Chapter 3: Systems of Many Particles

Medical Equipment I

2008-2009

Introduction

- Is it possible to use classical mechanics to describe systems of many particles ?
- Example: particles in 1 mm^3 of blood
  - Compute translational motion in 3D

$$v_i(t+\Delta t) = v_i(t) + F_i \Delta t / m \quad , \quad (i = x, y, z)$$

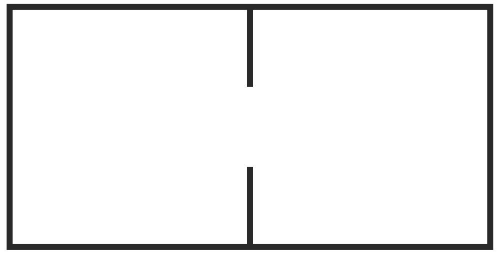
  - 6 multiplications + 6 additions / particle
  - For 10^{19} particle, 10^{20} operations required/interval
  - 10^8 s (3 years) on a 1G operations/s computer !!

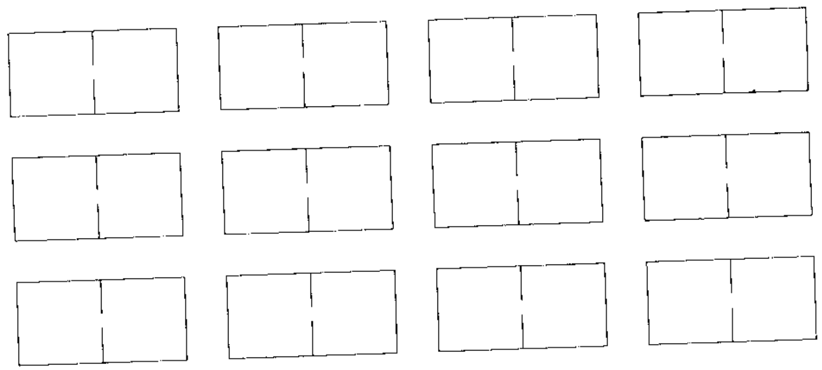
Statistical Mechanics

- Do not care about individual molecules
  - Impossible to trace practically
- Average macroscopic properties over many particles are what we need
- Such properties are studied under statistical physics / statistical mechanics
  - e.g., Pressure, Temperature, etc.
  - Average and probability distribution

Gas Molecules in a Box

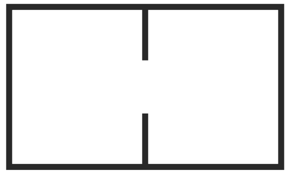
- Total number of molecules = N
- Box with imaginary partition
- Particles in left half = n
- P(n) can be computed from an ensemble of boxes





Gas Molecules in a Box

- Example: N=1
  - P(0)= 0.5 , P(1)= 0.5



- Example: N=2

Molecule 1	Molecule 2	n	$P(n;2)$
R	R	0	$\frac{1}{4}$
R	L	1	$\frac{1}{2}$
L	R	1	
L	L	2	$\frac{1}{4}$

Gas Molecules in a Box

- Example: N=3

Molecule 1	Molecule 2	Molecule 3	n	$P(n;3)$
R	R	R	0	$\frac{1}{8}$
R	R	L	1	
R	L	R	1	$\frac{3}{8}$
L	R	R	1	
L	L	R	2	
L	R	L	2	$\frac{3}{8}$
R	L	L	2	
L	L	L	3	$\frac{1}{8}$

