HW 2: Due September 24

1. **Discrete System**: Consider a system which consists of 3 coins. Each coin has two sides Heads (H) and Tails (T), which are assigned values of 2 and 1, respectively. Let the 3 coins be tossed and let us consider the following outcome : H, T, T $(2, 1, 1)$. We denote this outcome as the *microstate* of the system. A *macrostate* of the system is defined as the sum of the values of all the faces in the outcome. For example, the macrostate of the system for the outcome H, T, T is 2+1+1 = 4.

   (a) What are all the possible *microstates* and *macrostates* of the system?

   (b) If it is known that the *macrostate* of the system is 5, what are the accessible(admissible) *microstates* of the system? Remark: We denote this set of accessible microstates as the (statistical) ensemble corresponding to the macrostate of 5. In class, we have mentioned that an ensemble is a collection of replicas of the same system, where 'same' refers to certain (macroscopic) constraints. From this exercise, it should be noted that the systems in a given ensemble may be in different microstates but correspond to the same macrostate.

2. **Alternate Microcanonical Ensemble:** Our working definition of the microcanonical ensemble is:

$$\rho(\boldsymbol{y}) = \begin{cases} \frac{1}{V(E+\Delta)-V(E)} & E \leq H(\boldsymbol{y}) \leq E + \Delta \\ 0 & \text{otherwise}\,. \end{cases}$$

   (a) Argue that this can be expressed as:

$$\rho(\boldsymbol{y}) = \frac{\Theta(E + \Delta - H(\boldsymbol{y})) - \Theta(E - H(\boldsymbol{y}))}{V(E + \Delta) - V(E)}\,,$$

   where Θ is the Heaviside step function.

   (b) Show that this implies that one also has

$$\rho(\boldsymbol{y}) = \frac{\delta(E - H(\boldsymbol{y}))}{\Omega(E)}\,,$$

   where δ is the Dirac-delta function.

3. **Continuous System**: Consider a one-particle system moving in 1-dimension with the following Hamiltonian

$$H(x,p) \;=\; \frac{p^2}{2m} + \frac{1}{2}x^2\,, \tag{1}$$

   where x and p denote the position and momentum of the particle, respectively. Draw the statistical ensemble corresponding to the macrostate of H = 2 in the phase space; i.e. accurately sketch the subspace of Γ, the x-p plane occupied by this ensemble.

4. The logarithm of the phase space density is known as the index of probability, η, where

$$\eta = \log(\rho)\,.$$

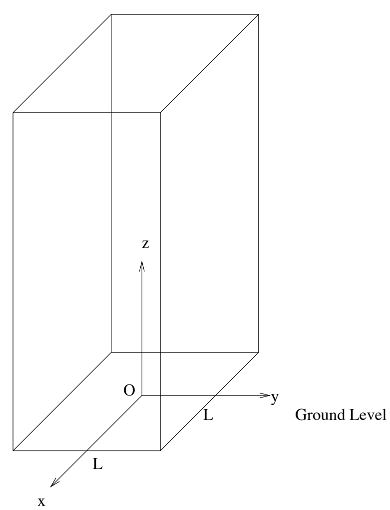
Consider a micro-canonical ensemble and show that the phase space average of $-\eta$ is simply $\overline{-\eta} = \log(\Omega(E)\Delta)$. Thus the expectation value of the negative of the index of probability is the logarithm of the accessible phase space volume. This then is a (logarithmic) measure of how much variability in state (uncertainty) exists in the micro-canonical ensemble. As we shall see later, $\overline{-\eta}$ is intimately related to the concept of entropy.

(See equation sheet on bSpace for some handy formulae for the following problems.)

5. Consider a point mass m with position $\boldsymbol{r} = x\boldsymbol{e}_x + y\boldsymbol{e}_y + z\boldsymbol{e}_z$, where its height above the ground is $z = \boldsymbol{r}\cdot\boldsymbol{e}_z$. The total energy of this particle is given by

$$H(\boldsymbol{r},\boldsymbol{p}) \;=\; \frac{\boldsymbol{p}\cdot\boldsymbol{p}}{2m} + mgz\,, \tag{2}$$

where $\boldsymbol{p}$ is the momentum vector and g is the acceleration due to gravity. Implicit, in this expression is the constraint that $z \geq 0$ and that $x, y \in (-L/2, L/2)$.



Assume a canonical phase-space distribution for this particle given by

$$\rho(\boldsymbol{r},\boldsymbol{p}) \;=\; C\exp(-\frac{H}{k_B T})\,, \tag{3}$$

where $k_B = 1.3806504 \times 10^{-23}$ J/K is Boltzmann constant, T is the absolution temperature of the surroundings (the heat bath) and C is the normalization constant.

(a) Calculate the mean height of the particle above the ground? Express it in terms of m, g, k_B and T.

(b) Assume the particle is a Helium atom with mass $4.0026/N_A$ g and the surrounding temperature is 300 K. What is the mean height? [Note: $N_A = 6.022 \times 10^{23}$ is Avagadro's number.]

(c) Assume that the particle has mass 10 kg and the surrounding temperature is 300 K. What is the mean height now? Does this correlate with your physical intuition?

6. **(Externally controlled system: Canonical)** Consider a system described by a Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p}; \mathcal{A}(t))$, which is at equilibirum with a heat bath with parameter θ and thus has phase space distribution $\rho(\boldsymbol{q}, \boldsymbol{p}; \mathcal{A}(t)) = \exp[-H(\boldsymbol{q}, \boldsymbol{p}; \mathcal{A}(t))/\theta] / \int_\Gamma \exp[-H(\boldsymbol{q}, \boldsymbol{p}; \mathcal{A}(t))/\theta]\, d\boldsymbol{q}d\boldsymbol{p}$ at all times t. Noting that $U = \int_\Gamma H \rho\, d\boldsymbol{q}d\boldsymbol{p}$ and that $\dot{U} = \dot{W} + \dot{Q}$, show that in general during a process where $\mathcal{A}$ changes there will be an exchange of heat between the system and the heat bath at a rate:

$$\dot{Q} = \frac{1}{\theta}\left[\overline{\frac{\partial H}{\partial \mathcal{A}}}\,\overline{H} - \overline{\frac{\partial H}{\partial \mathcal{A}} H}\right]\dot{\mathcal{A}}\,.$$

Since in general the mean of a product of two functions is not equal to the product of the means, there will will always be an exchange of heat in this setting.

7. Consider a system (discrete) which only takes on three states $\{1, 2, 3\}$ with energies $\epsilon = H(1)$, $2\epsilon = H(2)$, and $4\epsilon = H(3)$. The system is in equilibrium with a heat bath with parameter $\theta = 2\epsilon$.

(a) Compute the internal energy and entropy of the system.

(b) Suppose one performs "mechanical" work on the system such that $H(2) = 3\epsilon$ but $H(1)$ and $H(3)$ do not change. Compute the change in internal energy and entropy of the system.

(c) Suppose instead of mechanical work, heat work is performed on the system such that θ changes to 3ϵ. Compute the change in internal energy and entropy of the system.

(d) Suppose both the mechanical and heat work are performed on the system. Compute the change in internal energy and entropy of the system.