Universität Heidelberg
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Single-shot quantum thermodynamics

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`http://www.mpmueller.net/lecture2.html`

Exercises 9

(to hand in: **Thursday, January 22**, 2015)

In these exercises, we will be concerned with thermal operations and their relation to the concept of d-majorization (or relative majorization how it is called as well.) When we speak of thermal operations on this sheet, we will always assume that we start with diagonal states. This is not the most general setting, but it is a simplification we have to make since the classification of thermal operations for general states is an open question until now. However, for diagonal states, a result is known, and we will prove it on this sheet (at least for the qubit case).

Furthermore, we will always assume that the system we trace out in the thermal operation is just the heat bath. That is, in contrast to the most general case, the Hamiltonian and dimension of the quantum system under consideration will not change. (Compare the notes on Lecture 9, pages 4&5.)

Problem 33 (Constructing thermal operations): (10 points)

Assume that you have a quantum system with Hamiltonian H_S and a heat bath system with Hamiltonian H_B, and look at the combined Hamiltonian $H = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_B$. Assume furthermore that H is non-degenerate.

(i) Show that unitary matrices with $[H, U] = 0$ have to be diagonal as well, and are thus of the form $U = \mathrm{diag}(e^{i\theta_1}, \ldots, e^{i\theta_n})$. Why is non-degeneracy of H here important?

Now let γ_B be the Gibbs state of the heat bath (which is diagonal since we choose the basis of our vector space in such a way) and ρ_S be a diagonal state of our quantum system (see comment on top).

(ii) Show that under the assumptions on H from above, we have

$$U\,(\rho_S \otimes \gamma_B)\,U^\dagger = \rho_S \otimes \gamma_B$$

for all U with $[U, H] = 0$, and thus as well

$$\mathrm{Tr}_B\left[U\,(\rho_S \otimes \gamma_B)\,U^\dagger\right] = \rho_S.$$

This means that in the case that H is non-degenerate, the only thermal operation we can have is the identity. You have already seen in Problem 29 that it is in general possible to obtain non-trivial thermal operations. We will shortly repeat the results from there, and then generalize this.

The given Hamiltonians add up to H, and possible unitaries U with $[H, U] = 0$ are of the form

$$H = \begin{pmatrix} 0 & & & \\ & \Delta E & & \\ & & \Delta E & \\ & & & 2\Delta E \end{pmatrix} + \mathbb{1}E \qquad \text{and} \qquad U = \begin{pmatrix} 1 & & \\ & U_{2\times 2} & \\ & & 1 \end{pmatrix},$$

where $U_{2\times 2}$ is some arbitrary two-dimensional unitary matrix. If we now choose $U_{2\times 2} = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, and $\sigma = \mathrm{diag}(s_1, s_2, s_3, s_4)$ is some matrix on the combined system, we have

$$U\sigma U^\dagger = \mathrm{diag}(s_1, s_3, s_2, s_4).$$

Since the second and third level of our Hamiltonian had the same energy, we were able to find a unitary that interchanges the second and third diagonal elements of the state σ.
The generalization is the following statement: If you have a permutation P that leaves the vector $\vec{E}$ of energy eigenvalues of some Hamiltonian $H = \mathrm{diag}(\vec{E})$ invariant, we can find a unitary matrix U with $[H, U] = 0$ that permutes the diagonal elements of some $\sigma = \mathrm{diag}(s_1, \ldots, s_n) = \mathrm{diag}(\vec{s})$ as the permutation P. That means

$$U\sigma U^\dagger = \mathrm{diag}(P\vec{s}).$$

(iii) Describe how you would construct this type of unitary starting from the example discussed above. Use that each permutation can be written as a successive application of the exchange of just two components, and that the product of unitary matrices is again unitary.

