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

   Entropic principle *Entropy is the logarithm of the number of states that the system can be found in. In a spontaneous process, the entropy of the system can not decrease, it either increases or at most remains constant. The entropy of a part of a system can decrease as long as this decrease is compansated by an increase of the entropy by at least an equal amount in some other part of the system.*

   Closed system *A closed system is a system which does not interact with any other system by any means. It is a completely isolated system*

   Subsystem *A subsystem is a small but still macroscopic part of a larger system*

   Distribution function *Distribution function is a measure of the probability that the system will be in a particular state. In classical mechanics, it is the probability density that the system will have position* (p, q) *in phase space. In quantum mechanics it gives us the probability density that the system will be found at a specific state*

   Microcanonical distribution function *For a closed system, the total energy, total linear momentum, and total angular momentum are conserved. Hence given these values, the probability that the system will be observed in a state which does not have these valuse is zero. These conserved quantities can be considered as constraints imposed on the states of our system. Hence the probability that the system will be observed in a state which does not respect these constraints are zero. If one assumes that the probability that the system will be in a given state that respects these constraints is constant for all states respecting these constraints, the distribution function can be written as:*

$$\rho = constant \times \delta(E - E_0)\delta(\vec{P} - \vec{P}_0)\delta(\vec{M} - \vec{M}_0) \tag{1}$$

   where each delta function makes sure that the distribution function is zero for any system that does not have the given energy, momentum and angular momentum, respectively.

2. Consider N identical non-interacting 1D harmonic oscillators. The en-

ergy levels of the system will be given by:

$$E = \hbar\omega \left(\sum_{i=1}^{N} n_i + \frac{N}{2} \right) \tag{2}$$

a For N=2, calculate the total number of states that have energies less then or equal to $E = \hbar\omega(M + \frac{N}{2})$.
<u>*Solution:*</u>
The number of states that have the energy less then the given energy is equivalent to the number of integer pairs (n_1, n_2) such that $n_1 + n_2 \leq M$. To find this number, first consider the related problem of finding the number of integer pairs (n_1, n_2) such that $n_1 + n_2 = M'$.

n_1 can take any value from $n_1 = 0$ upto and including $n_1 = M'$. Once n_1 is fixed, n_2 is also fixed. Hence the total number of pairs (n_1, n_2) such that $n_1 + n_2 = M'$ is $M' + 1$.

Then the total number of integer pairs (n_1, n_2) such that $n_1 + n_2 \leq M$ is given by

$$\begin{aligned}
\Gamma(E) &= \sum_{M'=0}^{M} (M' + 1) \\
&= \frac{M(M+1)}{2} + M + 1 \\
&= \frac{M^2 + M + 2M + 2}{2} \\
&= \frac{M^2}{2} \left(1 + \frac{2}{M}\right) \left(1 + \frac{1}{M}\right)
\end{aligned} \tag{3}$$

Note that only for $M >> 2$ which is the total number of harmonic oscilators, this reduces to:

$$\Gamma(E) \simeq \frac{M^2}{2!} \tag{4}$$

which is the result that we one obtains using the areas.

b Generalize the previous result for arbitrary N and obtain an expression for $\Gamma_N(E)$.
<u>*Solution:*</u>

For the case of the N harmonic oscilators, the exact number $\Gamma(E)$ can be written as:

$$\Gamma_N(E) = \sum_{n_N=0}^{M} \sum_{n_{N-1}=0}^{M-1} \cdots \sum_{n_1=0}^{M-\sum_{i=2}^{N-1} n_i} 1 \tag{5}$$

where we have used a reasoning similar to that in the privious case, i.e. n_N can take any value from $n_N = 0$ upto and including $n_N = M$. Onca a value is assigned to n_N, n_{N-1} can take any value from 0 upto and including $M - n_N$, etc. To obtain an approximate answer valid for large M, the summations can be replaced by integrations. Hence

$$\Gamma_N(E) \simeq \int_0^M dn_N \int_0^{M-n_{N+1}} dn_{N-1} \cdots \int_0^{M-\sum_{i=2}^{M} n_i} dn_1 1 \tag{6}$$

I will show that

$$\Gamma_N(E) = \frac{M^N}{N!} \tag{7}$$

using induction on N. For $N = 2$, we have shown in the previous section that $\Gamma_2(E)$ is given in the form Eq. (7).

