PYU33P15: Statistical Thermodynamics
Continuous Assessment CA1 due 05/10/2021

Ruaidhrí Campion
19333850
JS Theoretical Physics

1.

a)

Since the minimum value r can take is 0, if we let all r_i be equal to 0 then we have

$$\begin{aligned} n_{\text{min}}\hbar\omega &= \sum_{i=1}^{N} r_i\hbar\omega \\ &= 0, \end{aligned}$$

and so $n_{\text{min}} = 0$.

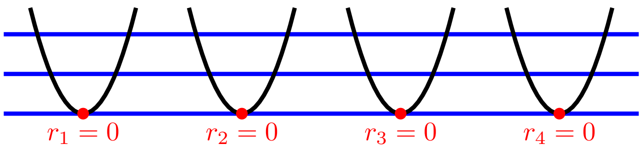
Since r_i can take any positive integer value, then there is theoretically no limit as to what the sum of all r_i can take, and so $n_{\text{max}} = \infty$.

Therefore n can be any non-negative integer, i.e. $n = 0, 1, 2, \ldots$

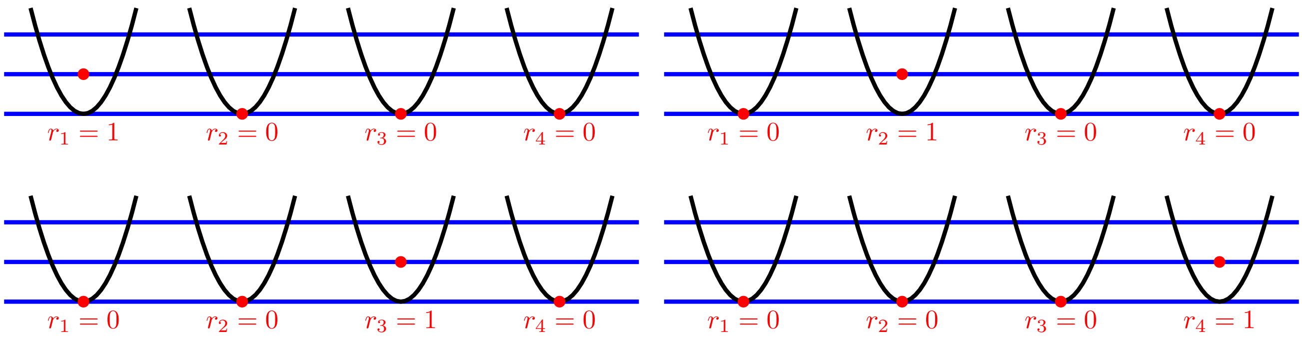
b)

The lowest three energy levels 0, $\hbar\omega$, $2\hbar\omega$ correspond to $n = 0, 1, 2$. We keep a constant $N = 4$.

