Exercise 3.1 Reduced density matrix - partial trace

Partial trace is an important concept in the quantum mechanical treatment of multi-partite systems, and is the natural generalisation of the concept of marginal distributions in classical probability theory.
Assume two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with orthonormal bases $\{\xi_j : j = 1, ..., m\}$ and $\{\eta_k : k = 1, ..., n\}$, respectively, and vector $|\Psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$ given by

$$|\Psi\rangle_{AB} = \sum_{j,k} C_{j,k}|\xi_j\rangle|\eta_k\rangle$$

Reduced density matrix of a system A is defined via a partial trace on the whole system:

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \sum_{k=1}^{n}\langle\eta_k|\rho_{AB}|\eta_k\rangle \tag{1}$$

a) *Show that the reduced state on a system A can be written as:*

$$\rho_A = \sum_{j,k,r} C_{jk}\overline{C}_{rk}|\xi_j\rangle\langle\xi_r|$$

and deduce that the matrix of ρ_A with respect to the basis $\{\xi_j\}$ can be written as $CC^\dagger$, where C is the $m \times n$ matrix with entries C_{jk}, and $C^\dagger$ its transpose. Also show that the matrix of ρ_B is $C^\dagger C$. Deduce that ρ_A and ρ_B must have same non-negative eigenvalues.

b) *Show that ρ_A is a valid density operator by proving it is:*

1) *Hermitian: $\rho_A = \rho_A^\dagger$.*
2) *Positive: $\rho_A \geq 0$.*
3) *Normalised: $Tr(\rho_A) = 1$.*

1) *Hermitian: $\rho_A = \rho_A^\dagger$.*
Remember that ρ_{AB} can always be written as

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

where $c_{ij;kl} = c^\dagger_{kl;ij}$ is hermitian.
The reduced density operator ρ_A is then given by

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

as can easily be verified. Hermiticity of ρ_A follows from

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

2) *Positive:* $\rho_A \geq 0$.

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

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

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

3) *Normalised:* $Tr(\rho_A) = 1$.

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

c) *Find ρ_A and ρ_B in the case when H_A and H_B have orthonormal bases $\{v_0, v_1, v_2\}$ and $\{\omega_1, \omega_2\}$, respectively (hence $m = 3, n = 2$), and the (unnormalised) state ψ is given by*

$$|\Psi\rangle_{AB} = |v_0\rangle(|\omega_1\rangle - |\omega_2\rangle) + |v_1\rangle|\omega_1\rangle + |v_2\rangle|\omega_2\rangle$$

Show that ρ_A and ρ_B have the same non-zero eigenvalues.

d) *Calculate the reduced density matrix of the system A in the Bell state*

$$|\Psi\rangle_{AB} = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right).$$

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

$$\begin{aligned}
\rho_{AB} = |\Psi\rangle\langle\Psi| &= \frac{1}{2}\Big(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11| \Big) \\
\mathrm{Tr}_B(\rho_{AB}) &= \frac{1}{2}\Big(|0\rangle\langle 0| + |1\rangle\langle 1| \Big) = \frac{1}{2}\mathbb{1}_A.
\end{aligned}$$

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

1) *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 $\mathcal{X}, \mathcal{Y} = \{0, 1\}$.
Using $P_X(x) = \sum_y P_{XY}(x, y)$, we obtain

$$P_X(0) = 0.5, \quad P_X(1) = 0.5.$$

2) *How can we represent* P_{XY} *in form of a quantum state?*
A probability distribution $P_Z = \{P_Z(z)\}_z$ may be represented by a state

$$\rho_Z = \sum_z P_Z(z) |z\rangle\langle z|, \tag{3}$$

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 $\mathcal{H}_X \mathcal{H}_Y$ in state

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

3) *Calculate the partial trace of* P_{XY} *in its quantum representation.*
The reduces state of qubit X is

$$\rho_X = \frac{1}{2}\big(|0\rangle\langle 0| + |1\rangle\langle 1|\big).$$

Notice that the reduced states of this classical state and the Bell state are the same, 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.

f) *Can you think of an experiment to distinguish the bipartite states of parts* b) *and* c)*?*
One could for instance measure the two states in the Bell basis,

$$|\psi_1\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \qquad |\psi_2\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}},$$
$$|\psi_3\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \qquad |\psi_4\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

The Bell state we analised 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.

