PHYS 6107. Spring 2002.

HOMEWORK #1 $\sum = 300\ pts$

DUE: Feb. 26 by 5 p.m. (in Dr. Marchenkov's mail box)

As anticipated, this homework is a large one, therefore, start working on it right away. As a reminder, I encourage you to talk about these problems with other students. I am also happy to answer any questions that you might have concerning this assignment. Remember, the purpose of the homework is ***training****; therefore, the relative wait of the homework in the final grade is relatively low.*

> *I hear, I know.*
> *I see, I remember.*
> *I do, I understand.*
>
> Confucius

> *In theory there is no difference between theory and practice.*
> *In practice there is.*
>
> Yogi Berra

I. Probability (20pts)

Problem I.1 (5 pts)

Don't worry, your instructor does not believe that grades are random.

Experts on college examinations often state that 10% of a class should get grades of "A". That is the practically the same as saying that the probability of one student getting a grade of "A" is one in ten, or 1/10, or 0.1. Assume that probability is correct, and that grades on examinations are completely random (like throwing dice). Then, in a class of 24 students (such as this one) what is the probability that 12 students will get grades of "A" on an examination?

Problem I.2 (5 pts)

Suppose an event characterized by a probability p occurs n times in $N \geq n$ trials. Show that the probability of n such occurrences is

$$w(n) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}$$

Problem I.3 (10 pts)

The meaning of "never".

Aldous Huxley, who wrote "Brave New World", supposedly said that "six monkeys, set to strum unintelligently on typewriters for millions of years, would be bound in time to write all the books in the British Museum". Really?? Here is a problem:

Suppose that 10^{10} monkeys have been seated at typewriters throughout the age of the universe, $\sim 10^{18}$ s. (The current world population, according to the World POPClock Projection of 2/10/02 at 1:42:14 AM EST is 6,204,622,005. See, e.g., http://www.census.gov/cgi-bin/ipc/popclockw.) We even suppose that a monkey can hit 10 typewriter keys per second. A typewriter may have 44 keys; we further accept lowercase letters in place of capital letters. Assuming that Shakespeare's *Hamlet* has 10^5 characters, will the monkeys hit upon *Hamlet*?

1. Find the probability that any given sequence of 10^5 characters typed at random will come out in the correct sequence (i.e., the sequence of *Hamlet*).
2. Find the probability that a *Monkey-Hamlet* will emerge in the age of the universe.

II. Basic Concepts of Statistical Mechanics (40 pts)

Problem II.1 (10 pts)

Do particles flow from high μ to low μ or *vice versa*? Explain your reasoning.

Problem II.2 (15 pts)

Commuter blues.

Traffic jams have some interesting physics associated with them. (See for example: "Origin of synchronized traffic flow on highways and its dynamic phase transitions" Phys. Rev. Lett. **81**, 1130 (1998).) In a simple model, suppose the probability a car has speed in the range $(v, v+dv)$ is

$$f(v)dv = Av\exp\left(-\frac{v}{v_0}\right)dv$$

Here v_0 is a characteristic speed and A is a normalization constant.

1. Find A.
2. What is the average speed?
3. Is the average speed the same as the most probable speed?
4. Roughly plot the distribution function.

Problem II.3 (15 pts)

Large fluctuations.

Mixture of two different gases, containing equal number N of atoms of each of the species, is sealed in a 1 liter container. Estimate N, such that the probability for the species to separate during the lifetime of the Universe (about 10^{10} years) is comparable to unity.

*[**Hint:** think carefully how to define such a probability.]*

III. Elements of Ensembles Theory (240 pts)

Problem III.1 (15 pts)

Non-interacting (ideal) systems.

The grand canonical potential allows the treatment of systems of variable numbers of particles. We may exploit this in the study of systems of non-interacting (or weakly-interacting) identical particles in the following way. We focus attention on a single-particle state, which we label by k. The state of the entire system is specified when we know how many particles are in each different (single-particle) quantum state.

many-particle state $\equiv \{n_1, n_2, \ldots, n_k, \ldots\}$

Energy of state $\equiv \sum_k n_k \varepsilon_k$

No. of particles $\equiv \sum_k n_k$.

Here ε_k is the energy of the k_{th} single-particle state. Note that ε_k are independent of the number of particles.

Prove the relation for the partition sum. Starting from the expression for the Gibbs distribution function (i.e. grand canonical ensemble) for a many-particle system, write down the grand partition function Ξ and show how it may be expressed as the product of Ξ_k, the grand partition function for the subsystem comprising particles in the k_{th} single-particle state.

REMEMBER THIS RESULT.

Problem III.2 (15 pts)

Prove that the energy fluctuations in the grand canonical ensemble are related to those in the canonical ensemble via:

$$\left\langle (\Delta E)^2 \right\rangle = \left\langle (\Delta E)^2 \right\rangle_{canonical} + \left[\left(\frac{\partial \langle E \rangle}{\partial N} \right)_{T,V} \right] \left\langle (\Delta N)^2 \right\rangle.$$

Problem III.3 (20 pts)

Alternative derivation of equilibrium distribution functions.

