Statistical Mechanics

Lecture two

Third stage

First semester

Statistical Mechanics

Introduction

Introduction to Statistical Mechanics:

Statistical mechanics or statistical thermodynamics is a branch of Physics that applies probability theory, which contains mathematical tools for dealing which large populations, to the study of the thermodynamic behavior of systems composed of a large number of particles .

Statistical thermodynamic or statistical Mechanics is a link between Microscopic properties and a bulk Macroscopic properties.

Statistical mechanics is available tool, which relates microscopic parameters to the macroscopic properties of a system that consists of a large number of molecules or colloidal particles.

Statistical mechanics, is a branch of Physics that combines the principles and procedures of statics with the laws of both classical and quantum mechanics, particularly with respect to the field of thermodynamics.

Statistical mechanics provides a framework for relating the microscopic properties of individual atoms and molecules to the macroscopic bulk properties of materials.

The description of physical phenomena in terms of statistical treatment of the behavior of large numbers of atoms or molecules, especially **with regard to** the distribution of energy among them.

The Kinetic theory of heat is one example of statistical mechanics; the laws of thermodynamics can all be explained using statistical mechanics.

Why statistical mechanics?

The object of statistical mechanics is the study of the properties of physical systems containing a very large number of particles (Avogadro's constant). In fact, this constant relates microscopic quantity to macroscopy quantities.

Why do we study statistical mechanics?

W e apply statistical mechanics to solve for real systems (a system for many particles). For example for an ideal gas, we assume that the molecules are none interchange, i.e. they do not affect each others energy levels.

At $T>0$, the systems possesses a total energy , E, so,

How is the energy E distributed among the particles?

How the particles are distributed over the energy levels?

We apply statistical mechanics to provide the answer and thermodynamic demands that the entropy be maximum at equilibrium.

Thermodynamics is concerned about heat and the direction of heat flow, whereas statistical mechanics gives a microscopic perspective of heat in terms of the structure of matter.

statistical mechanics, branch of physics that combines the principles and procedures of statistics with the laws of both classical and quantum mechanics, particularly with respect to the field of thermodynamics. It aims to predict and explain the measurable properties of macroscopic systems on the basis of the properties and behavior of the microscopic constituents of those systems.

Statistical mechanics interprets, for example, thermal energy as the energy of atomic particles in disordered states and temperature as a quantitative measure of how energy is shared among such particles. Statistical mechanics draws heavily on the laws of probability so that it does not concentrate on the behavior of every individual particle in a macroscopic substance but on the average behavior of a large number of particles of the same kind.

The fundamental postulate of statistical mechanics is: **An isolated system in equilibrium is equally likely to occupy any of its accessible states**.

Classification of statistical mechanics

Classical statistical mechanic

Classical particles

Maxwell -Boltzmann

Distinguishable particles

Quantum statistical mechanic

Quantum particles

Bose-Enestine Statistics

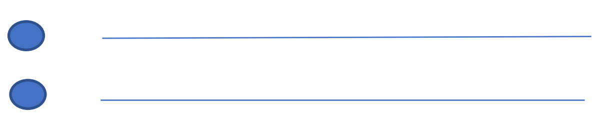
Fermi-Dirac Statistics

Indistinguishable particles

Distinguishable particles& Indistinguishable particles

Distinguishable particles:(classical particles)

The particles having distinct wave function known as distinguishable particles.



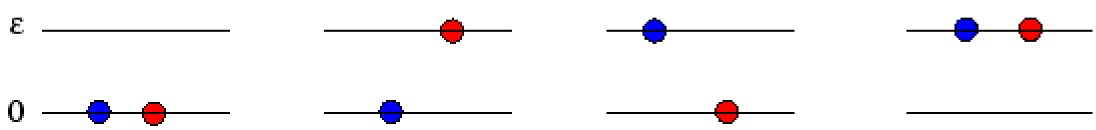
No overlapping of wave function of particles, they also called classical particles.

They don't obey Hiesenberg Uncertainty principle

Hence we can determine the conjugate Co-ordinate position an momentum precisely at the same time for these particles.

They follow up Maxwell-Boltzmann Statistics.

