Phys 430 - 1^{st} HOMEWORK

1. Discuss the following concepts (just writing formulas is not enough, use words)

   Ergodic principle

   Solution:
   Given the values of the conserved quantities of the system, such as the energy, the linear momentum, and the angular momentum, the system can not be observed in a system which does not have those values. Ergodic principle states that the probability that the system can be observed in any other system is uniform, i.e. constant for all other states.

   Ensemble

   Solution:
   In short, an ensemble of a system is an infinite set of dublicates of the original system. In more detail, one can think of the phase trajectory of a given system, and follow this phase trajectory. One picks up points on this phase trajectory with equal time spacing. Afterwards, instead of following the phase trajectory of a single system for infinite amount of time, one can follow the "flow" of all these points in phase space. Hence it is obvious that the time average of any quantity is equal to the ensemble average.

   Distribution function

   Solution
   In "phase space," one can talk about the probability that a particular system will be in or near a state in phase space. This probability is determined by the distiobution function in phase space.

   Microcanonical Distribution Function

   Solution:
   Making the ergodic hypothesis, the probability that the system will be observed in any state which does not respect the initial values of the conserved quantities is zero. The probability that the system will be in any one of the "allowed states" (allowed by the conservation laws) is uniform. This distribution function is called the microcanonical distribution function. The energy, linear momentum and angular momentum is conserved in this distribution and have the predefined values.

Subsystem

Solution:

Any part of a larger system which is small but still macroscopic is called a subsystem of the larger system. The requirement that the subsystem is macroscopic is important to assure that the interaction of a subsystem with the rest of the system is small. In this sense even a microscopic part of the larger system can be considered a subsystem if its interactions with the rest of the system is negligable compared to the total energy of the subsystem.

2. Suppose you have N books of equal mass and 3 shelves to place the books onto. Let the potential energy of a book on shelf 1 be zero, of a book on shelf 2 be U_0 and the potential energy of a book on shelf 3 be $2U_0$.

   (i) If there is no restriction on the way you can distribute the books on the shelves, in how many ways can you distribute the books on the shelves?

   Solution:

   Each book can be placed in 3 different shelves. Since there are N shelves, all the books can be distributed in 3^N different ways. (Note that the ordering of the books on the shelves is being ignored)

   (ii) Assume that all possible distributions of the books among the shelves are equally probable. What is the probability, P_n that the books will have a total potential energy $U = nU_0$? (It is enough that you write an expression which would let you calculate the probability)

   Solution

   Let $\Gamma(n)$ be the number of states that have the energy $U = nU_0$. Then

$$P_n = \frac{\Gamma(n)}{3^N} \tag{1}$$

   Thus the problem is reduced to finding $\Gamma(n)$. In order to find $\Gamma(n)$, let n_i, $i = 1,\ 2,\ 3$ be the number of books on the i^{th} shelf. Then

$$n_1 + n_2 + n_3 = N$$

   and

$$n_2 + 2n_3 = n$$

are the constraints that the n_i should satisfy. For a given set of (n_1, n_2, n_3), there are

$$\Gamma(n_1, n_2, n_3) = \begin{pmatrix} N \\ n_1 \end{pmatrix} \begin{pmatrix} N - n_1 \\ n_2 \end{pmatrix}$$

states that have the given set (n_1, n_2, n_3). Summing this number over all $\Gamma(n_1, n_2, n_3)$ consistent with the given constraints, one obtains $\Gamma(n)$, i.e.

$$\Gamma(n) = \sum_{n_1=0}^{N} \sum_{n_2=0}^{N} \sum_{n_3=0}^{N} \Gamma(n_1, n_2, n_3) \delta_{n_1+n_2+n_3,N} \delta_{n_2+2n_3,N} \tag{2}$$

where the Kronecker deltas assure that it is only the n_i consistant with the constraints that contribute to the sum. Thus, the probability P_n can be written as

$$P_n = \frac{1}{3^N} \sum_{n_1=0}^{N} \sum_{n_2=0}^{N} \sum_{n_3=0}^{N} \begin{pmatrix} N \\ n_1 \end{pmatrix} \begin{pmatrix} N - n_1 \\ n_2 \end{pmatrix} \delta_{n_1+n_2+n_3,N} \delta_{n_2+2n_3,N} \tag{3}$$

which is an expression that can be easily evaluates using programs such as mathematica.