Exercise 3.2 State Distinguishability

One way to understand the cryptographic abilities of quantum mechanics is from the fact that non-orthogonal states cannot be perfectly distinguished.

a) *In the course of a quantum key distribution protocol, suppose that Alice randomly chooses one of the following two states and transmits it to Bob:*

$$|\phi_0\rangle = \tfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \qquad or \qquad |\phi_1\rangle = \tfrac{1}{\sqrt{2}}(|0\rangle + i|1\rangle). \tag{4}$$

Eve intercepts the qubit and performs a measurement to identify the state. The measurement consists of the orthogonal states $|\psi_0\rangle$ *and* $|\psi_1\rangle$*, and Eve guesses the transmitted state was* $|\phi_0\rangle$ *when she obtains the outcome* $|\psi_0\rangle$*, and so forth. What is the probability that*

Eve correctly guesses the state, averaged over Alice's choice of the state for a given measurement? What is the optimal measurement Eve should make, and what is the resulting optimal guessing probability?

The probability of correctly guessing, averaged over Alice's choice of the state is

$$p_{\text{guess}} = \tfrac{1}{2}(|\langle\psi_0||\phi_0\rangle|^2 + |\langle\psi_1||\phi_1\rangle|^2) \tag{5}$$

To optimize the choice of measurement, suppose $|\psi_0\rangle = \alpha|0\rangle + \beta|1\rangle$ for some $\alpha, \beta \in \mathbb{C}$ such that $|\alpha|^2 + |\beta|^2 = 1$. Then $|\psi_1\rangle = -\beta^*|0\rangle + \alpha^*|1\rangle$ is orthogonal as intended. Using this in (5) gives

$$p_{\text{guess}} = \frac{1}{2}\left(\left|\frac{\alpha^* + \beta^*}{\sqrt{2}}\right|^2 + \left|\frac{i\alpha - \beta}{\sqrt{2}}\right|^2\right) \tag{6}$$

$$= \tfrac{1}{2}(1 + 2\text{Re}\left[\left(\tfrac{1-i}{2}\right)\alpha\beta^*\right]). \tag{7}$$

If we express α and β as $\alpha = ae^{i\theta}$ and $\beta = be^{i\eta}$ for real a, b, θ, η, then we get

$$p_{\text{guess}} = \tfrac{1}{2}(1 + 2ab\text{Re}\left[\left(\tfrac{1-i}{2}\right)e^{i(\theta-\eta)}\right]). \tag{8}$$

To maximize, we ought to choose $a = b = \frac{1}{\sqrt{2}}$, and we may also set $\eta = 0$ since only the difference $\theta - \eta$ is relevant. Now we have

$$p_{\text{guess}} = \tfrac{1}{2}(1 + \text{Re}\left[\left(\tfrac{1-i}{2}\right)e^{i\theta}\right]) \tag{9}$$

$$= \tfrac{1}{2}(1 + \tfrac{1}{\sqrt{2}}\text{Re}\left[e^{-i\pi/4}e^{i\theta}\right]), \tag{10}$$

from which it is clear that the best thing to do is to set $\theta = \pi/4$ to get $p_{\text{guess}} = \frac{1}{2}(1+\frac{1}{\sqrt{2}}) \approx$ 85.4%. The basis states making up the measurement are $|\psi_0\rangle = \frac{1}{\sqrt{2}}(e^{i\pi/4}|0\rangle + |1\rangle)$ and $|\psi_1\rangle = \frac{1}{\sqrt{2}}(-|0\rangle + e^{-i\pi/4}|1\rangle)$.

b) *Now suppose Alice randomly chooses between two states separated by an angle θ on the Bloch sphere. What is the measurement which optimizes the guessing probability? What is the resulting probability of correctly identifying the state?*

The point of this exercise is to show that thinking in terms of the Bloch sphere is a lot more intuitive than just taking a brute force approach as we did in the solution of the previous exercise. Let $\hat{n}_0$ and $\hat{n}_1$ be the Bloch vectors of the two states. Call $\hat{m}$ the Bloch vector associated with one of the two basis vectors of the measurement, specifically the one which indicates that the state is $|\phi_0\rangle$ (the other is associated with $-\hat{m}$). The guessing probability takes the form

$$p_{\text{guess}} = \tfrac{1}{2}(|\langle\psi_0||\phi_0\rangle|^2 + |\langle\psi_1||\phi_1\rangle|^2) \tag{11}$$

$$= \tfrac{1}{2}\left(\tfrac{1}{2}(1 + \hat{n}_0 \cdot \hat{m}) + \tfrac{1}{2}(1 - \hat{n}_1 \cdot \hat{m})\right) \tag{12}$$

$$= \tfrac{1}{4}\left(2 + \hat{m} \cdot (\hat{n}_0 - \hat{n}_1)\right) \tag{13}$$

The optimal $\hat{m}$ lies along $\hat{n}_0 - \hat{n}_1$ and has unit length, i.e.

