Fall 2024: Final Project
COM-309: Quantum Information Processing

This homework should be done by teams of two students. The implementation should be done with PennyLane **AND** Qiskit. Only one of the team's students should upload on Moodle a PDF with the answers to the theory questions and the two notebooks. The name of the two students and their SCIPER should be written in the PDF.

1 Werner state

The goal of this mini-project is to study the entanglement properties of mixed states. A mixed state ρ can be seen as a statistical mixture of pure states,

$$\rho = \sum_i p_i \left|\phi_i\right\rangle \left\langle\phi_i\right|, \quad p_i \in [0,1], \quad \sum_i p_i = 1 \tag{1}$$

and can be represented by density matrices which are positive semi-definite, self-adjoint matrices of trace 1.

In this mini-project, we will focus on a specific class of states, called the Werner states. A Werner state ρ_W is a convex combination of the completely mixed state $\mathbf{I}$ and the maximally entangled Bell state $\rho_{11} = \left|B_{11}\right\rangle \left\langle B_{11}\right|$ where $\left|B_{11}\right\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$. This mixture will depend on a parameter $w \in [0,1]$ such that

$$\rho_W(w) = (1-w)\frac{\mathbf{I}}{4} + w\rho_{11}. \tag{2}$$

Question Theory 1: Give the matrix representation of $\rho_W(w)$, compute its eigenvalues, and check that $\rho_W(w)$ is a valid state.

Solution.

$$\rho_W(w) = \begin{pmatrix} \frac{1-w}{4} & 0 & 0 & 0 \\ 0 & \frac{1+w}{4} & -\frac{w}{2} & 0 \\ 0 & -\frac{w}{2} & \frac{1+w}{4} & 0 \\ 0 & 0 & 0 & \frac{1-w}{4} \end{pmatrix}$$

Its eigenvalues are $\frac{1-w}{4}$ with eigenvectors $\left|00\right\rangle, \frac{|01\rangle+|10\rangle}{\sqrt{2}}, \left|11\right\rangle$ and $\frac{1+3w}{4}$ with eigenvector $\frac{|01\rangle-|10\rangle}{\sqrt{2}}$. We can trivially verify that $\rho_W(w) = \rho_W(w)^{\top,*}$ and $\operatorname{Tr}\rho_W(w) = 1$; $\rho_W(w) \succeq 0$ follows from the fact that all its eigenvalues are nonnegative. Therefore, $\rho_W(w)$ is indeed a valid state. $\square$

Werner state can be constructed with the following circuit

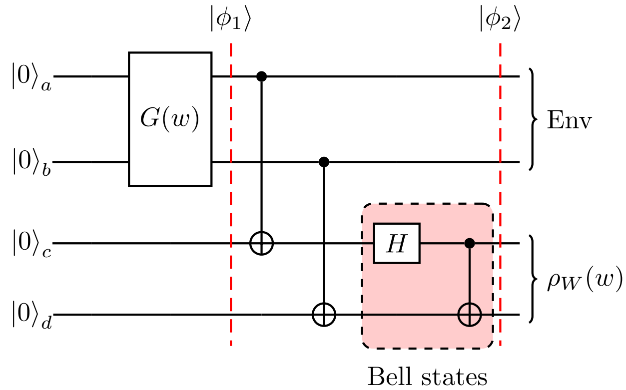

Figure 1: How to prepare Werner states

where $G(w)$ is the unitary such that $G(w)|00\rangle = \sqrt{\frac{1-w}{4}}(|00\rangle + |01\rangle + |10\rangle) + \sqrt{\frac{1+3w}{4}}|11\rangle$. The two qubits a and b can be considered as the environment acting on our system, the two qubits c and d. In the red box in Figure 1, you can recognize the Bell state preparation.

Question Theory 2: Compute the state $|\phi_2\rangle$ and check that $\rho_W(w) = \mathrm{Tr}_{a,b}(|\phi_2\rangle\langle\phi_2|)$.