(iii) Using the expression that you have obtained in part (ii), plot the probability P_n for $N = 5$, $N = 20$ and $N = 40$. (Do use computers to do these plots. You can use mathematica, or maple (both available in orca.cc.metu.edu.tr, or any other program). Normalize your plots so that the maximum value of your plots is 1 and the x axes goes from 0 to 1 so that you will see that as N increases, the graph gets narrower)
Solution:
In Fig. (1) is shown the probability distribution for the reduced potential energy, defined as $\frac{U}{U_{max}}$ where $U_{max} = 2NU_0$ is the maximum energy that the system can have. As is clearly seen, the distribution gets narrower as the N increases. The average value is seen to be $\langle U \rangle = NU_0 = \frac{U_{max}}{2}$. The variation of the average energy, i.e. the width of the curve, changes from about 60% for $N = 5$ to about 10% for $N = 100$ which is already a large decrease in the fluctuations even if the number $N = 100$ is not macroscopically large.

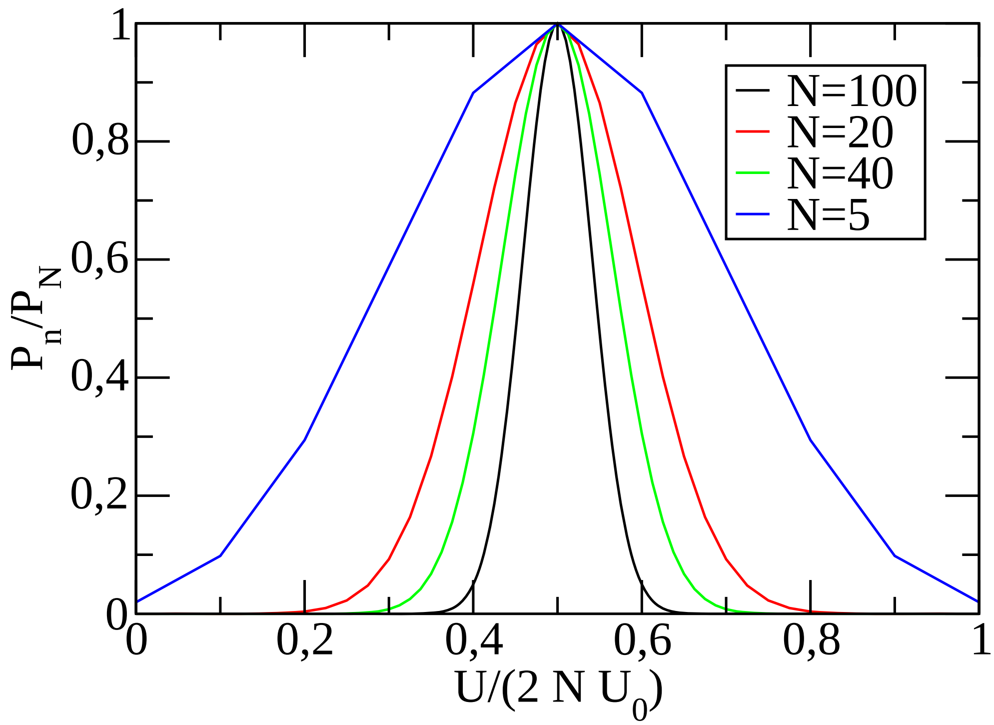

Figure 1: Plot of P_n for various values of N where $n = \frac{U}{U_0}$

(iv) For $N = 10$, what is the entropy of the system if the potential energy of the system is known to be $U = 15U_0$? (take the Boltzman constant $k = 1$)

Solution:

For $N = 10$ and $n = 15$, one can solve for the constraints to find $n_2 = 5 - 2n_1$ and $n_3 = 5 + n_1$. Thus the possible values of the triples (n_1, n_2, n_3) are $(0, 5, 5)$, $(1, 3, 6)$, and $(2, 7, 1)$. The number of states that have the corresponding numbers are $\Gamma(0, 5, 5) = 252$, $\Gamma(1, 3, 6) = 840$ and $\Gamma(2, 7, 1) = 360$. Thus the total number of states that have the energy $U = 15U_0$ is $\Delta\Gamma(15U_0) = 1452$, and the entropy $S = \ln \Delta\Gamma(15U_0) \simeq 7.28$

3. Consider two different quantum systems: system A and system B. Both of the systems can be only in two different states. If the wave function of the whole system is given by

$$\Psi = a_1 \Psi_A^1 \Psi_B^1 + a_2 \Psi_A^1 \Psi_B^2 + a_3 \Psi_A^2 \Psi_B^2 \tag{4}$$

where $|a_1|^2 + |a_2|^2 + |a_3|^2 = 1$ and Ψ_X^i $(X = A,\ B,\ i = 1,\ 2)$ is the wavefunction of the i^{th} state of the X system. What is the quantum statistical matrix of system A? What is the quantum statistical matrix of system B?

