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Statistical Mechanics

PHYS 5163 Homework Assignment 1

Problems: {1,2,3,4}

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Problem 1:

Three fun, independent parts related to probabilities

(a) A game show contestant is presented with three closed doors. Behind two of the doors are goats and behind the third is a fancy new car. The contestant would prefer getting the car... The game goes as follows:

(1) The contestant goes to a door but does not open it.

(2) The host, who knows which door has the car behind it, goes to one of the other doors, opens it, and reveals a goat.

(3) The contestant is given the choice to either stay with the door first picked or to switch.

What is the contestant's probability to win the car when they stay and when they switch?

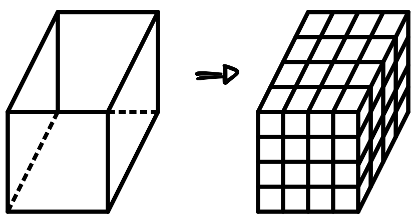
At the onset the probability is 1/3, so if the contestant stays after revealing the goat the probability will be $P = 1/3$.

Because probabilities must sum to 1, if the contestant switches the probability is 2/3.

$$\boxed{\text{Staying}: P = \frac{1}{3}, \ \text{Switching}: P = \frac{2}{3}}$$

(b) Imagine you take a blue painted cube and cut it into 64 equal pieces. What is the probability $P_n (n = 0, 1, 2, 3)$ that a little cube, picked at random, has n painted faces?

When we cut our cube into 64 pieces we have a new cube that will be a $4 \times 4 \times 4$. Amongst the remaining 64 little cubes, it is only at most possible to have 3 sides painted.



This means that for $n=0$ (0 painted faces) there are at most only 8 pieces that won't be painted. The pieces in the core.

For $n=1$, there will be 24 pieces that have only one side painted, the pieces in the middle.

For $n=2$, there will be 24 pieces that have two sides painted, the center pieces.

For $n=3$, there will be 8 pieces that have three sides painted, the corner pieces.

$$n=0, \ P_0 = \frac{8}{64} = \frac{1}{8} \ ; \ n=1, \ P_1 = \frac{24}{64} = \frac{3}{8} \ ; \ n=2, \ P_2 = \frac{24}{64} = \frac{3}{8} \ ; \ n=3, \ P_3 = \frac{8}{64} = \frac{1}{8}$$

$$\boxed{P_0 = \frac{1}{8}, P_1 = \frac{3}{8}, P_2 = \frac{3}{8}, P_4 = \frac{1}{8}}$$

Problem 1: Continued

(c) You are given four coins, each having equal and independent probability to be a quarter, nickel, dime, or penny. What is the probability that you just made 37 cents?

The probability of receiving a Quarter, Dime, Nickel, or penny is 1/4. The only combination with 4 coins that will make 37 cents is

Quarter, Dime, Penny, Penny.

It doesn't matter which order they come in only that we have this combination. With 4 choices and 4 selections we will have 4^4 combinations ($4^4 = 256$) total. The combinations for these are:

1.) QDPP	4.) DQPP	7.) PPDQ	10.) PPQD
2.) QPDP	5.) DPQP	8.) PDPQ	11.) PQPD
3.) QPPD	6.) DPPQ	9.) PDQP	12.) PQDP

With 12 combinations above, with 256 total possibilities this means the probability will be

$$P = \frac{12}{256} = \frac{3}{64} \approx 4.6875\,\%$$

The final probability of making 37 cents is:

$$\boxed{P = 3/64 \;,\; P = 4.6875\%}$$

Problem 1: Review

Procedure:

- - Initial probability is 1/3 → Opens door, probability is 1/2
  - Using the above logic we just sum the probabilities to find that the answer after switching is 2/3
- - This is is simply a counting game
  - Add up the occurrences and then divide by the total number of cubes (64)
- - There is only one combination where this can happen,

    $$Q, D, P, P$$

    we then count permutations of this with

    $$\mathcal{N} = \frac{N!}{\prod_i n_i!}$$

    where N is the total number of slots (4 in our case) and n is how many times one of variables in the slot is repeated. For instance there are two pennies so for $n_p = 2$.
  - Because there are 4 choices and 4 selections this means there are $\tilde{\mathcal{N}} = 4^4 = 256$ combinations when picking these coins
  - Take the number of permutations for 37 cents and divide it by the total number of combinations. Namely

    $$\mathcal{P} = \frac{\mathcal{N}}{\tilde{\mathcal{N}}}$$

Key Concepts:

