Exercises - Week 8

Problem 8.1: Thermal states, free energy, and the Maximum Entropy Principle (6 points)

In thermodynamic equilibrium the Helmholtz free energy is defined as:

$$F := E - 1/\beta S,$$

where E is the internal energy and S the entropy. We can apply the same formula to a general quantum state ρ, not necessarily in thermal equilibrium, by identifying $E := \mathrm{Tr}[\rho H]$, $S(\rho)$ as the state's von Neumann entropy, and β as the ambient inverse temperature (i.e., β is given as an external parameter).

i) Show that the thermal state γ_β can be expressed as $\gamma_\beta = \exp[\beta(\tilde{F} - H)]$ with $\tilde{F} = -\beta^{-1} \ln Z$ where Z is the canonical partition sum. Then show that $\tilde{F} = F$.
Hint: Note that H is an operator but $\tilde{F}$ is a number. You can formally write $\tilde{F}$ as $\tilde{F}\mathbf{I}$ where $\mathbf{I}$ is the identity on the same Hilbert space that the Hamiltonian H acts on.

ii) For a general state ρ, show that $F(\rho) = \beta^{-1} R(\rho||\gamma_\beta) + F(\gamma_\beta)$ where R is the quantum relative entropy.

iii) The Maximum Entropy Principle states that for a system with a fixed internal energy E we should assign the equilibrium state γ_β with β determined by $E = \mathrm{Tr}[H\gamma_\beta]$.
Use Klein's inequality (i.e., $R(\rho||\sigma) \geq 0 \;\forall\; \rho, \sigma$) to show that the entropy difference $\Delta S = S(\rho) - S(\gamma_\beta)$ is lower bounded by 0 for all states ρ which have the same internal energy as γ_β, i.e., $E = \mathrm{Tr}[\gamma_\beta H] = \mathrm{Tr}[\rho H]$. Recall that the quantum relative entropy implies 'identity of indiscernibles' (i.e., $R(\rho||\sigma) = 0 \Leftrightarrow \rho = \sigma$) to conclude that γ_β is the unique maximum entropy state among all states with the same internal energy.

Problem 8.2: Passivity (5 points)

If a state π is passive with respect to a Hamiltonian H its energy cannot be reduced by any cyclic unitary operation. However, if π is not thermal it can be *activated* by combining multiple identical copies as $\rho_N = \pi^{\otimes N}$. The energy of this activated state ρ_N is then not minimal with respect global cyclic unitary transformations. We denote any corresponding globally passive state π_N (i.e., $\pi_N = U_N \pi^{\otimes N} U_N^\dagger$ where U_N minimises $\mathrm{Tr}[U\pi^{\otimes N}U^\dagger H_N]$; H_N is the sum of the N local Hamiltonians H; and π_N, U, and U_N act on the N-partite space).
Remark: Note that U_N and π_N are only unique up to degeneracies in H_N. For simplicity, we choose only π_N that are diagonal in the same basis as H_N.

i) For a Hamiltonian $H = |e_1\rangle\langle e_1| + \frac{4}{3}|e_2\rangle\langle e_2|$ (with ground state $|e_0\rangle$) and state $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{6}|1\rangle\langle 1| + \frac{1}{3}|2\rangle\langle 2|$, find the corresponding passive state π (i.e., the state $\pi = U\rho U^\dagger$ with the lowest energy). Assume that $\{|i\rangle\}$ is an orthonormal basis that does not commute with the energy eigenbasis.

ii) Taking the same Hamiltonian $H = |e_1\rangle\langle e_1| + \frac{4}{3}|e_2\rangle\langle e_2|$ and the passive state $\pi = 0.5|e_0\rangle\langle e_0| + 0.3|e_1\rangle\langle e_1| + 0.2|e_2\rangle\langle e_2|$, what is the minimal number of copies n required to activate π as $\pi^{\otimes n}$?

iii) Returning to the case of a general passive state π which is not N-passive from the introduction paragraph to this problem, show that any globally passive state π_N is separable.

Problem 8.3: Ergotropy (8 points)

For a given Hamiltonian H and state ρ the energy difference between ρ and the corresponding passive state π is called *ergotropy* $\mathcal{W}$:

$$\mathcal{W}(\rho, H) := \min_U \mathrm{Tr}[(\rho - U\rho U^\dagger)H] \tag{1}$$

i) For a generic Hamiltonian H and state ρ:

$$H = \sum \epsilon_i |e_i\rangle\langle e_i|, \text{ with } \epsilon_{i+1} \geq \epsilon_i \; \forall \, i, \tag{2}$$

$$\rho = \sum \lambda_i |R_i\rangle\langle R_i|, \text{ with } \lambda_{i+1} \leq \lambda_i \; \forall \, i. \tag{3}$$

Express π in terms of the eigenvalues $\{\lambda_i\}$ and the energy eigenstates; express the optimal unitary $\tilde{U}$ in terms of the orthonormal bases $\{|e_i\rangle\}$ and $\{|R_i\rangle\}$. Then express $\mathcal{W}(\rho, H)$ in terms of the eigenvalues $\{\epsilon_i\}$ and $\{\lambda_i\}$, and the two eigenbases.

ii) For a quantum system with Hamiltonian H consider two qubit states ρ and σ with the same energy. Show that $S(\rho) \geq S(\sigma)$ implies $\mathcal{W}(\rho, H) \leq \mathcal{W}(\sigma, H)$ and vice versa.

iii) This intuition does not carry over to systems of larger dimensions. Demonstrate this by defining a qutrit Hamiltonian and two qutrit states, ρ and σ, with $\mathrm{Tr}[H\rho] = \mathrm{Tr}[H\sigma]$, $S(\rho) > S(\sigma)$, but $\mathcal{W}(\rho, H) > \mathcal{W}(\sigma, H)$.
Hint: You can solve this by finding two passive states π and π' with $S(\pi) < S(\pi')$ but $E(\pi) > E(\pi')$.
You may start your argument with the Hamiltonian $H = |e_1\rangle\langle e_1| + 9|e_2\rangle\langle e_2|$ (with ground state $|e_0\rangle$) and state $\pi' = \frac{1}{2}(|e_0\rangle\langle e_0| + |e_1\rangle\langle e_1|)$.

iv) Show that in general, for any Hamiltonian H, and states ρ and σ, with $\mathrm{Tr}[\rho H] = \mathrm{Tr}[\sigma H]$ and majorisation $\rho \succ \sigma$ implies $\mathcal{W}(\rho, H) \geq \mathcal{W}(\sigma, H)$.
Remark: Majorisation between quantum states is defined between the vectors of the states' eigenvalues.