In classical mechanics all the particles(fundamental and composite particles, atoms, molecules, electrons,……ect) in the system are considered distinguishable. As a consequence changing the position of any particle in the system leads to a completely different configuration of the entire system. Further more is no restriction on placing more than one particle in any given state. Classical statistic is called Maxwell-Boltzmann Statistics or (M-B statistic).



Distinguishable particles

Particles can be labeled 1,2,3,……. Or a,b,c,……. We can also called localized particles(mean particle can be located).
For two particle system the total wave function will be written as;

Particle 1 → statement a , particle 2 → statement b

$$\varphi_{(1,2)}=\varphi_{(1)}\ \varphi_{(2)}$$

Qus. Take electron in the system ,Can particles be distinguishable.

If you take the system identical may be moves in many waves you can located, if you press individual particles in system then it will be identical and be indistinguishable particles.

(identical and localized)

consider a system of N distinguishable particles, it is possible to label them as i=1,2,3,…….N. in such a system if is the energy of the particle, then the total energy(E) of the N non interacting particles is given by

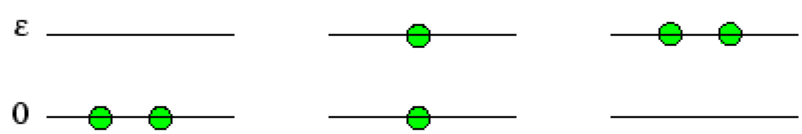
$$E=\sum_i \varepsilon i$$

Localized particles are distinguishable because they are fixed in space. For an isolated system, the volume, energy E, and total number of particles, N are fixed.

Indistinguishable particles

The particles having overlap wave functions are indistinguishable particles.

identical particles (also called indistinguishable or indiscernible particles) are **particles that cannot be distinguished from one another, even in principle**, Or Identical particles — Two particles are said to be identical if all their intrinsic properties (e.g., mass, electrical charge, spin, colour, ...) are exactly the same.



Indistinguishable particles

Mixing wave function called quantum particles.

They follow quantum statistics.

They will obey Hiesenberg Uncertainty principle

we cant determine the conjugate Co-ordinate position an momentum precisely at the same time.

They are also called Non -localized particles.

Indistinguishability is seen for identical particles(charge, mass, volume, size, shape) electron .electron, proton .proton.

In the case of distinguishable particles εi represents to the energy of i th particle.

In the case of indistinguishable particles let $\varepsilon(s)$ represent the possible values of the energy of any one of the indistinguishable particle in its sth quantum state. Thus each particle can have energy $\varepsilon 1$, $\varepsilon 2$, ………..let

n_s = the number of particles in state s

In terms of n_s the total energy of the system on non interacting particles can be written as:

$$E=\sum_i n_s \,\varepsilon(s)$$

Where the summation is for particles, we have s= 1,2,3,…..

There are N distinguishable quantum harmonic oscillator at 1-D lattice sites,

$$N=\sum_s Ns$$

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

They are oscillating quantum mechanically

Quantum particle can be distinguishable

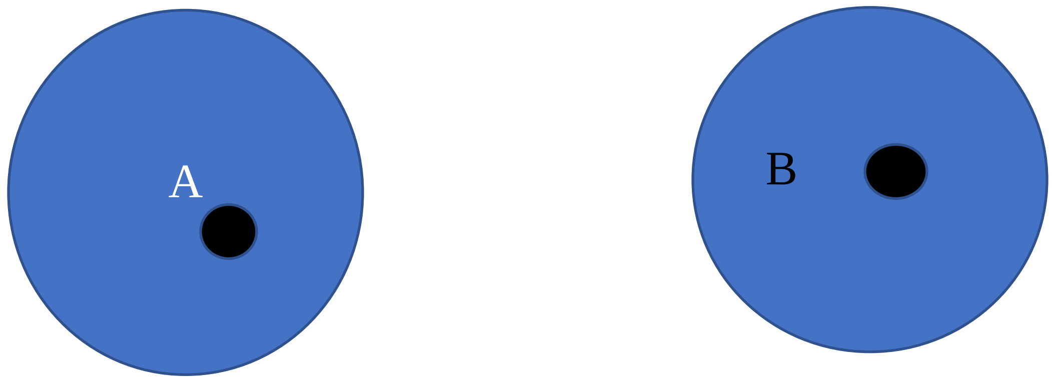


Figure 1: This figure represents two distant identical particles, as well as the spread of their respective wave functions. Each one of them occupies a distinct region of space, arbitrarily labelled A and B, thus allowing us to distinguish these identical particles, just as in a classical case.

