PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #1 SOLUTIONS

(1) Compute the information entropy in the Fall 2012 Physics 140A grade distribution. See http://www-physics.ucsd.edu/students/courses/fall2012/physics140a/index.html.

Solution :

$\sum_n N_n = 49$	A+	A	A-	B+	B	B-	C+	C	C-	D	F
N_n	2	10	3	8	11	2	7	1	0	4	1
$-p_n \log_2 p_n$	0.188	0.468	0.247	0.427	0.484	0.188	0.401	0.115	0	0.295	0.115

Table 1: F12 Physics 140A final grade distribution.

Assuming the only possible grades are A+, A, A-, B+, B, B-, C+, C, C-, D, F (11 possibilities), then from the chart we produce the entries in Tab. 1. We then find

$$S = -\sum_{n=1}^{11} p_n \log_2 p_n = 2.93 \text{ bits}$$

For maximum information, set $p_n = \frac{1}{11}$ for all n, whence $S_{\text{max}} = \log_2 11 = 3.46$ bits.

(2) Study carefully problem #11 from the worked examples to chapter 1 of the lecture notes. Suppose I have three bags. Initially, bag #1 contains a quarter, bag #2 contains a dime, and bag #3 contains two nickels. At each time step, I choose two bags randomly and randomly exchange one coin from each bag. The time evolution satisfies $P_i(t+1) = \sum_j Y_{ij} \, P_j(t)$, where $Y_{ij} = P(i\,,\,t+1\,|\,j\,,\,t)$ is the conditional probability that the system is in state i at time $t+1$ given that it was in state j at time t.

(a) How many configurations are there for this system?

(b) Construct the transition matrix Y_{ij} and verify that $\sum_i Y_{ij} = 1$.

(c) Find the eigenvalues of Y (you may want to use something like `Mathematica`).

(d) Find the equilibrium distribution P_i^{eq}.

Solution :

(a) There are seven possible configurations for this system, shown in Table 2 below.

	1	2	3	4	5	6	7
bag 1	Q	Q	D	D	N	N	N
bag 2	D	N	Q	N	Q	D	N
bag 3	NN	DN	NN	QN	DN	QN	DQ
g	1	2	1	2	2	2	2

Table 2: Configurations and their degeneracies for problem 3.

(b) The transition matrix is

$$Y = \begin{pmatrix} 0 & \frac{1}{6} & \frac{1}{3} & 0 & 0 & \frac{1}{6} & 0 \\ \frac{1}{3} & \frac{1}{6} & 0 & \frac{1}{6} & \frac{1}{3} & 0 & \frac{1}{6} \\ \frac{1}{3} & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & 0 & \frac{1}{3} & \frac{1}{6} \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{3} \end{pmatrix}$$

(c) Interrogating `Mathematica`, I find the eigenvalues are

$$\lambda_1 = 1 \quad , \quad \lambda_2 = -\tfrac{2}{3} \quad , \quad \lambda_3 = \tfrac{1}{3} \quad , \quad \lambda_4 = \tfrac{1}{3} \quad , \quad \lambda_5 = \lambda_6 = \lambda_7 = 0\,.$$

(d) We may decompose Y into its left and right eigenvectors, writing

$$Y = \sum_{a=1}^{7} \lambda_a \, | \, R^a \, \rangle \langle \, L^a \, |$$

$$Y_{ij} = \sum_{a=1}^{7} \lambda_a \, R^a_i \, L^a_j$$

The full matrix of left (row) eigenvectors is

$$L = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -2 & 1 & 2 & -1 & -1 & 1 & 0 \\ -1 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 & -1 & 1 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 1 & 0 \\ -1 & -1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

The corresponding matrix of right (column) eigenvectors is

$$R = \frac{1}{24}\begin{pmatrix} 2 & -3 & -6 & 0 & 4 & 1 & -5 \\ 4 & 3 & 0 & -6 & -4 & -1 & -7 \\ 2 & 3 & -6 & 0 & 4 & -5 & 1 \\ 4 & -3 & 0 & 6 & -4 & -7 & -1 \\ 4 & -3 & 0 & -6 & -4 & 5 & 11 \\ 4 & 3 & 0 & 6 & -4 & 11 & 5 \\ 4 & 0 & 12 & 0 & 8 & -4 & -4 \end{pmatrix}$$

Thus, we have $RL = LR = \mathbb{I}$, *i.e.* $R = L^{-1}$, and

$$Y = R\,\Lambda\,L\ ,$$

with $\Lambda = \text{diag}\big(1\,,\,-\frac{2}{3}\,,\,\frac{1}{3}\,,\,\frac{1}{3}\,,\,0\,,\,0\,,\,0\big)$.

