PHY 341/641
Thermodynamics and Statistical Physics

Lecture 11

Some further comments about probability theory and a beginning discussion of methodologies of statistical mechanics. (Chapters 3&4 in STP)

A. Poisson distribution and other distributions
B. Examples of macrostates and microstates

Schedule and assignments

Note: This schedule may need to be modified -- please check for changes and additions frequently.

No.	Lecture Date	Topic	Text Sections	Problem Assignments	Assignment Due Date
1	1/18/2012	Introductory concepts	1.1-1.5	HW 1	1/23/2012
2	1/20/2012	Introductory concepts	1.6-1.12	HW 2	1/23/2012
3	1/23/2012	First Law of Thermodynamics	2.1-2.11	HW 3	1/25/2012
4	1/25/2012	Second Law of Thermodynamics	2.12-2.14	HW 4	1/27/2012
5	1/27/2012	Entropy	2.15-2.19	HW 5	1/30/2012
6	1/30/2012	Thermodynamic Potentials	2.20-2.21	HW 6	2/1/2012
7	2/01/2012	Thermodynamic Potentials	2.22-2.24	HW 7	2/3/2012
8	2/03/2012	Introduction to probability theory	3.1-3.3	HW 8	2/6/2012
9	2/06/2012	Probability distributions	3.4-3.5	HW 9	2/8/2012
10	2/08/2012	Continuous distributions/Central limit theorem	3.6-3.10	HW 10	2/10/2012
11	2/10/2012	Introduction to statistical mechanics	4.1-4.2	HW 11	2/13/2012
12	2/13/2012	Enumeration of microstates	4.3	HW 12	2/15/2012
	2/15/2012				
	2/17/2012				
	2/20/2012				
	2/22/2012				
	2/24/2012				
	2/27/2012	APS			
	2/29/2012	APS			

Poisson probability distribution –
Approximation to binomial distribution for small p

$$\text{Full binomial distribution: } P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

$$\text{Assume} \quad N >> n \qquad\qquad p << 1$$

$$\frac{N!}{n!(N-n)!} \approx \frac{N^n}{n!}$$

$$\ln q^{N-n} = (N-n)\ln(1-p) \approx -(N-n)p \approx -Np$$

$$P_N(n) \approx \frac{N^n}{n!} p^n e^{-Np} = \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle}$$

$$\text{Check:} \qquad \langle n \rangle = \sum_{n=0}^{\infty} n \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle} = \langle n \rangle$$

Other probability distributions:

Continuous distributions $\quad p(x) \equiv \text{probability distribution}$

$$\int_{-\infty}^{\infty} p(x)dx = 1$$

Probability for x in given range: $P(a \le x \le b) = \int_a^b p(x)dx$

Average value of any function for $f(x)$: $\langle f \rangle = \int_{-\infty}^{\infty} f(x)\, p(x)dx$

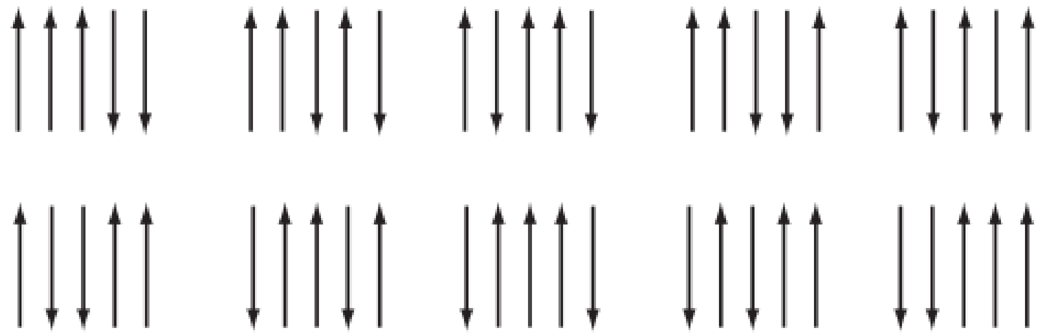
Example:

$$p(x) = \frac{1}{\pi}\frac{\gamma}{(x-a)^2 + \gamma^2}$$

Some methodologies of statistical mechanics

Example: Isolated closed system in a particular "macrostate"; analyze possible "microstates"

System 1: N=5 spins, where s_n=+1 or -1 and Σs_n=1



Ω=10

$$P_i = \frac{1}{\Omega}$$

$$\langle s_n \rangle = \sum_{i=1}^{\Omega} s_{n,i} P_i = \frac{1}{\Omega}\left[6(+1) + 4(-1)\right] = \frac{1}{5}$$

Note: If the magnetic moment of each spin is μs_i, then in a magnetic field B, this system has fixed energy E=-μB.