- - Switching your choice after the first door is opened improves your overall odds of winning
  - Probability is what we want divided by how many possibilities
- - This part is having us count up the number of sides that are painted and dividing by the total number of cubes to determine the probability
- - We can count the number of permutations for <u>distinguishable</u> selections with the equation for $\mathcal{N}$
  - Once we know the number of selections we use $\mathcal{P}$ to calculate the probability

Variations:

- - We can be given a different number of doors
    * This would just cause a slight change in the numbers that we use to calculate the probabilities
- - The cube could be cut into a different number of pieces or a different shape
    * This then would change the number of pieces with painted and unpainted sides etc
    * We would use the same procedure but with different numbers
- - We could be given a different total change
    * This would change the combinations, choices, and selections for the coins
    * We would use the same procedure for counting the combinations

Problem 2:

Make sure to carefully define your notation.

(a) Write down the classical and quantum mechanical ideal gas Hamiltonian for a system consisting of K point particles (atoms or molecules).

The Hamiltonian for an ideal gas is:

$$\text{Classically: } H = \sum_i \frac{P_i^2}{2m_i} + V \quad , \quad \text{Quantum Mechanically: } \tilde{H} = \sum_i \frac{\tilde{P}_i^2}{2m_i} + V$$

Classically And Quantum Mechanically this is:

$$\boxed{\vec{H}_C = \sum_i \frac{\vec{P}_i^2}{2m} + V \ , \ \tilde{H}_Q = \sum_i \frac{\tilde{P}_i^2}{2m} + V}$$

(b) Write down the classical and quantum mechanical Hamiltonian for a system that consists of eigth structureless partciles of mass m and five structureless particles of mass M. Each mass-m particle interacts with all other mass-m particles through the two-body potential V_{mm}. Each mass-M particle interacts with all other mass-M particles through the two-body potential V_{MM}. Each mass-m particle interacts with each mass-M particle through the two-body potential $V_m M$.

To simplify this, we will write it as a sum. The Classical Hamiltonian for this is,

$$\boxed{\vec{H}_C = \sum_i^8 \frac{\vec{P}_{im}^2}{2m} + \sum_i^5 \frac{\vec{P}_{iM}^2}{2M} + \sum_{i<j}^8 V_{mm}(\vec{r}_{im}, \vec{r}_{jm}) + \sum_{i<j}^5 V_{MM}(\vec{r}_{iM}, \vec{r}_{jM}) + \sum_{i=1}^8 \sum_{j=1}^5 V_{mM}(\vec{r}_{im}, \vec{r}_{jM})}$$

Where we say $r_{im} \to$ position vector of i^{th} particle with mass m. And vice versa. The Quantum Mechanical Version of this is

$$\boxed{H_Q = \sum_i^8 \frac{\hbar^2 \vec{\nabla}_{i,m}^2}{2m} + \sum_i^5 \frac{\hbar^2 \vec{\nabla}_{i,M}^2}{2M} + \sum_{i<j}^8 V_{mm}(\vec{r}_{im}, \vec{r}_{jm}) + \sum_{i<j}^5 V_{MM}(\vec{r}_{iM}, \vec{r}_{jM}) + \sum_{i=1}^8 \sum_{j=1}^5 V_{mM}(\vec{r}_{im}, \vec{r}_{jM})}$$

(c) Consider a system that consists of an equal number of electrons and protons.

(i) Write down the classical and quantum mechanical Hamiltonian for this system.

(ii) What equilibrium state are you expecting the system to be in the low temperature regime?

(iii) What equilibrium state are you expecting the system to be in the high temperature regime?

(iv) What equilibrium state are you expecting the system to be in at room temperature?