Solution.

$$\begin{aligned}
|\phi_1\rangle &= \left(\sqrt{\frac{1-w}{4}}(|00\rangle + |01\rangle + |10\rangle) + \sqrt{\frac{1+3w}{4}}|11\rangle\right) \otimes |00\rangle \\
\mathrm{CNOT}_{b,d}\mathrm{CNOT}_{a,c}|\phi_1\rangle &= \sqrt{\frac{1-w}{4}}(|0000\rangle + |0101\rangle + |1010\rangle) + \sqrt{\frac{1+3w}{4}}|1111\rangle \\
|\phi_2\rangle &= \sqrt{\frac{1-w}{4}}(|00\rangle|B_{00}\rangle + |01\rangle|B_{01}\rangle + |10\rangle|B_{10}\rangle) + \sqrt{\frac{1+3w}{4}}|11\rangle|B_{11}\rangle
\end{aligned}$$

Thus,

$$\begin{aligned}
\mathrm{Tr}_{a,b}(|\phi_2\rangle\langle\phi_2|) = \frac{1-w}{4}\Bigg(&\mathrm{Tr}(|00\rangle\langle 00|)|B_{00}\rangle\langle B_{00}| + \mathrm{Tr}(|01\rangle\langle 01|)|B_{01}\rangle\langle B_{01}| \\
&+ \mathrm{Tr}(|10\rangle\langle 10|)|B_{10}\rangle\langle B_{10}|\Bigg) + \frac{1+3w}{4}\mathrm{Tr}(|11\rangle\langle 11|)|B_{11}\rangle\langle B_{11}| \\
&= \frac{1-w}{4}(|B_{00}\rangle\langle B_{00}| + |B_{01}\rangle\langle B_{01}| + |B_{10}\rangle\langle B_{10}|) + \frac{1+3w}{4}|B_{11}\rangle\langle B_{11}| \\
&= \frac{1-w}{4}\mathbf{I} + w\rho_{11}
\end{aligned}$$

□

Question Implementation 1: Implement the circuit to construct Werner states in Pennylane and Qiskit. How to implement $G(w)$ is given in the notebooks.

2 Separability and the Peres criterion

A pure state $|\psi\rangle_{c,d}$ is a product state if it can be decomposed as the tensor product of $|\psi_1\rangle_c$ and $|\psi_2\rangle_d$ such that $|\psi\rangle = |\psi_1\rangle_c \otimes |\psi_2\rangle_d$. The state is otherwise entangled. This notion can be generalized to mixed states.

A mixed state ρ is *separable* if it can be written in the form

$$\rho_{c,d} = \sum_i p_i \rho_c^{(i)} \otimes \rho_d^{(i)}, \quad p_i \in [0,1], \quad \sum_i p_i = 1. \tag{3}$$

You can easily check that a product state is separable.

One can identify if a state is separable or not thanks to the **Peres criterion**: A two-qubit state $\rho_{c,d}$ is entangled if and only if $(\mathbf{I}_c \otimes T_d)\rho_{c,d}$ has a negative eigenvalue. Here, T_d is the operator that applies a transposition to the system d. In higher dimension, this criterion does not hold.

Question Theory 3: Prove that for a separable state $\rho_{c,d}$, $(\mathbf{I}_c \otimes T_d)\rho_{c,d}$ has only nonnegative eigenvalues. We will admit the other direction of the proof. *Hint 1:* What can you say about the eigenvalues of the transpose matrix ? *Hint 2:* Remind that for a semi-positive definite matrix M, for any $|\phi\rangle$, we have $\langle\phi| M |\phi\rangle \geq 0$.

Solution. If $\rho_{c,d}$ is separable, $(\mathbf{I}_c \otimes T_d)\rho_{c,d} = \sum_i p_i \rho_c^{(i)} \otimes \rho_d^{(i)T}$. For any square matrix, its eigenvalues are equal to the eigenvalues of its transpose matrix. (Since they have the same characteristic polynomial). Since for each i, $\rho_c^{(i)}$ and $\rho_d^{(i)}$ are positive semidefinite matrices, the eigenvalues of $\rho_c^{(i)} \otimes \rho_d^{(i)T}$ are non negative.

