

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

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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	1/16/2012	Introductory concepts	1.1-1.5	001.1	1/23/2012
2	1/20/2012	Introductory concepts	1.6-1.12	001.2	1/23/2012
3	1/23/2012	First Law of Thermodynamics	2.1-2.11	001.3	1/26/2012
4	1/25/2012	Second Law of Thermodynamics	2.12-2.14	001.4	1/27/2012
5	1/27/2012	Entropy	2.15-2.19	001.5	1/30/2012
6	1/30/2012	Thermodynamic Potentials	2.20-2.21	001.6	2/1/2012
7	2/1/2012	Thermodynamic Potentials	2.22-2.24	001.7	2/5/2012
8	2/5/2012	Introduction to probability theory	3.1-3.3	001.8	2/6/2012
9	2/6/2012	Probability distributions	3.4-3.5	001.9	2/6/2012
10	2/10/2012	Continuous distributions/Central limit theorem	3.6-3.10	001.10	2/10/2012
11	2/10/2012	Introduction to statistical mechanics	4.1-4.2	001.11	2/13/2012
12	2/13/2012	Enumeration of microstates	4.3	001.12	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			

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Poisson probability distribution –

Approximation to binomial distribution for small p

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

$$\text{Assume } N \gg n \quad p \ll 1$$

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

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

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

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

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Other probability distributions:

Continuous distributions $p(x) \equiv$ probability distribution

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

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

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

Example:

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

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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 $\sum s_n = 1$

$$\begin{array}{cccccc} \uparrow\uparrow\uparrow\downarrow & \uparrow\uparrow\uparrow\downarrow & \uparrow\uparrow\uparrow\downarrow & \uparrow\uparrow\uparrow\downarrow & \uparrow\uparrow\uparrow\downarrow & \Omega=10 \\ \uparrow\downarrow\uparrow\uparrow & \downarrow\uparrow\uparrow\uparrow & \downarrow\uparrow\uparrow\uparrow & \downarrow\uparrow\uparrow\uparrow & \downarrow\uparrow\uparrow\uparrow & P_i = \frac{1}{\Omega} \end{array}$$

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

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

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

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

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:

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

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Einstein solid with $N=2$, $E_A=5$, $\Omega_A=6$ Einstein solid with $N=2$, $E_B=1$, $\Omega_B=2$

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

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.

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

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

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Now, allow the barrier to accommodate energy transfer

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

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

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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 5, 1 4, 2 3, 3	7	0	0, 0	1	7	7/84
5	5, 0 4, 1 3, 2	6	1	1, 0 0, 1	2	12	12/84
4	4, 0 3, 1 2, 2	5	2	2, 0 1, 1	3	15	15/84
3	3, 0 2, 1 1, 2	4	3	3, 0 2, 1 1, 2	4	16	16/84
2	2, 0 1, 1	3	4	4, 0 3, 1 2, 2	5	15	15/84
1	1, 0 0, 1	2	5	5, 0 4, 1 3, 2 2, 3	6	12	12/84
0	0, 0	1	6	6, 0 5, 1 4, 2 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 $E_{tot} = E_A + E_B = 6$ 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 .

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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:

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

$$\Omega_{\text{tot}} = 84$$

This example suggests a measure of "missing information"

$$S = k \ln \Omega$$

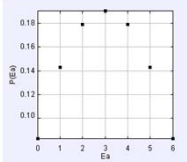
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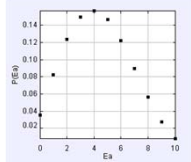
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Simulation program [stp EinsteinSolids.jar](#)

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



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



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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

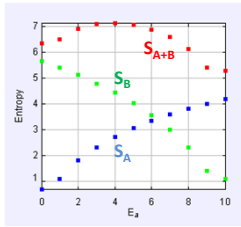
Table 4.5: The number of microstates of subsystems A and B for total energy $E_{\text{tot}} = E_A + E_B = 10$ and $N_A = 3$ and $N_B = 4$. The number of states was determined using (4.3). There are a total of 8008 microstates. The most probable energy of subsystem A is $E_A = 4$ and the fraction of microstates 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.

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Simulation [stp_EntropyEinsteinSolid.jar](#)



$$S = k \ln \Omega$$

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