In this exercise sheet, we will explore the information-processing aspects of thermodynamics.

Exercise 1.   The non-equilibrium quantum free energy

Consider a quantum system in state ρ and with Hamiltonian H. Its non-equilibrium quantum free energy is a functional defined as

$$F(\rho) = kTS(\rho\|\tau) - kT \log Z, \tag{1}$$

where $\tau = e^{-\beta H}/Z$ is the thermal state you saw in the preliminaries, with $\beta = (kT)^{-1}$ the inverse temperature and $Z = \mathrm{Tr}[e^{-\beta H}]$ is the partition function. $S(X\|Y)$ is the quantum relative entropy

$$S(X\|Y) = \mathrm{Tr}[X(\log X - \log Y)]. \tag{2}$$

In this exercise we will study some of its properties.

(a) For what states does the non-equilibrium free energy recover its equilibrium version?

(b) Recall from equilibrium thermodynamics that the Helmholtz free energy is defined as $F_{\mathrm{eq}} = U - TS$, with U the internal energy and S the entropy. Can you write an analogous expression for the non-equilibrium free energy, involving the (quantum) average energy and the von Neumann entropy?

(c) Prove that the non-equilibrium contribution $kTS(\rho\|\tau)$ is always non-negative.

   Hint: Given the function $\theta(x,y) = x\log(x/y)$, it holds that

   $$\theta(x_1 + x_2, y_1 + y_2) \le \theta(x_1, y_1) + \theta(x_2, y_2). \tag{3}$$

(d) Prove that for a bipartite state ρ_{AB} one can neatly split its non-equilibrium free energy into a component from A only, one from B only and a term measuring the overall correlations between A and B (Hint: look up quantum mutual information).

(e) Take an initial state ρ_S. Suppose you are allowed to bring in any thermal state τ_B at fixed temperature T (but with arbitrary Hamiltonian H_B) and perform an arbitrary unitary interaction U_{SB} involving both S and B. Before and after this interaction, the total Hamiltonian is $H_S \otimes I_B + I_S \otimes H_B$. Define the average extracted work W as the average overall energy change under this process. Prove that $W \le F(\rho_S) - F(\rho_S')$, where ρ_S' in the state of S after the interaction. Compare with the situation in equilibrium thermodynamics and intuitively discuss when the quantum bound can be saturated.

Exercise 2.   Properties of thermal operations

We defined in class the set of thermal operations $\mathcal{C}$ on a system with Hamiltonian H_S and with respect to a background (inverse) temperature β. Here we will prove some of its core properties.

(a) (Thermal fixed point) Prove that the thermal state is fixed: $\mathcal{C}(\tau_S) = \tau_S$, where $\tau_S = e^{-\beta H_S}/Z_S$.

(b) (Time-translation symmetry) Prove that the following symmetry property is satisfied for every ρ_S and time t:
$$\mathcal{C} \circ \mathcal{U}_t(\rho_S) = \mathcal{U}_t \circ \mathcal{C}(\rho_S), \tag{4}$$
where $\mathcal{U}_t(X) = e^{-iH_S t} X e^{iH_S t}$.

(c) (Coherence non-generation) Prove that for every state incoherent state ρ_{SA} with Hamiltonian $H_S \otimes I_A + I_S \otimes H_A$, one has that $\mathcal{C} \otimes \mathcal{I}_A(\rho_{SA})$ is incoherent too ($\mathcal{I}_A$ is the identity channel).

(d) (Mode maps into mode) For every mode of coherence ω, and every state ρ_S
$$\mathcal{C}(\rho_S^{(\omega)}) = \mathcal{C}(\rho_S)^{(\omega)}. \tag{5}$$

(e) Are properties (b), (c), (d) equivalent?

(f) (Convexity) Prove that thermal operations are a convex set, meaning that if $\mathcal{C}_1$ and $\mathcal{C}_2$ are thermal operations also $p\mathcal{C}_1 + (1-p)\mathcal{C}_2$ for $p \in [0,1]$ is a thermal operation.

Exercise 3. Constructing thermal monotones

Suppose that $\sigma = \mathcal{C}(\rho)$, where $\mathcal{C}$ is a thermal operation. Let $\vec{x}$ and $\vec{y}$ be the vectors of populations (occupation of energy levels) of ρ and σ, respectively.