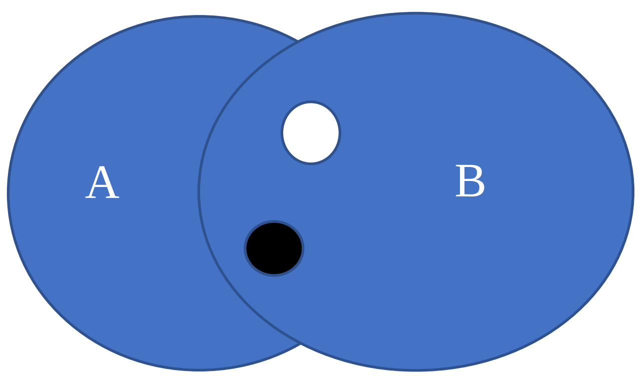


Figure 2: This figure represents two identical particles in a situation where their respective wave functions overlap. It is no longer unambiguous which region of space each particle occupies. The particles are indistinguishable — a purely quantum effect — and must now obey the Symmetrization Postulate: there are symmetry restrictions to the states describing the joint system.

Important point; don't judge system by wording Distinguishable particles& Indistinguishable look at energy of individual particles, if it is discrete then the particles are quantum approach and if it is continuous then use classical statistics.

Indistinguishable particles

Fermions

Fermi particle

Particle having half integral spin

$S=\frac{1}{2},\frac{3}{2},\frac{5}{2},\ldots \ldots$

e, p, N, elementary particles

Fermi-Derac Statistics

Bosons

Bose Particles having integral spin

S= 0,1,2,3,…………

Photons, Mesons

Bose-Einstein Statistics

Fermi-Derac Statistic

The total wave function for fermions system should be Anti-Symmetry

$\Psi_{tot} \rightarrow$ anti-symmetry

$\Psi_{tot} = S_{pecial} \,.\, \Psi_{spin}$

The wave function for the Boson system should be symmetry

$\Psi_{tot} \rightarrow$ symmetry

$\Psi_{tot}(2,1) = \Psi_{tot}(1,2)$

S_{pecial} continuous character $n \; l \; m_l \; m_s$

$\Psi(2,1) = -\Psi(1,2)$ anti-symmetry in character

Difference between Distinguishable & Indistinguishable

Distinguishable	Indistinguishable
Identical	Non Identical
Localized	Non Localized
	discreet energy

Name	Symbol	Value
Principle quantum number	n	$n=1,2,3,\ldots..$
Angular momentum Quantum number	l	for $n=3$ $l=0,1,2$(s, p, d)
Magnetic quantum number	m_l	$l=2$ $m_l=-2,-1,0,1,2$
Spin quantum number	m_s	
For an electron	$s=\frac{1}{2}$, so	$m_s = -\frac{1}{2}, +\frac{1}{2}$

Bose-Einstein Statistics

In Bose-Einstein Statistics (B-E Statistics) interchanging any two particles of the system leaves the resultant system in a symmetric state. That's, the wave function of the system before inter changing equals the wavefunction of the system after interchanging.

It is important to emphasize that the wave function of the system has not changed itself. There is no restriction to the number of particles that can be placed in a single state (accessible to the system). It is found that the particles that obey Bose-Einstein Statistics are the ones which have integer spins, which are there fore called Bosons. Examples of Bosons include photons and helium-4 atoms.

Fermi-Derac Statistic

Interchanging any two particles of the system leaves the resultant system in an anti-symmetric.
This shows that Fermi-Derac Statistics, more than one particles cannot occupy a single state accessible to the system. This is called Pauli's Exclusion Principle. Its found that particles with half-integer spin(or fermions) obey the Fermi-Derac Statistics. This includes electrons, protons.