The *isobaric-isothermal ensemble* is a statistical ensemble with fixed pressure, temperature and number of particles. In this ensemble, the volume can fluctuate, e.g., due to being bounded by flexible walls. The probability of finding the system with a volume V in quantum state i (with corresponding energy value $E_{i,V}$) is denoted $w_{i,V}$. (For correctness, we assume that allowed values of V form a discrete set.)

The approach that we have followed in class thus far begins with a statistical characterization of equilibrium states and then arrives at distribution laws. Alternatively, one could begin with the second law of phenomenological thermodynamics and the Gibbs entropy formula $S = -\sum_{i,V} w_{i,V} \ln\left(w_{i,V}\right)$ rather than deducing them from the principle of equal weights.

1 By maximizing the entropy subject to the constrains

$$\sum_{i,V} w_{i,V} = 1$$

$$\sum_{i,V} w_{i,V} E_{i,V} = \langle E \rangle$$

$$\sum_{i,V} w_{i,V} V_{i,V} = \langle V \rangle$$

(where $\langle E \rangle$ and $\langle V \rangle$ are the *observed* mean energy and volume, respectively) show that

$$w_{i,V} = \frac{\exp\left(-\beta E_{i,V} - \gamma V\right)}{Z_0}$$

2 Give thermodynamic identifications of the parameters β,γ. Basically, form the differential of the entropy S and compare with the combined first and second laws of thermodynamics.

3 Calculate $\left\langle (\Delta V)^2 \right\rangle$ in this ensemble.

Problem III.4 (25 pts)

A gas of N particles lives in a two-dimensional surface – a sphere. Find the energy $E = E(T, A)$, where A is the surface area, and the equation of state. The equation of state is the relation connecting the pressure, volume, and the temperature of a system in the state of thermal equilibrium: $f(p,V,T)=0$.

Problem III.5 (25 pts)

Zipper.

A zipper has N links; each link has a state in which it is closed with energy 0 and a state in which it is open with energy ε. We require that the zipper only unzip from one side (say from above) and that the link can only open if all links above it are already open. (This model is sometimes used for DNA molecules.)

1 Find the partition function.

2 Find the average number of open links $\langle n \rangle$ and show that for low temperatures $(T \ll \varepsilon)$, $\langle n \rangle$ is independent of N.

Problem III.6 (25 pts)

Equivalency of ensembles.

Consider a system of N identical but distinguishable particles, each of which has two states, with energies $\pm\varepsilon$ available to it. Use the microcanonical, canonical, and grand canonical ensembles to calculate the mean entropy per particle as a function of the mean energy per particle in the limit of a very large system. Verify that all three ensembles yield identical results in this limit.

Problem III.7 (35 pts)

Binary chain.

A lattice in one dimension has N sites and is at temperature T. At each site there is an atom, which can be in either of two energy states: $E_i = \pm\varepsilon$. When L consecutive atoms are in the $+\varepsilon$ state, we say that they form a cluster of length L (provided that the atoms adjacent to the ends of the cluster are in the $-\varepsilon$ state). Using the canonical ensemble, in the limit $N \to \infty$:

1 Explain why the canonical ensemble can be used for such a system.

2 Calculate the probability w_L that a given site belongs to a cluster of length L.

3 Calculate the mean length of a cluster $\langle L \rangle_T$ and determine its low- and high-temperature limits.

*[**Hint**: Choose a particular site on the lattice. Write the conditions when this site belongs to a cluster of length L. How many sites to the left and to the right belong to the same cluster?]*

Problem III.8 (40 pts)

Degenerate systems.

Consider a system of N identical but distinguishable particles, each of which has two energy levels with energy 0 or $\varepsilon > 0$. The upper energy level has a g-fold degeneracy while the lower level is non-degenerate. The total energy of the system is E.

1. Using the microcanonical ensemble, find the occupation numbers n_+ and n_0 in terms of the temperature of the system (where n_+ corresponds to the upper level and n_0 to the lower one).
2. Consider the case $g=2$. If the system has energy $E=0.75N\varepsilon$ and brought into contact with a bath at constant temperature $T=500\ K$, in what direction does heat flow? In order to answer this question, sketch the entropy as a function of energy.

Problem III.9 (40 pts)

3-level system.

A system of N three-level particles has a Hamiltonian of the form

$$H=-h\sum_{i=1}^{N}S_i \qquad S_i=1,0,-1$$

where h is a positive constant. (This might represent the energy levels of spin-1 particles in an applied magnetic field.)

1. If n_S is the average number of particles in the state $S \quad (S=1,0,-1)$, use the microcanonical ensemble to find the ratio ${n_{-1}}/{n_1}$ in terms of the temperature in the limit $N\to\infty$. Hence find the Helmholtz free energy $F(T,N)$.
2. Check you answer for $F(T,N)$ by using the canonical ensemble (which is much easier!).
3. Identify the limits in which the information on the state of the system is maximum (when we know exactly the state of every particle) and minimum (each particle has equal probabilities of occupying all three energy levels). And find the entropy in these cases.

Appendix:

You may find useful *Stirling's approximation:*

$$\ln N! \approx N \ln N - N$$