For any h convex function in $\mathbb{R}$, define the f-divergence
$$f(\vec{x}) = \sum_i g_i h(x_i/g_i), \tag{6}$$
where $g_i = e^{-\beta E_i}/Z$. Prove that
$$f(\vec{x}) \geq f(\vec{y}), \tag{7}$$
so that each f can be interpreted as a generalized free energy.

Exercise 4. Work cost of processes on a quantum computer

Consider a quantum computer with a register of n qubits described by the trivial Hamiltonian $H = 0$. Assume that the quantum computer can perform standard unitary gates at no work cost on the register. Suppose furthermore that the quantum computer has two functions RESET_ZERO$_k$ and EXTRACT_WORK$_k$ defined as follows. The function RESET_ZERO$_k$ transforms the k-th qubit to the $|0\rangle$ state, regardless of the k-th qubit's initial state, at a work cost equal to $kT \ln 2$ where T is some fixed temperature and k is Boltzmann's constant. The function EXTRACT_WORK$_k$ is such that if the k-th qubit is in the $|0\rangle$ state, then it is transformed to the maximally mixed state while extracting $kT \ln 2$ work. (I.e., the functions RESET_ZERO$_k$ and EXTRACT_WORK$_k$ operate on the k-th qubit like the reset procedure and the work extraction process do on a Szilárd engine.)

(a) Suppose that when you turn on your quantum computer, the memory register is uninitialized. We model this situation by assuming that the register is in a maximally mixed state. How much work is required to restore the memory register to the computational all-zero state $|0\rangle^{\otimes n}$? How about if you would like to initialize it in the all-one state $|1\rangle^{\otimes n}$? How about if you would like to prepare a given fixed computational basis state $|x_1\rangle|x_2\rangle \ldots |x_n\rangle$?

(b) Find protocols and their associated work cost in order to achieve the following tasks:

  (i) Suppose three qubits of the memory are entangled in the GHZ state

  $$|GHZ\rangle = \frac{(|000\rangle + |111\rangle)}{\sqrt{2}}.$$

  Find a protocol that resets the first qubit to $|0\rangle$ while leaving the reduced state of the second and third qubits unchanged.

  (ii) Suppose three qubits of the memory are in the classically correlated state

  $$\rho = \frac{1}{3}|000\rangle\langle 000| + \frac{2}{3}|111\rangle\langle 111|.$$

  Find a protocol that resets the first qubit to $|0\rangle$ while leaving the reduced state of the second and third qubits unchanged.

  (iii) Implement a MEASURE$_{k,\ell}$ function that will set the ℓ-th qubit to the classical value of the k-th qubit in the computational basis, i.e., such that:

  $$\text{MEASURE}_{k,\ell}\big(|i\rangle\langle i|_k|j\rangle\langle j|_\ell\big) = |i\rangle\langle i|_k|i\rangle\langle i|_\ell \quad \forall i,j.$$

(c) Using the entropic bounds introduced in the lecture, determine the optimal work cost of the tasks (i), (ii), and (iii). Are the protocols you found optimal? If not, try to find optimal ones.

Exercise 5. Entropy and Observers in Gibbs' paradox

When two different gases mix, the system acquires a contribution to the entropy, the *entropy of mixing*, in addition to the entropy associated with each gas. Gibbs' paradox refers to the discontinuity when we take the gases to be arbitrarily similar. At which point are they no longer two different gases and is the entropy of mixing no longer present? Here, we study an example presented in Jaynes' excellent treatment of the subject.[1]

(a) A box contains two volumes V_1 and V_2 of identical argon gases at the same pressure and temperature. We remove the separator that keeps the gases apart, allowing them to mix freely. What is the entropy change of the full system?

(b) Suppose that the two volumes of argon gas are in fact two different kinds of argon, $A1$ and $A2$. But these two different types of argon haven't been discovered yet and it still looks like we're mixing two volumes of identical argon gases. $A1$ and $A2$ are identical in all physical aspects (mass, charge, etc.), except that $A2$ is soluble in Whifnium, a hypothetical substance that hasn't been discovered yet. Consider the mixing process as in (a). What is the entropy change of the full system? Explain your answer.

(c) 100 years later, we've discovered Whifnium and we know there are two types of Argon, $A1$ and $A2$. Consider the mixing process as in (a). What is the entropy change of the full system? Explain your answer.

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[1] https://link.springer.com/chapter/10.1007/978-94-017-2219-3_1