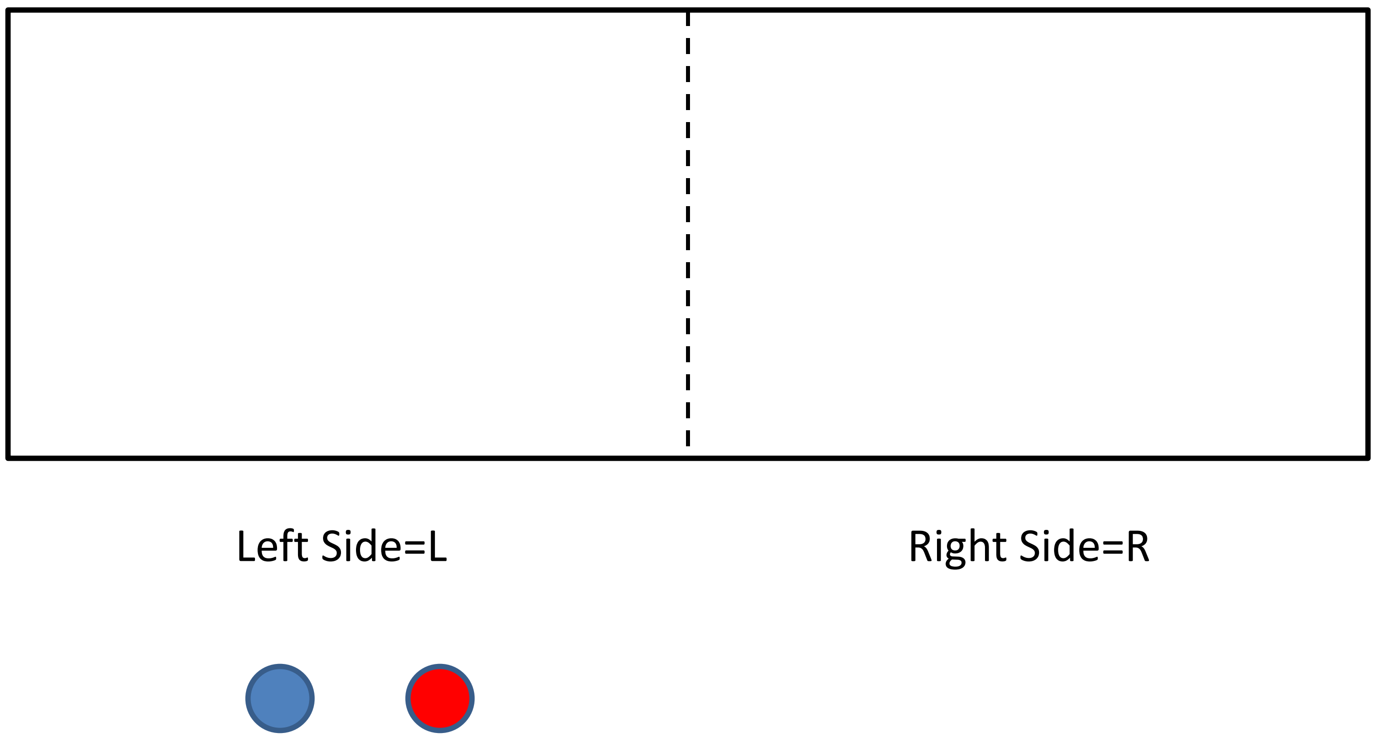
Lecture 8 Topics

- Statistical mechanics
  - Micro vs. macro states
  - Equilibrium states
- New statistical definitions (using Harmonic Oscillators)
  - Energy states
  - Average energy
  - Occupation number
  - Density of states
- Probability distribution
  - Maxwell-Boltzman
  - Bose-Einstein
  - Fermi-Dirac
  - Fermi Energy