We must first account for the coulomb interactions between the point particles

$$V_{int}(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_n ; \vec{R}_1, \vec{R}_2 \ldots \vec{R}_n) = \sum_{i<j}^n V_{ee}(\vec{r}_{ij}) + \sum_{i<j}^n V_{pp}(\vec{R}_{ij}) + \sum_i^n \sum_j^n V_{ep}(|\vec{r}_i - \vec{R}_j|)$$

Accounting for these interactions the Hamiltonians are then

Problem 2: Continued

$$\boxed{\hat{H}_C = \sum_i^8 \frac{\hat{p}_i^2}{2m} + \sum_i^5 \frac{\hat{p}_i^2}{2m} + V_{int}(\ldots) \quad , \quad H_Q = \sum_i^8 \frac{\hbar^2 \vec{\nabla}^2_{i,m}}{2m} + \sum_i^5 \frac{\hbar^2 \vec{\nabla}^2_{i,m}}{2m} + V_{int}(\ldots)}$$

In the low temperature regime, the equilibrium state will most likely be bonded molecules.

In the high temperature regime, the equilibrium state will most likely be protons separating from nuetrons, something like the time of recombination.

And at room temperature the equilibrium state is most likely unbound molecules and will have energy low compared to the binding energy

Problem 2: Review

Procedure:

- – For a Classical Hamiltonian use $\vec{p}$ and for the Quantum version use $\tilde{\mathbf{p}}$
- – First take into account the different interactions between masses m and M for the two body potentials
  – The only difference between the Classical Hamiltonian the Quantum version is that Classically we use vectors and Quantum Mechanically we use operators
  – Use $-i\hbar\vec{\nabla}_{j,(m,M)}$ in place of $\vec{p}$ for the Quantum version
- – Write out the different Coulomb interactions between the electrons and protons for this system
  – Write out the Classical and Quantum Hamiltonians with these new interactions

Key Points:

- – The largest difference between Quantum Mechanical Hamiltonians and Classical versions is that Classical Hamiltonians use vectors and Quantum versions use operators
- – In this part we must account for the two different masses of the particles. This is done by creating two separate sums for the momentum part and having separate interactions for the potentials.
  – We write out three separate interactions for the potentials. One for each $(m, m), (M, M), (m, M)$.
  – Our indices will range between 1 to 8 for m and 1 to 5 for M
  – The correct operator to use in place of $\vec{p}$ is $-i\hbar\vec{\nabla}$
- – Similar to part (b), the largest difference is that this potential is now the Coulomb potential and not the Two-Body potential
  – Low temperatures result in bonded molecules
  – High temperatures have unbound molecules like the time of recombination
  – The binding energy is greater compared to energy in the room and the molecules are likely unbound

Variations

- This problem cannot be altered too much other than changing the number of m and M particles. Because of this we would use almost the exact same procedure but with a slightly different system if asked to.

Problem 3:

Consider a non-interacting classical gas of three-level atoms with energy levels $0, \epsilon$, and 10ϵ. Further assume that there exists some "magic" mechanism by which the number of atoms in the single-particle state with energy 0 is equal to the number of atoms in the single-particle state with energy ϵ.

(a) Treating N, E, and V as macro-variables, derive a condition that ensures that the system is characterized by a negative temperature.

we need to come up with an expression for the entropy. To do this, we first calculate the number of microstates with

$$\Omega = \frac{N!}{\prod_{i=1} N_i!}$$

$$\Omega = \frac{N!}{N_0! \cdot N_\epsilon! \cdot N_{10\epsilon}!}, \quad N_0 = N_\epsilon \doteq n \quad \therefore \quad \Omega = \frac{N!}{(n!)^2 \cdot N_{10\epsilon}!}$$

The entropy is then calculated with $(N_{10\epsilon} = N - 2n)$

$$S = k\log(\Omega) = k\log\left(\frac{N!}{(n!)^2((N-2n)!)}\right)$$

We now wish to apply the Stirling approximation: $\log(N!) = N\log(N) - N$. This then becomes

$$S = k\left[\log(N!) - 2\log(n!) - \log((N-2n)!)\right] \Rightarrow \log(N!) = N\log(N) - N + \text{other terms}$$

$$S = k[N\log(N) - \cancel{N} - 2n\log(n) + \cancel{2n} - (N-2n)\log(N-2n) + \cancel{N} - \cancel{2n}]$$

$$S = k[N\log(N) - N\log(N-2n) - 2n\log(n) + 2n\log(N-2n)] = k\left(N\log\left(\frac{N}{N-2n}\right) - 2n\log\left(\frac{N-2n}{N}\right)\right)$$

