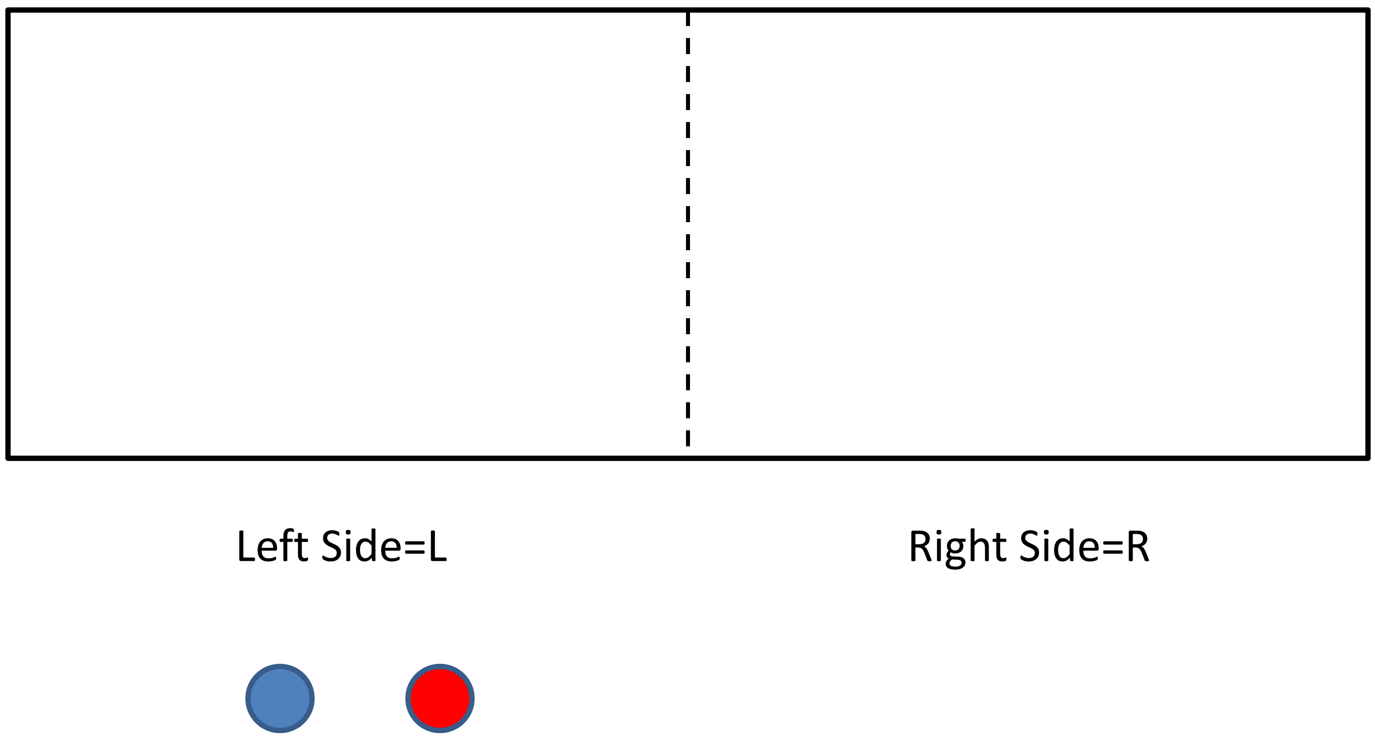
Lecture 8 Topics

- 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

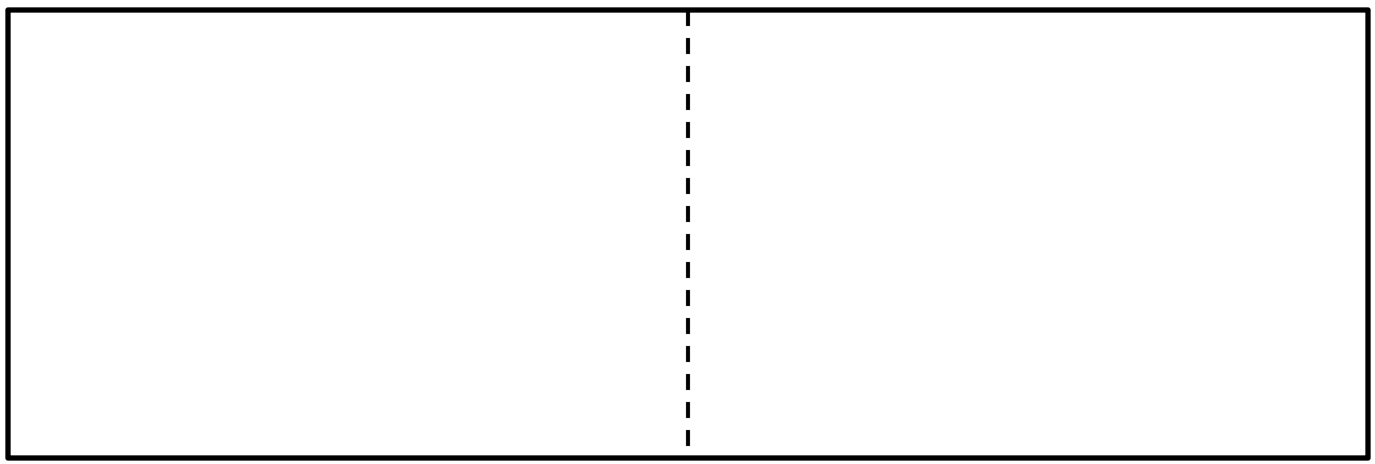
Statistical Mechanics

- Describing and predicting properties and behaviors of a system that contains MANY, MANY particles
- Use averages, like $\bar{E}$
- Averages can be pretty precise as N becomes really large