The right eigenvector corresponding to the $\lambda = 1$ eigenvalue is the equilibrium distribution. We therefore read off the first column of the R matrix:

$$(P^{\text{eq}})^{\text{t}} = \begin{pmatrix} \frac{1}{12} & \frac{1}{6} & \frac{1}{12} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} \end{pmatrix}\ .$$

Note that

$$P^{\text{eq}}_i = \frac{g_i}{\sum_j g_j}\ ,$$

where g_j is the degeneracy of state j (see Tab. 2). Why is this so? It is because our random choices guarantee that $Y_{ij}\,g_j = Y_{ji}\,g_i$ for each i and j (*i.e.* no sum on repeated indices). Now sum this equation on j, and use $\sum_j Y_{ji} = 1$. We obtain $\sum_j Y_{ij}\,g_j = g_i$, which says that the $|\,g\,\rangle$ is a right eigenvector of Y with eigenvalue 1. To obtain the equilibrium probability distribution, we just have to normalize by dividing by $\sum_j g_j$.

(3) A system consists of N 'molecules'. Each molecule consists of four 'spins': σ, μ_1, μ_2, and μ_3, where each spin polarization can takes values ± 1. The molecular Hamiltonian is

$$\hat{h} = J\sigma(\mu_1 + \mu_2 + \mu_3) - H\big(3\sigma - \mu_1 - \mu_2 - \mu_3\big)\ .$$

(a) Enumerate all the molecular energy states along with their degeneracies.

(b) Find the molecular partition function $\zeta(T, H)$.

(c) Compute the magnetic susceptibility $\chi(T, H = 0)$.

Solution :

(a) The states and their degeneracies are listed in Tab. 3 below. Note that there $\hat{h}$ exhibits permutation symmetry among the (μ_1, μ_2, μ_3) states.

(b) Accordingly,

$$\zeta(T, H) = 2\,e^{-3\beta J} + 2\,e^{+3\beta J}\cosh(6\beta H) + 6\,e^{-\beta J}\cosh(2\beta H) + 6\,e^{+\beta J}\cosh(4\beta H)\ .$$

σ	(μ_1, μ_2, μ_3)	g	E
$+$	$(+,+,+)$	1	$+3J$
$+$	$(+,+,-)$	3	$+J-2H$
$+$	$(+,-,-)$	3	$-J-4H$
$+$	$(-,-,-)$	1	$-3J-6H$
$-$	$(+,+,+)$	1	$-3J+6H$
$-$	$(+,+,-)$	3	$-J+4H$
$-$	$(+,-,-)$	3	$+J+2H$
$-$	$(-,-,-)$	1	$+3J$

Table 3: States and their degeneracies g.

(c) The molecular magnetization is

$$\begin{aligned} m &= -\frac{\partial f}{\partial H} = \frac{1}{\beta}\frac{\partial \ln \zeta}{\partial H} \\ &= \frac{6\,e^{3\beta J}\sinh(6\beta H) + 6\,e^{-\beta J}\sinh(2\beta H) + 12\,e^{\beta J}\sinh(4\beta H)}{e^{-3\beta J} + e^{3\beta J}\cosh(6\beta H) + 3\,e^{-\beta J}\cosh(2\beta H) + 3\,e^{\beta J}\cosh(4\beta H)} \\ &= \frac{18\,e^{3\beta J} + 6\,e^{-\beta J} + 24\,e^{\beta J}}{\cosh(3\beta J) + 3\cosh(\beta J)} \cdot \beta H + \mathcal{O}(H^3)\,. \end{aligned}$$

