Purification and Partial Trace Notes

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Definitions

Definition (Partial Trace)**.** *Let ρ_{AB} be a density matrix defined on $\mathcal{H}_A \otimes \mathcal{H}_B$. Further, let $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ be bases for $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. Then,*

$$\mathrm{Tr}_A[\rho_{AB}] \coloneqq \sum_i \left(\langle i_A| \otimes \mathbb{1}_B\right) \rho_{AB} \left(|i_A\rangle \otimes \mathbb{1}_B\right)$$
$$\mathrm{Tr}_B[\rho_{AB}] \coloneqq \sum_j \left(\mathbb{1}_A \otimes \langle j_B|\right) \rho_{AB} \left(\mathbb{1}_A \otimes |j_B\rangle\right)$$

Definition (Purification)**.** *Let ρ_A be a density matrix defined on $\mathcal{H}_A$ with decomposition*

$$\rho_A = \sum_i p_i \, |\phi_i\rangle\!\langle\phi_i| \,,$$

where $p_i \geq 0$, $\sum_i p_i = 1$, and the $|\phi_i\rangle \in \mathcal{H}_A$ need not be orthogonal. Let $\{|j_B\rangle\}$ be an orthonormal basis for another Hilbert space $\mathcal{H}_B$. Then,

$$|\psi_{AB}\rangle \coloneqq \sum_j \sqrt{p_i}\, |\phi_i\rangle \, |j_B\rangle$$

is a pure state on $\mathcal{H}_A \otimes \mathcal{H}_B$.

1 Notes

Consider a pure state on $\mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^2 \otimes \mathbb{C}^2$,

$$|\Psi\rangle = c_{00}\,|00\rangle + c_{01}\,|01\rangle + c_{10}\,|10\rangle + c_{11}\,|11\rangle\,; \qquad |c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c_{11}|^2 = 1.$$

The reduced density matrices are

$$\rho_A = \begin{pmatrix} |c_{00}|^2 + |c_{01}|^2 & c_{00}c_{10}^* + c_{01}c_{11}^* \\ c_{00}^*c_{10} + c_{01}^*c_{11} & |c_{10}|^2 + |c_{11}|^2 \end{pmatrix}$$

$$\rho_B = \begin{pmatrix} |c_{00}|^2 + |c_{10}|^2 & c_{00}c_{01}^* + c_{10}c_{11}^* \\ c_{00}^*c_{01} + c_{10}^*c_{11} & |c_{01}|^2 + |c_{11}|^2 \end{pmatrix}$$

with determinants

$$d_A := \det \rho_A = \left(\left|c_{00}\right|^2 + \left|c_{01}\right|^2\right)\left(\left|c_{10}\right|^2 + \left|c_{11}\right|^2\right) - \left|c_{00}c_{10}^* + c_{01}c_{11}^*\right|^2$$

$$d_B := \det \rho_B = \left(\left|c_{00}\right|^2 + \left|c_{10}\right|^2\right)\left(\left|c_{01}\right|^2 + \left|c_{11}\right|^2\right) - \left|c_{00}c_{01}^* + c_{10}c_{11}^*\right|^2.$$

Note

$$0 \le d_A, d_B \le \frac{1}{4}$$

The eigenvalues are

$$\lambda_\pm^{A(B)} = \frac{1}{2}\left(1 \pm \sqrt{1 - 4d_{A(B)}}\right).$$

and the corresponding eigenvectors are labeled $\left|\lambda_\pm^{A(B)}\right\rangle$.

Let $\{|\phi_+\rangle, |\phi_-\rangle\}$ be an orthonormal basis for $\mathcal{H}_B$. Purify ρ_A as

$$\begin{aligned}
\left|\tilde{\Psi}_{AB}\right\rangle &= \sqrt{\lambda_+^A}\left|\lambda_+^A\right\rangle|\phi_+\rangle + \sqrt{\lambda_-^A}\left|\lambda_-^A\right\rangle|\phi_-\rangle \\
&= \left(\sqrt{\lambda_+^A}\left\langle 0_A\middle|\lambda_+^A\right\rangle\langle 0_B|\phi_+\rangle + \sqrt{\lambda_-^A}\left\langle 0_A\middle|\lambda_-^A\right\rangle\langle 0_B|\phi_-\rangle\right)|00\rangle \\
&+ \left(\sqrt{\lambda_+^A}\left\langle 0_A\middle|\lambda_+^A\right\rangle\langle 1_B|\phi_+\rangle + \sqrt{\lambda_-^A}\left\langle 0_A\middle|\lambda_-^A\right\rangle\langle 1_B|\phi_-\rangle\right)|01\rangle \\
&+ \left(\sqrt{\lambda_+^A}\left\langle 1_A\middle|\lambda_+^A\right\rangle\langle 0_B|\phi_+\rangle + \sqrt{\lambda_-^A}\left\langle 1_A\middle|\lambda_-^A\right\rangle\langle 0_B|\phi_-\rangle\right)|10\rangle \\
&+ \left(\sqrt{\lambda_+^A}\left\langle 1_A\middle|\lambda_+^A\right\rangle\langle 1_B|\phi_+\rangle + \sqrt{\lambda_-^A}\left\langle 1_A\middle|\lambda_-^A\right\rangle\langle 1_B|\phi_-\rangle\right)|11\rangle
\end{aligned}$$