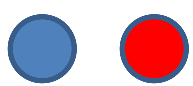
Example



Example



Left Side=L　　　　Right Side=R

Two Particle System 

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

Particle 1	Particle 2	Number of particles in the right side
L	L	0
L	R	1
R	L	1
R	R	2

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L	R	1
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R	R	2

Number of particles in the right side	Number of states	Probability =Number of states/total number of possible states
0	1	¼
1	2	2/4
2	1	¼

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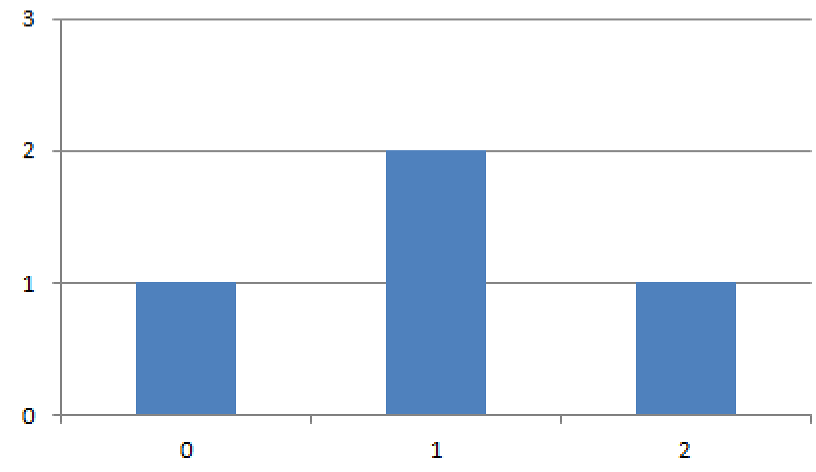

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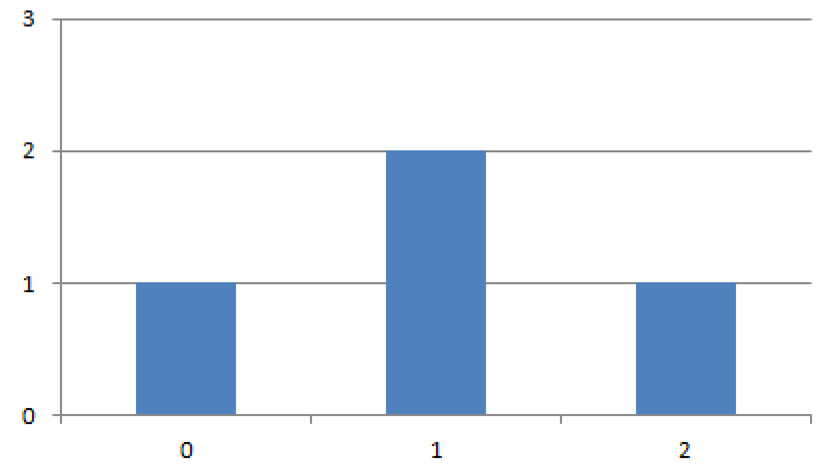