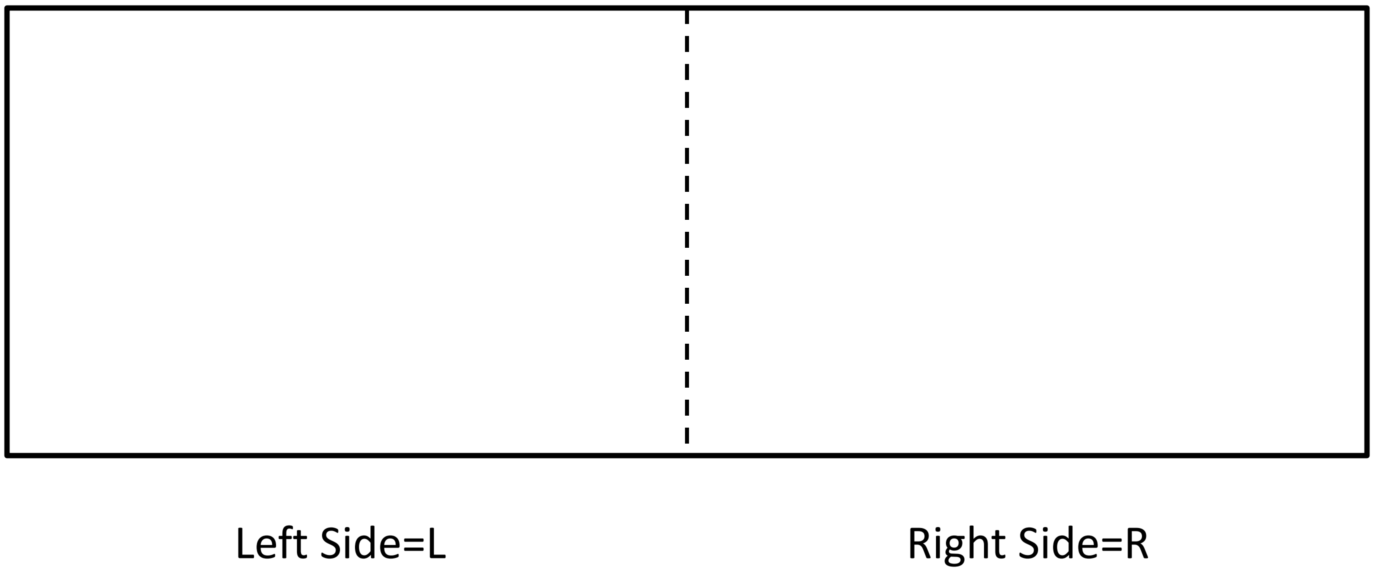
Statistical Mechanics

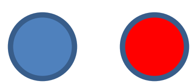
- Describing and predicting properties and behaviors of a system that contains MANY, MANY particles
- Use averages
- Averages can be pretty precise as N becomes really large

Example



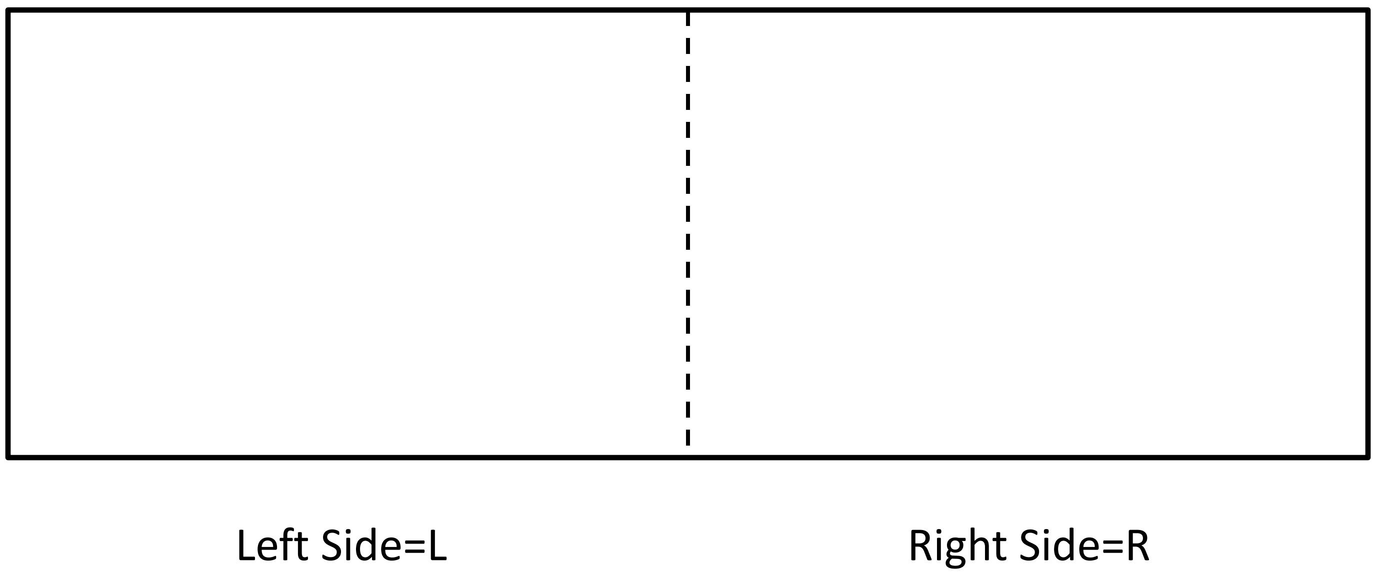
Example

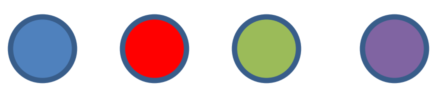


Two Particle System 

- How many possible states related to the number of particles in the right side?
- How many possible arrangements for each state?

Example



Four Particle System 

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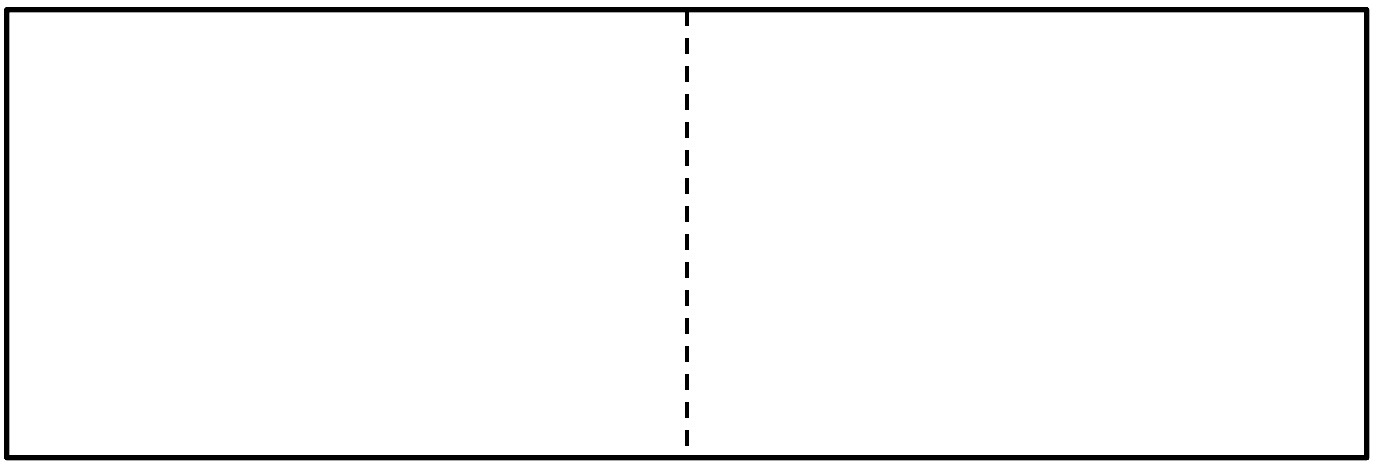
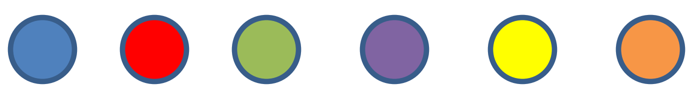