Problem 34 (Thermal operations for the qubit via the harmonic oscillator): (15 points)

In this exercise, we want to prove the following statement: A diagonal qubit state can be mapped to another diagonal qubit state via thermal operations if and only if there exists a stochastic matrix mapping the vectors of diagonal elements into each other and leaving the vector of diagonal elements of the system's Gibbs state invariant.
First remember Problem 29 from Exercise sheet 7, where it was shown that thermal operations cannot produce any off-diagonal terms. This means that thermal operations are linear maps from diagonal matrices to diagonal matrices, and thus can as well be seen as linear maps from vectors to vectors since they just map the vector of diagonal elements to another vector of diagonal elements. Thus we can write them down as a stochastic matrix (stochastic since the normalization of the matrix and thus of the vector of diagonal elements is preserved) which also leaves the vector of diagonal elements of the Gibbs state of the system invariant (why?).
Let us show this explicitly again, with the system and environment of Problem 27 as already used above.

$$H_S = \begin{pmatrix} 0 & 0 \\ 0 & \Delta E \end{pmatrix}, \qquad H_B = \begin{pmatrix} E & 0 \\ 0 & E + \Delta E \end{pmatrix}, \qquad \gamma_B = \begin{pmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{pmatrix} \quad \text{and } \Delta E > 0.$$

Let us denote the thermal operation from density matrices to density matrices by Φ,

$$\Phi(\rho_S) = \mathrm{Tr}_B \left[U \left(\rho_S \otimes \gamma_B \right) U^\dagger \right],$$

and U is the unitary chosen in the above exercise that interchanges the second and third component.
Now let us check where the density matrices $\mathrm{diag}(1, 0)$ and $\mathrm{diag}(0, 1)$ are mapped to.

(i) Show that $\Phi(\mathrm{diag}(1, 0)) = \gamma_B$ and $\Phi(\mathrm{diag}(0, 1)) = \gamma_B$.

(ii) Argue why the stochastic matrix B_Φ corresponding to Φ is $B_\Phi = \left(\begin{smallmatrix} \gamma_1 & \gamma_1 \\ \gamma_2 & \gamma_2 \end{smallmatrix}\right)$, where $\gamma_S = \gamma_B = \mathrm{diag}(\gamma_1, \gamma_2)$. Check that it is stochastic and Gibbs-preserving.

Now we are referring to yet another previous problem. On the last sheet, you parametrized all two-by-two matrices leaving some vector invariant. Let us choose this vector to be $\vec{\gamma} = (\gamma_1, \gamma_2)$, then all $\vec{\gamma}$ preserving matrices can be written as

$$\begin{pmatrix} 1-t & \gamma_1/\gamma_2\, t \\ t & 1-\gamma_1/\gamma_2\, t \end{pmatrix} \qquad \text{with} \qquad 0 < t < \gamma_2/\gamma_1.$$

We need the condition $t < \gamma_2/\gamma_1$ since $\Delta E > 0$, and thus $\gamma_1 > \gamma_2$, and without this restriction on t the matrix would not be stochastic anymore.
So for each environment and specific unitary used in some thermal operation on a qubit, we can give some parameter t to describe to which $\vec{\gamma}$-preserving matrix this thermal operation corresponds.

(iii) To what value of t does the above stochastic matrix B_Φ correspond? Argue that for some general environment and unitary in the thermal operation, we just need to calculate $\mathrm{Tr}_B \left[U \left(\mathrm{diag}(1,0) \otimes \gamma_B\right) U^\dagger\right]$ to determine the corresponding value of t.

We will now choose an environment and a unitary to get close to the maximal value $t = \gamma_2/\gamma_1$. We choose H_S as above and the heat bath Hamiltonian as

$$H_B = \begin{pmatrix} 0 & & & & \\ & \Delta E & & & \\ & & 2\,\Delta E & & \\ & & & \ddots & \\ & & & & (n-1)\Delta E \end{pmatrix} \quad \text{with} \quad \gamma_B = \begin{pmatrix} \delta_1 & & & & \\ & \delta_2 & & & \\ & & \delta_3 & & \\ & & & \ddots & \\ & & & & \delta_n \end{pmatrix} \quad \text{and} \quad \delta_i = e^{-\beta(i-1)\Delta E}/Z.$$