Gas Molecules in a Box

- Histogram representation

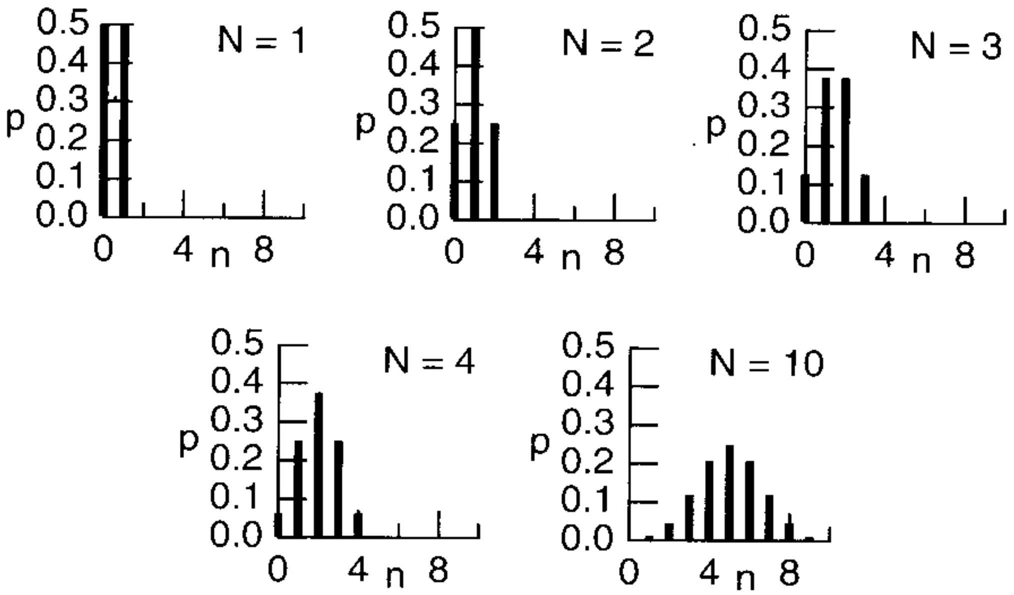
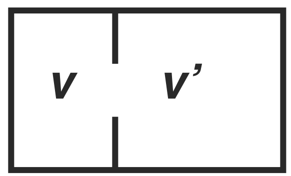


FIGURE 3.2. Histograms of $P(n; N)$ for different values of N.

Gas Molecules in a Box

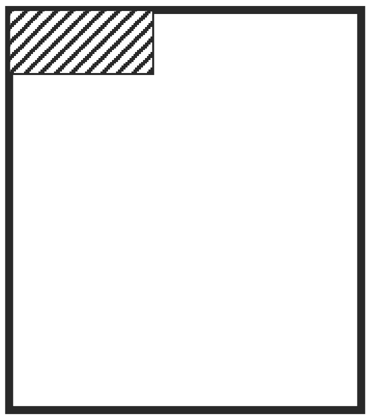
- General case: binomial distribution
- Assume a general box partitioning into two volumes v (left) and v' (right) such that $p=v/V$, $q= v'/V$, then $p+q=1$
- Probability of n particles in volume v given by

$$P(n;N,p) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}$$



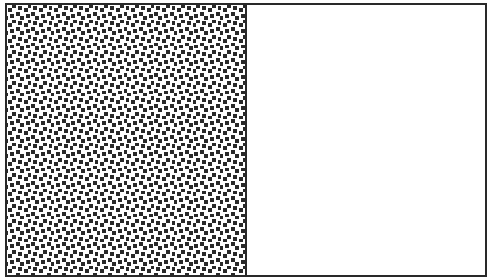
Microstates and Macrostates

- Microstates: all information about a system
  - Position and velocity of all molecules
- Macrostates: average properties
  - Number of molecules in each half
- Example: Toys in a room
  - Microstate: position of every toy
  - Macrostate: “picked-up” or “mess”

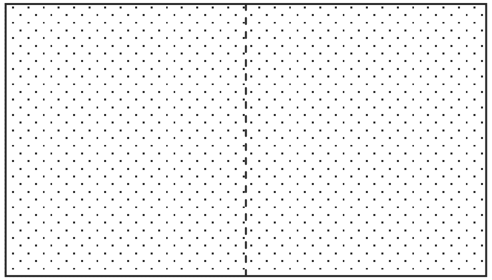


Gas Box Example

- Partition in between



- Partition suddenly removed
  - Many more microstates available
  - Improbable to remain all on left
  - Equilibium: half on each side
  - Macroscopic states not changing with time
  - Most random, most probable



