# P653 HW2

**Due Sept 8, 2005**

**Problem 1. Information Theoretic Definition of Entropy**

Entropy is a measure of the uncertainty in an ensemble. Here we will use some simple information theoretic ideas (due to Shannon) to calculate the entropy for a generic ensemble – even one which is not in equilibrium.

Our setup is that we know that our system is in one of $N$ states, and that each state $i$ occurs in the ensemble with probability $p_i$.

Suppose we measure that the system is in state $i$. Let us assume that we can quantify the amount that we learn from this measurement. Call this $k_i$. Clearly $k_i$ is larger if the probability $p_i$ is smaller. We will define $k_i$ so that it is only a function of the probability $p_i$, ie

$$k_i = k(p_i).$$

We will define the entropy of information $S_I$ (for the remainder of this question we drop the $I$) to be the average amount of information gained from a measurement:

$$S = \sum_i p_i k(p_i).$$

**1.1.** Entropy, as a state variable is extensive. Suppose we build a larger system out of two independant subsystems $A$ and $B$. The entropy of the whole should be

$$S = S_A + S_B,$$

where $S_A$ and $S_B$ are the entropies of the parts.

Use this relationship to derive a functional relationship that $k$ must obey.

[Hint 1: Recall that independance means that the probability of $A$ being in state $i$ and $B$ being in state $j$ is $p_{ij} = p_i p_j$.]

[Hint 2: You will need to use that $\sum_i p_i = 1$.]

**Solution 1.1.** The entropy of the whole is

$$\begin{aligned} S &= \sum_{ij} p_{ij} k(p_{ij}) = \sum_i p_i k(p_i) + \sum_j p_j k(p_j) \\ &= \sum_{ij} p_i p_j \left[k(p_i) + k(p_j)\right], \end{aligned}$$

where we have used the fact that $\sum_i p_i = 1$. Equating terms in the sum, we have that

$$k(xy) = k(x) + k(y).$$

**1.2.** Show that this functional relationship is obeyed by

$$k(x) = -k \log(x),$$

for any constant $k$.

Prove that these are the only solutions to this relationship. [Feel free to assume that k(x) is differentiable, and you may use standard uniqueness theorems.]

**Solution 1.2.** It is obvious that the suggested form obeys the functional relationship. To prove uniqueness, we first set $x = y = 1$ to find that $k(1) = 0$. We then let $y = 1 + \delta$ where $\delta$ is an infinetesmal. To lowest order in $\delta$ one finds

$$\delta x k'(x) = \delta k'(1).$$

The uniqueness of the solution to this differential equation gives the desired result.

**1.3.** We need that the entropy will be maximized in equilibrium. What constraint does that place on the sign of $k$?

**Solution 1.3.** Suppose we have the equilibrium $p_i$'s. If we let $p_1 \to p_1 + \delta$ and $p_2 \to p_2 - \delta$ the entropy changes be

$$\Delta S = -k\delta \log(p_1 p_2) > 0.$$

Since $p_j < 0$, this requires that $k > 0$.

As the notation might suggest, we will take the constant $k$ to be Boltzmann's constant. We have therefore arrived at the definition

$$S_I = -k_b \sum_i p_i \log p_i,$$

where the $I$ stands for information.

**1.4.** Show that the thermodynamic entropy in the microcannonical ensemble is equal to the information entropy.

**Solution 1.4.** In the microcannonical ensemble, $p_i = 1/\Omega$, where $\Omega$ is the number of states. Therefore

$$S_I = -k_b \sum_i p_i \log(p_i) = -k_b \log(1/\Omega) = k_b \log(\Omega), \tag{1}$$

which is the definition of the microcannonical entropy.

**1.5.** Show that the thermodynamic entropy in the cannonical ensemble is equal to the information entropy.

**Solution 1.5.** In the cannonical ensemble, $p_i = e^{-\beta E_i}/Z$, where $Z = e^{-\beta F}$ is the partition function. The information entropy is

$$S_I = k_b \sum_i \frac{e^{-\beta E_i}}{Z}(\beta E_i - \log Z) = \frac{1}{T}(\langle E \rangle - F), \tag{2}$$

which is the thermodynamic entropy.

**Problem 2. Maximum Entropy Principle** Consider the set of all possible states $i$ of a system. Each of these state contains a given number of particles $N_i$ and has energy $E_i$. We define an ensemble of these states by specifying the probability $p_i$ for the system to be in a given state.

Find the $p_i$'s for the ensemble which maximizes the entropy $S_I$ subject to the constraint that the expectation value of the energy and particle number are fixed,

$$\langle E \rangle = \sum_i p_i E_i$$

$$\langle N \rangle = \sum_i p_i N_i$$

[Don't forget that the probabilities are constrained by $\sum_i p_i = 1$.]

