PHYS 403 Problem Set 3

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Question I1.

$$H = mgz + \frac{1}{2}mv^2.$$

Question I2. Because the v velocity term is independent of the height z, we can treat the Hamilton as $H = mgz$ (more precisely, the $e^{\frac{1}{2}mv^2}$ terms would cancel between the energy and partition function).

$$p(z) = \frac{1}{Z}e^{-\beta mgz} = \frac{e^{-\beta mgz}}{\int_0^\infty e^{-\beta mgz'}dz'}.$$

Question I3. We can assume that density is proportional to the probability at a given elevation. Thus:

$$\frac{p(z_{\text{Mt Everest}})}{p(z_{\text{Sea Level}})} = e^{-\beta mg(z_{\text{Mt Everest}} - z_{\text{Sea Level}})} = e^{-4.6528\cdot 10^{-26}\cdot 9.81\cdot 8848/(270\cdot 1.381\cdot 10^{-23}}) = 0.34.$$

This makes sense. According to Wikipedia the atmosphere pressure there is around 33.7kPa, which compared to atmospheric pressure of 101.325kPA is a ratio of 0.33 (which given we're assuming sea level and Mount Everest have the same temperature is surprisingly close).

Question II1. Just summing over the possibilities explicitly:

$$Z = e^{-\beta\cdot 0} + 2e^{\beta\epsilon_b} + e^{-\beta(-2\epsilon_b + U)}.$$

Question II2. For the number of electrons, we can can compute the expected value, where Z is defined as before:

$$\langle \text{\# Electrons}\rangle = \frac{1}{Z}\left(2e^{\beta\epsilon_b} + 2e^{-\beta(-2\epsilon_b+U)}\right).$$

The plot of this function can be seen in figure 1. Note that the question asks for graphs of temperature but specifies the range in terms of k_BT, so to keep the numbers nicer the x axis is k_BT.

Next for the energy, we can write out a similar expression, the graph is in figure 2:

$$\langle E\rangle = \frac{1}{Z}\left(-2\epsilon_b e^{\beta\epsilon_b} + (-2\epsilon_b + U)e^{-\beta(-2\epsilon_b+U)}\right).$$

Finally, for heat capacity, we can find it in terms of $\langle E\rangle$:

$$C = \frac{\partial\langle E\rangle}{\partial T}.$$

Numerical differention was used to calculate this derivative in figure 3, although in theory it would be a simple quotient rule application. Here is the code used:

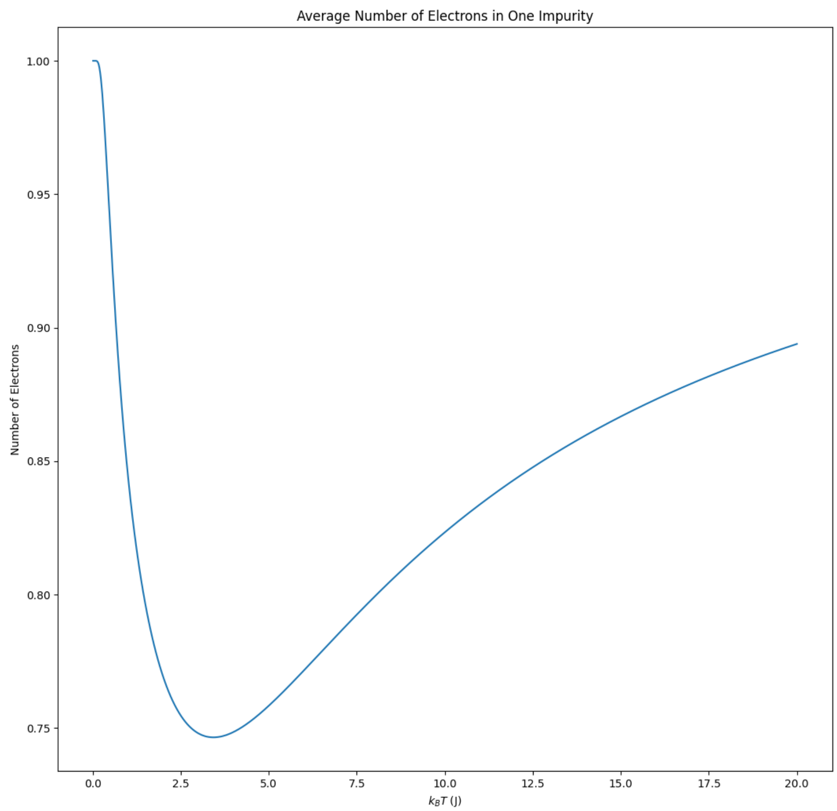

Figure 1: Graph for question II2a.