Left Side=L   Right Side=R

Four Particle System 

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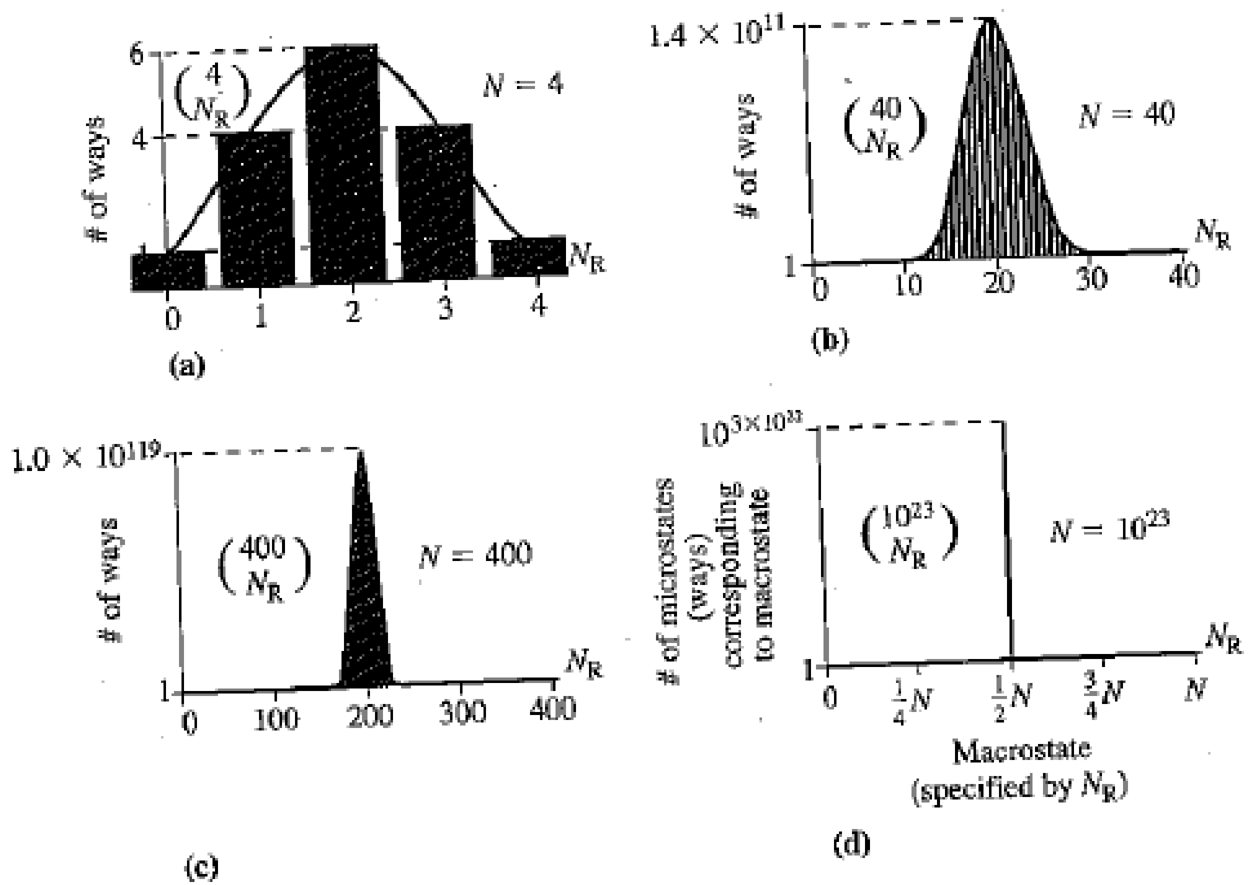
- How many possible arrangements for each state?

How does N affect the distribution?

Figure 9.3 Number of ways of distributing particles on two sides of a room: variation as total number of particles increases from 4 to 10^{23}.