Define U^A by

$$U^A|0_A\rangle = \left|\lambda_+^A\right\rangle; \quad U^A|1_A\rangle = \left|\lambda_-^A\right\rangle,$$

and

$$\det U_A := e^{i\theta_A}.$$

Define also V^B by

$$V^B|0_B\rangle = |\phi_+\rangle; \quad V^B|1_B\rangle = |\phi_-\rangle$$

Then,

$$\begin{aligned}
\left\langle 0_A\middle|\lambda_+^A\right\rangle &= \langle 0_A|U^A|0_A\rangle =: U_{00}^A \\
\left\langle 1_A\middle|\lambda_+^A\right\rangle &= \langle 1_A|U^A|0_A\rangle =: U_{10}^A \\
\left\langle 0_A\middle|\lambda_-^A\right\rangle &= \langle 0_A|U^A|1_A\rangle =: U_{01}^A \\
\left\langle 1_A\middle|\lambda_-^A\right\rangle &= \langle 1_A|U^A|1_A\rangle =: U_{11}^A \\
\langle 0_B|\phi_+\rangle &= \langle 0_B|V^B|0_B\rangle =: V_{00}^B \\
\langle 1_B|\phi_+\rangle &= \langle 1_B|V^B|0_B\rangle =: V_{10}^B
\end{aligned}$$

$$\langle 0_B|\phi_-\rangle = \langle 0_B|V^B|1_B\rangle =: V^B_{01}$$
$$\langle 1_B|\phi_-\rangle = \langle 1_B|V^B|1_B\rangle =: V^B_{11}$$

and,

$$\begin{aligned}\left|\tilde{\Psi}_{AB}\right\rangle = &\left(\sqrt{\lambda^A_+}U^A_{00}V^B_{00} + \sqrt{\lambda^A_-}U^A_{01}V^B_{01}\right)|00\rangle \\ &+\left(\sqrt{\lambda^A_+}U^A_{00}V^B_{10} + \sqrt{\lambda^A_-}U^A_{01}V^B_{11}\right)|01\rangle + \\ &+\left(\sqrt{\lambda^A_+}U^A_{10}V^B_{00} + \sqrt{\lambda^A_-}U^A_{11}V^B_{01}\right)|10\rangle + \\ &+\left(\sqrt{\lambda^A_+}U^A_{10}V^B_{10} + \sqrt{\lambda^A_-}U^A_{11}V^B_{11}\right)|11\rangle\,.\end{aligned}$$

Demanding $\left|\tilde{\Psi}_{AB}\right\rangle = |\Psi_{AB}\rangle$ gives

$$\begin{aligned}\sqrt{\lambda^A_+}U^A_{00}V^B_{00} + \sqrt{\lambda^A_-}U^A_{01}V^B_{01} &= C_{00}\\ \sqrt{\lambda^A_+}U^A_{00}V^B_{10} + \sqrt{\lambda^A_-}U^A_{01}V^B_{11} &= C_{01}\\ \sqrt{\lambda^A_+}U^A_{10}V^B_{00} + \sqrt{\lambda^A_-}U^A_{11}V^B_{01} &= C_{10}\\ \sqrt{\lambda^A_+}U^A_{10}V^B_{10} + \sqrt{\lambda^A_-}U^A_{11}V^B_{11} &= C_{11}\end{aligned}$$

$$\Longrightarrow \begin{pmatrix}\sqrt{\lambda^A_+}U^A_{00} & 0 & \sqrt{\lambda^A_-}U^A_{01} & 0\\ 0 & \sqrt{\lambda^A_+}U^A_{00} & 0 & \sqrt{\lambda^A_-}U^A_{01}\\ \sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_-}U^A_{11} & 0\\ 0 & \sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_-}U^A_{11}\end{pmatrix}\begin{pmatrix}V^B_{00}\\ V^B_{10}\\ V^B_{01}\\ V^B_{11}\end{pmatrix} = \begin{pmatrix}c_{00}\\ c_{01}\\ c_{10}\\ c_{11}\end{pmatrix}.$$

