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  $\rho$  and with Hamiltonian H. Its non-equilibrium quantum free energy is a functional defined as

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

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

$$S(X||Y) = Tr[X(\log X - \log Y)].$$
(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  $F_{eq} = U TS$ , 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

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

- (d) Prove that for a bipartite state  $\rho_{AB}$  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  $\rho_S$ . Suppose you are allowed to bring in any thermal state  $\tau_B$  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  $W \leq F(\rho_S) - F(\rho'_S)$ , where  $\rho'_S$  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 C on a system with Hamiltonian  $H_S$  and with respect to a background (inverse) temperature  $\beta$ . 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  $\rho_S$  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  $\rho_{SA}$  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  $\omega$ , and every state  $\rho_S$ 

$$\mathcal{C}(\rho_S^{(\omega)}) = \mathcal{C}(\rho_S)^{(\omega)}.$$
(5)

- (e) Are properties (b), (c), (d) equivalent?
- (f) (Convexity) Prove that thermal operations are a convex set, meaning that if  $C_1$  and  $C_2$  are thermal operations also  $pC_1 + (1-p)C_2$  for  $p \in [0,1]$  is a thermal operation.

# Solution

EXERCISE 1 (a) For thermal state  $c = \varepsilon$ ,  $S(\varepsilon|\varepsilon) = 0$ so  $F(\varepsilon) = -kT \log Z$ (b) F(e) = kT(Tre[eloge] - Tr[eloge]) $-kT \cos 2$   $s(e) = -Ta[e \cos e] = -kT S(e) - kT Tre \left[ e \cos \frac{-H/kT}{Z} \right]$ - KTRog Z = Tor[eH] - KTS(e) = <H7e - KTS(e) (c)  $e = \sum_{n} p_{i} \left[ \frac{1}{2\pi i} \frac{1}{2\pi i} \right] = \sum_{j} e_{j} \left[ \frac{1}{3} \frac{1$ S(elle) = Tre[eloge] - Tre[eloge]  $= \sum_{i=1}^{2} P_{i} \cdot \log P_{i} - \sum_{i=1}^{2} P_{i} \cdot \log (P_{i}) (\langle x_{i}|y_{i} \rangle)^{2}$   $= \sum_{i=1}^{2} \left[ P_{i} \cdot \log P_{i} - P_{i} \cdot \log \sum_{i=1}^{2} P_{i} \cdot (\langle x_{i}|y_{i} \rangle)^{2} \right]$  $= \sum_{n} P_{n} \cdot \Theta_{n} \frac{P_{n}}{re_{j}} := S(\underline{P} | \underline{r}) \cdot \underline{r}_{j}$ 

x70, B70 Then  $S(PIIE) = \overline{\Sigma}\Theta(Pi, ei)$  $\geq \Theta(\Sigma_{p_{1}}, \Sigma_{r_{1}}) = \Theta(1, 1) = 0.$ So S(elle) 20. (d) HAB = HADAB + ALADHB  $S = 2_{AB} = 2_A B 2_B$ F(CAB) = KTS(CABNZADZB) - KTGOGZAB = - KTS(CAB) - KTT2[CAB Cog 2 3 23] - KT Cog ZA - KT Cog ZB = KT (S(PA) + S(PB) - S(PAB)) - KT Tr[CAlog CA] - KTlog ZA - KTS(CA)

-  $kTTr[e_Beog 2_B] - kTEog 2_B - kTS(e_B)$ = KT I(A:B) + F(CA) + F(CB) mitual info (e)  $\mathcal{C}_{SB} = \mathcal{C}_S \supset \mathcal{C}_B$  since  $H_{SB} = H_S \supset I_{B} + I_{S} \supset H_B$ W:= Ta [HSB ( CS DCB - U CS DCB UT)] = Tr[HSB(PSD2B)] - KTS(PSD2B) unitory soentropic - Tre [HSB Ues DrBUt] + kTS(Ues DrBUt) = F(es D 20) - F(U(es D 20)). Let es = Tre ese (cs B 20). CB = Tres CSB mituel info From (d)  $F(U(P_{s} D 2_{8})U^{\dagger}) = F(P_{s}') + F(2_{8}') - kTI(S':B')$ 5 F(C's) + F(2B) C mutuel info nou-negative F(X) minimel fore thermal state