1-D Harmonic Oscillators

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+\frac{1}{2}kx^2\,\psi(x)=\mathrm{E}\,\psi(x)$$

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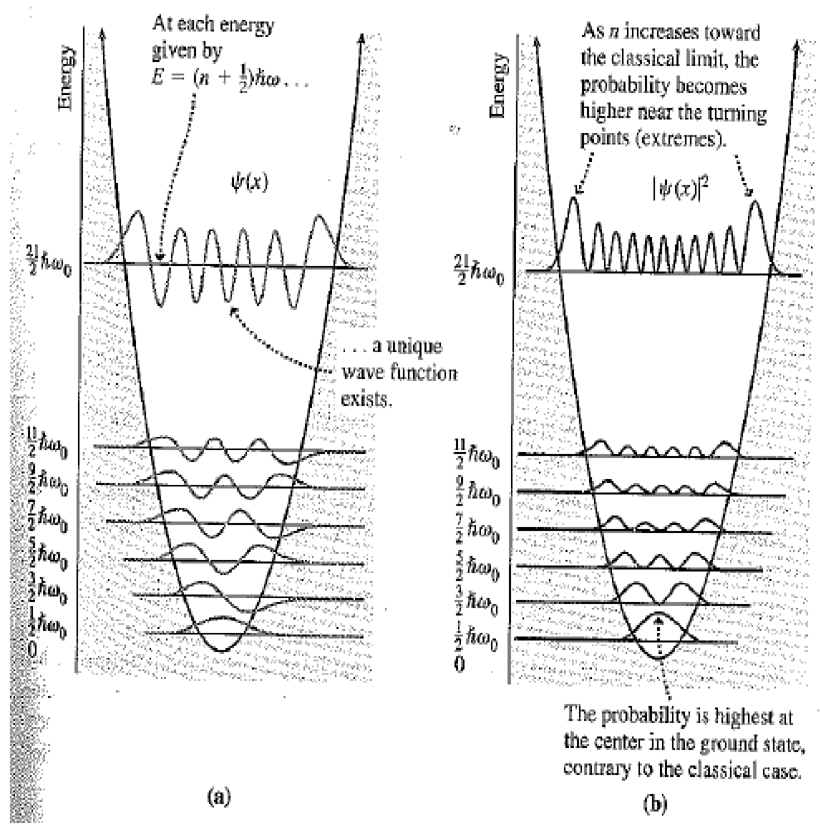
$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega_0$$

$$\psi_n(x)=\left(\frac{b}{2^n n!\sqrt{\pi}}\right)^{\frac{1}{2}}H_n(bx)e^{-\frac{1}{2}b^2x^2}$$



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$$\psi_n(x)=\left(\frac{b}{2^n n!\sqrt{\pi}}\right)^{\frac{1}{2}}H_n(bx)e^{-\frac{1}{2}b^2x^2}$$

Let's take:

$$E_n=n\hbar\omega_0$$

N particle 1d Harmonic Oscillators

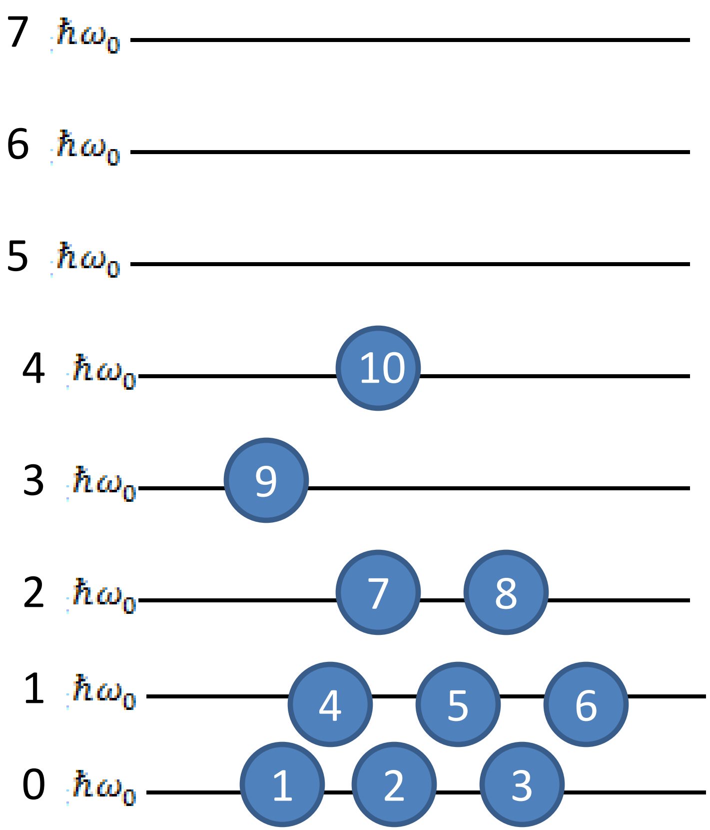
the energy of ith oscillator is in the n_ith energy level

$$E_{n_i} = n_i \hbar \omega_0$$

Total Energy = ?