System 2: "Einstein solid" with N=3, E=3

$$E = \sum_{k=1}^{N} \varepsilon_{n_k} \qquad \varepsilon_{n_k} = 0,1,2,\cdots$$

microstate	red	white	blue
1	1	1	1
2	2	0	1
3	2	1	0
4	1	0	2
5	1	2	0
6	0	1	2
7	0	2	1
8	3	0	0
9	0	3	0
10	0	0	3

$$\Omega = 10$$

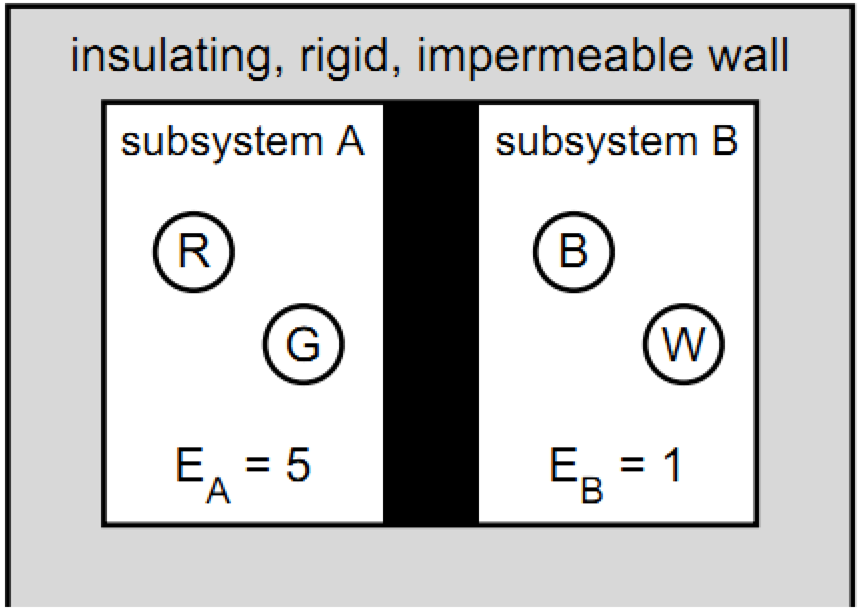
$$\langle \varepsilon_{n_k} \rangle = \frac{1}{10}(4\cdot 0 + 3\cdot 1 + 2\cdot 2 + 1\cdot 3) = 1$$

$$P(\varepsilon_{n_k} = 1) = \frac{3}{10}$$

More generally:

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

Einstein solid with N=2, E_A=5, Ω_A=6 Einstein solid with N=2, E_B=1, Ω_B=2



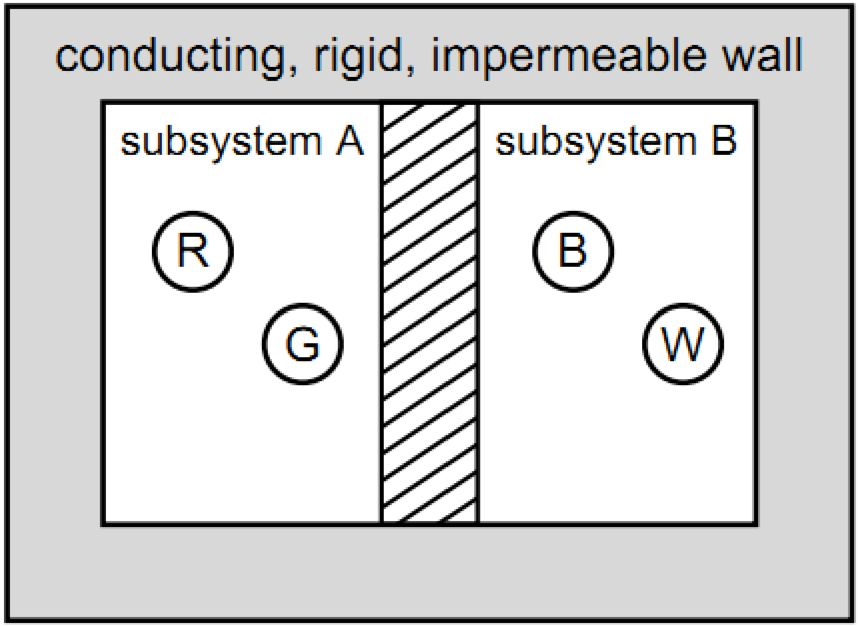
E_A	accessible microstates of A		E_B	accessible microstates of subsystem B	
5	5,0	0,5	1	1,0	0, 1
	4,1	1,4			
	3,2	2,3			