The matrix above is ove the form

$$\begin{pmatrix}\alpha\mathbb{1}_2 & \beta\mathbb{1}_2\\ \gamma\mathbb{1}_2 & \delta\mathbb{1}_2\end{pmatrix}$$

with

$$\alpha = \sqrt{\lambda^A_+}U^A_{00},\ \beta = \sqrt{\lambda^A_-}U^A_{01},\ \gamma = \sqrt{\lambda^A_+}U^A_{10},\ \delta = \sqrt{\lambda^A_-}U_{11},$$

and is easily invertible. Its determinant is simply

$$\alpha\delta - \beta\gamma = \sqrt{\lambda^A_+\lambda^A_-}\left(U^A_{00}U^A_{11} - U^A_{01}U^A_{10}\right) = \sqrt{d_A}e^{i\theta_A},$$

and the inverse is then

$$\frac{1}{\alpha\delta - \beta\gamma}\begin{pmatrix}\delta\mathbb{1}_2 & -\beta\mathbb{1}_2\\ -\gamma\mathbb{1}_2 & \alpha\mathbb{1}_2\end{pmatrix} = \frac{e^{-i\theta_A}}{\sqrt{d_A}}\begin{pmatrix}\sqrt{\lambda^A_-}U^A_{11} & 0 & -\sqrt{\lambda^A_-}U^A_{01} & 0\\ 0 & \sqrt{\lambda^A_-}U^A_{11} & 0 & -\sqrt{\lambda^A_-}U^A_{01}\\ -\sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_+}U^A_{00} & 0\\ 0 & -\sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_+}U^A_{00}\end{pmatrix}.$$

Solving for the Vs, we get

$$\begin{aligned}
\begin{pmatrix} V^B_{00} \\ V^B_{10} \\ V^B_{01} \\ V^B_{11} \end{pmatrix} &= \frac{e^{-i\theta_A}}{\sqrt{d_A}} \begin{pmatrix} \sqrt{\lambda^A_-}U^A_{11} & 0 & -\sqrt{\lambda^A_-}U^A_{01} & 0 \\ 0 & \sqrt{\lambda^A_-}U^A_{11} & 0 & -\sqrt{\lambda^A_-}U^A_{01} \\ -\sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_+}U^A_{00} & 0 \\ 0 & -\sqrt{\lambda^A_+}U^A_{10} & 0 & \sqrt{\lambda^A_+}U^A_{00} \end{pmatrix} \begin{pmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{pmatrix} \\
&= e^{-i\theta_A} \begin{pmatrix} \left(\lambda^A_+\right)^{-1/2} \left(U^A_{11}c_{00} - U^A_{01}c_{10}\right) \\ \left(\lambda^A_+\right)^{-1/2} \left(U^A_{11}c_{01} - U^A_{01}c_{11}\right) \\ \left(\lambda^A_-\right)^{-1/2} \left(-U^A_{10}c_{00} + U^A_{00}c_{10}\right) \\ \left(\lambda^A_-\right)^{-1/2} \left(-U^A_{10}c_{01} + U^A_{00}c_{11}\right) \end{pmatrix} \\
&= e^{-i\theta_A} \begin{pmatrix} \left(\lambda^A_+\right)^{-1/2} \begin{pmatrix} -c_{10} & c_{00} \\ -c_{11} & c_{01} \end{pmatrix} \begin{pmatrix} U^A_{01} \\ U^A_{11} \end{pmatrix} \\ \left(\lambda^A_-\right)^{-1/2} \begin{pmatrix} c_{10} & -c_{00} \\ c_{11} & -c_{10} \end{pmatrix} \begin{pmatrix} U^A_{00} \\ U^A_{10} \end{pmatrix} \end{pmatrix}
\end{aligned}$$

So...

$$\begin{aligned}
|\phi_+\rangle &= \frac{e^{-i\theta_A}}{\sqrt{\lambda^A_+}} \begin{pmatrix} -c_{10} & c_{00} \\ -c_{11} & c_{01} \end{pmatrix} \begin{pmatrix} U^A_{01} \\ U^A_{11} \end{pmatrix} \\
&= \frac{e^{-i\theta_A}}{\sqrt{\lambda^A_+}} \begin{pmatrix} -c_{10} & c_{00} \\ -c_{11} & c_{01} \end{pmatrix} \begin{pmatrix} \left\langle 0_A \middle| \lambda^A_- \right\rangle \\ \left\langle 1_A \middle| \lambda^A_- \right\rangle \end{pmatrix} \\
|\phi_-\rangle &= \frac{e^{-i\theta_A}}{\sqrt{\lambda^A_-}} \begin{pmatrix} c_{10} & -c_{00} \\ c_{11} & -c_{01} \end{pmatrix} \begin{pmatrix} U^A_{01} \\ U^A_{11} \end{pmatrix} \\
&= \frac{e^{-i\theta_A}}{\sqrt{\lambda^A_-}} \begin{pmatrix} c_{10} & -c_{00} \\ c_{11} & -c_{01} \end{pmatrix} \begin{pmatrix} \left\langle 0_A \middle| \lambda^A_+ \right\rangle \\ \left\langle 1_A \middle| \lambda^A_+ \right\rangle \end{pmatrix}
\end{aligned}$$