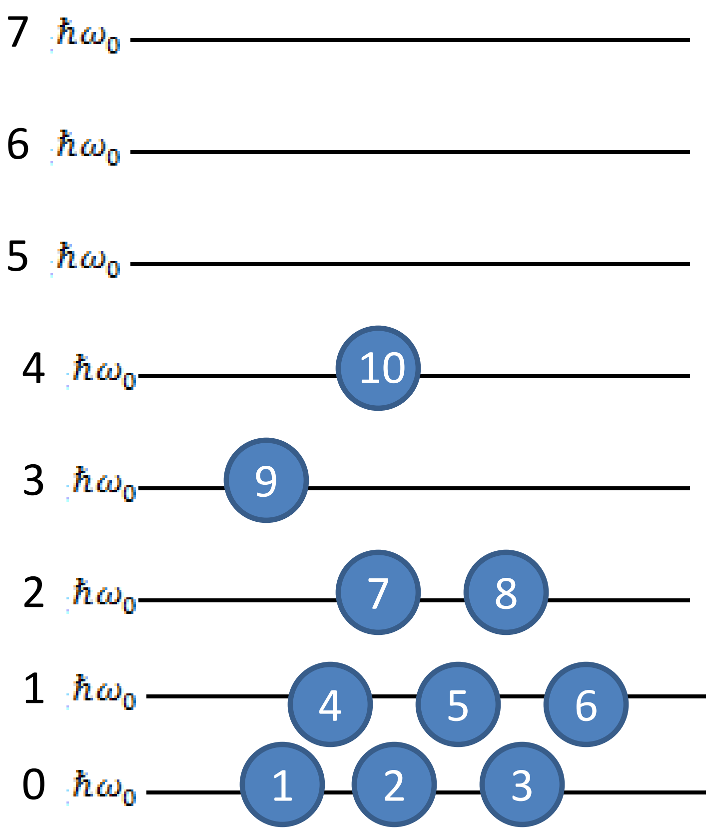
12 particle harmonic oscillator

Total energy



12 particle harmonic oscillator

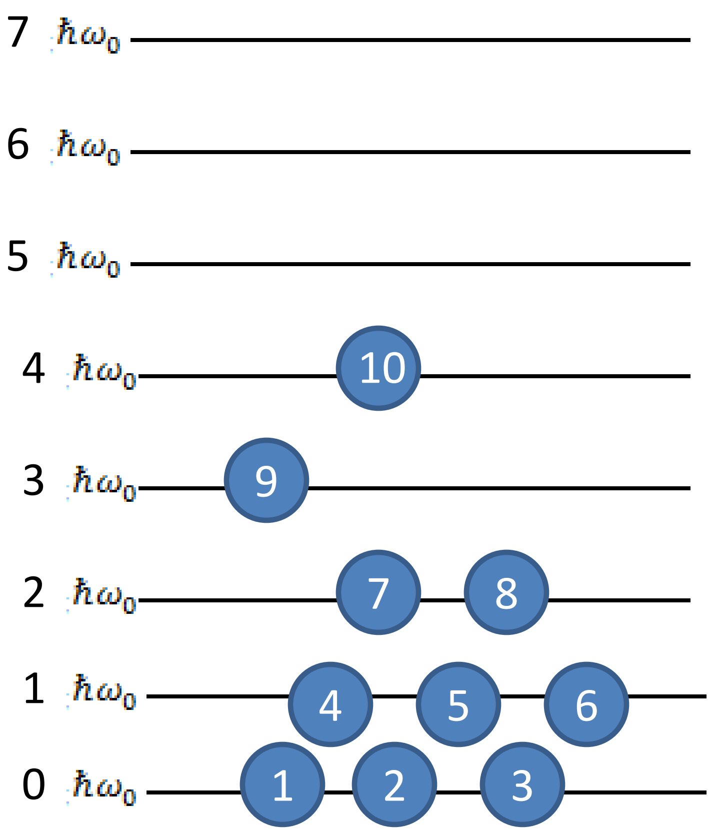
Total energy= 4+3+4+3=14 $\hbar\omega_0$



Energy unit $\hbar\omega_0$	Number of particles	Energy at that level
4	1	4
3	1	3
2	2	4
1	3	3
0	3	0

12 particle harmonic oscillator

Total energy=
(0+0+0+1+1+1+2+2+3+4) $\hbar\omega_0$



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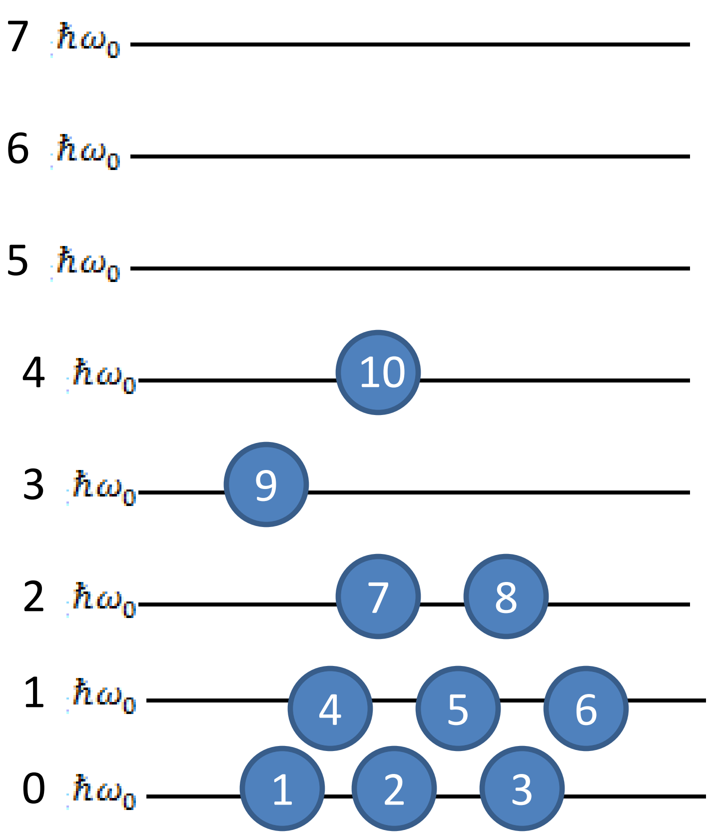
Total Energy = $E = \sum_{i=1}^{N} n_i \hbar \omega_0 = M \hbar \omega_0 \;\; where\, M = \sum_{i=1}^{N} n_i$

Suppose, N=10 and M=50, then average energy = ?