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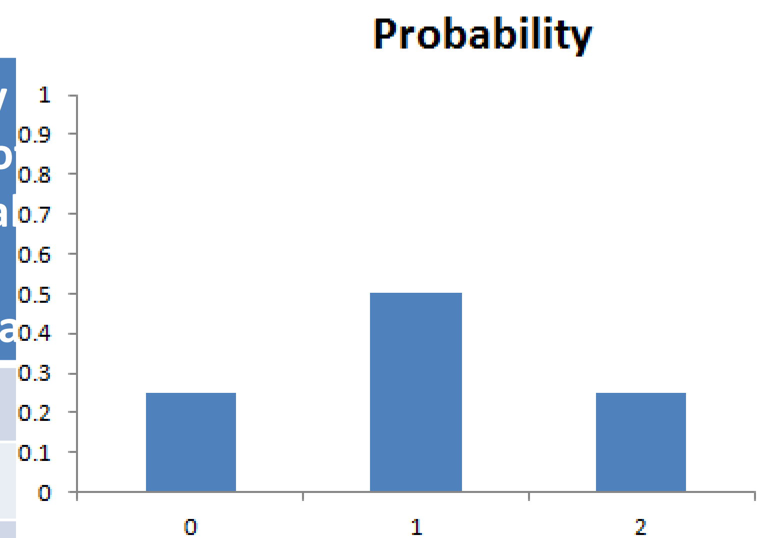
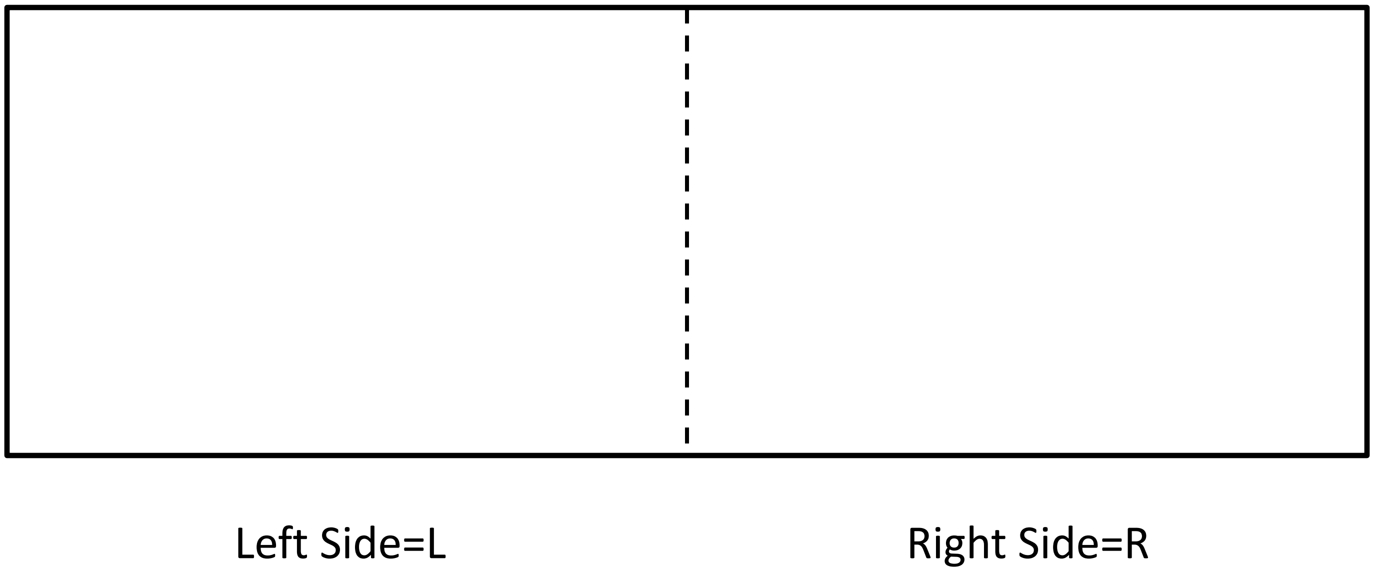
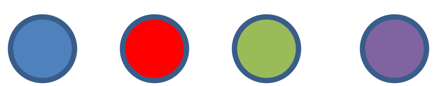


Example



Four Particle System 

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

Particle 1	Particle 2	Particle 3	Particle 4	No. of particles in the right side

No. of possibilities for a particle to be found in the right side:

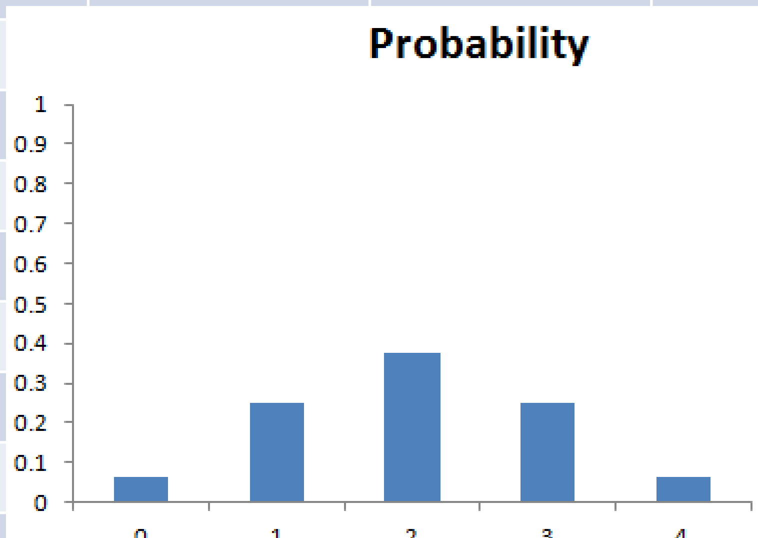
0:
1:
2:
3:
4:

Particle 1	Particle 2	Particle 3	Particle 4	No. of particles in the right side
L	L	L	L	0
L	L	L	R	1
L	L	R	L	1
L	L	R	R	2
L	R	L	L	1
L	R	L	R	2
L	R	R	L	2
L	R	R	R	3
R	L	L	L	1
R	L	L	R	2
R	L	R	L	2
R	L	R	R	3
R	R	L	L	2
R	R	L	R	3
R	R	R	L	3
R	R	R	R	4

No. of possibilities for a particle to be found in the right side:

0:1
1:4
2:6
3:4
4:1

Particle 1	Particle 2	Particle 3	Particle 4	No. of particles in the right side
L	L	L	L	0
L	L	L	R	1
L	L	R	L	1
L	L			
L	R			
L	R			
L	R			
L	R			
R	L			
R	L			
R	L	R	L	2
R	L	R	R	3
R	R	L	L	2
R	R	L	R	3
R	R	R	L	3
R	R	R	R	4