Table 4.2: The 12 equally probable microstates of the isolated composite system composed of subsystems A and B with $N_A = 2$, $E_A = 5$, $N_B = 2$, and $E_B = 1$. The 12 microstates consist of all combinations of the microstates of A and B.

$$E_{tot} = E_A + E_B = 6$$

$$\Omega_{tot} = \Omega_A \Omega_B = 12$$

Now, allow the barrier to accommodate energy transfer



$$E_{tot} = E_A + E_B = 6$$

$$\Omega_{tot} = \sum_{E_{tot}=6} \Omega_A(E_A)\Omega_B(E_B) = 84$$

E_A	microstates	$\Omega_A(E_A)$	E_B	microstates	$\Omega_B(E_B)$	$\Omega_A\Omega_B$	$P_A(E_A)$
6	6,0 0,6 5,1 1,5 4,2 2,4 3,3	7	0	0,0	1	7	7/84
5	5,0 0,5 4,1 1,4 3,2 2,3	6	1	1,0 0,1	2	12	12/84
4	4,0 0,4 3,1 1,3 2,2	5	2	2,0 0,2 1,1	3	15	15/84
3	3,0 0,3 2,1 1,2	4	3	3,0 0,3 2,1 1,2	4	16	16/84
2	2,0 0,2 1,1	3	4	4,0 0,4 3,1 1,3 2,2	5	15	15/84
1	1,0 0,1	2	5	5,0 0,5 4,1 1,4 3,2 2,3	6	12	12/84
0	0,0	1	6	6,0 0,6 5,1 1,5 4,2 2,4 3,3	7	7	7/84

Table 4.3: The 84 equally probable microstates accessible to the isolated composite system composed of subsystems A and B after the removal of the internal constraint. The total energy is $E_{\text{tot}} = E_A + E_B = 6$ with $N_A = 2$ and $N_B = 2$. Also shown are the number of accessible microstates in each subsystem and the probability $P_A(E_A)$ that subsystem A has energy E_A.

Note that, for the constrained system:

$$\langle E_A \rangle = 5 \quad \text{(by design)}$$

$$\Omega_{\text{tot}} = 12$$

For the system with thermal exchange:

$$\langle E_A \rangle = 0 \cdot \frac{7}{84} + 1 \cdot \frac{12}{84} + 2 \cdot \frac{15}{84} + 3 \cdot \frac{16}{84} + 4 \cdot \frac{15}{84} + 5 \cdot \frac{12}{84} + 6 \cdot \frac{7}{84} = 3$$

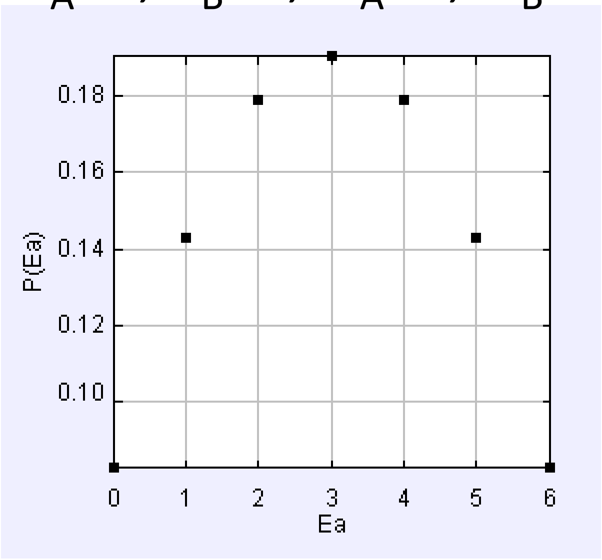
$$\Omega_{tot} = 84$$

This example suggests a measure of "missing information"