12 particle harmonic oscillator



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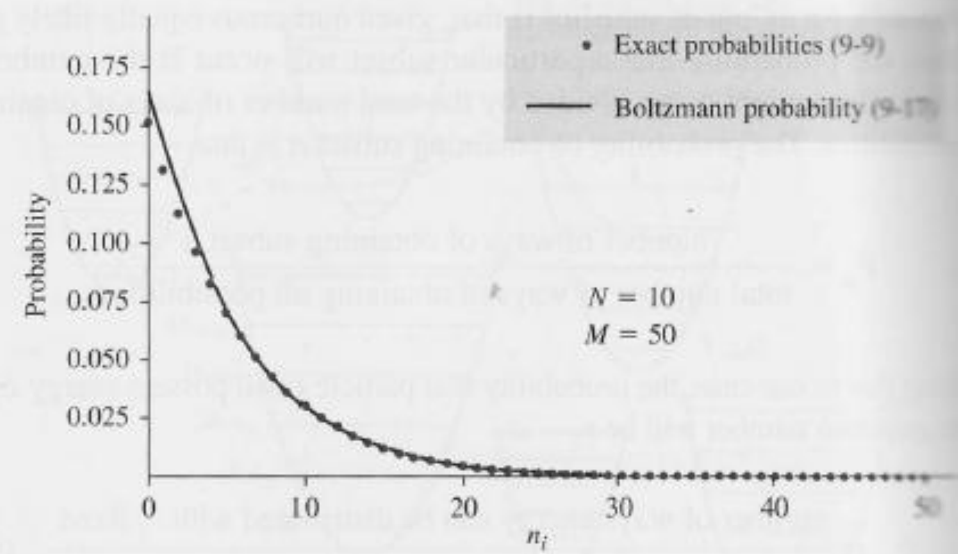
Suppose, N=10 and M=50, then average energy = $\bar{E} = \frac{E}{N} = \frac{50\hbar\omega_0}{10} = 5\hbar\omega_0$

Probability using the exact math expression= $P_{n_i} = \binom{(M - n_i) + N - 1}{(M - n_{i)}} / \binom{M + N - 1}{M}$

N particle 1d Harmonic Oscillators

the energy of ith oscillator

Figure 9.6 Probabilities of a given oscillator being in its n_i state, and Boltzmann probability.



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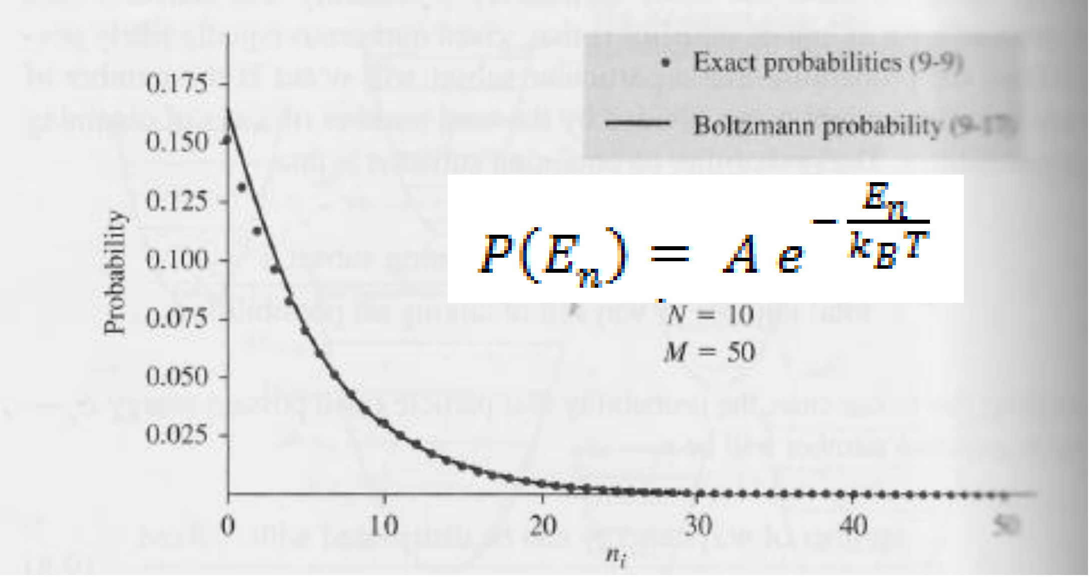

$$P(E_n) = A\, e^{-\frac{E_n}{k_B T}}$$

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Boltzman Distribution/Probability

Boltzman probability: $P(E_n) = A\, e^{-\frac{E_n}{k_B T}}$

$$k_B T(when\ T = 300K, room\ temperature) = \left(1.38x10^{-23}\,\frac{J}{K}\right)(300K) = 4.14\,x\,10^{-21} J = 0.026\ eV$$

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$$\sum P(E_n) = \sum_n A\, e^{-\frac{E_n}{k_B T}} = 1 \rightarrow A = \frac{1}{\sum_n e^{-\frac{E_n}{k_B T}}}$$

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$$D(E) \equiv \frac{dn}{dE}$$

→ When E spacing is very close

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Apply Boltzman Probability to HO

$$E_n = n\hbar\omega_0$$

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$$\bar{E} = \sum E_n P(E_n)$$