0:1
1:4
2:6
3:4
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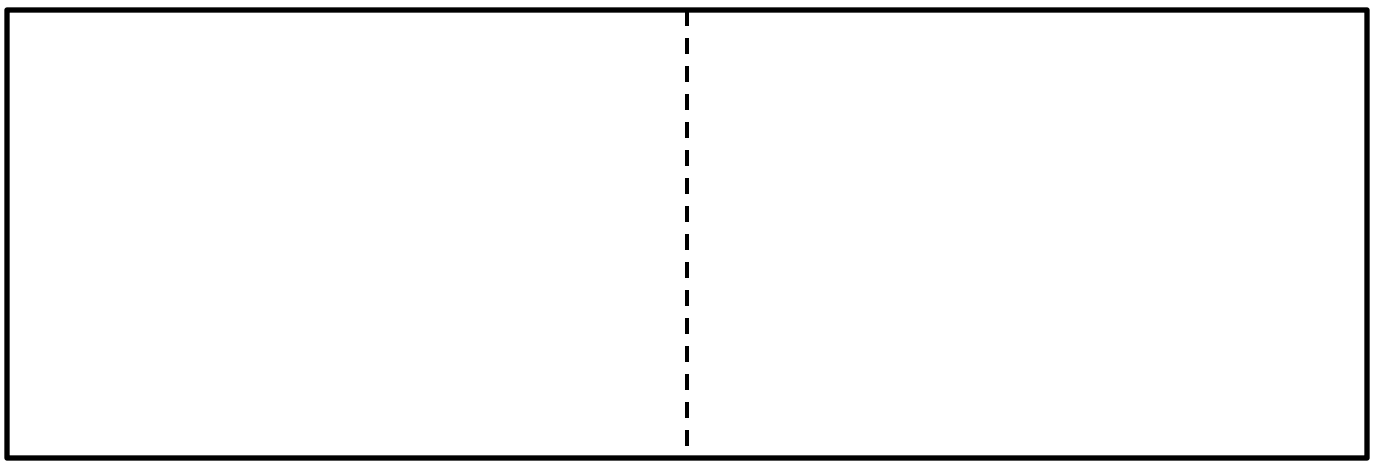
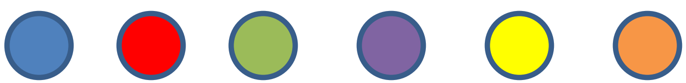
$$\binom{N}{N_R} = \frac{N!}{N_R!\,(N-N_R)!}$$

Example



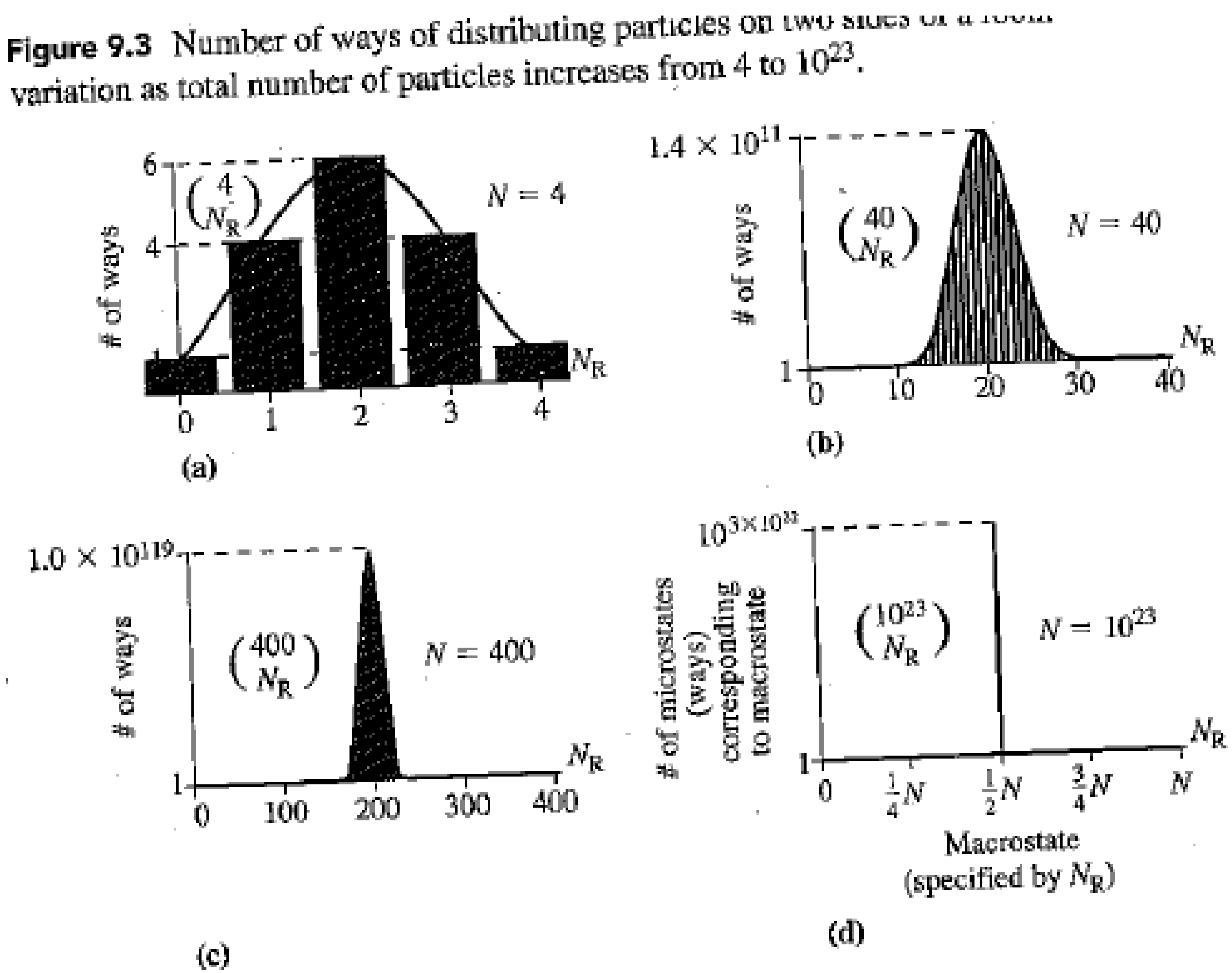
Left Side=L Right Side=R

Six Particle System



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

How does N affect the distribution?