Thus, the corresponding Hamiltonian $H = H_S + H_B$ is given as

$$H = \left(\begin{array}{cccc|cccc} 0 & & & & & & & \\ & \Delta E & & & & & & \\ & & \ddots & & & & & \\ & & & (n-1)\Delta E & & & & \\ \hline & & & & \Delta E & & & \\ & & & & & 2\,\Delta E & & \\ & & & & & & \ddots & \\ & & & & & & & n\,\Delta E \end{array}\right) \quad \text{and} \quad \mathrm{diag}(1,0)\otimes\gamma_B = \left(\begin{array}{cccc|cccc} \delta_1 & & & & & & & \\ & \delta_2 & & & & & & \\ & & \ddots & & & & & \\ & & & \delta_n & & & & \\ \hline & & & & 0 & & & \\ & & & & & 0 & & \\ & & & & & & \ddots & \\ & & & & & & & 0 \end{array}\right)$$

(iv) Argue, using the result (iii) of Problem 33 above, that there exists a unitary U such that

$$\mathrm{Tr}_B \left[U \left(\mathrm{diag}(1,0) \otimes \gamma_B\right) U^\dagger\right] = \mathrm{diag}(\delta_1, \delta_2 + \cdots + \delta_n).$$

(v) Use the geometric series and the normalization condition to calculate $t = \sum_{i=2}^n \delta_i$ and show that for $n \to \infty$ we have $t \to \gamma_2/\gamma_1 = e^{-\beta\Delta E}$.

Now we are nearly done. We can explicitly give Hamiltonians and unitaries for the environment either corresponding to $t = 0$ (the identity), $t = \gamma_2$, or some other value arbitrarily close to $t = \gamma_2/\gamma_1$. But how does this help us with constructing a unitary and an environment for an arbitrary $t \in [0, \gamma_2/\gamma_1)$? Here is how: Remember the matrix $U_{2\times 2}$ chosen in the above exercise to be $\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$? We could as well choose it to be $\left(\begin{smallmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{smallmatrix}\right)$. Continuously varying the parameter α, we can get from $t = 0$ to $t = \gamma_2$. Furthermore, if we build a general unitary as done in (iii) of Problem 33 above, we can exchange all swaps of two components with these rotations, giving us a way to continuously interpolate from the identity ($t = 0$) to the t value of some permutation. This means that we can get all t if we just choose the dimension n of the environment large enough.

What we have shown in this exercise is that for the qubit, the problem of interconvertibility under thermal operations is reduced to the concept of d-majorization. This is still true for larger systems; however, then a more general proof is needed, as you have seen in the lecture.

Problem 35 (Monotones for d-majorization): (5 points)

Remember Problem 12, where you have shown that all Rényi entropies are Schur concave. Some similar set of functions with an analogous property exists for d-majorization. Check the lecture notes of Lecture 11 online, and have a look at the theorem on page 6.
Define the *relative Rényi entropies* as

$$D_\alpha(p\|q) := \frac{\operatorname{sign}\alpha}{\alpha - 1} \log \sum_{i=1}^{n} p_i^\alpha q_i^{1-\alpha} \qquad \text{with } \alpha \in \mathbb{R}\backslash\{1\},$$

where we set $0^0 := 0$ and $\operatorname{sign}\alpha := \left\{ \begin{array}{cc} 1 & \alpha \geq 0 \\ -1 & \alpha < 0 \end{array} \right\}$. Use the aforementioned theorem to show that

$$(p, d) \succ (p', d') \quad \Rightarrow \quad D_\alpha(p\|d) \geq D_\alpha(p'\|d') \quad \text{for all } \alpha,$$

and

$$\lim_{\alpha \to 1} D_\alpha(p\|q) = D(p\|q),$$

where $D(p\|q)$ is the standard relative entropy (Kullback-Leibler divergence).