The entropy then becomes,

$$S = kN\log\left(\frac{N}{N-2n}\right) - 2kn\log\left(\frac{N-2n}{N}\right)$$

Now that we have our entropy, we wish to use the inverse temperature equation to determine when it will be negative

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V}$$

we now wish to express the total energy

$$E = 0 \cdot n + \epsilon n + 10\epsilon(N-2n) = \epsilon n + 10\epsilon N - 20\epsilon n = 10\epsilon N - 19\epsilon n \quad \therefore \quad E = 10\epsilon N - 19\epsilon n$$

$$\frac{E}{\epsilon} = 10N - 19n, \quad 19n = 10N - \frac{E}{\epsilon} \quad \therefore \quad n = \frac{1}{19}\left(10N - \frac{E}{\epsilon}\right)$$

Problem 3: Continued

Our inverse temperature then becomes

$$\left(\frac{\partial S}{\partial E}\right)_{N,V} = \frac{\partial S}{\partial n}\frac{\partial n}{\partial E} \quad , \quad \frac{\partial S}{\partial n} = -2k\log\left(\frac{N-2n}{n}\right) - \frac{2k(2n+N)}{2n-N} \quad , \quad \frac{\partial n}{\partial E} = -\frac{1}{19\epsilon}$$

The temperature is then

$$T = \left(-2k\left(\log\left(\frac{N-2n}{n}\right) - 1\right)\right)^{-1} \quad , \quad \log\left(\frac{N-2n}{n}\right) - 1 = 0 \qquad 0 < \frac{N-2n}{n} < 1 \quad \therefore \quad N > 3n$$

$$\boxed{T < 0, N > 3n}$$

(b) Provide a physical interpretation of the existence of the negative temperature in this system of three-level atoms.

As energy is added the system becomes more ordered and the entropy becomes less and less.

(c) Can negative temperatures be realized in any system? If your answer is "yes", explain. If your answer is "no", provide a necessary condition for negative temperatures to be realized?

Hint: Stirling's formula: $N! \approx N\log N - N$

Yes, negative temperatures can be recognized. For this to happen the system must possess an upper bound for the Energy or have Finite # of energy levels. So this can happen, but is not true for all Systems, and therefore this <u>cannot</u> happen in <u>reality</u>.

Problem 3: Review

Procedure:

- – Begin by calculating the entropy with
  $$S = k\log(\Gamma)$$
  where Γ is the number of microstates
  – Calculate Γ with
  $$\Gamma = \frac{N!}{\prod_i n_i!}$$
  where N is our total number of choices and n are how many particles are in each energy level
  – Once the entropy has been calculated, proceed to calculate the inverse temperature with
  $$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V}$$
  where
  $$\frac{\partial S}{\partial E} = \frac{\partial S}{\partial n}\frac{\partial n}{\partial E}.$$
  – Calculate the total E and then use the above equation to solve for T in terms of n
- – As energy is added the entropy will decrease
- – This cannot happen in reality

Key Concepts:

- – Since we are working in the microcanonical ensemble we will count the number of microstates and then use that with the entropy to find T
  – We can find a relationship for this system with temperature using the inverse temperature equation
  – We can calculate the inverse temperature once we have our entropy
  – We used the following equation to calculate the total energy
  $$E = \sum_i n_i \epsilon_i$$
- – As energy is added it will cause the entropy of the system to decrease
- – This in theory can happen if their is an upper bound on the energy or if there are a finite number of energy levels
  – Since there is not a finite number of energy levels or bounded energy this cannot happen in reality

Variations

- – We can be given a different initial system (i.e there are more particles with different energies etc.)
    * This would most likely cause a difference in the microstate equation where everything else after that would be the same procedure with different values
  – We could be asked to find a different relationship for a different condition
    * This would cause us to evaluate our T function differently at the end
- – Because this question is qualitative it would have to be a brand new question where we could possibly be asked about a different temperature value
- – Same as part (b)

Problem 4:

1200 particles are to be distributed among three energy levels with energies ϵ_1, ϵ_2, and ϵ_3: $\epsilon_1 = 1\,\text{eV}$, $\epsilon_2 = 2\,\text{eV}$, and $\epsilon_3 = 3\,\text{eV}$. The total energy of the system is fixed at 2400 eV and each possible microstate is equally probable.