Now we will assume that Eq. (7) is valid for N and show that this implies that Eq. (7) is also true for $N + 1$. First note that

$$\begin{aligned} \Gamma_{N+1}(M) &= \int_0^M dn_{N+1} \int_0^{M-n_{N+1}} dn_N \cdots \int_0^{M-\sum_{i=2}^{M} n_i} dn_1 1 \\ &= \int_0^M dn_{N+1} \Gamma_N(M - n_{N+1}) \end{aligned} \tag{8}$$

We have already assume that Eq. (7) is valid for N and hence

$$\begin{aligned} \Gamma_{N+1}(M) &= \int_0^M dn_{N+1} \Gamma_N(M - n_{N+1}) \\ &= \int_0^M dn_{N+1} \frac{(M - n_{N+1})^N}{N!} \\ &= - \left. \frac{(M - n_{N+1})^{N+1}}{(N+1)!} \right|_0^M \\ &= \frac{M^{N+1}}{(N+1)!} \end{aligned} \tag{9}$$

Thus Eq. (7) is also valid for $N+1$, therefore it is valid for any integer N. Then expressing M in terms of energy, one obtains:

$$\Gamma_N(E) = \frac{1}{N!}\left(\frac{E}{\hbar\omega} - \frac{N}{2}\right)^N \tag{10}$$

c Calculate the total number of states, $\Delta\Gamma$ that the system can be in if the total energy is exactly $E = \hbar\omega(M + \frac{N}{2})$. How is this result related to $\Gamma(E)$

Solution:

To calculate exactly the number of states that have the given energy is equivalent to the problem of finding the number of N-tuples of integers $\{n_1, n_2, \cdots, n_N\}$ such that $\sum_{i=1}^{N} n_i = M$.

To find this number, consider M spheres arranged on a line, and $N-1$ walls that devide these M spheres into N sections, some sections might involve no spheres. If one identifies n_i with the number of spheres in the i^{th} section, then by construction, $\sum_{i=1}^{N} n_i = M$. Then the problem that we were trying to solve is equivalent to the number of distinct orderings of these M spehers and $N-1$ walls. Since the walls are identical, and also the walls are identical, their exchange does not give us a new ordering. Hence, the total number of distinct ways that these $M+N-1$ objects can be ordered is given by:

$$\Delta\Gamma_N(M) = \frac{(M+N-1)!}{(N-1)!M!} \tag{11}$$

Note that for $M >> N$, the ratio

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

contains $N-1$ factors which are equal to M plus a number smaller then N which we neglect. Hence, we can write this as:

$$\Delta\Gamma_N(M) \simeq \frac{M^{N-1}}{(N-1)!} \tag{12}$$

or

$$\Delta\Gamma_N(E) \simeq \frac{1}{(N-1)!}\left(\frac{E}{\hbar\omega} - \frac{N}{2}\right)^{N-1} \tag{13}$$

also note that

$$\Gamma_N(E+\hbar\omega)-\Gamma_N(E)\simeq\frac{\partial\Gamma_N(E)}{\partial E}\Delta E=\Delta\Gamma_N(E) \tag{14}$$

where $\Delta E=\hbar\omega$ so that there is exactly one energy eigenvalue between E and $E+\Delta E$

d Calculate entropy, S. What is the temperature T of the state?
<u>Solution:</u>
The entropy S is the logarith of $\Delta\Gamma(E)$ devided by the Boltzman constant k, hence

$$\begin{aligned} S(E) &= k\ln\Delta\Gamma(E) \\ &= k\left((N-1)\ln\left(\frac{E}{\hbar\omega}-\frac{N}{2}\right)-\ln(N-1)!\right) \\ &= Nk\left(\ln\left(\frac{E}{\hbar\omega}-\frac{N}{2}\right)-\ln N+1\right) \\ &= Nk\left(\ln\left(\frac{E}{N\hbar\omega}-\frac{1}{2}\right)+1\right) \end{aligned} \tag{15}$$

where we have used the Stirling's approximation and neglected 1 in comparison with N.

In terms of entropy $S(E)$, the temperature is defined as

$$T=\left(\frac{\partial S}{\partial E}\right)_T^{-1} \tag{16}$$

Using the expression for entropy, one obtains:

$$T=\frac{E-\frac{N\hbar\omega}{2}}{Nk} \tag{17}$$

or $E=NkT+N\frac{\hbar\omega}{2}$.

e What is the probability that a particular harmonic oscillator is in the n^{th} excited state?
<u>Solution:</u>
The probability can be written as

$$\begin{aligned} p(n) &= \frac{\Delta\Gamma_{N-1}(E-\epsilon_n)}{\Delta\Gamma_N(E)} \\ &= e^{\frac{1}{k}(S_{N-1}(E-\epsilon)-S_N(E))} \end{aligned} \tag{18}$$

where ϵ_n is the energy of the n^{th} excited state of the harmonic oscillator, and we have used the definition of entropy.