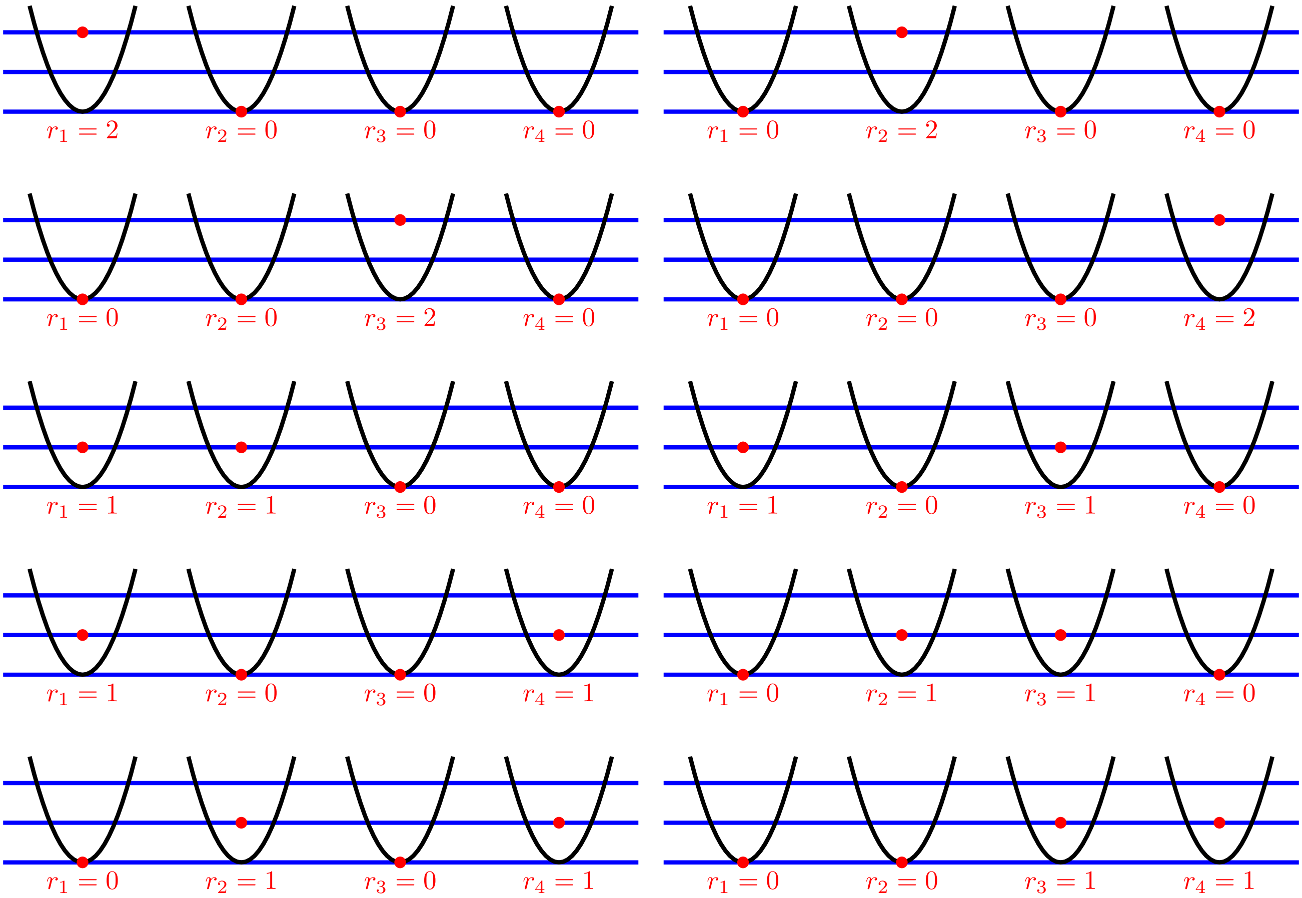
$$\Phi(4, 0) = \frac{(4+0-1)!}{0!(4-1)!} = 1 \text{ microstate} \qquad n = 0 \implies \sum_{i=1}^{4} r_i = 0$$



$$\Phi(4, 1) = \frac{(4+1-1)!}{1!(4-1)!} = 4 \text{ microstates} \qquad n = 1 \implies \sum_{i=1}^{4} r_i = 1$$



$$\Phi(4,2) = \frac{(4+2-1)!}{2!(4-1)!} = 10 \text{ microstates} \qquad\qquad n = 2 \implies \sum_{i=1}^{4} r_i = 2$$



c)

