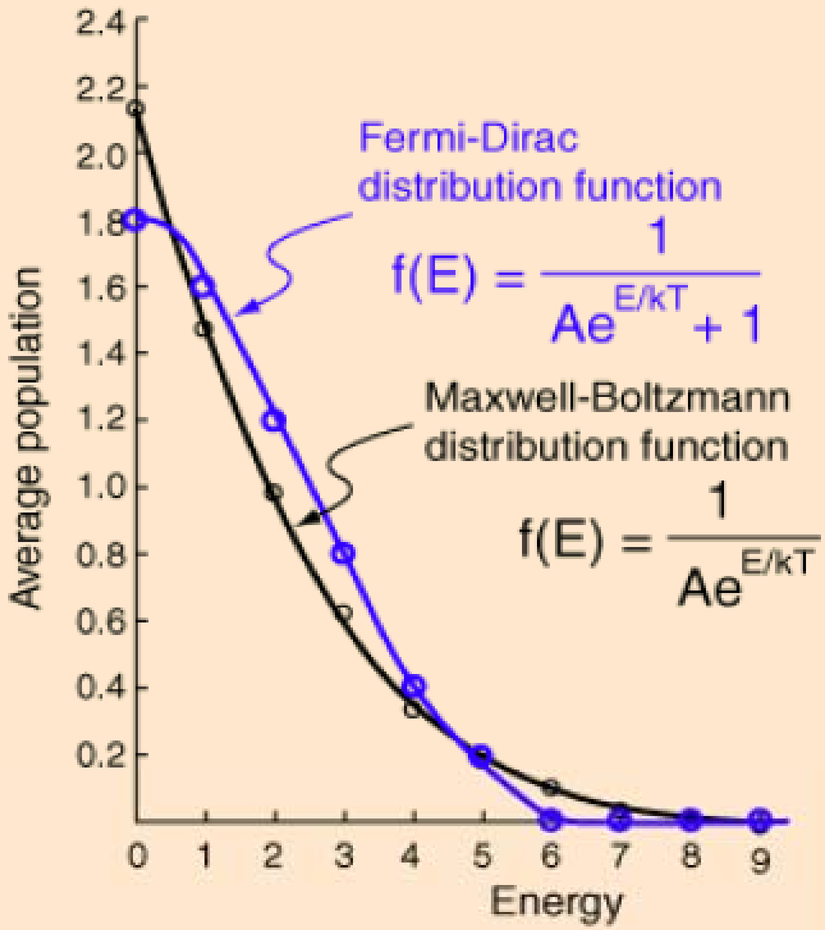
The average occupancy per energy level

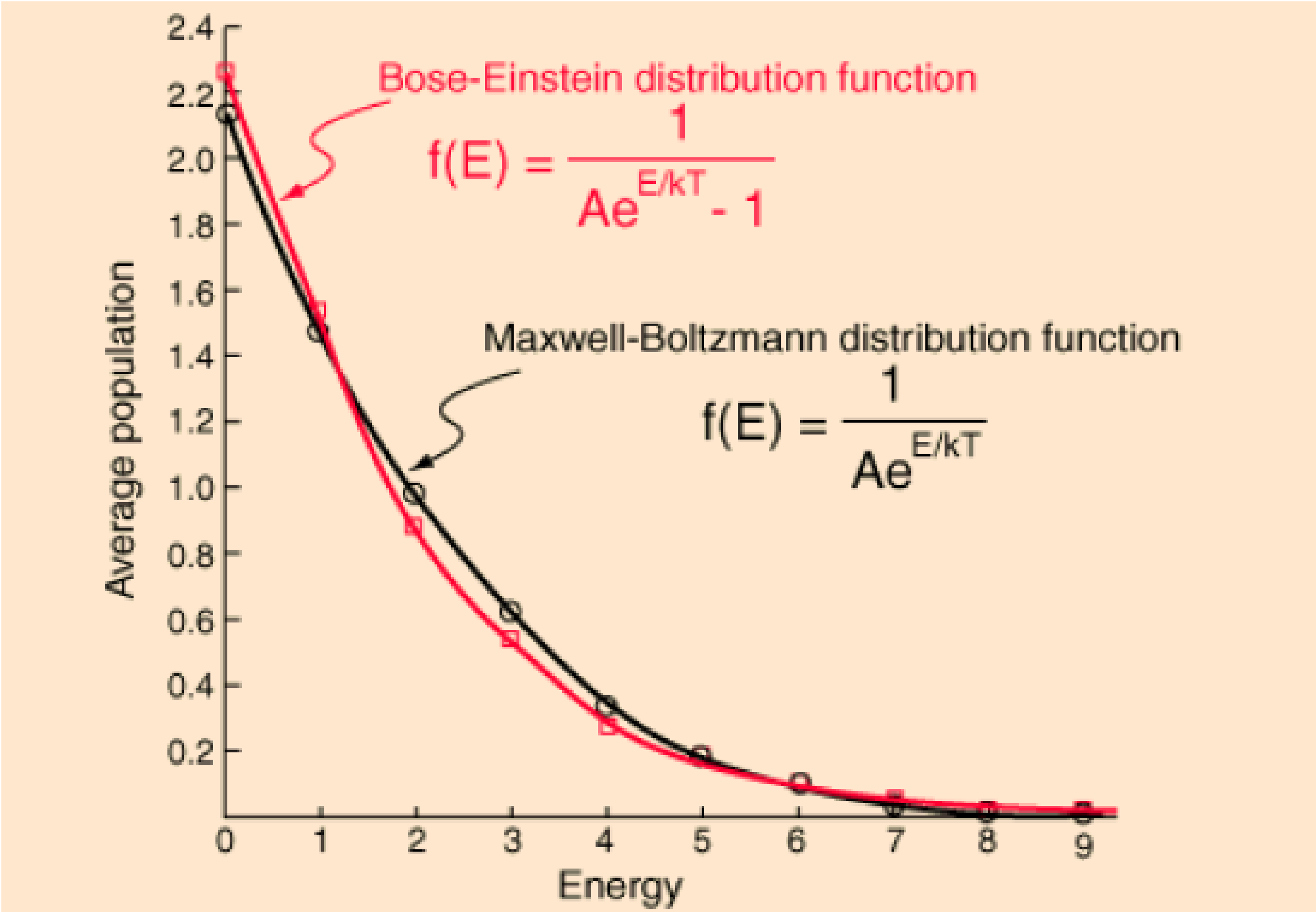
the sum of the numbers of particles in a given energy state over all the 5 distributions divided by 5.

$$n_0 = 9/5 = 1.8$$

$$\ldots\ldots\ n_1,\ n_2, n_3, \ldots\ldots.$$

| E | Average number Maxwell-Boltzmann | Average number Bose-Einstein | Average number Fermi-Dirac |
|---|---|---|---|
| 0 | 2.143 | 2.269 | 1.8 |
| 1 | 1.484 | 1.538 | 1.6 |
| 2 | 0.989 | 0.885 | 1.2 |
| 3 | 0.629 | 0.538 | 0.8 |
| 4 | 0.378 | 0.269 | 0.4 |
| 5 | 0.210 | 0.192 | 0.2 |
| 6 | 0.105 | 0.115 | 0 |
| 7 | 0.045 | 0.077 | 0 |
| 8 | 0.015 | 0.038 | 0 |
| 9 | 0.003 | 0.038 | 0 |




Bose-Einstein distribution function
$f(E) = \frac{1}{Ae^{E/kT} - 1}$
Maxwell-Boltzmann distribution function
$f(E) = \frac{1}{Ae^{E/kT}}$
Average population
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
1
2
3
4
5
6
7
8
9
Energy

# PHEW…!!

REFERENCES:

1. REAF, F : “Fundamentals Of Statistical And Thermal Physics”, McGraw-Hill.

2. KITTEL & KROMER: “Thermal Physics”, W.H. Freeman & Company.