**Solution 2.1.** We need to introduce three Lagrange multipliers $[\beta, \mu, F]$ to account for the three constraints of fixed energy, number, and probability. We therefore need to minimize the function

$$L = \frac{S}{k_B} - \beta\left[(\langle E \rangle - E) - \mu(\langle N \rangle) - N\right] + (\beta F + 1)(\sum_i p_i - 1). \tag{3}$$

Taking the derivative with respect to $p_i$ yields

$$\frac{\partial L}{\partial p_i} = [-\log p_i - 1] - \beta\left[E_i - \mu N_i\right] + (\beta F + 1) = 0. \tag{4}$$

Solving for $p_i$ gives

$$p_i = \frac{e^{-\beta(E_i - \mu N_i)}}{\mathcal{Z}}, \tag{5}$$

where $\mathcal{Z} = e^{-\beta F}$.

**Problem 3. Microscopic origin of dissipation**

Here we look at a simple model of a dissipative classical system, namely an oscillator coupled to an oscillator bath. For a quantum treatment, see Feynman and Vernon, Ann. Phys. **24**, 118 (1963).

Consider a harmonic oscillator with position $X$, momentum $P$, and frequency $\Omega$, linearly coupled to a bath of other oscillators with positions $x_i$, momenta $p_i$ and frequencies $\omega_i$. This system obeys a Hamiltonian

$$H = \frac{P^2}{2M} + \frac{1}{2}M\Omega^2 X^2 + \sum_i \left(\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 x_i^2\right) + \sum_i \lambda_i x_i X.$$

**3.1.** Write the equations of motion for $x_i$, $p_i$, $X$, and $P$.

**Solution 3.1.**

$$\begin{aligned}
\dot{x}_i &= p_i/m_i \\
\dot{p}_i &= -m_i\omega_i^2 x_i - \lambda_i X \\
\dot{X} &= P/M \\
\dot{P} &= -M\Omega^2 X - \sum_i \lambda_i x_i
\end{aligned}$$

**3.2.** Fourier transform these equations of motion, using the convention

$$A(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t} A(\omega).$$

**Solution 3.2.**

$$\begin{aligned}
-i\omega x_i &= p_i/m \\
-i\omega p_i &= -m_i\omega_i^2 x_i - \lambda_i X \\
-i\omega X &= P/M \\
-i\omega P &= -M\Omega^2 X - \sum_i \lambda_i x_i
\end{aligned}$$

**3.3.** Eliminate $p_i(\omega)$ to write $x_i(\omega)$ as a function of $X(\omega)$.

**Solution 3.3.**

$$x_i = \frac{\lambda_i}{m_i(\omega^2 - \omega_i^2)} X$$

**3.4.** Eliminate $x_i(\omega)$ and $P$ from the equations for $X$, to arrive at an equation of the form,

$$[\omega^2 - \Omega^2 - F(\omega)]X = 0.$$

What is $F(\omega)$?

**Solution 3.4.**

$$F(\omega) = \sum_i \frac{\lambda_i^2}{Mm_i(\omega^2 - \omega_i^2)}.$$

**3.5.** It is convenient to introduce a "spectral density"

$$J(E) = \sum_i \frac{\lambda_i^2}{m_i\omega_i} 2\pi\delta(E - \omega_i)$$

which encodes all relevant information about the oscillator bath. Verify that

$$F(\omega) = \frac{1}{2M} \int \frac{dE}{2\pi} \frac{1}{\omega - E} \left[J(E) - J(-E)\right].$$

**Solution 3.5.** The formula is readily verified by substituting $J(E)$ into the right hand side.

**3.6.** In the limit of a large bath, one can assume that $J(E)$ is smooth. We will concentrate on an *ohmic* bath, where $J(E) = \alpha E$ for small $E$. To be concrete, we will take

$$J(E) = \begin{cases} \alpha E & |E| < E_c \\ 0 & |E| > E_c \end{cases}$$

Furthermore, we will assume that $E_c$ is the largest energy in the problem. Explicitly calculate $F(\omega)$, neglecting terms of order $\omega/E_c$. It may be useful to recall that

$$\frac{1}{x-y} = \frac{P}{x-y} - i\pi\delta(x-y),$$

though this example has been cooked up so that one does not have to explicitly use this formula.

**Solution 3.6.**

$$\begin{aligned} F &= \frac{\alpha}{2\pi M} \int_{-E_c}^{E_c} \frac{dE\,E}{\omega - E} \\ &= \frac{\alpha}{2\pi M} (-2E_c + \omega \log\left(\frac{1+\omega/E_c}{-1+\omega/E_c}\right) \\ &= \frac{\alpha}{2\pi M} (-2E_c - i\pi\omega + \omega\mathcal{O}(\omega/E_c)). \end{aligned}$$

It should be apparent that to this order in $\omega/E_c$, this result is actually independent of the form of the cutoff.

**3.7.** Substituting this expression for $F$ into equation of motion for $X$ should give the equations of motion for a damped harmonic oscillator. What is the frequency $\bar{\Omega}$ of this oscillator? Note that in most experimental realizations of this system there is no way to measure the bare frequency $\Omega$. Only the renormalized frequency $\bar{\Omega}$ is physical.

**Solution 3.7.**

$$\bar{\Omega}^2 = \Omega^2 - \frac{\alpha E_c}{\pi M}$$