$$
\begin{aligned}
S &= k_B \ln \Phi && \text{(entropy definition)}\\
&= k_B \ln\left(\frac{(N+n-1)!}{n!(N-1)!}\right) && \text{(substituting } \Phi = \tfrac{(N+n-1)!}{n!(N-1)!}\text{)}\\
&= k_B[\ln((N+n-1)!) - \ln(n!(N-1)!)] && (\ln\left(\tfrac{a}{b}\right) = \ln(a) - \ln(b))\\
&= k_B[\ln((N+n-1)!) - \ln(n!) - \ln((N-1)!)] && (\ln(ab) = \ln(a)\ln(b))\\
&\approx k_B[(N+n-1)\ln(N+n-1) - (N+n-1) - n\ln(n) + n - (N-1)\ln(N-1) + N - 1]\\
& && (\ln(a!) \approx a\ln(a) - a)\\
&\approx k_B[(N+n)\ln(N+n) - (N+n) - n\ln(n) + n - N\ln(N) + N] && (N \gg 1)\\
&= k_B\left[N\ln\left(N\left(1+\frac{n}{N}\right)\right) + n\ln\left(N\left(1+\frac{n}{N}\right)\right) - n\ln\left(N\left(\frac{n}{N}\right)\right) - N\ln(N)\right]\\
& && \text{(expanding, factoring and cancelling)}\\
&= k_B\left[N\ln(N) + N\ln\left(1+\frac{n}{N}\right) + n\ln(N) + n\ln\left(1+\frac{n}{N}\right) - n\ln(N) - n\ln\left(\frac{n}{N}\right) - N\ln(N)\right]\\
& && (\ln(ab) = \ln(a) + \ln(b))\\
&= k_B\left[N\ln\left(1+\frac{n}{N}\right) + n\ln\left(1+\frac{n}{N}\right) - n\ln\left(\frac{n}{N}\right)\right] && \text{(cancelling)}\\
&= k_B N\left[\left(1+\frac{n}{N}\right)\ln\left(1+\frac{n}{N}\right) - \frac{n}{N}\ln\left(\frac{n}{N}\right)\right] && \text{(factoring)}
\end{aligned}
$$

d)

Since we can write the energy $U = n\hbar\omega$, we can rearrange to find $n = \frac{U}{\hbar\omega}$. Substituting into our expression for S in c) gives us

$$S(U,N) = k_B N\left[\left(1+\frac{U}{N\hbar\omega}\right)\ln\left(1+\frac{U}{N\hbar\omega}\right) - \frac{U}{N\hbar\omega}\ln\left(\frac{U}{N\hbar\omega}\right)\right].$$

e)

$$\begin{aligned}
\frac{1}{T} &= \left(\frac{\partial S}{\partial U}\right)_{V,N} && \text{(known expression)}\\
&= k_B N\left[\frac{1}{N\hbar\omega}\ln\left(1+\frac{U}{N\hbar\omega}\right) + \left(1+\frac{U}{N\hbar\omega}\right)\frac{1}{1+\frac{U}{N\hbar\omega}}\frac{1}{N\hbar\omega} - \frac{1}{N\hbar\omega}\ln\left(\frac{U}{N\hbar\omega}\right) - \frac{U}{N\hbar\omega}\frac{N\hbar\omega}{U}\frac{1}{N\hbar\omega}\right]\\
&&& \text{(calculating and substituting } \tfrac{\partial S}{\partial U}\text{)}\\
&= k_B N\left[\frac{1}{N\hbar\omega}\left(\ln\left(1+\frac{U}{N\hbar\omega}\right) - \ln\left(\frac{U}{N\hbar\omega}\right)\right)\right] && \text{(factoring and cancelling)}\\
&= \frac{k_B}{\hbar\omega}\left[\ln\left(1+\frac{U}{N\hbar\omega}\right) - \ln\left(\frac{U}{N\hbar\omega}\right)\right] && \text{(rearranging factors)}\\
\frac{\hbar\omega}{k_B T} &= \ln\left(\frac{N\hbar\omega}{U}+1\right) && \text{(rearranging, } \ln(a)-\ln(b)=\ln\left(\tfrac{a}{b}\right)\text{)}\\
e^{\frac{\hbar\omega}{k_B T}} &= \frac{N\hbar\omega}{U}+1 && \text{(exponent of both sides)}\\
U &= \frac{N\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}}-1} && \text{(rearranging)}
\end{aligned}$$

2.