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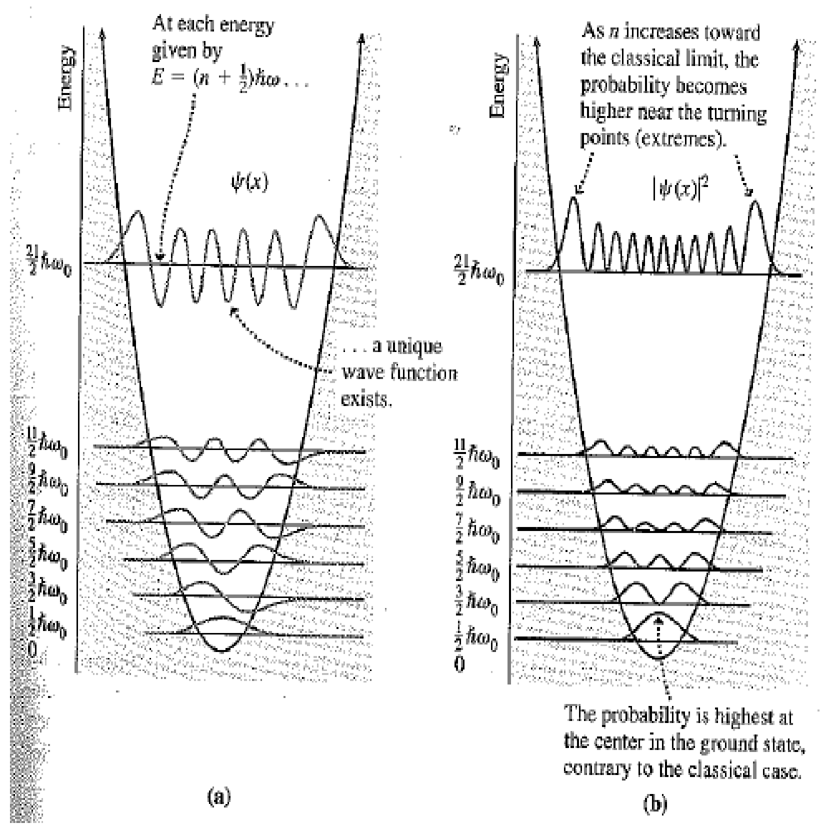
$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega_0$$

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



1-D Harmonic Oscillators

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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

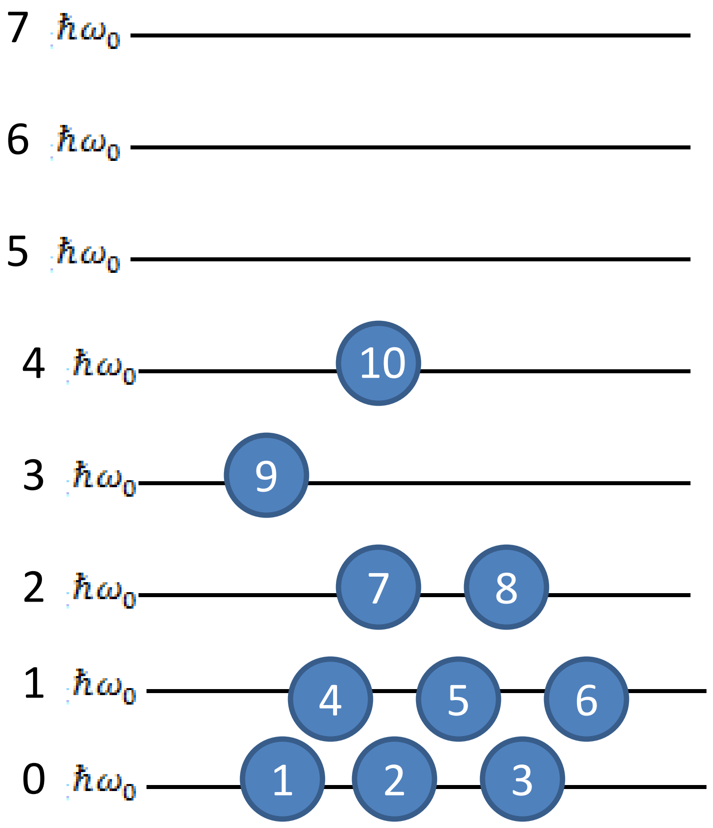
the energy of ith oscillator is in the n_ith energy level

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

Total Energy = ?