Fermions are particles with half integral spin angular momentum and they obey Pauli's Exclusion Principle i.e no two particles can occupy same state at the same time.
Examples of Fermions are: Electrons, protons, neutrons, neutrinos etc.

Microstate and Macro state

Macro state

A macro state is defined by the macroscopic properties of the system, such as temperature, pressure, volume, etc. For each macro state, there are many microstates which result in the same macro state.

A macro state is defined by specifying the value of every macroscopic variable. There may be huge number of microstates all corresponding to the same microstate.

Specification of macroscopic(thermodynamical) variables for the system, is defining microstate for a system.

A system in general many microstate.

Macro state, is specified by the number of particles in each of energy levels of the system.

Or is defined as a state of the system where the distribution of particles over the energy level is specified.

If N_i is the number of particles that occupy the i^{th} energy level. If there are n energy level, then

$$\sum_{i=1}^{n} N_i = N$$

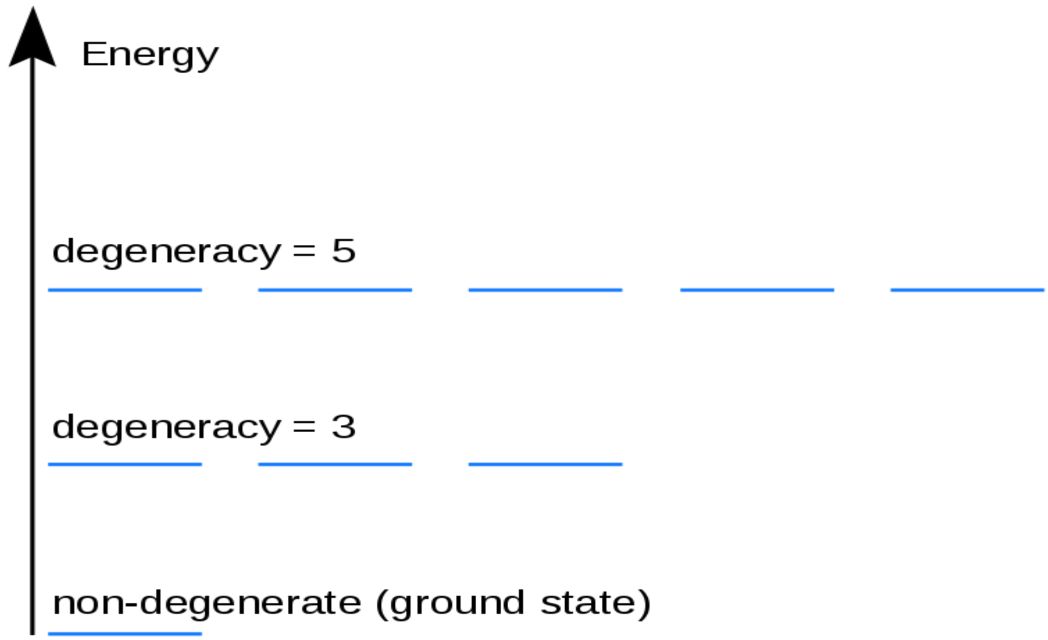
A macrostate is defined by (N_1,N_2,N_3,……….N_n)

Microstate for a system

A microstate are defined corresponding to particular microstate.
Microstate; is defined as a state of the system where all the parameters of the constituents(particles) are specified.
Is specified by the number of particles in each energy state.
The various internal distinct arrangements of the system in a particular macrostate, are known as a microstate of system, corresponding to that microstate.
Microstate for thermodynamical system is in general very very large number.

A microstate is specified by the number of particles in each quantum state.

In general, there will be more than one quantum state for each energy level, a situation called ***Degeneracy***.



Degenerate states in a quantum system

Accessible microstate

The microstate allowed under a constraint on systems are accessible microstate.

Most probable microstates

A system can have many macrostates And there exit very large number of microstates corresponding to each microstate.

Macrostates microstate

A	30000
B	100000
C	1000000
D	600
E	10000

The macrostate having largest number of microstate is most probable macrostate in this example its…..C

The **difference** between microstate and macrostate is that **microstate refers to the microscopic configuration of a thermodynamic system, whereas macrostate refers to the macroscopic properties of a thermodynamic system**.