(a) Assume that the particles are distinguishable. What is the number of microstates? Express your result in terms of N_1, where N_1 denotes the number of particles in the energy level ϵ_1. What is the most probable value of N_1?

The total number of particles is 1200, so mathematically this means:

$$N_1 + N_2 + N_3 = 1200$$

We know that the total energy in our system is 2400 eV, mathematically this means:

$$N_1 + 2N_2 + 3N_3 = 2400\text{ eV} \qquad \text{w/ } E_{Tot} = \sum_{n=1}^{\infty} nN_n$$

We wish to calculate the total number of microstates in terms of N_1. The equation for total number of microstates for a K-level system is

$$\Omega = \frac{N!}{\prod_{j=1}^{K} N_j!}.$$

So we need to solve for Ω only in terms of N_1 and N. Ω is then

$$\Omega = \frac{N!}{(N_1)!(N_2)!(N_3)!}.$$

We now solve for N_2 in terms of N_1

$$N_3 = 1200 - N_2 - N_1 \rightarrow N_1 + 2N_2 + 3(1200\text{ eV} - N_2 - N_1) = 2400\text{ eV}$$

$$N_1 + 2N_2 + 3600\text{ eV} - 3N_2 - 3N_1 = 2400\text{ eV}$$

$$-2N_1 - N_2 = -1200\text{ eV} \quad \therefore \quad N_2 = 1200\text{ eV} - 2N_1$$

Taking this and putting it in the original equation yields

$$N_1 + (1200\text{ eV} - 2N_1) + N_3 = 1200\text{ eV} \rightarrow -N_1 + N_3 = 0 \quad \therefore \quad N_1 = N_3$$

Using the above result we get our number of microstates to be

$$\boxed{\Omega = \frac{1200!}{(N_1!)^2(1200 - 2N_1)!}}$$

Problem 4: Continued

We now wish to find the most probable value of N_1. We do this by extremizing the entropy and solving for N_1

$$S = K\log(\Omega).$$

We first need to apply the Stirling formula ; $N! = N\log(N) - N$.

$$N_1! = N_1\log(N_1) - N_1 \;,\; (1200-2N_1)! = (1200-2N_1)\log(1200-2N_1) - (1200-2N_1)$$

This then means the entropy then becomes

$$S = K\log\left(\frac{1200}{(N_1!)^2(1200-2N_1)!}\right) = K\left(\log(1200) - 2\log(N_1!) - \log((1200-2N_1)!)\right) \;,\; N! = N\log(N) - N$$

$$S = K\log(1200) - K\left(2\log(N_1\log(N_1) - N_1) + \log((1200-2N_1)(\log(1200-2N_1) - 1)\right)$$

Using mathematica to simplify S we get

$$S = -K\left(2N_1\log\left(\frac{N_1}{1200}\right) + (1200-2N_1)\log\left(\frac{1200-2N_1}{1200}\right)\right) \qquad (*)$$

We now take (*) and extremize it for N_1

$$\frac{\partial S}{\partial N_1} = -K\left(2\log\left(\frac{N_1}{1200}\right) + 2 - 2\log\left(\frac{1200-2N_1}{1200}\right) - \cancel{(1200-2N_1)}\frac{\overset{2}{\cancel{1}}}{(600-N_1)}\right) \rightarrow \frac{\partial S}{\partial N_1} = 0$$

$$0 = -K\left(2\log\left(\frac{N_1}{1200}\right) - 2\log\left(\frac{1200-2N_1}{1200}\right)\right) = \log\left(\frac{N_1}{1200}\right) - \log\left(\frac{1200-2N_1}{1200}\right)$$

$$0 = \log\left(\frac{N_1}{1200-2N_1}\right) \Rightarrow \frac{N_1}{1200-2N_1} = 1 \quad \therefore \quad 3N_1 = 1200 \quad \therefore \quad N_1 = 400$$

The most probable value of N_1 is then

$$\boxed{N_1 = 400}$$

Problem 4: Continued

(b) Assume that the particles are identical bosons (quantum particles that are described by a fully symmetric many-body wave function). What is the number of microstates? What is the most probable value of N_1?