Solution:

Consider any operator $\mathcal{O}_A$ which acts only on the subsystem A. Consider the matrix element of this operator in the given state:

$$\begin{aligned} \langle \mathcal{O}_A \rangle & \int d^3x_1 d^3x_2 \Psi^*(x1, x2) \mathcal{O}_A \Psi(x1, x2) \\ &= \int d^3x_1 d^3x_2 \left(a_1^* \Psi_A^{1*}(x1) \Psi_B^{1*}(x_2) + a_2^* \Psi_A^{1*}(x_1) \Psi_B^{2*}(x_2) + a_3^* \Psi_A^2(x_1) \Psi_B^{2*}(x_2) \right) \mathcal{O}_A \\ & \left(a_1 \Psi_A^1(x_1) \Psi_B^1(x_2) + a_2 \Psi_A^1(x_1) \Psi_B^2(x_2) + a_3 \Psi_A^2(x_1) \Psi_B^2(x_2)) \right) \end{aligned} \tag{5}$$

Using the fact that $\mathcal{O}_A$ acts only on x_1 and not on x_2, one can integrate over x_2 using the normalization of the functions Ψ_B^n to obtain:

$$\begin{aligned} \langle \mathcal{O}_A \rangle & \int d^3x_1 d^3x_2 \Psi^*(x1, x2) \mathcal{O}_A \Psi(x1, x2) \\ &= |a_1|^2 \mathcal{O}_A^{11} + \mathcal{O}_A^{11} + a_2^* a_3 \mathcal{O}_A^{12} + a_3^* a_2 \mathcal{O}_A^{21} + |a_3|^2 \mathcal{O}_A^{22} \end{aligned} \tag{6}$$

where

$$\mathcal{O}_A^{nm} = \int d^3x_1 \Psi_A^{n*}(x_1) \mathcal{O}_A \Psi_A^m(x_1) \tag{7}$$

This can be written in matrix form as:

$$\langle \mathcal{O}_A \rangle = Tr \left[\begin{pmatrix} |a_1|^2 + |a_2|^2 & a_2 a_3^* \\ a_2^* a_3 & |a_3|^2 \end{pmatrix} \begin{pmatrix} \mathcal{O}_A^{11} & \mathcal{O}_A^{12} \\ \mathcal{O}_A^{21} & \mathcal{O}_A^{22} \end{pmatrix} \right] = Tr \rho_A \mathcal{O}_A \tag{8}$$

where $\mathcal{O}_A$ is the matrix corresponding to the operator $\mathcal{O}_A$ and

$$\rho_A = \begin{pmatrix} |a_1|^2 + |a_2|^2 & a_2 a_3^* \\ a_2^* a_3 & |a_3|^2 \end{pmatrix} \tag{9}$$

is the quantum statistical matrix of the subsystem A

In order to obtain the quantum statistical matrix for the subsystem B, one needs to do the same analysis using an operator, $\mathcal{O}_B$, acting only on subsystem B.

$$\begin{aligned}
\langle\mathcal{O}_B\rangle & \int d^3x_1 d^3x_2 \Psi^*(x1,x2)\mathcal{O}_A\Psi(x1,x2) \\
= & \int d^3x_1 d^3x_2 \left(a_1^*\Psi_A^{1*}(x1)\Psi_B^{1*}(x_2) + a_2^*\Psi_A^{1*}(x_1)\Psi_B^{2*}(x_2) + a_3^*\Psi_A^2(x_1)\Psi_B^{2*}(x_2)\right)\mathcal{O}_B \\
& \left(a_1\Psi_A^1(x_1)\Psi_B^1(x_2) + a_2\Psi_A^1(x_1)\Psi_B^2(x_2) + a_3\Psi_A^2(x_1)\Psi_B^2(x_2))\right) \qquad (10)
\end{aligned}$$

Using the fact the the operator $\mathcal{O}_B$ acts only on x_2, one can integrate over x_1 to obtain:

$$\langle\mathcal{O}_B\rangle = |a_1|^2\mathcal{O}_B^{11} + a_1^*a_2\mathcal{O}_B^{12} + a_2^*a_!\mathcal{O}_B^{21} + |a_2|^2\mathcal{O}_B^{22} + |a_3|^2\mathcal{O}_B^{22} \qquad (11)$$

which can be written in matrix form:

$$\langle\mathcal{O}_B\rangle = Tr\left[\begin{pmatrix} |a_1|^2 & a_1a_2^* \\ a_1^*a_2 & |a_2|^2+|a_3|^2 \end{pmatrix}\begin{pmatrix} \mathcal{O}_B^{11} & \mathcal{O}_B^{12} \\ \mathcal{O}_B^{21} & \mathcal{O}_B^{22} \end{pmatrix}\right] = Tr\rho_B\mathcal{O}_B \qquad (12)$$

where $\mathcal{O}_B$ is the matrix corresponding to the operator and

$$\rho_B = \begin{pmatrix} |a_1|^2 & a_1a_2^* \\ a_1^*a_2 & |a_2|^2+|a_3|^2 \end{pmatrix} \qquad (13)$$

is the quantum statistical matrix of the subsystem B.