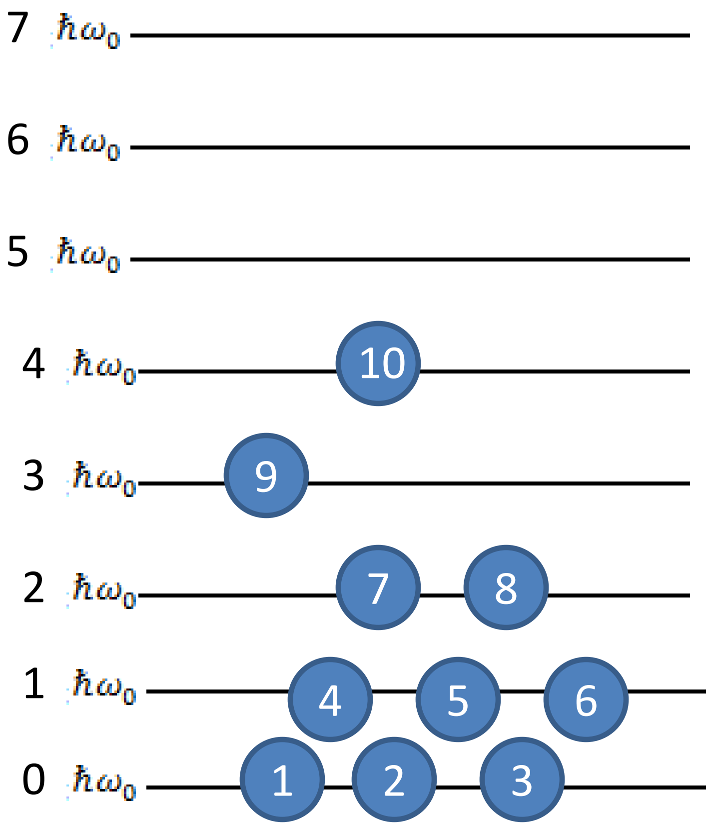
12 particle harmonic oscillator

Total energy



12 particle harmonic oscillator

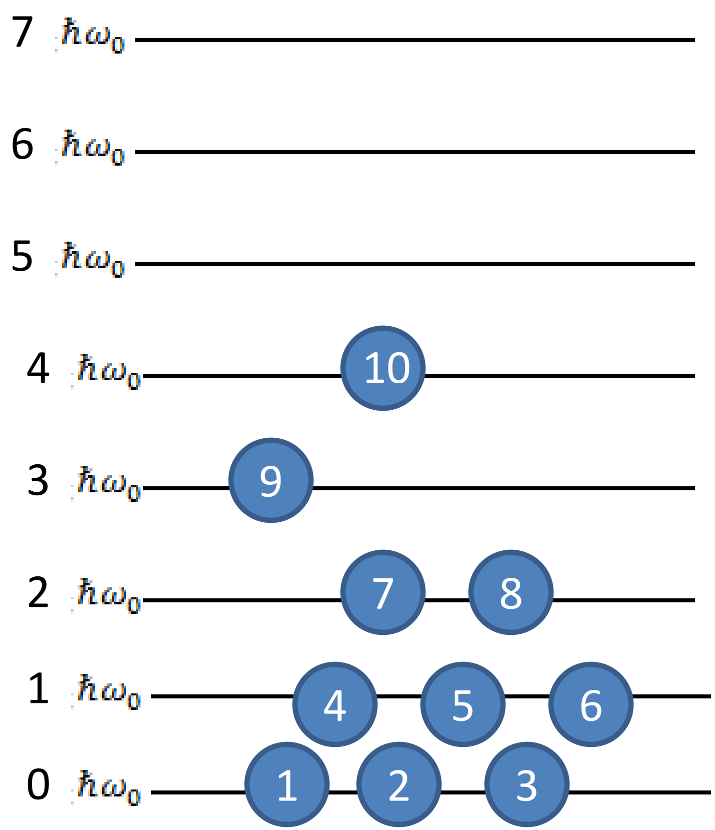
Total energy= 4+3+4+3=14 $\hbar\omega_0$



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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1	3	1+1+1
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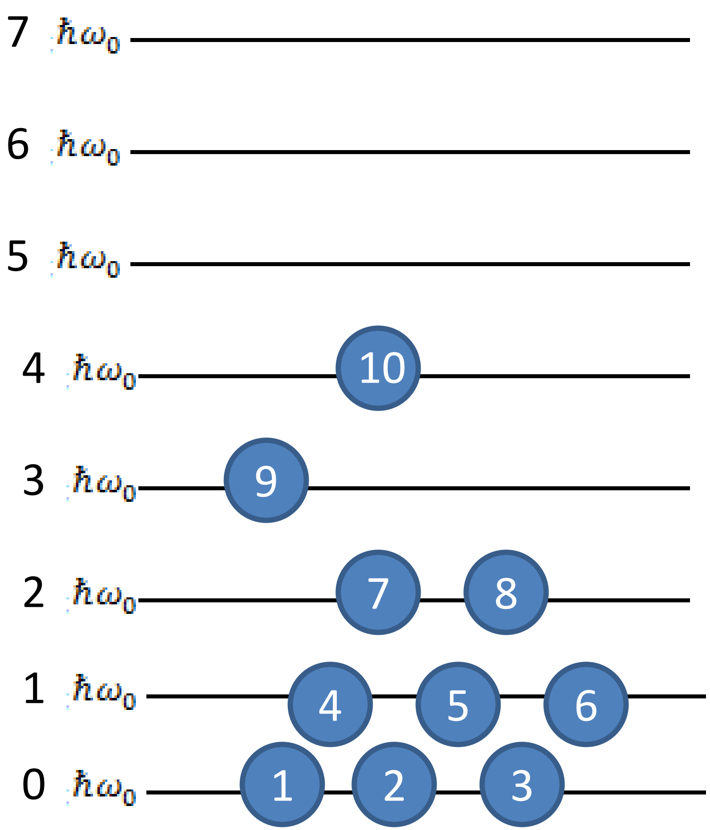

