In this first problem sheet, we will recap on some concepts that you might have learned in previous courses.

Exercise 1. Unitary and Hermitian operators

Let $\mathcal{H}$ be a Hilbert space and $A, B \in End(\mathcal{H}, \mathcal{H})$ operators in that Hilbert space. Here you have to prove some of their properties.
Note: the operator exponential is given by the power series:

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$$

(a) Show that $(e^A)^\dagger = e^{A^\dagger}$.

(b) Suppose that $[A, B] = AB - BA = 0$, that is, the operators A and B commute. Prove that $e^{A+B} = e^A e^B$.

(c) Show that if the operator A is Hermitian ($A = A^\dagger$) , then $U = e^{iA}$ is unitary ($UU^\dagger = U^\dagger U = \mathbb{I}$). Show also that for a collection $\{A_j\}_j$ of Hermitian operators , $U = \bigotimes_j e^{iA_j}$ is unitary.

Hint: Make use of the results in (a) and (b).

(d) Show that if U is a unitary, then there exists a Hermitian operator A such that $U = e^{iA}$.

(e) Suppose that V is both unitary and Hermitian. Show that the only possible eigenvalues for V are ± 1 and that $V^2 = \mathbb{I}$.

(f) Show that adding $\alpha \mathbb{1}$, where $\alpha \in \mathbb{R}$, to a Hamiltonian of a system only induces a global phase, and thus we can always shift the energy of the ground state of the Hamiltonian to zero.

(g) Suppose that A and B are Hermitian operators which commute $[A, B] = 0$. Show that in that case there exists a basis in which both A and B are diagonal, or block-diagonal.

Exercise 2. Trace and partial trace

The trace of an operator $A : \mathcal{H} \to \mathcal{H}$ is defined as $\operatorname{tr}(A) = \sum_j \langle j|A|j\rangle$, where $\{|j\rangle\}_j$ is an orthonormal basis in $\mathcal{H}$. Show that the trace operation is:

(a) Linear: $\operatorname{tr}(\alpha A + \beta B) = \alpha \operatorname{tr}(A) + \beta \operatorname{tr}(B)$ for all operators A, B and coefficients $\alpha, \beta \in \mathbb{C}$;

(b) Cyclic: $\operatorname{tr}(ABC) = \operatorname{tr}(BCA)$ for all operators A, B, C;

(c) Basis-independent: $\operatorname{tr}(UAU^\dagger) = \operatorname{tr}(A)$ for all operators A and arbitrary unitaries U.

The partial trace is an important concept in the quantum mechanical treatment of multi-partite systems, and it is the natural generalisation of the concept of marginal distributions in classical probability theory. Let ρ_{AB} be a density matrix on the bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. We define the *reduced state* (or *marginal*) on $\mathcal{H}_A$ as the partial trace over $\mathcal{H}_B$,

$$\rho_A := \operatorname{tr}_B(\rho_{AB}) = \sum_j (\mathbb{1}_A \otimes \langle j|_B)\ \rho_{AB}\ (\mathbb{1}_A \otimes |j\rangle_B),$$

where $\{|j\rangle_B\}_j$ is an orthonormal basis of $\mathcal{H}_B$.

(d) Show that ρ_A is a valid density operator by proving it is:

  (i) Hermitian: $\rho_A = \rho_A^\dagger$.
  (ii) Positive: $\rho_A \geq 0$.
  (iii) Normalised: $\operatorname{tr}(\rho_A) = 1$.

(e) Calculate the reduced density matrix of system A in the Bell state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \quad \text{where} \quad |ab\rangle = |a\rangle_{\mathrm{A}} \otimes |b\rangle_{\mathrm{B}}. \tag{1}$$

(f) Consider a classical probability distribution P_{XY} with marginals P_X and P_Y.

  (i) Calculate the marginal distribution P_X for

$$P_{XY}(x,y) = \begin{cases} 0.5 & \text{for } (x,y) = (0,0), \\ 0.5 & \text{for } (x,y) = (1,1), \\ 0 & \text{else,} \end{cases} \tag{2}$$

  with alphabets $\mathcal{X}, \mathcal{Y} = \{0,1\}$.
  (ii) How can we represent P_{XY} in form of a quantum state?
  (iii) Calculate the partial trace of P_{XY} in its quantum representation.

(g) Can you think of an experiment to distinguish the bipartite states of parts (b) and (c)?

Exercise 3. Composability of thermal states

Given a system with Hamiltonian

$$H = \sum_i E_i |i\rangle\langle i|,$$

and a temperature T, we define the *thermal state*

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

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

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

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two systems with the joint Hamiltonian

$$H_{AB} = H_A \otimes \mathbb{I}_B + \mathbb{I}_A \otimes H_B \quad \text{(the systems don't interact)}$$

(a) Show that in this case the thermal state of the joint system can be written as a tensor product of thermal states on individual subsystems:

$$\tau_{AB} = \tau_A \otimes \tau_B, \quad \text{or} \quad \frac{e^{-\frac{H_{AB}}{kT}}}{Z_{AB}} = \frac{e^{-\frac{H_A}{kT}}}{Z_A} \otimes \frac{e^{-\frac{H_B}{kT}}}{Z_B}$$

(b) Generalize the statement in (a) for the thermal state of n non-interacting subsystems.