Using Hint 2, for two semidefinite positive matrices A, B, and for any $|\phi\rangle$, we have $\langle\phi| A + B |\phi\rangle = \langle\phi| A |\phi\rangle + \langle\phi| B |\phi\rangle \geq 0$ and thus $A + B$ is semidefinite.

We could also have used a similar fact for Hermitian matrices. For two hermitian matrices H_1 and H_2, we have $\lambda_{min}(H_1 + H_2) \geq \lambda_{min}(H_1) + \lambda_{min}(H_2)$ where $\lambda_{min}(\cdot)$ is the smallest eigenvalue. We can prove this property. Since H_1 and H_2 are hermitian, they can be written $H_i = \sum_j \lambda_j(H_i) |x_j^i\rangle \langle x_j^i|$ where $(|x_j^i\rangle)_j$ form a basis and the $(\lambda_j(H_i))_j$ are real. Then for any state $|\phi\rangle = \sum_j \phi_j^1 |x_j^1\rangle = \sum_j \phi_j^2 |x_j^2\rangle$, we have

$$\begin{aligned}
\langle\phi| H_1 + H_2 |\phi\rangle &= \langle\phi| H_1 |\phi\rangle + \langle\phi| H_2 |\phi\rangle && (4)\\
&= \sum_j \sum_{j'} \phi_j^1 \phi_{j'}^1 \langle x_j^1| H_1 |x_{j'}^1\rangle + \sum_j \sum_{j'} \phi_j^2 \phi_{j'}^2 \langle x_j^2| H_2 |x_{j'}^2\rangle && (5)\\
&= \sum_j (\phi_j^1)^2 \lambda_j(H_1) + \sum_j (\phi_j^2)^2 \lambda_j(H_2) && (6)\\
&\geq \lambda_{min}(H_1) + \lambda_{min}(H_2) && (7)
\end{aligned}$$

Choosing $|\phi\rangle$ as the eigenvector of the smallest eigenvalue of $H_1 + H_2$ gives the result. With this property, we find that the smallest eigenvalue of $\rho_{c,d}$ is nonnegative, and thus all the other eigenvalues are also. □

Question Implementation 2: Implement the Peres criterion to the Werner state for $w \in [0,1]$. For which w is $\rho_W(w)$ separable?

To implement $\mathbf{I}_c \otimes T_d$ it might be useful to note that the action of $\mathbf{I}_c \otimes T_d$ on a general state $\rho = \sum_{ijkl} \rho_{kl}^{ij} |ij\rangle \langle kl|$ is

$$\begin{aligned}
(\mathbf{I}_c \otimes T_d)\rho &= (\mathbf{I}_c \otimes T_d) \sum_{ijkl} \rho_{kl}^{ij} |ij\rangle \langle kl| \\
&= (\mathbf{I}_c \otimes T_d) \sum_{ijkl} \rho_{kl}^{ij} |i\rangle \langle k|_c \otimes |j\rangle \langle l|_d \\
&= \sum_{ijkl} \rho_{kl}^{ij} |i\rangle \langle k|_c \otimes |l\rangle \langle j|_d \\
&= \sum_{ijkl} \rho_{kj}^{il} |i\rangle \langle k|_c \otimes |j\rangle \langle l|_d \,.
\end{aligned}$$

Question Theory 4: Check your implementation by studying the eigenvalues of $(\mathbf{I}_c \otimes T_d)\rho_W(w)$.

Solution.

$$(\mathbf{I}_c \otimes T_d)\rho_W(w) = \begin{pmatrix} \frac{1-w}{4} & 0 & 0 & -\frac{w}{2} \\ 0 & \frac{1+w}{4} & 0 & 0 \\ 0 & 0 & \frac{1+w}{4} & 0 \\ -\frac{w}{2} & 0 & 0 & \frac{1-w}{4} \end{pmatrix}$$