Total energy=
(0+0+0+1+1+1+2+2+3+4) $\hbar\omega_0$

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

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N particle 1d Harmonic Oscillators

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

N particle 1d Harmonic Oscillators

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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 = $\bar{E} = \frac{E}{N} = \frac{50\hbar\omega_0}{10} = 5\hbar\omega_0$

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

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

Suppose, N=10 and M=50, t

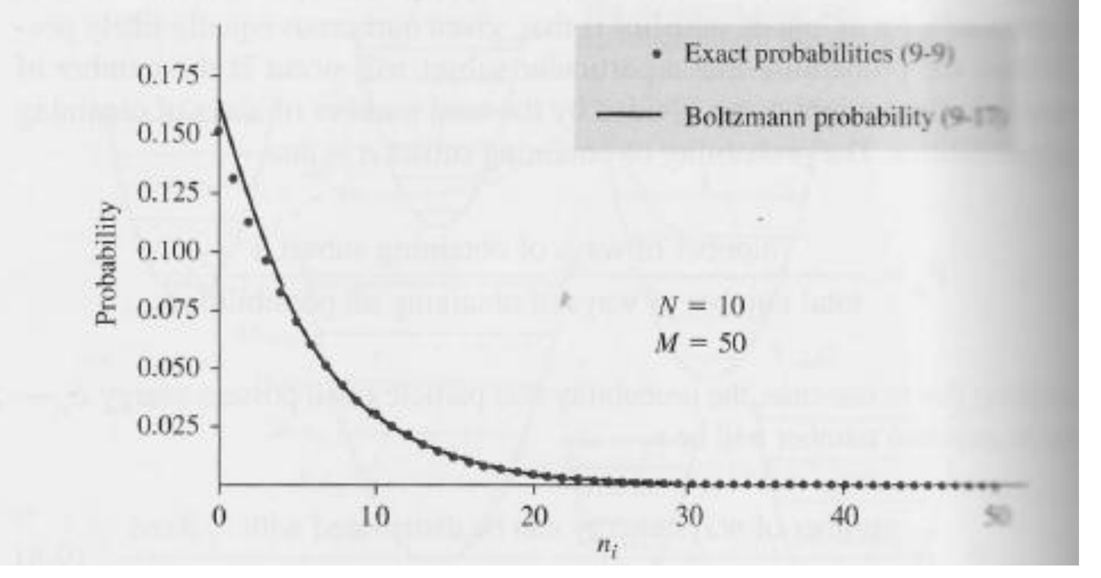

Figure 9.6 Probabilities of a given oscillator being in its n_i state, and Boltzmann probability.

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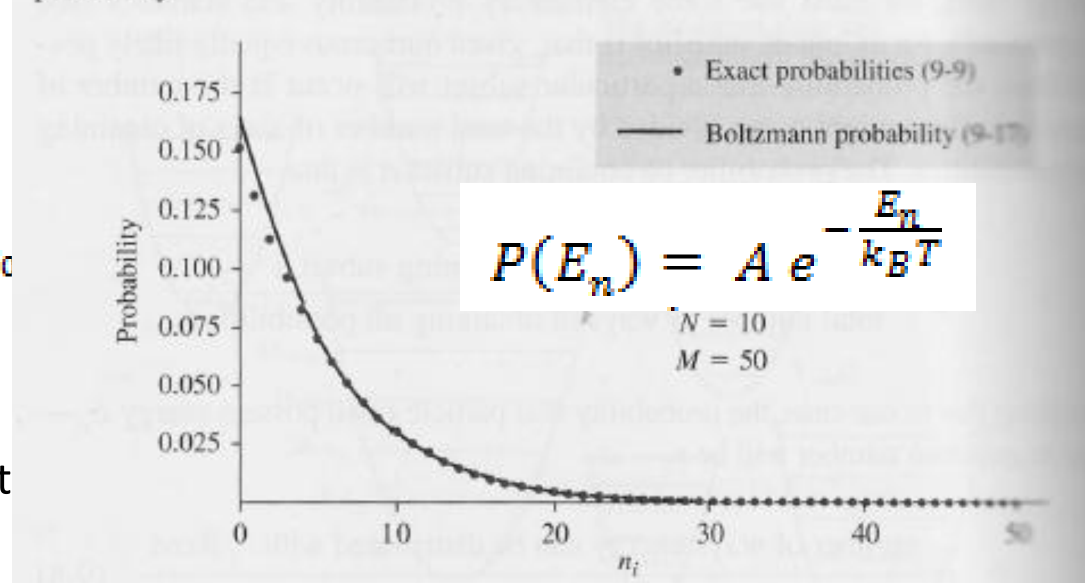
Figure 9.6 Probabilities of a given oscillator being in its n_i state, and Boltz probability.



