UNIVERSITY OF CALIFORNIA BERKELEY
Department of Civil Engineering
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Structural Engineering,
Mechanics and Materials
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HW 2: Due September 17

Understanding ensembles

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. **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.

Liouville's Theorem and Statistical Equilibrium

3. Consider a N-particle system where each particle moves in 1-dimension. The particles are connected with springs in a periodic fashion such that the system's Hamiltonian is given by:

$$H(x_1, \cdots, x_N, p_1, \cdots, p_N) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N-1} \frac{1}{2}K(x_i - x_{i+1})^2 + \frac{1}{2}K(x_1 - x_N)^2 , \tag{2}$$

   where m_i is the mass of atom i and k is a constant.

   (a) What are the equations of motion for this system?

(b) Consider the following phase-space distribution

$$\rho(\mathbf{y},t) = \frac{e^{-\frac{1}{k_B T}\left(\sum_{i=1}^{N}\frac{p_i^2}{2m_i} + \sum_{i=1}^{N-1}\frac{1}{2}K(x_i - x_{i+1})^2 + \frac{1}{2}K(x_1 - x_N)^2\right)}}{\int_\Gamma e^{-\frac{1}{k_B T}\left(\sum_{i=1}^{N}\frac{p_i^2}{2m_i} + \sum_{i=1}^{N-1}\frac{1}{2}K(x_i - x_{i+1})^2 + \frac{1}{2}K(x_1 - x_N)^2\right)} \mathrm{d}\mathbf{y}} \tag{3}$$

where $\mathbf{y} = (x_1, \cdots, x_n, p_1, \cdots, p_N)$ is a point in phase-space. Here, k_B and T are constants (Boltzmann's constant and temperature, respectively).

Is the choice of phase-space distribution given by equation (3) valid? If it is valid, is the system in statistical-equilibrium?

Liouville' Theorem for Non-Hamiltonian Systems

4. In class, we have derived the local form of Liouville's theorem for Hamiltonian systems. Derive the local form of the Liouville' theorem for non-Hamiltonian systems, *i.e.*, for systems whose equations of motion are not derivable from a prescribed Hamiltonian. Express the local form in terms of the phase-space distribution function ρ and the phase-space variables $\mathbf{y}$ and $\dot{\mathbf{y}}$. (Hint: Start from the same global form as used in the derivation in class, but look where you specialized it for Hamiltonian systems).

   Using this *new* local form, specialize the theorem to the case of Hamiltonian systems and express it in terms of the Hamiltonian H, distribution function ρ, and phase-space variables $\mathbf{y}$. You should recover the local form of Liouville's theorem that was derived in class for a Hamiltonian system.