In this preliminary exercise 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 $(e^A)^\dagger = e^{A^\dagger}$.*

Solution

$$(e^A)^\dagger = \sum_{n=0}^{\infty} \frac{1}{n!} (A^n)^\dagger = \sum_{n=0}^{\infty} \frac{1}{n!} (A^\dagger)^n = e^{A^\dagger}.$$

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

Solution The operators A and B commute, hence $AB = BA$ – which means that the order does not matter for these operators when they are multiplied, and we can use the binomial theorem in a usual way:

$$\begin{aligned} e^{A+B} &= \sum_{n=0}^{\infty} \frac{1}{n!} (A+B)^n = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{m=0}^{n} C_n^m A^m B^{n-m} = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{m=0}^{n} \frac{n!}{m!(n-m)!} A^m B^{n-m} \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{1}{m!(n-m)!} A^m B^{n-m} = e^A e^B. \end{aligned}$$

In the last step, we have used the Cauchy formula for the product of two series.

(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.*

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

Solution From (a) it follows that $U^\dagger = e^{-iA^\dagger} = e^{-iA}$. Then since $[A, A] = 0$ (every operator commutes with itself),

$$U^\dagger U = e^{-iA} e^{iA} = e^{-iA+iA} = \mathbb{I}.$$

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

Solution Let us write U in its diagonal form: $U = WDW^\dagger$ where $D = diag(e^{i\alpha_1}, e^{i\alpha_2}, \dots)$ with $\alpha_j \in \mathbb{R}$, and W is a unitary. Let us choose $H = W diag(\alpha_1, \alpha_2, \dots)W^\dagger$. H is Hermitian, as α_j are real, and

$$e^{iH} = \sum_{n=0}^{\infty} \frac{1}{n!}(W diag(\alpha_1, \alpha_2, \dots)W^\dagger)^n = \sum_{n=0}^{\infty} \frac{i^n}{n!} W diag(\alpha_1, \alpha_2, \dots)^n W^\dagger$$
$$= W e^{i \cdot diag(\alpha_1, \alpha_2, \dots)} W^\dagger = WDW^\dagger = U.$$

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

Solution From the definitions of Hermitian and unitary operators it follows that $\mathbb{I} = V^\dagger V = VV = V^2$. Suppose that $|\phi\rangle$ is an eigenvector of V, corresponding to the eigenvalue λ: $V|\phi\rangle = \lambda|\phi\rangle$. The complex conjugate reads $\langle\phi|V^\dagger = \langle\phi|\lambda^*$; the product of these two expressions gives

$$\lambda\lambda^* = \langle\phi|V^\dagger V|\phi\rangle = 1 \Rightarrow |\lambda|^2 = 1.$$

Additionally, note

$$\lambda^* = \langle\phi|V^\dagger|\phi\rangle = \langle\phi|V|\phi\rangle = \lambda$$

Hence, λ is real, and $|\lambda|^2 = 1$, which means $\lambda = \pm 1$.

(f) *Show that adding $\alpha\mathbb{I}$, 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.*

Solution Suppose that we initially have a Hamiltonian H, and we add a term $\alpha\mathbb{I}$: $H' = H + \alpha\mathbb{I}$. First, let us note that H' has the same set of eigenfunctions $\{|\psi\rangle_i\}_i$ as H:

$$H'|\psi\rangle_i = (H + \alpha\mathbb{I})|\psi\rangle_i = H|\psi\rangle_i + \alpha|\psi\rangle_i = (E_i + \alpha)|\psi\rangle_i$$

All eigenvalues shift by α for H', therefore we can always choose the parameter α such that the energy of the ground state E_0 is equal to 0.
The evolution of the system is governed by a unitary U':

$$U' = e^{-iH't} = e^{-iHt - i\alpha\mathbb{I}t} \overset{[H,\mathbb{I}]=0}{=} e^{-iHt}e^{-i\alpha t}$$

Hence, for the evolution of the state we only acquire a phase factor $e^{-i\alpha t}$.

(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.*

Solution Let us consider an eigenbasis of A: $\{|\psi_i^(j)\rangle\}_{i,j}$, where we take into account that some eigenvalues of A can be degenerate:

$$A|\psi_i^{(j)}\rangle = \lambda_i|\psi_i^{(j)}\rangle \quad \forall j.$$

For all eigenvectors of A $|\phi\rangle$ it holds that

$$AB|\phi\rangle = BA|\phi\rangle = \lambda_i B|\phi\rangle.$$

Hence, $B|\phi\rangle$ is an eigenvector of A, with an eigenvalue λ_i. If λ_i is non-degenerate, then $B|\phi\rangle$ can only differ from $|\psi_i\rangle$ by a constant factor: $B|\phi\rangle = \mu_i|\psi_i\rangle$, and $|\psi_i\rangle$ is an eigenstate of B. This gives us both A and B having a diagonal element in their representation in $\{|\psi_i^(j)\rangle\}_{i,j}$.