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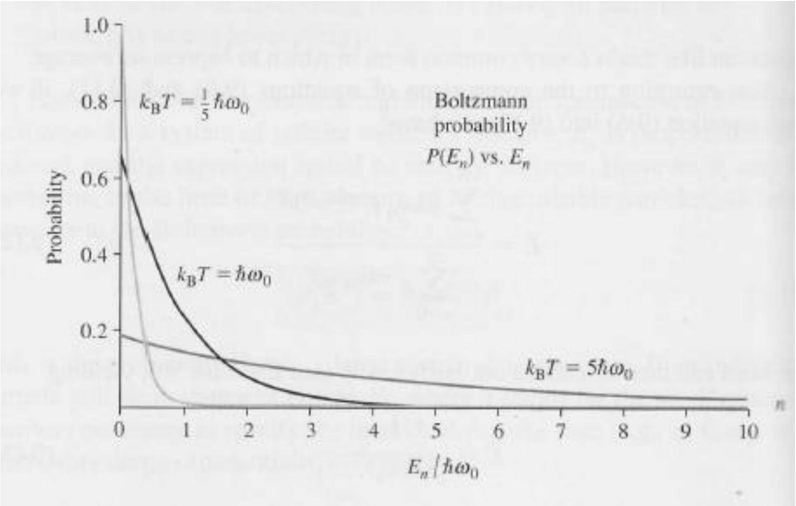

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When energy is closely spaced

$$E = n\hbar\omega_0$$
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Density of states: $$\frac{dn}{dE} = D\left(E\right)$$

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Since $\int_0^\infty x^m e^{-bx}dx = \frac{m!}{b^{m+1}}$

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Three types of distribution

Distribution	Occupation index	Particles	Identical particles?	Spin	Distingui-shable?	Exclusion principle?
Boltzman	$\frac{1}{Be^{E/k_B T}}$	Classical	Yes	Any spin	Yes	No
Bose-Einstein	$\frac{1}{Be^{E/k_B T} - 1}$	Bosons	Yes	0 or integer spin	No	No
Fermi-Dirac	$\frac{1}{Be^{E/k_B T} + 1}$	Fermions	Yes	1/2	No	Yes

When N is REALLY large, like 10^{23}

System requirement

- Conservation of particles

$$\sum \mathcal{N}(E_i) = \mathcal{N}(E_1) + \mathcal{N}(E_2) + \cdots + \mathcal{N}(E_k) = N$$

- Conservation of energy

$$\sum \mathcal{N}(E_i)E_i = \mathcal{N}(E_1)E_1 + \mathcal{N}(E_2)E_2 + \cdots + \mathcal{N}(E_k)E_k = E$$

- Example: 4 (a, b, c, d) particles with total energy of $2\hbar\omega_0$.
  - Consider $E_i = n_i\hbar\omega_0$

Maxwell-Boltzman

n	10 possible ways	No. of possibilities where a particle can have n quantum number (#)	Probability of a particle having the n quantum number (P=#/40)	Probable number of particles to have the n quantum number P x 4
2				
1				
0				
	Total	40	1.0	4.0

Maxwell-Boltzman

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2	*a*	*b*	*c*	*d*									
1					*ab*	*ac*	*ad*	*bc*	*bd*	*cd*			
0	*bcd*	*acd*	*abd*	*abc*	*cd*	*bd*	*bc*	*ad*	*ac*	*ab*			
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2	*a*	*b*	*c*	*d*							4	0.1	0.4
1					*ab*	*ac*	*ad*	*bc*	*bd*	*cd*	12	0.3	1.2
0	*bcd*	*acd*	*abd*	*abc*	*cd*	*bd*	*bc*	*ad*	*ac*	*ab*	24	0.6	2.4
										Total	40	1.0	4.0

Bose-Einstein

n	Two possible ways		(#)	(P=#/8)	P x 4
2					
1					
0					
		Total	8	1.000	4.00

Bose-Einstein

n	Two possible ways		(#)	(P=#/8)	P x 4
2	X				
1		XX			
0	XXX	XX			
		Total	8	1.000	4.00

Bose-Einstein

n	Two possible ways		(#)	(P=#/8)	P x 4
2	X		1	0.125	0.50
1		XX	2	0.250	1.00
0	XXX	XX	5	0.625	2.50
		Total	8	1.000	4.00

Fermi-Dirac

n	1 possible way	(#)	(P=#/8)	P x 4
2				
1				
0				
	Total	4	1.0	4.0

Fermi-Dirac

n	1 possible way	(#)	(P=#/8)	P x 4
2				
1	XX			
0	XX			
	Total	4	1.0	4.0

Fermi-Dirac

n	1 possible way	(#)	(P=#/8)	P x 4
2		0	0.0	0.0
1	XX	2	0.5	2.0
0	XX	2	0.5	2.0
	Total	4	1.0	4.0

Probable Number Plotting

n	Maxwell-Boltzmann	Bose-Einstein	Fermi-Dirac
2	.4	0.5	0.0
1	1.2	1.0	2.0
0	2.4	2.5	2.0