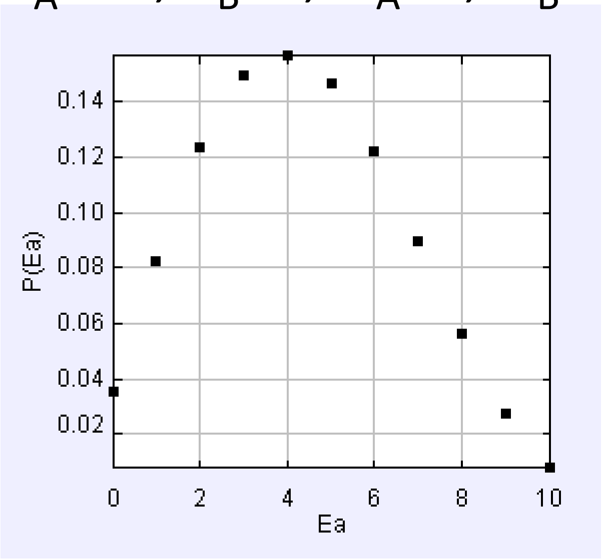
$$S = k \ln \Omega$$

Simulation program [stp_EinsteinSolids.jar]

E_A=5, E_B=1, N_A=2, N_B=2



E_A=10, E_B=0, N_A=3, N_B=4

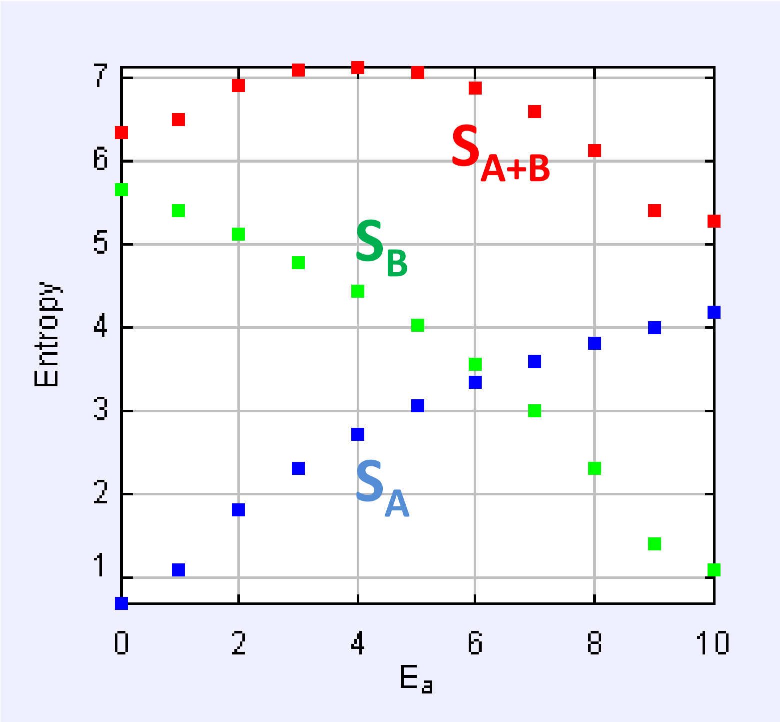


More results for E_A=10, E_B=0, N_A=3, N_B=4:

E_A	$\Omega_A(E_A)$	$\ln\Omega_A(E_A)$	T_A^{-1}	T_A	E_B	$\Omega_B(E_B)$	$\ln\Omega_B(E_B)$	T_B^{-1}	T_B	$\Omega_A\Omega_B$
10	66	4.19	na	na	0	1	0	na	na	66
9	55	4.01	0.19	5.22	1	4	1.39	1.15	0.87	220
8	45	3.81	0.21	4.72	2	10	2.30	0.80	1.24	450
7	36	3.58	0.24	4.20	3	20	3.00	0.63	1.60	720
6	28	3.33	0.27	3.71	4	35	3.56	0.51	1.94	980
5	21	3.05	0.31	3.20	5	56	4.03	0.44	2.28	1176
4	15	2.71	0.37	**2.70**	6	84	4.43	0.38	**2.60**	1260
3	10	2.30	0.46	2.18	7	120	4.79	0.34	2.96	1200
2	6	1.79	0.60	1.66	8	165	5.11	0.30	3.30	990
1	3	1.10	0.90	1.11	9	220	5.39	0.28	3.64	660
0	1	0	na	na	10	286	5.66	na	na	286

Table 4.5: The number of microstates of subsystems A and B for total energy $E_{\rm tot} = E_A + E_B = 10$ and $N_A = 3$ and $N_B = 4$. The number of states was determined using (4.3). There are a total of 8008 microstates. The most probable energy of subsystem A is $\tilde{E}_A = 4$ and the fraction of microstates associated with the most probable macrostate is $1260/8008 \approx 0.157$. This fraction will approach one as the number of particles in the systems become larger.

Simulation [stp_Entropy EinsteinSolid.jar]



$$S = k \ln \Omega$$