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

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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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Occupation number: $$\mathcal{N}(E_n)_{Boltman} = N\, P(E_n) = N\,\frac{e^{-\frac{E_n}{k_B T}}}{\sum_n e^{-\frac{E_n}{k_B T}}}$$

Boltzman Distribution/Probability

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Boltzman Distribution/Probability

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Density of states over (E, E+dE): $$D(E) \equiv \frac{dn}{dE}$$

→ When E spacing is very close

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Occupation number: $$\mathcal{N}(E_n)_{Boltman} = N\, P(E_n) = N \frac{e^{-\frac{E_n}{k_B T}}}{\sum_n e^{-\frac{E_n}{k_B T}}}$$

Density of states over (E, E+dE): $$D(E) \equiv \frac{dn}{dE}$$

→ When E spacing is very close

Apply Boltzman Probability to HO

$$E_n = n\hbar\omega_0$$

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

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

Apply Boltzman Probability to HO

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

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Apply Boltzman Probability to HO

$$E_n = n\hbar\omega_0$$

$$P(E_n) = \frac{e^{-\frac{E_n}{k_B T}}}{\sum_n e^{-\frac{E_n}{k_B T}}} = \frac{e^{-\frac{n\hbar\omega_0}{k_B T}}}{\sum_n e^{-\frac{n\hbar\omega_0}{k_B T}}}$$

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$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \; ; \; \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2}$$

Apply Boltzman Probability to HO

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Apply Boltzman Probability to HO

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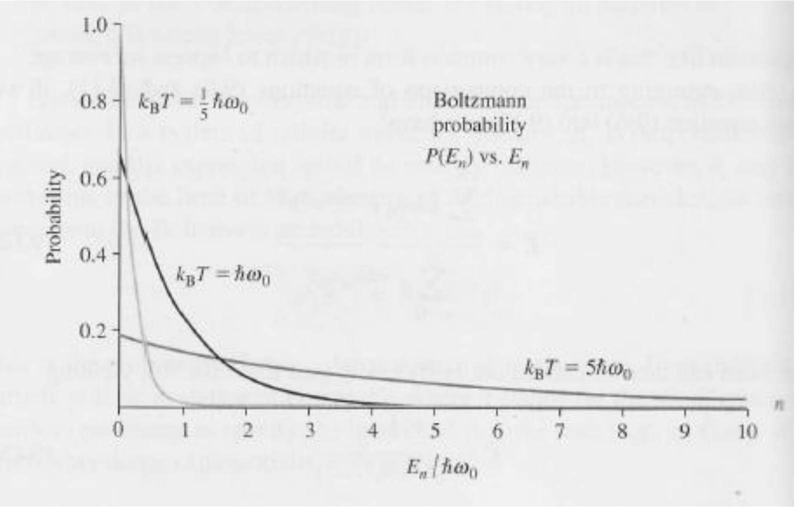

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$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \; ; \; \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2}$$

When energy is closely spaced

$$E = n\hbar\omega_0$$
$$n = \frac{E}{\hbar\omega_0}$$

Density of states: $\frac{dn}{dE} = D(E)$

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Average Energy: $\bar{E} = \frac{\int E\, \mathcal{N}(E) D(E) dE}{\int \mathcal{N}(E) D(E) dE}$

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Average Energy: $\bar{E} = \frac{\int E\,\mathcal{N}(E)D(E)dE}{\int \mathcal{N}(E)D(E)dE} = \frac{\int E\;NAe^{-E/k_BT}1/\hbar\omega_0 dE}{\int NAe^{-E/k_BT}1/\hbar\omega_0 dE} = k_BT$

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

When energy is closely spaced

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Average Energy: $\bar{E} = \frac{\int E\,\mathcal{N}(E)D(E)dE}{\int \mathcal{N}(E)D(E)dE} = \frac{\int E\ NAe^{-E/k_BT}1/\hbar\omega_0 dE}{\int NAe^{-E/k_BT}1/\hbar\omega_0 dE} = k_BT$

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

Compare with summation:

$$\bar{E} = \sum E_n P(E_n) = \frac{\sum_n n\hbar\omega_0 e^{-\frac{n\hbar\omega_0}{k_BT}}}{\sum_n e^{-\frac{n\hbar\omega_0}{k_BT}}} = \frac{\hbar\omega_0}{e^{\frac{n\hbar\omega_0}{k_BT}}-1}$$

When energy is closely spaced

$$E = n\hbar\omega_0$$

$$n = \frac{E}{\hbar\omega_0}$$

Density of states: $\frac{dn}{dE} = D(E) = \frac{1}{\hbar\omega_0}$

Average Energy: $\bar{E} = \frac{\int E\,\mathcal{N}(E)D(E)dE}{\int \mathcal{N}(E)D(E)dE} = \frac{\int E\,NAe^{-E/k_BT}1/\hbar\omega_0\,dE}{\int NAe^{-E/k_BT}1/\hbar\omega_0\,dE} = k_BT$

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

Compare with summation:

$$\bar{E} = \sum E_n P(E_n) = \frac{\sum_n n\hbar\omega_0 e^{-\frac{n\hbar\omega_0}{k_BT}}}{\sum_n e^{-\frac{n\hbar\omega_0}{k_BT}}} = \frac{\hbar\omega_0}{e^{\frac{n\hbar\omega_0}{k_BT}}-1} = k_BT$$