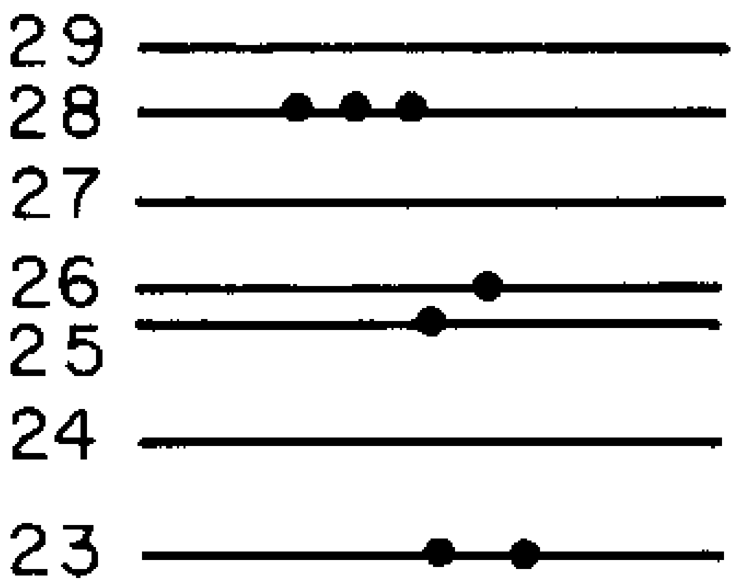
Microstates

- Energy levels defined by a set of quantum numbers = ***3N*** (in 3D)
  - Discrete levels
- Total number of quantum numbers required to specify state of all particles is called *degrees of freedom (f)*
- *Microstate*: specified if all quantum numbers for all particles are specified

First Law of Thermodynamics

- Total energy U = sum of particle energies

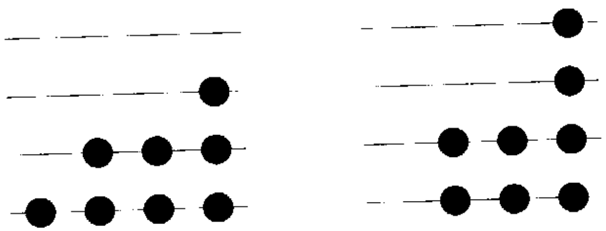
$$U = 2u_{23} + u_{25} + u_{26} + u_{28}$$



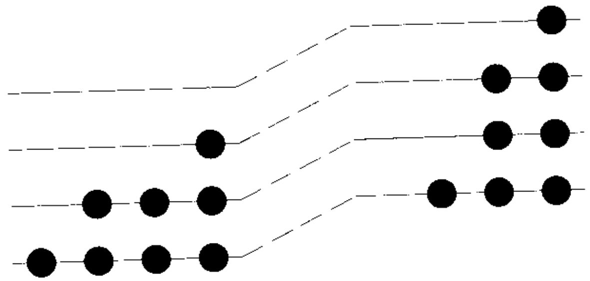
Exchange of Energy

- Exachange forms: Work and Heat

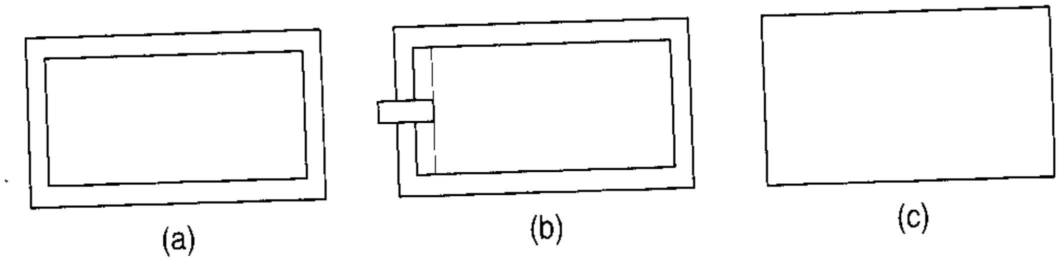
$$\Delta U = Q - W$$



No work – Heat added



Work done – no heat



Specifying Microstates and Macrostates

- Microstates
  - quantum numbers of each particle in the system
- Macrostates
  - All of external parameters
  - Total energy of the system

Basic Postulates

1. If an isolated system is found with equal probability in each one of its accessible microstates, it is in equilibrium
   - Converse is also true
2. If it is not in equilibrium, it tends to change with time until it is in equilibrium
   - Equilibrium is the most random, most probably state.

Assignment

- Problem assignment on web site