If λ_i is degenerate, then $B|\phi\rangle$ can be written as a combination of $\{|\psi_i^(j)\rangle\}_j$; B can be seen as acting internally in that subspace. This gives us A having a diagonal entries in its matrix representation in $\{|\psi_i^(j)\rangle\}_{i,j}$, and B having a block-diagonal entry.

Exercise 2. *Trace and partial trace*

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

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

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

(c) Basis-independent: $\mathrm{Tr}\,(UAU^\dagger) = \mathrm{Tr}\,(A)$ *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 $\mathcal{H}_B$,*

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

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: $\mathrm{Tr}\,(\rho_A) = 1$.

Solution

(i) Remember that ρ_{AB} can always be written as

$$\rho_{AB} = \sum_{i,j,k,l} c_{ij;kl}\ |i\rangle\langle k|_A \otimes |j\rangle\langle l|_B, \tag{S.1}$$

for some bases $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and $c_{ij;kl} = c^\dagger_{kl;ij}$ is hermitian. The reduced density operator ρ_A is then given by

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \sum_{i,k}\sum_m c_{im;km}|i\rangle\langle k|_A \tag{S.2}$$

as can easily be verified. Hermiticity of ρ_A follows from

$$\rho_A^\dagger = \sum_{i,k}\sum_m c^\dagger_{im;km}\,(|i\rangle\langle k|_A)^\dagger = \sum_{i,k}\sum_m c_{km;im}|k\rangle\langle i|_A = \rho_A. \tag{S.3}$$

(ii) Since $\rho_{AB} \geq 0$ is positive, its scalar product with any pure state is positive. Let $|\psi\rangle_A$ an arbitrary pure state in $\mathcal{H}_A$ and define $|\Psi_m\rangle_{AB} = |\psi\rangle_A \otimes |m\rangle_B$, a state on $\mathcal{H}_A \otimes \mathcal{H}_B$:

$$\begin{aligned} 0 &\leq \sum_m \langle \Psi_m | \rho_{AB} | \Psi_m \rangle \\ &= \sum_m \langle \psi |_A \otimes \langle m |_B \rho_{AB} | \psi \rangle_A \otimes | m \rangle_B \\ &= \sum_m \sum_{i,j,k,l} c_{ij;kl} \langle \psi | i \rangle \langle k | \psi \rangle_A \langle m | j \rangle \langle l | m \rangle_B \\ &= \sum_{i,k} \sum_m c_{im;km} \langle \psi | i \rangle \langle k | \psi \rangle_A \\ &= \langle \psi | \rho_A | \psi \rangle \end{aligned} \tag{S.4}$$

Because this is true for any $|\psi\rangle$ on $mathcal H_A$, it follows that ρ_A is positive.

(iii) Consider

$$\begin{aligned} \operatorname{Tr}(\rho_A) &= \sum_{i,j} \sum_{m,n} c_{im;km} \langle n | i \rangle \langle k | n \rangle \\ &= \sum_{m,n} c_{nm;nm} = \operatorname{Tr}(\rho_{AB}) = 1. \end{aligned} \tag{S.5}$$

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

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle), \quad \textit{where} \quad |ab\rangle = |a\rangle_A \otimes |b\rangle_B. \tag{1}$$

Solution The reduced state is mixed, even though $|\Psi\rangle$ is pure:

$$\rho_{AB} = |\Psi\rangle\langle\Psi| = \frac{1}{2}\Big(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\Big) \tag{S.6}$$

$$\operatorname{Tr}_B \rho_{AB} = \frac{1}{2}\Big(|0\rangle\langle 0| + |1\rangle\langle 1|\Big) = \frac{\mathbb{I}_A}{2}. \tag{S.7}$$

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

(i) Calculate the marginal distribution P_X for

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

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.

Solution

(i) Using $P_X(\cdot) = \sum_{y \in \mathcal{Y}} P_{XY}(\cdot, y)$, we immediately obtain

$$P_X(0) = 0.5, \quad P_X(1) = 0.5. \tag{S.8}$$

(ii) A probability distribution $P_Z = \{P_Z(z)\}_z$ may be represented by a state

$$\rho_Z = \sum_z P_Z(z)|z\rangle\langle z| \tag{S.9}$$

for a basis $\{|z\rangle\}_z$ of a Hilbert space $\mathcal{H}_Z$. In this case we can create a two-qubit system with composed Hilbert space $\mathcal{H}_X \otimes \mathcal{H}_Y$ in state

$$\rho_{XY} = \frac{1}{2}\big(|00\rangle\langle 00| + |11\rangle\langle 11|\big). \tag{S.10}$$

(iii) The reduced state of qubit X is

$$\rho_X = \frac{1}{2}\big(|0\rangle\langle 0| + |1\rangle\langle 1|\big) = \frac{\mathbb{I}_X}{2}. \tag{S.11}$$

Notice that the reduced states of this classical state and the Bell state are the same whereas the state of the global state is very different – in particular, the latter is a pure state that can be very useful in quantum communication and cryptography whereas the former is not.