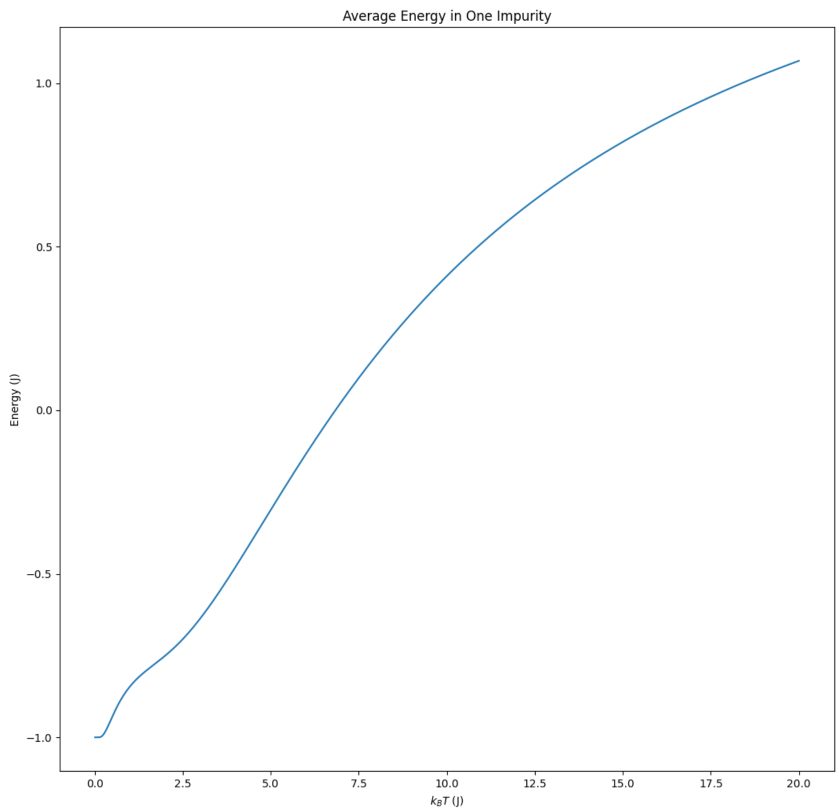

Figure 2: Graph for question II2b

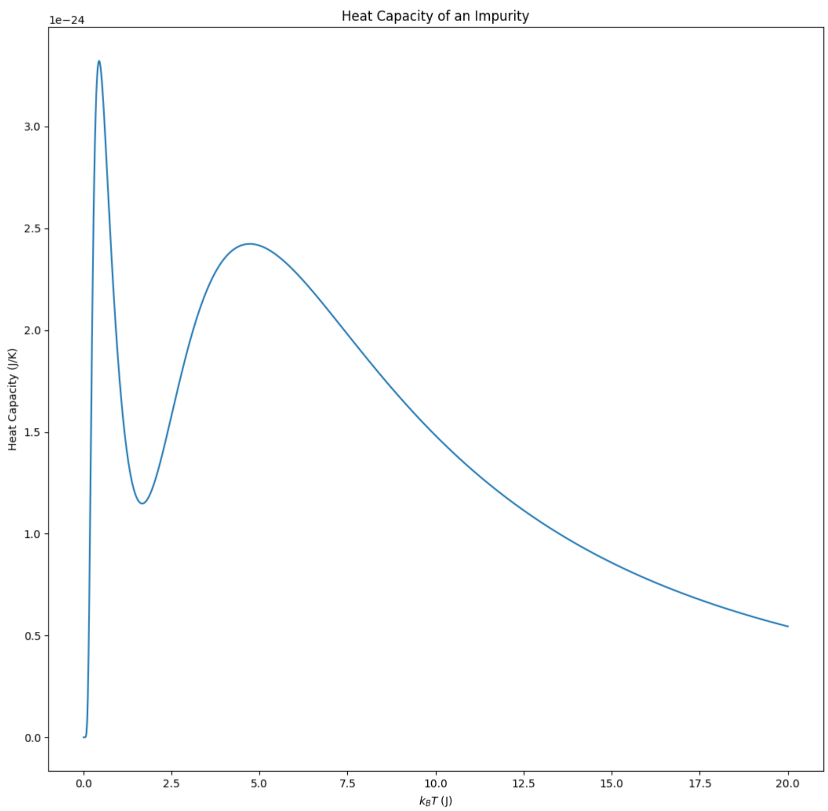

Figure 3: Graph for question II2c

```
import numpy as np
import matplotlib.pyplot as plt

eb = 1
U = 12
kb = 1.381e-23
T = np.linspace(0.01/kb, 20/kb, 1000)
dT = T[1] - T[0]

beta = 1/(kb*T)
Z = 1+2*np.exp(beta*eb)+np.exp(-beta*(-2*eb+U))


ne = 1/Z * (2*np.exp(beta*eb)+2*np.exp(-beta*(-2*eb+U)))

plt.plot(kb*T, ne)
plt.title("Average Number of Electrons in One Impurity")
plt.xlabel("$k_BT$ (J)")
plt.ylabel("Number of Electrons")
plt.show()

E = 1/Z * (-2*eb*np.exp(beta*eb)+(-2*eb+U)*np.exp(-beta*(-2*eb+U)))

plt.plot(kb*T, E)
plt.title("Average Energy in One Impurity")
plt.xlabel("$k_BT$ (J)")
plt.ylabel("Energy (J)")
plt.show()

C = np.gradient(E, dT)

plt.plot(kb*T, C)
plt.title("Heat Capacity of an Impurity")
plt.xlabel("$k_BT$ (J)")
plt.ylabel("Heat Capacity (J/K)")
plt.show()
```

Question III1. All that's relevant here is the energy levels:

$$Z = \sum_{n=0}^{\infty} e^{-\hbar\omega(n+1/2)/(k_BT)} = e^{-\hbar\omega/(2k_BT)} \frac{1}{1 - e^{-\hbar\omega/(k_BT)}}.$$

Question III2.

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z = \frac{\hbar\omega}{2} + \frac{\partial}{\partial \beta} \log\left(1 - e^{-\beta\hbar\omega}\right) = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}.$$

Question III3.

$$C = \frac{\partial}{\partial T}\langle E \rangle = \frac{(\hbar\omega)^2 e^{\hbar\omega/(k_BT)}}{k_BT^2\left(e^{(\hbar\omega)/(k_BT)} - 1\right)^2}.$$