PHYS 403 Problem Set 3

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11/02/24

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:

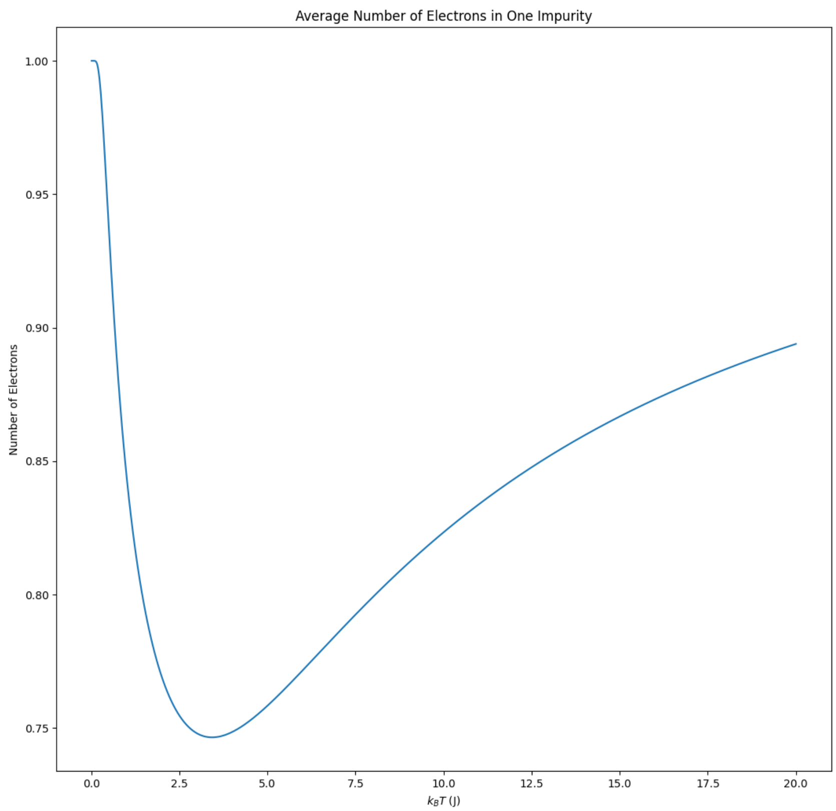

Figure 1: Graph for question II2a.