We conclude from F(eso 28) = F(es) + F(28)  $W_{EXT} \leq F(e_s) + F(r_s) - F(e'_s) - F(r_s)$ EXERCISE 2 (a) C(2s)=  $= T_{B} \left[ U(z_{S} \mathfrak{D} \mathfrak{Z}_{B}) \mathcal{O}^{\dagger} \right]$ But [U, Hs + Hz]=0  $\Rightarrow [U, 2s D 2B] = 0$ 11  $\mathcal{C}(\tau_s) = \operatorname{Tr}_{\mathcal{B}}[(\tau_s \mathcal{D} \tau_s) \cup \mathcal{U}^{\dagger}] = \tau_s.$ (b)  $\mathcal{U}_{t}^{s}(x) := \tilde{e}^{AH_{s}t} \times e^{AH_{s}t}$  $\mathcal{U}_{t}^{B}(x) := \tilde{e}^{AH_{s}t} \times e^{AH_{s}t}$  $\mathcal{C}(\mathcal{U}_{t}^{s}(e_{s})) = \operatorname{Tre}_{B}[\mathcal{U}(\mathcal{U}_{t}^{s}(e_{s}) \supset \mathcal{T}_{s})\mathcal{U}] =$  $= Tr_{B} \left[ \cup \left( \mathcal{U}_{t}^{S}(\boldsymbol{e}_{s}) \gg \mathcal{U}_{t}^{B}(\boldsymbol{e}_{s}) \right) \cup^{T} \right]$ thermal stationary

 $= \operatorname{Tr}_{\mathcal{B}} \left[ \bigcup \mathcal{U}_{s}^{\dagger} \mathfrak{D} \mathcal{U}_{s}^{\dagger} \left( e_{s} \mathfrak{D} \mathfrak{T}_{s} \right) \bigcup \right]$ =  $Tr_{B}\left[\bigcup_{a} -i(H_{S}+H_{B})t\right] = C_{S} B^{*}C_{B} e^{a(H_{S}+H_{B})t} \bigcup_{a}^{T} \\ commute \\ = commute \\ -iH_{S}t Tr_{B}\left[\bigcup_{a} (e_{s} \partial^{*}C_{B}) \bigcup_{a}^{T}\right] e^{aH_{S}t}$ cyclic property of trace on B  $= \mathcal{U}_t^{s}(\mathcal{C}(e_s)).$ (c) <u>CLAIM</u> <u>B</u> <u>C</u> <u>S</u> J<sub>A</sub> (C<sub>SA</sub>) incoherent for all and all <u>C</u> <u>SA</u>  $H_{SA} = H_S + H_A$  $\Leftrightarrow \mathcal{C}_{S} \circ \mathcal{U}_{t} = \mathcal{U}_{t} \circ \mathcal{C}_{S}$ Prof (=>> 3n porticular J\_SS'= (US & J's') (Is incoherent with  $H_{SA} = H \ge 1 - 1 \ge H^* \quad (S \simeq S^1)$ By the morse that map  $\mathcal{C}(\mathcal{P}_{s'}) = \operatorname{Tr}_{s'} \left[ \mathcal{J}_{ss'} \left( \mathcal{I} | \mathcal{D} \mathcal{P}_{s'} \right) \right]$ 

Then  $\mathcal{U}_{s} \circ \mathcal{C}(\mathcal{C}_{s'}) = \operatorname{Tre}_{s'} \left[ (\mathcal{U}_{s} \circ \mathcal{I}_{s'}) (\mathcal{I}_{ss'}) (\mathcal{I}_{ss'}) (\mathcal{I}_{ss'}) \right] =$  $= \operatorname{Ter}_{S^{1}}\left[\left(A_{S} \otimes \mathcal{U}_{S^{1}}^{*}\right)\left(\mathcal{U}_{S} \otimes \mathcal{U}_{S^{1}}^{*}\right)\left(\overline{\mathcal{I}_{SS^{1}}}\right)\left(A_{S} \otimes \mathcal{P}_{S^{1}}^{\top}\right)\right]$  $= \operatorname{Tr}_{S^{1}} \left[ \operatorname{T}_{S^{1}} \left( \operatorname{H}_{S^{2}} \mathcal{M}_{S^{1}} \left( \operatorname{P}_{S^{1}}^{\operatorname{Ts}^{1}} \right)^{T} \right) \right] = \operatorname{Co} \mathcal{U}_{S^{1}} \left( \operatorname{P}_{S^{1}} \right)^{T}$  $(\Longrightarrow) \mathcal{M}_{S} \otimes \mathcal{M}_{A} (\mathcal{C}_{S} \otimes \mathcal{J}_{A}) (\mathcal{C}_{SA}) = (\mathcal{C}_{S} \otimes \mathcal{J}_{A}) (\mathcal{U}_{S} \otimes \mathcal{U}_{A}) (\mathcal{C}_{SA})$  $= (\mathcal{E}_{S} \mathrel{\smbox{\tiny $D$}} \mathcal{T}_{A})(\mathcal{E}_{SA}).$ This thous coherence non - gen and covorion de ore equivalent. Since TD one convenent (see (b)), they satisfy adarence nou - gen. (1) We did not have time to cover Hus! See Def 11 & Theorem 13 of axiv 1807. 11549. This also completes the onswer to question (e) Properties (b), (c), (d) one equivalent. (f)Appendix C axiv 1410,4572.

