Exercise 1. ***Energy preservation***

Suppose that the system is characterized by a Hamiltonian H, and a unitary operation U is applied.

(a) *Show that if $[U, H] = 0$, then the unitary preserves the energy of the system.*

Solution The energy of the system after the unitary is applied (we use the circularity of trace and $HU = UH$):

$$E' = \mathrm{tr}(H\rho') = \mathrm{tr}(HU\rho U^\dagger) = \mathrm{tr}(UH\rho U^\dagger) = \mathrm{tr}(U^\dagger UH\rho) = \mathrm{tr}(H\rho) = E.$$

(b) *Consider a four-level system with a Hamiltonian $H = \Delta|1\rangle\langle 1| + \Delta|2\rangle\langle 2| + 2\Delta|3\rangle\langle 3|$, written in the energy eigenbasis $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$. Come up with one non-trivial unitary U_{pres} which would preserve the energy of the system for any state, and identify the common eigenbasis of U and H. Find another unitary $U_{non\text{-}pres}$ which would not preserve the energy of the system for any state.*

Solution The Hamiltonian of the system is degenerate: the states $|1\rangle$ and $|2\rangle$ correspond to the same energy Δ:

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 \\ 0 & 0 & \Delta & 0 \\ 0 & 0 & 0 & 2\Delta \end{pmatrix}$$

Since the levels $|1\rangle$ and $|2\rangle$ have the same energy, swapping their populations will not change the net energy:

$$U_{\text{pres}} = (|1\rangle\langle 2| + |2\rangle\langle 1|) + (|0\rangle\langle 0| + |3\rangle\langle 3|) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The common eigenbasis of U and H is: $\{|0\rangle, \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), |3\rangle\}$.

If we additionally swap the populations of the levels $|0\rangle$ and $|3\rangle$, the unitary is no longer energy-preserving:

$$U_{\text{non-pres}} = (|1\rangle\langle 2| + |2\rangle\langle 1|) + (|0\rangle\langle 3| + |3\rangle\langle 0|) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

(c) *Give an example of an initial state of the system, for which the energy would still be preserved after applying $U_{non\text{-}pres}$.*

Solution For the example we have given, the energy would still be preserved if, for instance, $\rho = |1\rangle\langle 1|$. Then the state of the system after the application of U is $\rho\prime = |2\rangle\langle 2|$, and

$$E = \mathrm{tr}(\rho H) = \Delta$$
$$E' = \mathrm{tr}(\rho' H) = \Delta.$$

Exercise 2. *Temperature of a qubit*

Consider a qubit with Hamiltonian $H = \Delta|1\rangle\langle 1|$, with the energy gap $\Delta = 1$ for simplicity. Recall that the thermal state at temperature T is given by

$$\tau(T) = \frac{e^{-\frac{H}{kT}}}{Z},$$

where k is a constant (Boltzmann constant), and Z is the normalization factor, which is called the partition function:

$$Z(T,H) = \sum_i e^{-\frac{E_i}{kT}}.$$

For simplicity of notation, we can define the inverse temperature $\beta = \frac{1}{kT}$.

(a) *What is the temperature of the state $\rho = |0\rangle\langle 0|$ (the ground state)? And of $\rho = |1\rangle\langle 1|$ (the excited state)? And of the maximally mixed state $\rho = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2$? Place these three states on the β axis.*

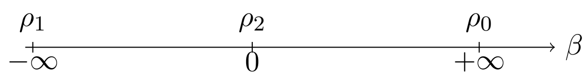
Solution In the energy eigenbasis, the thermal state of the qubit has only diagonal elements:

$$\tau(\beta) = \frac{1}{1+e^{-\beta\Delta}} \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta\Delta} \end{pmatrix}.$$

This means any state which is diagonal in the energy basis, can be represented as a thermal state – the remaining trick is to choose the appropriate inverse temperature β. Some examples are given below:

$$\rho_0 = |0\rangle\langle 0| \qquad \beta_0 = +\infty$$
$$\rho_1 = |1\rangle\langle 1| \qquad \beta_1 = -\infty$$
$$\rho_2 = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \qquad \beta_2 = 0.$$

On the β axis:



(b) *Take the following two states that are close to the maximally mixed state, $\epsilon > 0$:*

$$\rho_+ = \left(\frac{1}{2}+\epsilon\right)|0\rangle\langle 0| + \left(\frac{1}{2}-\epsilon\right)|1\rangle\langle 1| \tag{1}$$
$$\rho_- = \left(\frac{1}{2}-\epsilon\right)|0\rangle\langle 0| + \left(\frac{1}{2}+\epsilon\right)|1\rangle\langle 1|. \tag{2}$$

Find the temperatures $\beta_\pm$ corresponding to the above states, using $\epsilon << 1$ to expand to first order approximations.

Solution The temperature of the state ρ_+ is defined by (we are keeping only first order terms w.r.t. ϵ):

$$\frac{1}{2} + \epsilon = \frac{1}{1 + e^{-\beta_+ \Delta}} \Rightarrow \beta_+ = -\frac{1}{\Delta} \ln \left(\frac{\frac{1}{2} - \epsilon}{\frac{1}{2} + \epsilon} \right)$$
$$\beta_+ = \frac{1}{\Delta} (\ln(1 + 2\epsilon) - \ln(1 - 2\epsilon) \approx \frac{4\epsilon}{\Delta}.$$

Analogously, for ρ_- we find:

$$\beta_- = \frac{1}{\Delta} (\ln(1 - 2\epsilon) - \ln(1 + 2\epsilon) \approx -\frac{4\epsilon}{\Delta}.$$

(c) *Continuing from the above, look at the limit $\epsilon \to 0$ to argue that β is continuous w.r.t. the populations, while $T = (k\beta)^{-1}$ is not, which is why it is more natural to work with β in quantum thermodynamics. (Another way to argue this is to show that the limit $T \to 0$ is not the same from the left and right, by showing that the states in either limit are very different).*

Solution We see that the left and right limits of β at $\epsilon = 0$ both converge to 0:

$$\lim_{\epsilon \to 0} \beta_+ = \lim_{\epsilon \to 0} \beta_- = 0.$$

However, if we look at the variable T, its right and left limits at $\epsilon = 0$ do not coincide:

$$\lim_{\epsilon \to 0} T_+ = \lim_{\epsilon \to 0} \frac{1}{k\beta_+} = +\infty$$
$$\lim_{\epsilon \to 0} T_- = \lim_{\epsilon \to 0} \frac{1}{k\beta_-} = -\infty$$

This justifies why it is more natural to work with β when talking about populations of the states.