Microstate vs Macrostate

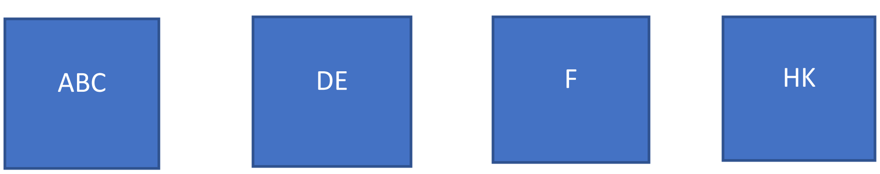
More Information Online WWW.DIFFERENCEBETWEEN.COM

	Microstate	Macrostate
DEFINITION	Microstate is a term that describes the microscopic properties of a thermodynamic system	Macrostate is a term that describes the macroscopic properties of a thermodynamic system
PROPERTIES	Microscopic	Macroscopic
NATURE	Changes of microstate show very slight or no effect on macrostate	Changes in macrostate are the average of large changes of microstates
EXAMPLES	Changes in quantum state	Temperature, pressure, volume and density

Distinguish between **microstate &macrostate**

Let the cell in the phase space are $c_1, c_2, c_3, \ldots\ldots\ldots\ldots c_j$

$N_1=3$ $\qquad$ $N_2=2$ $\qquad$ $N_3=1$ $\qquad$ $N_j=2$



Cell 1 Cell 2 Cell 3 Cell j

The phase points are labeled A,B,C,D,F,H,K

A particular microstate is specified by
Phase points ABC in cell 1
Phase points DE in cell 2
Phase points F in cell 3
Phase points HK in cell j

The corresponding macrostate is specified by the total number Ni of the phase points,

N_1 =3 phase points in cell 1
N_2 =2 phase points in cell 2
N_3 =1 phase points in cell 3
N_j =2 phase points in cell j

Definitions

The following terms are commonly used in statistical mechanic.

Configuration.

Each way in which the molecules of a substance can be distributed. Two types of distribution in statistical mechanics.

i- **Ordered distribution.**
In such case the number of possible configurations of the molecules is the minimum.

ii- **Disordered distribution.**
In this case the number of possible configuration the maximum.

Accessible microstate.

Any microstate of a system which is its quantum state in which the system can be found without breaking any conditions imposed by the macroscopic information about the system.

Degeneracy.

This is the number of accessible microstate.
(an energy level contains more than one energy state)

Non degenerate.

A system is said to be nondegenerate if no two particles in the system have the same energy.

Assembly.

Denote a number N of identical entities, such as molecules, atoms, electrons.

Ensembles

In kinetic theory ensemble means, a collection of a huge number of particles can regard as a system.

In statistical mechanics ensemble means, a collection or ensemble of a huge number of systems.

Ensemble approaches.

There are three important thermodynamic ensembles;

***Microcanonical Ensemble:**

Isolated system with fixed energy E and number particles, N. Each of the members of the ensemble are required to have the same total energy and particles number.

***Canonical Ensemble:**
A statistical ensemble where the energy is not known exactly but the number of particles is fixed N canonical ensemble described a closed system.

***Grand canonical ensemble**.(Nothing is Fixed),
Where neither the energy nor particle number are fixed. The grand canonical ensemble is appropriate for describing an open system. Consist of open assemblies that ca exchange both energies and particles with a reservoir.

What is the difference between Classical and Quantum Statistics?

The following is the difference between classical and quantum statistics;
In classical statistics,
1- The total number of assembly is constant.
2- The energy is continuous.

3- All systems are distinguishable and obeys Maxwell-Boltzmann statistics .
In quantum statistics,
1- The energy is discrete $E_n = \hbar w(n + 1/2)$
2- All particles are indistinguishable.
3-There are two types of quantum statistics.
a- Bose-Einstein statistics (Bosons), not obey Pauli exclusion principle.

b- Fermi-Dirac statistics (Fermions) obey Pauli exclusion principle.