# Exercise 3. Constructing thermal monotones

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

$$f(\vec{x}) \ge f(\vec{y}),\tag{7}$$

so that each f can be interpreted as a generalized free energy.

**Solution** This is a tool to construct  $\vec{g}$ -Schur-convex functions on  $(\mathbb{R}^n, \succ)$  from convex functions on  $\mathbb{R}$ : Let  $h : \mathbb{R} \to \mathbb{R}$  be convex. Then the function f

$$f(\vec{x}) = \sum_{i=1}^{n} g_i h\left(\frac{x_i}{g_i}\right),$$

is  $\vec{g}$ -Schur-convex. We prove the statement for h convex. As we have seen,  $\vec{x} \succ_g \vec{y}$  if and only if  $y_i = \sum_{j=1}^n G_{i|j} x_j$ , with  $\sum_{j=1}^n G_{i|j} \frac{g_j}{g_i} = 1$  and  $\sum_{i=1}^n G_{i|j} = 1$ . Then,

$$f(\vec{y}) = \sum_{i=1}^{n} g_i h\left(\sum_{j=1}^{n} G_{i|j} \frac{x_j}{g_i}\right) = \sum_{i=1}^{n} g_i h\left(\sum_{j=1}^{n} \left[G_{i|j} \frac{g_j}{g_i}\right] \frac{x_j}{g_j}\right) \le \sum_{j=1}^{n} g_j h\left(\frac{x_j}{g_j}\right) = f(\vec{x}).$$

## 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<sub>k</sub> and EXTRACT\_WORK<sub>k</sub> defined as follows. The function RESET\_ZERO<sub>k</sub> 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<sub>k</sub> 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<sub>k</sub> and EXTRACT\_WORK<sub>k</sub> 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⟩<sup>⊗n</sup>? How about if you would like to initialize it in the all-one state |1⟩<sup>⊗n</sup>? How about if you would like to prepare a given fixed computational basis state |x<sub>1</sub>⟩|x<sub>2</sub>⟩...|x<sub>n</sub>⟩?

**Solution** Resetting *n* qubits from a maximally mixed state to the all-zero state costs  $kT \ln(2)$  work per bit, according to Landauer's principle, for a total cost of  $nkT \ln(2)$ .

The same principle applies whether you'd like to reset to one or reset to zero, costing  $kT \ln(2)$  work per qubit. So you need to pay  $nkT \ln(2)$  regardless of which pure state you'd like to reset to, such as the all-one state or any fixed computational basis state  $|x_1\rangle|x_2\rangle \dots |x_n\rangle$ .

- (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.

**Solution** Here is a possible protocol (other protocols are possible):

1. Apply a C-NOT gate on qubits 2 and 3 to obtain the state

$$\frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)_{1,2} \otimes |0\rangle_3 ; \qquad (S.1)$$

2. Extract work from the first two qubits, leaving them maximally mixed (extract  $2 \times kT \ln(2)$  work). The state is now

$$\frac{1}{4}\mathbb{1}_{1,2}\otimes|0\rangle\langle0|_3; \qquad (S.2)$$

3. Reset the first qubit to zero, paying  $kT \ln(2)$  work. The state is now

$$|0\rangle\langle 0|_1 \otimes \frac{1}{2}\mathbb{1}_2 \otimes |0\rangle\langle 0|_3 ;$$
 (S.3)

4. Apply a C-NOT gate on the second and third qubits to obtain

$$|0\rangle\langle 0|_1 \otimes \left(\frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|\right)_{2,3} , \qquad (S.4)$$

achieving the desired transformation. In total, we've extracted  $kT \ln(2)$  work. This protocol is optimal as can be seen by the entropic bound

$$\frac{W_{\text{cost}}}{kT\ln(2)} = H_{\text{max},0}(1|2,3) = \log \left\| \text{tr}_1(|GHZ\rangle\langle GHZ|) \right\|_{\infty}$$
$$= \log \left\| \frac{1}{2} |00\rangle\langle 00| + \frac{1}{2} |11\rangle\langle 11| \right\|_{\infty} = \log \frac{1}{2} = -1 , \qquad (S.5)$$

noting that the projector onto the support of  $|GHZ\rangle\langle GHZ|$  is simply  $|GHZ\rangle\langle GHZ|$ .

