UNIVERSITY OF CALIFORNIA BERKELEY
Department of Civil Engineering
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Structural Engineering,
Mechanics and Materials
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HW 3: Due October 3

Fluctuations

1. **Small systems:** Let us a consider a 1-dimensional harmonic oscillator with a Hamiltonian

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

where p is the momentum and x is the position. Here, m is the mass and k is the spring constant. If the 1-dimensional oscillator follows the canonical distribution at temperature T,

   (a) calculate the average energy $\bar{H}$.

   (b) calculate the relative standard deviation of energy in the ensemble, *i.e.*, calculate $\frac{\sqrt{\overline{\Delta H^2}}}{\overline{H}}$ (a.k.a. the coefficient of variation), where $\Delta H = H - \overline{H}$.

2. **Large systems:** For 0.01 moles of an ideal gas ($\sim$ 2 dl at STP) which is in contact with a heat bath at a temperature T,

   (a) calculate the average energy $\bar{H}$.

   (b) calculate the relative standard deviation of energy in the ensemble, *i.e.*, calculate $\frac{\sqrt{\overline{\Delta H^2}}}{\overline{H}}$.

Can you see any difference between small and large systems in terms of the relative standard deviation of energy in the canonical ensemble?

Remark: The standard deviations from the averages are also called "fluctuations". These fluctuations are important in the study of phase-transitions, obtaining estimates of continuum quantities like heat capacity, viscosity, thermal conductivity etc.

Heat Capacity

3. The constant-volume heat capacity is given by

$$C_V = \frac{\partial \overline{H}}{\partial T}(V, T) \tag{2}$$

   (a) For an ideal gas consisting of N molecules, calculate the heat capacity using (2).

   (b) In the class, we have seen that heat capacity can be expressed in terms of fluctuations of energy in the canonical ensemble. Use that expression and obtain the expression for heat capacity.

Remark: It is remarkable that a continuum quantity like heat capacity can be expressed in terms of fluctuations of quantities in a statistical ensemble.

4. (Discrete Two Level System) Consider a system that can only be in two energetic states ϵ and $\epsilon + \Delta$. Assume that the system is in thermal equilibrium with a heat bath with absolute temperature T.
   (a) Write down the partition function for this system.
   (b) What is the mean energy of the system?
   (c) What is the heat capacity for the system? $[c = dU/dT]$

Thermo-Mechanical Properties

5. Consider a single particle of mass m moving in one-dimension between two walls at separation L; i.e. $q \in [0, L]$. The Hamiltonian for the particle is given as

$$H(q,p) = \frac{p^2}{2m} + V_1(q) + V_2(q)\,,$$

where are the interaction potentials of the particle with the walls are

$$\begin{aligned} V_1(q) &= \begin{cases} +\infty & q < 0 \\ -U & 0 \leq q < a \\ 0 & a \leq q \end{cases} \\ V_2(q) &= \begin{cases} +\infty & q > L \\ -U & L - a < q \leq L \\ 0 & x \leq L - a\,. \end{cases} \end{aligned}$$

Note that the potential favors the particle being within a distance a of either wall.

Determine an expression for the heat capacity, $c = \partial \overline{H}/\partial T$, of the system as a function of the distance between the wall. Consider $L = \lambda \cdot a$ and plot $c/(k_B/2)$ versus $\lambda \in [1.0, 2.0]$ for values of $U/k_B T \in \{0.3, 1.0, 3.0\}$. By examining plots of $V_1(q) + V_2(q)$ for the various values of λ argue why the heat capacity goes to zero at the extremes of the given range, why it peaks, and why the heat capacity is nearly constant at the higher temperature.

Remark: This problem is an example of the influence of mechanical loading on thermal properties.