The eigenvalues are $\frac{1+w}{4}$ with eigenvectors $|01\rangle, |10\rangle, 1/\sqrt{2}(|00\rangle - |11\rangle)$ and $\frac{1-3w}{4}$ with $1/\sqrt{2}(|00\rangle + |11\rangle)$ The smallest eigenvalues is $\frac{1-3w}{4}$ which is negative for $w > 1/3$. $\square$

3 Bell (CHSH) inequality

In the lectures, we discussed the Bell inequalities. They are derived in relation to the experiments on quantum systems: if the results of an experiment can be explained by the local hidden-variable (LHV) model, such inequality should be satisfied. Its violation shows that in fact, LHV theory does not hold. Particularly, we looked at the CHSH inequality: in the corresponding experiment, Alice and Bob shared the two-qubit (pure) *Bell* state $|\Psi\rangle$ and estimated the correlation coefficient $\chi = \langle\Psi|\,\mathcal{B}\,|\Psi\rangle$ by measuring the observable

$$\mathcal{B} = A\otimes B + A\otimes B' - A'\otimes B + A'\otimes B',$$

where A, A', B, B' are observables

$$A = |\alpha\rangle\langle\alpha| - |\alpha_\perp\rangle\langle\alpha_\perp|\,,\quad A' = |\alpha'\rangle\langle\alpha'| - |\alpha'_\perp\rangle\langle\alpha'_\perp|\,,$$
$$B = |\beta\rangle\langle\beta| - |\beta_\perp\rangle\langle\beta_\perp|\,,\quad B' = |\beta'\rangle\langle\beta'| - |\beta'_\perp\rangle\langle\beta'_\perp|\,.$$

and $\{|\alpha\rangle, |\alpha_\perp\rangle\}$, $\{|\alpha'\rangle, |\alpha'_\perp\rangle\}$, $\{|\beta\rangle, |\beta_\perp\rangle\}$, $\{|\beta'\rangle, |\beta'_\perp\rangle\}$ are pairs of orthogonal states. The CHSH inequality states that $|\chi_{\text{LHV}}| \le 2$, but in practice, with certain choice of configuration $\alpha, \alpha', \beta, \beta'$, $|\chi_{\text{QM}}|$ can reach up to $2\sqrt{2}$! In fact, one can prove that for any two-qubit pure *entangled* state $|\Psi\rangle$ there exists such configuration that the CHSH inequality is violated.

However, now we consider mixed states as well, so the correlation coefficient is now expressed as

$$\chi = \operatorname{Tr}(\rho\mathcal{B})\,.$$

Question Theory 5: In homework 6, you have shown that the inequality $\langle\Psi|\,\mathcal{B}\,|\Psi\rangle \le 2\sqrt{2}$ holds for *any pure state* $|\Psi\rangle \in \mathbb{C}^2\otimes\mathbb{C}^2$ (Tsirelson's bound). i.e. $\chi(w) \le 2\sqrt{2}$, holds. Using this, show that it holds for arbitrary two-qubit mixed state as well, i.e. $\chi(w) \le 2\sqrt{2}$.

Solution. Using the representation of a mixed state from above,

$$\chi(w) = \operatorname{Tr}(\rho\mathcal{B}) = \operatorname{Tr}\left(\sum_i p_i\,|\phi_i\rangle\langle\phi_i|\,\mathcal{B}\right) = \sum_i p_i \operatorname{Tr}(|\phi_i\rangle\langle\phi_i|\,\mathcal{B}) = \sum_i p_i\,\langle\phi_i|\,\mathcal{B}\,|\phi_i\rangle \le$$
$$\underset{\text{bound}}{\overset{\text{Tsirelson's}}{\le}} \sum_i p_i\cdot 2\sqrt{2} = 2\sqrt{2}\cdot\underbrace{\left(\sum_i p_i\right)}_{=1} = 2\sqrt{2}.$$

□

One can show that if the mixed state ρ is separable, the CHSH inequality is satisfied. This does not work in reverse: mixed non-separable states can satisfy CHSH inequality for any configuration. In this problem, we will see this with the example of Werner states, i.e. we will measure correlation coefficient

$$\chi(w) = \operatorname{Tr}(\rho_W(w)\,\mathcal{B})\,.$$

Question Theory 6: Show that the optimal configuration $\alpha, \alpha', \beta, \beta'$ does not depend on value of w.

