Question 1

```
import numpy as np
import math
```

```
def analytical(b,h,w):
    z = (math.exp(-b*h*w*0.5)/(1-math.exp(-b*h*w)))
    return z

def en(h,w,n):
    e = h*w*(n+0.5)
    return e

def sum_equation(b,h,w,n):
    results_sum = 0
    for i in range(n + 1):
        results = math.exp(-b*en(h,w,i))
        results_sum = results_sum + results
    return results_sum

energy_levels = [1,10,100]
```

a)

```
print("Analytical Result: " + str(analytical(1,1,1)))
print(" ")
print("Numerical Results:")
for i in energy_levels:
    print("for " + str(i) + " energy levels: " + str(sum_equation(1,1,1,i)))
```

```
Analytical Result: 0.9595173756674719

Numerical Results:
for 1 energy levels: 0.8296608198610632
for 10 energy levels: 0.9595013500953602
for 100 energy levels: 0.9595173756674712
```

The analytical result is greater than the numerical results. The numerical results increases as the energy level increases. The numerical results seem to converge around 0.9595 at energy level of n = 10

b)

```
print("Analytical Result: " + str(analytical(0.1,1,1)))
print(" ")
print("Numerical Results:")
for i in energy_levels:
    print("for " + str(i) + " energy levels: " + str(sum_equation(0.1,1,1,i)))
```

```
Analytical Result: 9.995834548290834

Numerical Results:
for 1 energy levels: 1.8119374009257718
for 10 energy levels: 6.668510269734563
for 100 energy levels: 9.995423923853489
```

The analytical result is greater than the numerical results. The numerical results increases as the energy level increases. The numerical results seem to converge around 9.995 at energy level of n = 100

For $\beta = 1$, The numerical results converge at lower energy levels (n = 10) compared to $\beta = 0.1$ where the numerical results converge at a higher energy level (n = 100). Since the equation for β is $\beta = 1/KT$ where T is temperature, as the temperature increases, the numerical results will converge at higher energy levels.

Question ②

$$S = -K_B \sum_n p_n \ln p_n$$

$$S = K_B \ln \Omega \qquad Z = \sum_n e^{-\beta E_n}$$

$$p_n = \frac{e^{-\beta E_n}}{Z} \qquad \beta = \frac{1}{K_B T}$$

$$S = -k_B \sum_n \left(\frac{e^{-\beta E_n}}{Z}\right) \ln\left(\frac{e^{-\beta E_n}}{Z}\right)$$

$$S = \frac{-k_B}{Z} \sum_n e^{-\beta E_n} \ln\left(\frac{e^{-\beta E_n}}{Z}\right)$$

$$S = \frac{-k_B}{Z} \sum_n e^{-\beta E_n} \left[-\beta E_n - \ln Z\right]$$

$$S = \frac{-k_B}{\cancel{\sum_n e^{-\beta E_n}}} \cancel{\sum e^{-\beta E_n}} \left[-\beta E_n - \ln Z\right]$$

$$S = K_B \ln Z + K_B \beta E_n$$

$$S = K_B \ln Z + \cancel{K_B}\left(\frac{1}{\cancel{K_B} T}\right) E_n$$

$$S = K_B \ln Z + \frac{E_n}{T}$$

Question ③

$\delta E = E - \langle E \rangle$

$(\delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2$

$$(\delta E)^2 = (E - \langle E \rangle)^2 = (E - \langle E \rangle)(E - \langle E \rangle)$$
$$= \langle E^2 \rangle - E\langle E \rangle - E\langle E \rangle + \langle E \rangle^2$$
$$= \langle E^2 \rangle - 2E\langle E \rangle + \langle E \rangle^2$$
$$= \langle E^2 \rangle - 2\langle E \rangle\langle E \rangle + \langle E \rangle^2$$
$$= \langle E^2 \rangle - 2\langle E \rangle^2 + \langle E \rangle^2$$
$$\boxed{= \langle E^2 \rangle - \langle E \rangle^2}$$

Question ④

show that $U_N = \sum_{i=1}^{N} U_i$

$$U = \frac{1}{Z} \sum E_N e^{N - \beta E_N} = -\frac{\partial \ln Z}{\partial \beta}$$

$$U = \frac{-\partial \ln Z}{\partial \beta}$$

$$Z = \frac{e^{-\beta \hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}$$

$$\ln Z = N\left[-\frac{1}{2}\beta\hbar\omega - \ln(1 - e^{-\beta\hbar\omega})\right]$$

for N individual harmonic oscillators

$$Z = \left[\frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}\right]^N$$

$$-\frac{\partial \ln Z}{\partial \beta} = -N\left[-\frac{1}{2}\hbar\omega - \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\right]$$

$$\boxed{U = N\hbar\omega\left[\frac{1}{2} + \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\right]}$$