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

$$\rho=\frac{1}{3}|000\rangle\langle000|+\frac{2}{3}|111\rangle\langle111|$$

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

**Solution** Here is a possible protocol (other protocols are possible):

1. Apply a C-NOT gate between the first and second qubit to obtain the state

$$|0\rangle\langle 0|_1 \otimes \left(\frac{1}{3}|00\rangle\langle 00| + \frac{2}{3}|11\rangle\langle 11|\right), \qquad (S.6)$$

achieving the desired process at no work cost.

This protocol is optimal, as can be seen by the entropic bound. The projector onto the support of the state is

$$\Pi_{1,2,3}^{\rho} = |000\rangle\langle 000| + |111\rangle\langle 111| . \tag{S.7}$$

The entropic bound then reads

$$\frac{W_{\text{cost}}}{kT\ln(2)} = H_{\text{max},0}(1|2,3) = \log \left\| \text{tr}_1(|000\rangle\langle 000| + |111\rangle\langle 111|) \right\|$$
$$= \log \left\| |00\rangle\langle 00| + |11\rangle\langle 11| \right\| = \log(1) = 0 .$$
(S.8)

(iii) Implement a MEASURE<sub>k,l</sub> 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:

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

**Solution** Here's a possible protocol:

- 1. Reset the qubit  $\ell$  to the  $|0\rangle$  state, paying  $kT \ln(2)$  work.
- 2. Apply a C-NOT gate between the k-th and the  $\ell$ -th qubits, thus correlating the  $\ell$ -th qubit with the value of the k-th qubit. This achieves the desired process.

Note that the total work cost of this measurement process is  $kT \ln(2)$ . The only work that was required was to prepare the ancilla qubit that will store the measurement result, the process itself of correlating the ancilla with the k-th qubit doesn't require work.

We can write the process we want to implement as

$$\mathcal{E}((\cdot)_{k,\ell}) = \sum_{i,j} \langle i,j | (\cdot) | i,j \rangle_{k,\ell} | i,i \rangle \langle i,i |_{k,\ell} .$$
(S.9)

(The protocol above doens't exactly implement this process, because it handles states with coherences differently. To achieve the process  $\mathcal{E}$ , you can simply add a dephasing operation to make sure the output is classical; the dephasing costs no additional work.)

The minimal work cost is then given (for any full-rank  $\sigma$ ) by

$$W_{\text{cost}}(\mathcal{E}, \sigma) = \log \left\| \mathcal{E}(\mathbb{1}_{k,\ell}) \right\| = \log \left\| \sum_{i,j} \langle i, j | \mathbb{1} | i, j \rangle_{k,\ell} | i, i \rangle \langle i, i |_{k,\ell} \right\|$$
$$= \log \left\| 2 \sum_{i} |i, i \rangle \langle i, i |_{k,\ell} \right\| = \log 2 = 1 , \qquad (S.10)$$

where the factor 2 comes from the summation over 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.

**Solution** See solutions in part (b).

## 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.<sup>1</sup>

(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?

**Solution** Thermodynamics ascribes zero entropy change to the mixing of two samples of argon at the same temperature and pressure.

(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.

**Solution** Even if we manage to get pure A1 in volume  $V_1$ , and pure A2 in volume  $V_2$ , we would have no way of detecting any difference in the resulting diffusion process, so we would still ascribe zero entropy change to the process.

(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.

**Solution** Now we can prepare two volumes of A1 and A2. We start the experiment with  $n_1 = \alpha n$  moles of A1, and  $n_2 = (1 - \alpha)n$  moles of A2, and due to our greater knowledge the diffusion results in entropy increase

$$\Delta S = \Delta S_1 + \Delta S_2 \text{ with}$$
$$\Delta S_1 = -n\alpha \log \alpha, \ \Delta S_2 = -n(1-\alpha)\log(1-\alpha).$$

If this entropy is more than a consequence of our knowledge increase, it has to have observable consequences, like work we could extract from the process. All in all, then the amount of useful work we can extract from a system depends on our "subjective" information about the state.

<sup>&</sup>lt;sup>1</sup>https://link.springer.com/chapter/10.1007/978-94-017-2219-3\_1