Solution. By linearity of trace,

$$\operatorname{Tr}\{\rho_W(w)(A\otimes B)\} = \frac{1-w}{4}\operatorname{Tr}\{\mathbf{I}(A\otimes B)\} + w\operatorname{Tr}\{\rho_{11}(A\otimes B)\} = w\operatorname{Tr}\{\rho_{11}(A\otimes B)\}$$

where the last equality follows from $\operatorname{Tr}\{\mathbf{I}(A\otimes B)\} = \operatorname{Tr}\{A\}\operatorname{Tr}\{B\} = 0$. Thus,

$$\begin{aligned}\chi(w) &= \operatorname{Tr}\{\rho_W(w)(A\otimes B)\} + \operatorname{Tr}\{\rho_W(w)(A\otimes B')\} - \operatorname{Tr}\{\rho_W(w)(A'\otimes B)\} + \operatorname{Tr}\{\rho_W(w)(A'\otimes B')\}\\ &= w\left(\operatorname{Tr}\{\rho_{11}(A\otimes B)\} + \operatorname{Tr}\{\rho_{11}(A\otimes B')\} - \operatorname{Tr}\{\rho_{11}(A'\otimes B)\} + \operatorname{Tr}\{\rho_{11}(A'\otimes B')\}\right)\\ &= w\operatorname{Tr}\{\rho_{11}\mathcal{B}\}\,,\end{aligned}$$

and maximization of $\chi(w)$ is equivalent to maximization of $\operatorname{Tr}\{\rho_{11}\mathcal{B}\}$. □

One can prove that $\alpha = \frac{\pi}{4}, \alpha' = 0, \beta = -\frac{\pi}{8}, \beta' = -\frac{3\pi}{8}$ is an optimal configuration.

Question Theory 7: For this configuration, express A, A', B, B' as a linear combination of Pauli matrices. This will be used later for Pennylane and Qiskit implementations of observables.

Solution. For any γ, as $|\gamma\rangle = (\cos\gamma, \sin\gamma)$, $|\gamma_\perp\rangle = (-\sin\gamma, \cos\gamma)$:

$$|\gamma\rangle\langle\gamma| - |\gamma_\perp\rangle\langle\gamma_\perp| = \begin{pmatrix} \cos^2\gamma & \cos\gamma\sin\gamma \\ \cos\gamma\sin\gamma & \sin^2\gamma \end{pmatrix} - \begin{pmatrix} \sin^2\gamma & -\sin\gamma\cos\gamma \\ -\sin\gamma\cos\gamma & \cos^2\gamma \end{pmatrix} = \begin{pmatrix} \cos(2\gamma) & \sin(2\gamma) \\ \sin(2\gamma) & -\cos(2\gamma) \end{pmatrix}$$

Thus,

$$A = X, A' = Z, B = \frac{1}{\sqrt{2}}(Z - X), B' = -\frac{1}{\sqrt{2}}(X + Z).$$

□

Question Implementation 3: Run the circuits and measure $\mathcal{B}$ to evaluate $\chi(w)$ for $w \in [0, 1]$. Draw a plot of this dependence; compare it to 2 (validity of the CHSH inequality bound) and Tsirelson's bound. More details are provided in the corresponding notebooks.

Question Theory 8: From the implementation, what is the value of $\chi(0)$ and $\chi(1)$? What are the values of w s.t. the CHSH inequality is satisfied? Compare them with the values of w for those when $\rho_W(w)$ is separable.

Solution. $\chi(0) = 0$, $\chi(1) = 2\sqrt{2}$. The CHSH inequality is satisfied for $w \leq \frac{1}{\sqrt{2}}$. The Peres criterion shows that the Werner state is separable only for $w \leq \frac{1}{3}$. Thus, while for $\frac{1}{3} < w \leq \frac{1}{\sqrt{2}}$, $\rho_W(w)$ is not separable, we cannot conclude this by simply using the CHSH inequality.

□