$$\hat{m} = \frac{\hat{n}_0 - \hat{n}_1}{\sqrt{(\hat{n}_0 - \hat{n}_1) \cdot (\hat{n}_0 - \hat{n}_1)}} \tag{14}$$

$$= \frac{\hat{n}_0 - \hat{n}_1}{\sqrt{2 - 2\cos\theta}}. \tag{15}$$

Therefore,

$$p_{\text{guess}} = \tfrac{1}{4}\left(2+\sqrt{2-2\cos\theta}\right) \tag{16}$$
$$= \tfrac{1}{2}\left(1+\sqrt{\frac{1-\cos\theta}{2}}\right) \tag{17}$$
$$= \tfrac{1}{2}\left(1+\sin\tfrac{\theta}{2}\right). \tag{18}$$

Finally, we should check that this gives sensible results. When $\theta = 0$, $p_{\text{guess}} = \frac{1}{2}$, as it should. On the other hand, the states $|\phi_k\rangle$ are orthogonal for $\theta = \pi$, and indeed $p_{\text{guess}} = 1$ in this case. In the previous exercise we investigated the case $\theta = \frac{\pi}{2}$ and here we immediately find $p_{\text{guess}} = \frac{1}{2}(1+\frac{1}{\sqrt{2}})$, as before.

Exercise 3.3 One-qubit POVM

Consider a single qubit and unit vectors $\vec{n_k}, k \in \{1, ..., n\}$ such that

$$\sum_k \lambda_k \vec{n_k} = 0$$

for $\lambda_k \in (0,1)$ and $\sum_k \lambda_k = 1$. Show that a measurement on a qubit defined by

$$F_k = 2\lambda_k | \uparrow_{\vec{n_k}}\rangle\langle\uparrow_{\vec{n_k}} |$$

is a POVM. Explain cases $N = 2$ and $N = 3$, and connect them to the Bloch sphere representation. For the case $N = 3$ think of suitable vectors $\vec{n_k}$ and extend above POVM measurement on a qubit to the orthogonal measurement on a qutrit in a suitable basis (Neumark's theorem is a generalisation of this fact).

One can trivially see that each F_k is positive, as λ_k's are positive and $| \uparrow_{\vec{n_k}}\rangle\langle\uparrow_{\vec{n_k}} |$ defines a projective measurement. As $| \uparrow_{\vec{n_k}}\rangle\langle\uparrow_{\vec{n_k}} |$ defines a density matrix of a projective measurement in the direction of $\vec{n_k}$ on the Bloch sphere, it can be written as

$$| \uparrow_{\vec{n_k}}\rangle\langle\uparrow_{\vec{n_k}} | = \frac{1}{2}(1+\vec{n_k}\cdot\vec{\sigma})$$

Then

$$\sum_k F_k = \sum_k \lambda_k(1+\vec{n_k}\cdot\sigma) = \sum_k \lambda_k + (\sum_k \lambda_k\vec{n_k})\cdot\vec{\sigma_k} = 1$$

Hence F_k's indeed define a POVM. In the case $N = 2$ we have $\vec{n_2} = -\vec{n_1}$, and the POVM is an orthogonal measurement along the $\vec{n_1}$ axis. In the case $N = 3$, if we restrict to the symmetric case, we have $\vec{n_1}+\vec{n_2}+\vec{n_3} = 0$ and $\lambda_1 = \lambda_2 = \lambda_3$, hence

$$F_k = \frac{1}{3}(1+\vec{n_k}\cdot\sigma) = \frac{2}{3}| \uparrow_{\vec{n_k}}\rangle\langle\uparrow_{\vec{n_k}} |$$

By Neumark's theorem, we can extend this POVM measurement on a qubit, to an orthogonal measurement on a qutrit. It is left as an exercise to show that if one chooses $\vec{n_1} = (0,0,1), \vec{n_2} = (\sqrt{3}/2, 0, -1/2), \vec{n_3} = (-\sqrt{3}/2, 0, -1/2)$ appropriate orthogonal measurement on a qutrit would be in the basis:

$$|u_1\rangle, |u_2\rangle, |u_3\rangle = \begin{pmatrix}\sqrt{2/3}\\ 0\\ \sqrt{1/3}\end{pmatrix}, \begin{pmatrix}\sqrt{1/6}\\ \sqrt{1/2}\\ -\sqrt{1/3}\end{pmatrix}, \begin{pmatrix}-\sqrt{1/6}\\ \sqrt{1/2}\\ \sqrt{1/3}\end{pmatrix}$$

If we would perform orthogonal measurement on a qutrit in this basis, an observer only having access to the two-dim subspace, would conclude that we have performed a POVM given by F_1, F_2, F_3.