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

Solution One could for instance measure the two states in the Bell basis,

$$\begin{aligned} |\psi_1\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \quad |\psi_2\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}, \\ |\psi_3\rangle &= \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \quad |\psi_4\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}. \end{aligned} \tag{S.12}$$

The Bell state we analysed corresponds to the first state of this basis, $|\Psi\rangle = |\psi_1\rangle$, and a measurement in the Bell basis would always have the same outcome. For the classical state, however, $\rho_{XY} = \frac{1}{2}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|)$, so with probability $\frac{1}{2}$ a measurement in this basis will output $|\psi_2\rangle$, and we will know we had the classical state. Of course, if we only have access to a single copy we will find out about the difference only with probability $\frac{1}{2}$. However, with arbitrarily many copies we will find out which state we have with very high probability after a few measurements.

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

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

(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:*

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

Solution Let us rewrite the Hamiltonian of AB in terms of eigenbases of A and B:

$$H_{AB} = \sum_i E_i^A |i\rangle\langle i| \otimes \mathbb{I}_B + \mathbb{I}_A \otimes \sum_j E_j^B |j\rangle\langle j|$$

It immediately follows that the eigenvalues of H_{AB} are $E_i^A + E_j^B$, $\forall i, j$. Then the thermal state on AB (here we denote $\beta = \frac{1}{kT}$)

$$\tau_{AB} = \frac{e^{-\beta H_{AB}}}{\sum_{i,j} e^{-\beta(E_i^A + E_j^B)}} = \frac{e^{-\beta H_A \otimes \mathbb{I}_B + \mathbb{I}_A \otimes H_B}}{\sum_{i,j} e^{-\beta(E_i^A + E_j^B)}} = \frac{e^{-\beta H_A \otimes \mathbb{I}_B}}{\sum_i e^{-\beta E_i^A}} \frac{e^{-\beta \mathbb{I}_A \otimes H_B}}{\sum_j e^{-\beta E_j^B}} =$$
$$= \frac{e^{-\beta H_A}}{Z_A} \otimes \frac{e^{-\beta H_B}}{Z_B} = \tau_A \otimes \tau_B.$$

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

Solution By induction from (a), for n non-interacting systems with local Hamiltonians $H_1, \ldots, H_n$ the thermal state is written as

$$\tau = \tau_1 \otimes \cdots \otimes \tau_n, \text{ where } \tau_j = \frac{e^{-\beta H_j}}{Z_j}.$$

Exercise 4. *Energy preservation*

Suppose that the system is characterized by a Hamiltonian H, and a unitary operation U is applied.

(a) *Show that if $[U, H] = 0$, then the unitary preserves the energy of the system.*

Solution The energy of the system after the unitary is applied (we use the circularity of trace and $HU = UH$):

$$E' = \mathrm{Tr}\left(()\, H\rho'\right) = \mathrm{Tr}\left(()\, HU\rho U^\dagger\right) = \mathrm{Tr}\left(()\, UH\rho U^\dagger\right) = \mathrm{Tr}\left(()\, U^\dagger UH\rho\right) = \mathrm{Tr}\left(()\, H\rho\right) = E.$$

(b) *Consider a four-level system with a Hamiltonian $H = \Delta|1\rangle\langle 1| + \Delta|2\rangle\langle 2| + 2\Delta|3\rangle\langle 3|$, written in the energy eigenbasis $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$. Come up with one non-trivial unitary U_{pres} which would preserve the energy of the system for any state, and identify the common eigenbasis of U and H. Find another unitary $U_{non\text{-}pres}$ which would not preserve the energy of the system for any state.*

Solution The Hamiltonian of the system is degenerate: the states $|1\rangle$ and $|2\rangle$ correspond to the same energy Δ:

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 \\ 0 & 0 & \Delta & 0 \\ 0 & 0 & 0 & 2\Delta \end{pmatrix}$$

Since the levels $|1\rangle$ and $|2\rangle$ have the same energy, swapping their populations will not change the net energy:

$$U_{\text{pres}} = (|1\rangle\langle 2| + |2\rangle\langle 1|) + (|0\rangle\langle 0| + |3\rangle\langle 3|) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The common eigenbasis of U and H is: $\{|0\rangle, \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), |3\rangle\}$.

If we additionally swap the populations of the levels $|0\rangle$ and $|3\rangle$, the unitary is no longer energy-preserving:

$$U_{\text{non-pres}} = (|1\rangle\langle 2| + |2\rangle\langle 1|) + (|0\rangle\langle 3| + |3\rangle\langle 0|) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

(c) *Give an example of an initial state of the system, for which the energy would still be preserved after applying $U_{non\text{-}pres}$.*

Solution For the example we have given, the energy would still be preserved if, for instance, $\rho = |1\rangle\langle 1|$. Then the state of the system after the application of U is $\rho\prime = |2\rangle\langle 2|$, and

$$E = \mathrm{Tr}\left(()\, \rho H\right) = \Delta$$
$$E' = \mathrm{Tr}\left(()\, \rho' H\right) = \Delta.$$