a)

$$\begin{aligned}
\mathbb{Z} &\equiv \sum_{N=0}^{\infty}\sum_{i_N} e^{\frac{N\mu - E_{i_N}}{k_B T}} && \text{(grand partition function definition)}\\
&= e^{\frac{0-0}{k_B T}} + e^{\frac{\mu-0}{k_B T}} + e^{\frac{\mu-E_2}{k_B T}} && (N=0 \implies E_{1_0}=0,\ N=1 \implies E_{1_1}=E_1=0, E_{2_1}=E_2,\ N \not\geq 3)\\
\mathbb{Z} &= 1 + e^{\frac{\mu}{k_B T}} + e^{\frac{\mu-E_2}{k_B T}} && \text{(simplifying)}
\end{aligned}$$

b)

$$\begin{aligned}
\langle N\rangle &= k_B T\frac{\partial \ln \mathbb{Z}}{\partial \mu} && \text{(given expression)}\\
&= \frac{k_B T}{\mathbb{Z}}\frac{\partial \mathbb{Z}}{\partial \mu} && \text{(simplifying derivative)}\\
&= \frac{k_B T}{1+e^{\frac{\mu}{k_B T}}+e^{\frac{\mu-E_2}{k_B T}}}\left(0+\frac{e^{\frac{\mu}{k_B T}}}{k_B T}+\frac{e^{\frac{\mu-E_2}{k_B T}}}{k_B T}\right) && \text{(calculating and substituting)}\\
\langle N\rangle &= \frac{e^{\frac{\mu}{k_B T}}+e^{\frac{\mu-E_2}{k_B T}}}{1+e^{\frac{\mu}{k_B T}}+e^{\frac{\mu-E_2}{k_B T}}} && \text{(multiplying and simplifying)}\\
&= \frac{\mathbb{Z}-1}{\mathbb{Z}} && \text{(simplifying)}
\end{aligned}$$

c)

The thermal average occupancy of the state at energy E_2 will be equal to the sum of all $e^{\frac{N\mu - E_{i_N}}{k_B T}}$ for N, E_{i_N} that correspond to this state being occupied, divided by the grand partition function. When $E_{i_N} = 0$, this state is not occupied, however when $E_{i_N} = E_2$, this state is occupied. Thus the only term in this sum corresponds to $N = 1$ and $E_{2_1} = E_2$, and so the thermal average occupancy is given by

$$\langle N(E_2) \rangle = \frac{e^{\frac{\mu - E_2}{k_B T}}}{1 + e^{\frac{\mu}{k_B T}} + e^{\frac{\mu - E_2}{k_B T}}} = \frac{e^{\frac{\mu - E_2}{k_B T}}}{\mathbb{Z}}.$$

d)

$$\begin{aligned}
\langle E_i \rangle &= \frac{1}{\mathbb{Z}} \sum_{N=0}^{\infty} \sum_{i_N} E_i e^{\frac{N\mu - E_i}{k_B T}} && \text{(expression for average of a thermodynamic quantity)} \\
&= \frac{1}{1 + e^{\frac{\mu}{k_B T}} + e^{\frac{\mu - E_2}{k_B T}}} \left(0 + E_1 e^{\frac{\mu - E_1}{k_B T}} + E_2 e^{\frac{\mu - E_2}{k_B T}} \right) && \text{(expanding sum for } N = 0, 1\text{)} \\
\langle E_i \rangle &= \frac{E_2}{1 + e^{\frac{\mu}{k_B T}} + e^{\frac{\mu - E_2}{k_B T}}} e^{\frac{\mu - E_2}{k_B T}} && (E_1 = 0\text{, simplifying)} \\
&= E_2 \langle N(E_2) \rangle && \text{(simplifying)}
\end{aligned}$$

e)

$$\begin{aligned}
\mathbb{Z}_{\text{new}} &\equiv \sum_{N=0}^{\infty} \sum_{i_N} e^{\frac{N\mu - E_{i_N}}{k_B T}} && \text{(grand partition function definition)} \\
&= e^{\frac{0-0}{k_B T}} + e^{\frac{\mu - 0}{k_B T}} + e^{\frac{\mu - E_2}{k_B T}} + e^{\frac{2\mu - (E_1 + E_2)}{k_B T}}
\end{aligned}$$

(first three terms as before but now including an extra term for $N = 2$, $E_{1_2} = E_1 + E_2$)

$$\mathbb{Z}_{\text{new}} = 1 + e^{\frac{\mu}{k_B T}} + e^{\frac{\mu - E_2}{k_B T}} + e^{\frac{2\mu - E_2}{k_B T}} \qquad \text{(simplifying)}$$