Note, even though part (b) mentions the many-body wave function, there is no need to explicitly construct wave functions to answer the questions.

The number of microstates is calculated with

$$\Omega \approx \frac{(N+M-1)!}{N!(M-1)!} \approx \frac{(N+M)!}{N!M!}$$

where N is the number of particles in the system, M is how many ways the particles can be re-arranged. In this case $N = 1200$ $M = 3$ $\therefore$

$$\Omega \approx \frac{(1200+3-1)!}{1200!(3-1)!} \approx \frac{1202!}{2\cdot 1200!} \approx \frac{1202\cdot 1201\cdot \cancel{1200!}}{2\cdot \cancel{1200!}} \approx 721{,}801$$

The total number of microstates is then

$$\boxed{\Omega = 721{,}801}$$

Again we maximize the entropy to find the most probable number of microstates for N_1

$$S = k\log(\Omega) = k\log\left(\frac{(N+M)!}{N!M!}\right) = k\left(\log((N+M)!) - \log(N!) - \log(M!)\right)$$

In this case $N = N_1 + N_2 + N_3$ and $M = 3$, so the entropy becomes

$$S = k(\log((N+3)!) - \log(N!) - \log(6)) = k((N+3)\log(N+3) - (N+3) - N\log(N) + N - \log(6))$$

$$= k((N+3)\log(N+3) - 3 - N\log(N) - 3\log(3) + 3) = k((N+3)\log(N+3) - N\log(N) - 3\log(3))$$

$$= k(N\log(N+3) - N\log(N)) = kN(\log(N+3) - \log(N)) = kN\log\left(\frac{N+3}{N}\right)$$

Our entropy is now,

$$S = kN\log\left(\frac{N+3}{N}\right) \qquad \text{w/ } N = N_1 + N_2 + N_3$$

Where we extremize and solve for N_1 to get the most probable value. We know from our prior definitions that

$$N_1 = N_3 \;\;\&\;\; N_2 = 1200 - 2N_1$$

With a maximum number of 1200 particles, this means N_1 can range between 0 and 600.

Problem 4: Review

Procedure:

- – Begin by using the equations

  $$N_1 + N_2 + N_3 = 1200\,\text{eV} \qquad N_1 + 2N_2 + 3N_3 = 2400\,\text{eV}$$

  along with the generic equation for counting microstates Γ

  $$\Gamma = \frac{N!}{\prod\limits_i n_i!}$$

  – Proceed to calculate the most probable value of N_1 by extremizing the entropy equation

  $$S = k\log(\Gamma)$$

- – Since we are using Bosons now the way we calculate microstates for Bosons is

  $$\Gamma_\gamma \approx \frac{(N+M-1)!}{N!(M-1)!} \approx \frac{(N+M)!}{N!M!}$$

  – We then extremize the entropy again to find the most probable value of N_1

Key Concepts:

- – Since we are working in the microcanonical ensemble we will count the number of microstates and then use that with the entropy to find the most probable value of N_1
  – We can use the relationship for the number of particles and the total energy to find a relationship for N
  – We extremize the entropy with respect to the variable we are examining the find the most probable value for that variable
  – These particles are <u>distinguishable</u> and that is why we can use the generic microstates equation for Γ
- – Since these particles are <u>indistinguishable</u> we cannot use the generic equation for microstates Γ
  – We once again extremize the entropy to find the most probable value for N_1 since we are working in the microcanonical ensemble
  – From deductive reasoning we can say that N_1 must range between 0 and 600

Variations:

- – We could be given a different arrangement of particles, or a different number of particles
  - ∗ We would then still have to calculate the number of microstates and eventually the entropy
  - ∗ The change will come from the relationships for the total energy and the total number of particles
- – We could once again have the same scenario in (a)
  - ∗ We would then do the same procedure with different values now

  – We could be given a different type of particle (For both (a) and (b))
  - ∗ This would then change how we counted microstates but would not affect the overall procedure for finding N_1