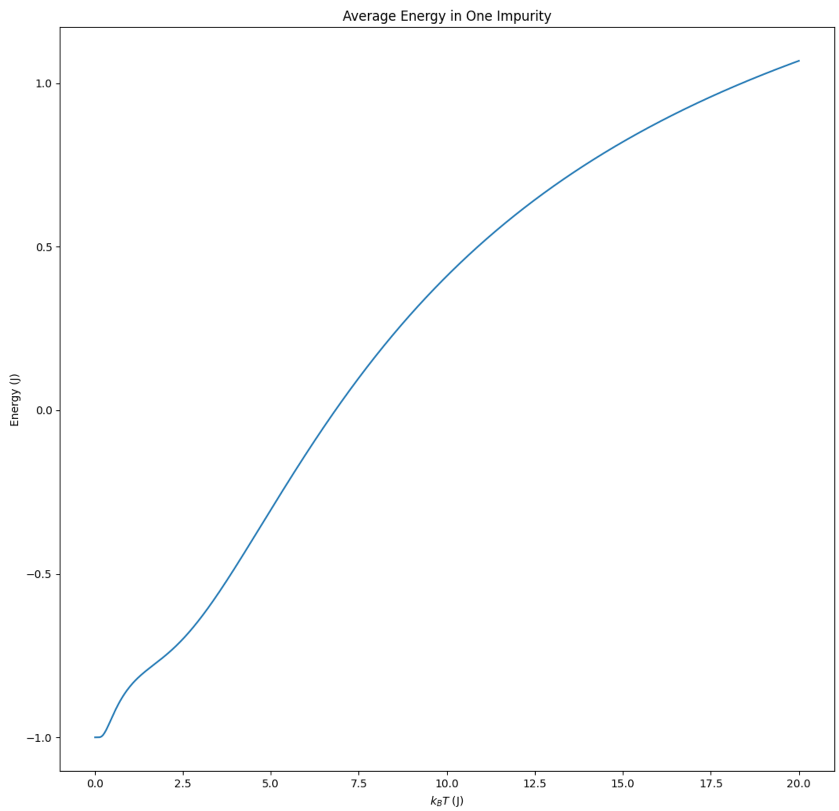

Figure 2: Graph for question II2b

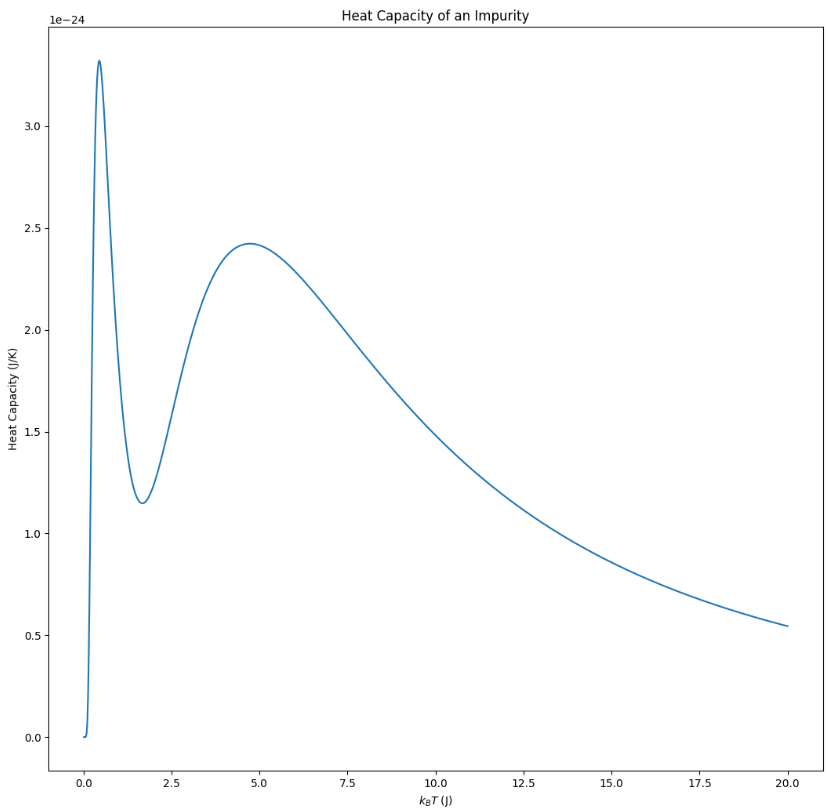

Figure 3: Graph for question II2c

```
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:

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

Question III2.

$$\langle E \rangle = -\frac{\partial}{\partial\beta} \log Z = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_BT}\right).$$

Question III3.

$$C = \frac{\partial}{\partial T}\langle E\rangle = k_B \left(\frac{\hbar\omega}{2k_B T}\right)^2 \frac{1}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)}.$$

See figure 4 for the graph, here is the code used to plot it:

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

T = np.linspace(0.01, 300, 1000)
hbar = 1.055e-24
omega = 1e3
kb = 1.381e-23

C = kb*(hbar*omega/(2*kb*T))**2/np.sinh(hbar*omega/(2*kb*T))**2

plt.plot(T, C)
plt.plot(T, T*0+kb)
plt.axvline(x=hbar*omega/2/kb, color='g', linestyle='-')
plt.title("Heat Capacity of Quantum Harmonic Oscillator")
plt.xlabel("Temperature (K)")
plt.ylabel("Heat Capacity (J/K)")
plt.show()
```

Question III4. From figure 4, we can see that the heat capacity increases monotonically to the classical prediction, which from the equipartition theorem is k_B (we're in 1 dimension with position and momentum). Roughly speaking this occurs when sinh is behaves linearly, which is when (order of magnitude) $T \approx \frac{\hbar\omega}{2k_B}$. This is confirmed from the graph, where the green line represents this transition.

Question III5. From the given graphs, it appears that the translational modes always behave classically and so contribute $\frac{3}{2}k_B$ to the heat capacity. The lowest modes from the rotation corresponds to $\lambda^{-1} \approx 0.2\text{cm}^{-1} \implies E = \frac{hc}{\lambda} = 0.2hc$. Similarly for the vibration modes we see that $E = \frac{hc}{\lambda} = 23.3hc$. The heat capacity is additive and we can get ω from E with $\omega = \frac{E}{\hbar}$, so using our previous result we can plot the total heat capacity in figure 5.

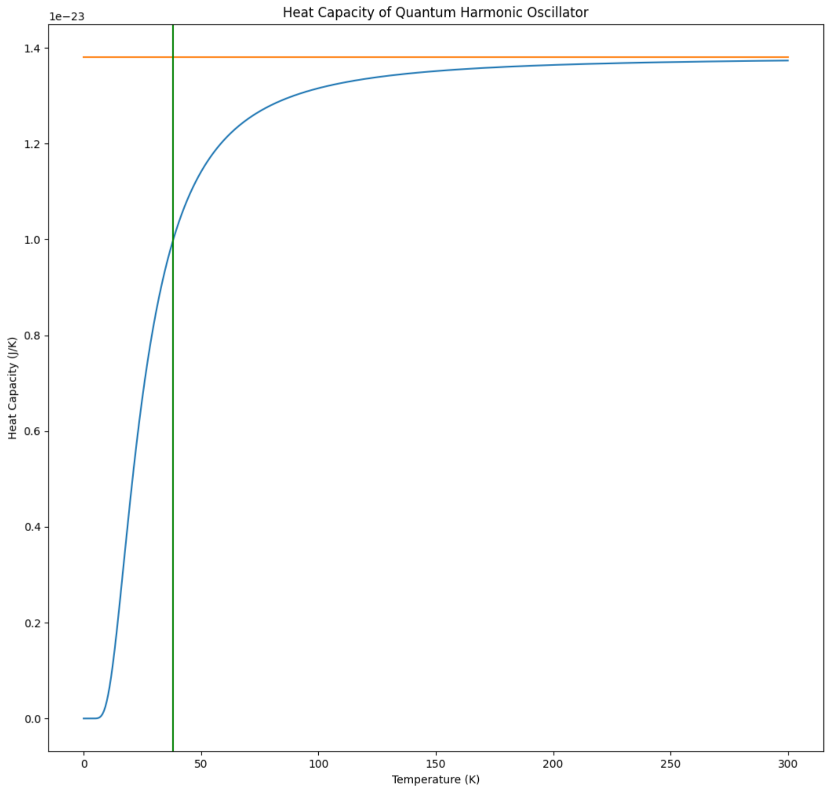

Figure 4: Graph for question III3. Here $\omega = 1000\text{rad/s}$, the orange line is $C = k_B$ and the green line is $T = \frac{\hbar\omega}{2k_B}$.

Figure 5: III5