Thus, the zero-field molecular susceptibility is

$$\chi(T, H=0) = \frac{\partial m}{\partial H} = \frac{18\,e^{3J/k_B T} + 6\,e^{-J/k_B T} + 24\,e^{J/k_B T}}{\cosh(3J/k_B T) + 3\cosh(J/k_B T)} \cdot \frac{1}{k_B T}\,.$$

Note that for $J = 0$ we obtain $\chi(T, H=0) = 12/k_B T$. For a single spin with magnetic moment p, *i.e.* $\hat{h} = -pH\sigma$, the susceptibility is $p^2/k_B T$. Thus for our system, when $J = 0$ we have one spin (σ) with $p = 3$ and three ($\mu_{1,2,3}$) with $p = 1$, hence the total susceptibility is $\chi = (3^2 + 1^2 + 1^2 + 1^2)/k_B T = 12/k_B T$.

(4) Consider a system of identical but distinguishable particles, each of which has a non-degenerate ground state with $\varepsilon_0 = 0$, and a $g-$fold degenerate excited state with energy $\varepsilon > 0$. Study carefully problems #1 and #2 from the worked example problems for chapter 4 of the lecture notes, where this system is treated in the microcanonical and ordinary canonical ensembles. Here you are invited to work out the results for the grand canonical ensemble.

(a) Find the grand partition function $\Xi(T, z)$ and the grand potential $\Omega(T, z)$. Express your answers in terms of the temperature T and the fugacity $z = e^{\mu/k_B T}$.

(b) Find the entropy $S(T, z)$.

(c) Find the number of particles, $N(T, z)$.

(d) Show how, in the thermodynamic limit, the entropy agrees with the results from the microcanonical and ordinary canonical ensembles.

Solution :

(a) There ordinary canonical partition function is clearly

$$Z(T,N) = \big(1 + ge^{-\varepsilon/k_\text{B}T}\big)^N ,$$

hence the grand partition function is

$$\Xi = \sum_{N=0}^{\infty} z^N Z(T,N) = \frac{1}{1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})} ,$$

where $z = \exp(\mu/k_\text{B}T)$ is the fugacity. The grand potential is

$$\Omega(T,z) = -k_\text{B}T \ln \Xi = k_\text{B}T \ln\Big(1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})\Big) .$$

(b) The entropy is $S = -\big(\frac{\partial\Omega}{\partial T}\big)_\mu$, so we must take care to allow $z = \exp(\mu/k_\text{B}T)$ to vary. The result is

$$S(T,\mu) = -k_\text{B} \ln\Big(1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})\Big) - \frac{\mu}{T} \cdot \frac{z(1 + g\,e^{-\varepsilon/k_\text{B}T})}{1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})} + \frac{\varepsilon}{T} \cdot \frac{zg\,e^{-\varepsilon/k_\text{B}T}}{1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})} .$$

(c) The particle number is

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_T = -\frac{z}{k_\text{B}T}\left(\frac{\partial\Omega}{\partial z}\right)_T = \frac{z(1 + g\,e^{-\varepsilon/k_\text{B}T})}{1 - z(1 + g\,e^{-\varepsilon/k_\text{B}T})} .$$

Thus,

$$z = \frac{1}{1 + N^{-1}} \cdot \frac{1}{1 + g\,e^{-\varepsilon/k_\text{B}T}} .$$

(d) Expressing the entropy $S(T,z)$ in terms of T and N, we find

$$S(T,N) = Nk_\text{B} \ln\big(1 + g\,e^{-\varepsilon/k_\text{B}T}\big) + \frac{N\varepsilon}{T}\,\frac{g\,e^{-\varepsilon/k_\text{B}T}}{1 + g\,e^{-\varepsilon/k_\text{B}T}} + k_\text{B} \ln(N+1) + Nk_\text{B} \ln\big(1 + N^{-1}\big) .$$

The first two terms are extensive, *i.e.* of order N^1. They agree with the results in example problem 4.2(c). The penultimate term is of order $\ln N$ and the last term is of order N^0, hence they are subleading and negligible in the thermodynamic limit.