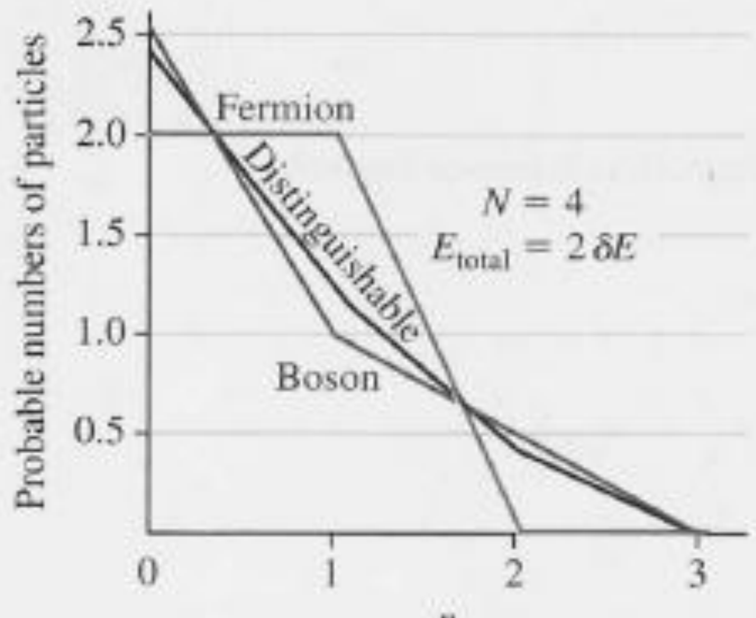


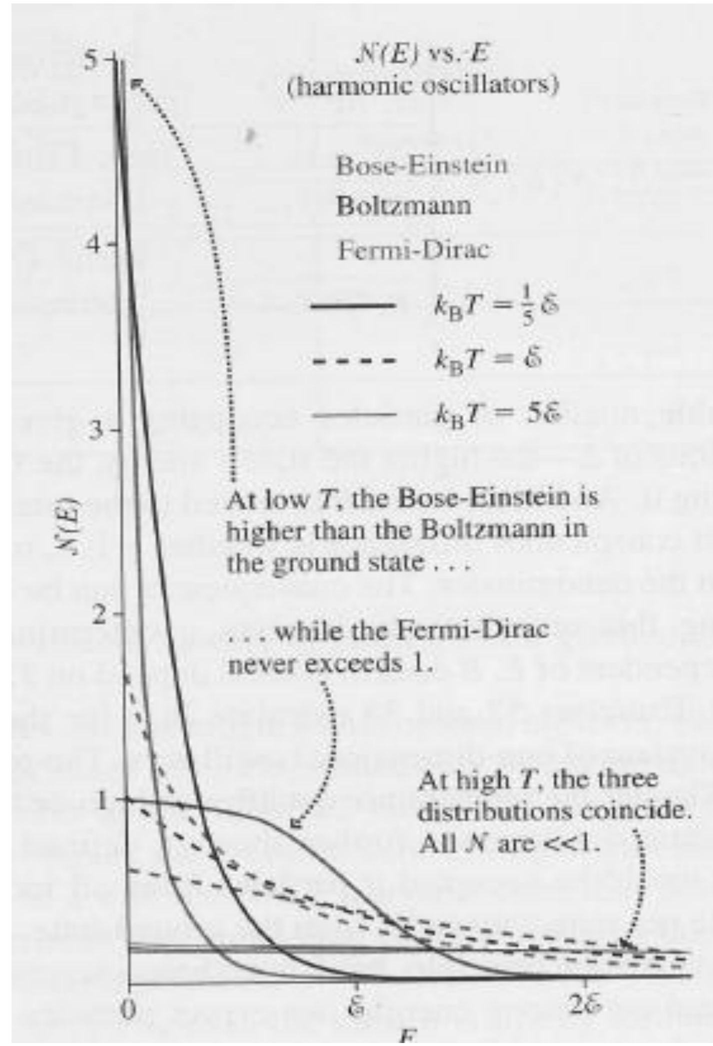
Figure 9.9 The probable number of particles at the allowed energies depends on whether the particles are bosons, fermions, or distinguishable.

Probability distribution comparison

As E increases

k_BT is larger than E

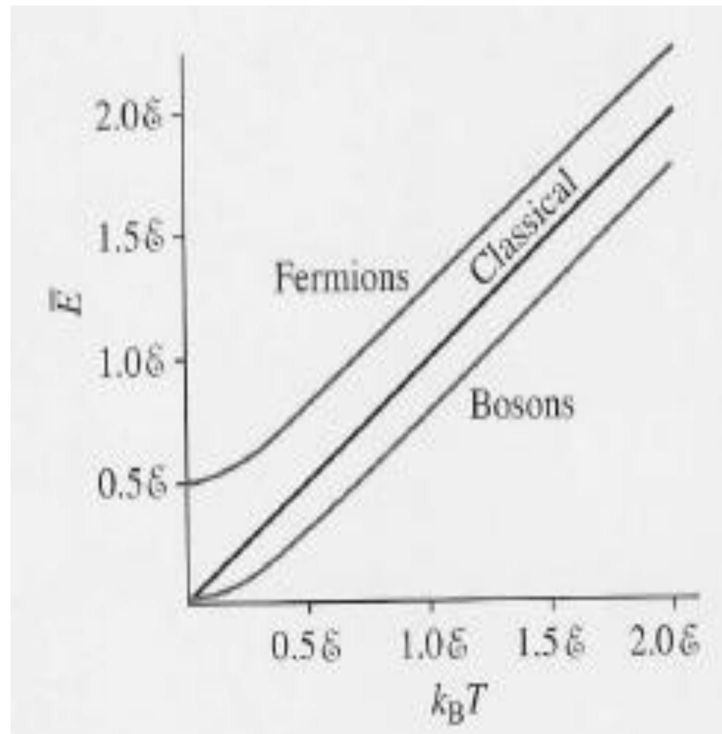
k_BT is smaller than E



Average energy

$k_B T$ is larger than E (high temp)

$k_B T$ is smaller than E (low temp)



Fermi Energy

$$\mathcal{N}(E_F) = \frac{1}{Be^{E/k_BT}+1} = \frac{1}{2} \quad \text{which makes } B = e^{-\frac{E_F}{k_BT}}$$

$$\mathcal{N}(E_F) = \frac{1}{e^{(E-E_F)/k_BT}+1}$$