Before going further, note that the entropy can be written as:

$$S_N(E) = Nk\left(\ln\left(\frac{M}{N}\right) + 1\right) \tag{19}$$

where $E = \hbar\omega(M + \frac{1}{2})$ Thus,

$$\begin{aligned}
\ln p(n) &= (N-1)\left(\ln\left(\frac{M-n}{N-1}\right) + 1\right) - N\left(\ln\left(\frac{M}{N}\right) + 1\right) \\
&= (N-1)\left(\ln\left(\frac{M}{N}\frac{N}{N-1}\frac{M-n}{M}\right) + 1\right) - N\left(\ln\left(\frac{M}{N}\right) + 1\right) \\
&= (N-1)\left[\ln\left(\frac{M}{N}\right) + 1\right] + (N-1)\left[-\ln\left(1 - \frac{1}{N}\right) + \ln\left(1 - \frac{n}{M}\right)\right] \\
&- N\left[\ln\left(\frac{M}{N}\right) + 1\right] \\
&\simeq -\left(\ln\left(\frac{M}{N}\right) + 1\right) + (N-1)\left[\frac{1}{N} - \frac{n}{M}\right] \\
&\simeq \ln\frac{N}{M} - 1 + 1 - \frac{1}{N} - \frac{N}{M}n \\
&\simeq \ln\frac{N}{M} - \frac{N}{M}n
\end{aligned} \tag{20}$$

where we have neglected terms of the order of N^{-1} with respect to terms of the order of 1. Expressing M in terms of E and then expressing E in terms of temperature, we obtain:

$$p(n) = \frac{N}{M}e^{-\beta\left(\epsilon_n - \frac{\hbar\omega}{2}\right)} \tag{21}$$

f Given a subsystem consisting of 2 harmonic oscillators, what is the probability that this subsystem has total energy, $\epsilon = \hbar\omega(n+1)$

Solution:

This problem can also be solved using the method of the previous section, i.e.

$$p(\epsilon) = \frac{\Delta\Gamma_2(\epsilon)\Delta\Gamma_{N-2}(E-\epsilon)}{\Delta\Gamma_N(E)} \tag{22}$$

There will be only 2 2 points to take into account: i) since we are specified energy and not the state, we have an extra factor of $\Delta\Gamma_2(\epsilon)$ and ii) since in general ϵ will be only a few units of energy, it can not be considered large, also 2 is not a large number, thus $\Delta\Gamma_2(\epsilon)$ has to be evaluated *exactly*. The rest is similar to the previous calculation.

But here, another method of solving will be considered. The probability that the first oscilator will be in the n_1^{th} state and the second oscilator will be in the n_2^{th} state is the product of each probabilities, i.e.

$$p_2(n_1, n_2) = p(n_1)p(n_2) \tag{23}$$

where $p(n)$ is calculated in the previous section. Thus

$$p_2(n_1, n_2) = \left(\frac{N}{M}\right)^2 e^{-\beta(\epsilon_1+\epsilon_2-\hbar\omega)} \tag{24}$$

Then the probability that the system will have total energy $\epsilon = \hbar\omega(n+1)$ is the sum of the probabilities that the system is in a state (n_1, n_2) such that $n_1 + n_2 = n$, i.e.

$$p_2(\epsilon) = \sum_{n_1,n_2} p_2(n_1, n_2) \tag{25}$$

where the sum is restricted to the values of n_1 and n_2 such that $n_1+n_2 = n$. Then

$$\begin{aligned} p_2(\epsilon) &= \sum_{n_1,n_2} \left(\frac{N}{M}\right)^2 e^{-\beta(\epsilon_1+\epsilon_2-\hbar\omega)} \\ &= \sum_{n_1,n_2} \left(\frac{N}{M}\right)^2 e^{-\beta(\epsilon-\hbar\omega)} \\ &= \left(\frac{N}{M}\right)^2 e^{-\beta(\epsilon-\hbar\omega)}\Delta\Gamma_2(\epsilon) \end{aligned} \tag{26}$$

where

$$\Delta\Gamma_2(\epsilon) = n + 1 = \frac{\epsilon}{\hbar\omega} + \frac{1}{2} \tag{27}$$

Hint: In calculating the probabilities, express you result in terms of temperature and try to obtain an expression which is proportional to $e^{-\frac{\epsilon}{kT}}$