Violation≠Quantum

Xingyu Guo\textsuperscript{a,b}\textsuperscript{1} and Chen-Te Ma\textsuperscript{a,b,c,d,e}\textsuperscript{2}

\textsuperscript{a} Guangdong Provincial Key Laboratory of Nuclear Science, Institute of Quantum Matter, South China Normal University, Guangzhou 510006, Guangdong, China.
\textsuperscript{b} Guangdong-Hong Kong Joint Laboratory of Quantum Matter, Southern Nuclear Science Computing Center, South China Normal University, Guangzhou 510006, Guangdong, China.
\textsuperscript{c} Asia Pacific Center for Theoretical Physics, Pohang University of Science and Technology, Pohang 37673, Gyeongsangbuk-do, South Korea.
\textsuperscript{d} School of Physics and Telecommunication Engineering, South China Normal University, Guangzhou 510006, Guangdong, China.
\textsuperscript{e} The Laboratory for Quantum Gravity and Strings, Department of Mathematics and Applied Mathematics, University of Cape Town, Private Bag, Rondebosch 7700, South Africa.

Abstract

The only entanglement quantity is concurrence in a 2-qubit pure state. The maximum violation of Bell’s inequality is monotonically increasing for this quantity. Therefore, people expect that pure state entanglement is relevant to the quantum violation. To understand the relation between violation and entanglement, we extend the study to three qubits. When only turning on one entanglement measure, the numerical result shows a contradiction to the expectation. The maximum violation does not have the same behavior as in 2-qubit pure states. Therefore, we conclude “Violation≠Quantum”. In the end, we propose the generalized $R$-matrix or correlation matrix for the new diagnosis of Quantum Entanglement. We demonstrate the evidence by restoring the monotonically increasing result.

\textsuperscript{1}e-mail address: guoxy@m.scnu.edu.cn
\textsuperscript{2}e-mail address: yefgst@gmail.com
1 Introduction

The black-body radiation problem and photoelectric effect do not have a proper interpretation from classical physics. The experimental results introduce discrete values or quantization to a characterization of objects. This surprising observation leads to wave-particle duality and the uncertainty principle. People combine all concepts to develop a fundamental theory at an atomic scale, Quantum Mechanics (QM) [1]. The modern description of a particle’s motion is not deterministic instead a probability amplitude (complex-valued wave function). The complex number and probabilistic interpretation introduce the philosophical problem of QM.

The indeterminism may imply that QM loses a complete description of nature. One naive idea is to introduce hidden variables to describe a more fundamental theory. Requiring the independence of separated measurement processes (local realism) can rule out non-physical cases (instantaneous interactions between separate events). The locality implies a constraint (Bell’s inequality) to correlations of two separated particles [2]. The quantum measurement observed the violation of Bell’s inequality [3]. At the time, the Bell test experiments still suffered some loopholes without conclusive results. Recently, the issues disappeared without changing the conclusion [4]. Hence the fact of violation shows the existence of quantumness.

When calculating expectation value of Bell’s operator in QM, ones used two largest eigenvalues of $R$-matrix to show an equivalent description of maximum violation [5]. The maximum violation is monotonically increasing with concurrence [6] for all possible pure states [7]. The concurrence is also positively correlated with entanglement entropy. Hence this result successfully shows that Quantum Entanglement is a necessary and sufficient condition of violation for 2-qubit.

Quantum Entanglement is a phenomenon in which a quantum state of each particle does not have an individual description. In Classical Mechanics (CM), the dynamics of particles only relies on a set of parameters. When Quantum Entanglement occurs, the observation also affects the dynamics. Therefore, the parameters of CM are not enough to show a consistent description. Hence Quantum Entanglement should be unique for distinguishing QM and CM. Because this phenomenon seems to violate local realism, it generates the broken of local hidden variable theory.
For a 2-qubit state, one only has one choice to perform a partial trace operation. Any higher dimensional qubit states have more than one choice. This problem shows the difference between 2-qubit and many-body. One main difficulty of many-body Quantum Entanglement is the multi-parameter characterization of Quantum Entanglement. One can use the Schmidt decomposition to describe a general 2-qubit pure state by one variable. Therefore, the diagnosis of Quantum Entanglement is easy. In other words, it is hard to use a similar way to generalize to a general n-qubit state [8, 9]. Currently, people showed the following general properties in a 3-qubit state:

- Using the generalized Schmidt decomposition [10] shows that five variables are enough for a general 3-qubit state [11].
- The local operations and classical communication (LOCC) shows two inequivalent entangled classes [12].
- One cannot ignore the three-body entanglement measure, 3-tangle, in a general study [13].
- A 3-qubit state is realizable in experiments [14, 15].

Therefore, a 3-qubit state contains more than one entanglement description from more than one variable. The genuine tripartite entanglement is a necessary ingredient. The progress of techniques provides an opportunity to study many-body Quantum Entanglement in both theory and experiments. Hence a simple study of exploring the possible generalization of many-body Quantum Entanglement is to show an analytical solution of 3-qubit states.

In this paper, we first consider all possible 3-qubit operators with a symmetric permutation. Our results justify that Quantum Entanglement is only necessary but not sufficient for violation. Necessity and sufficiency in a two-qubit pure state is only a coincidence. We then distinguish the maximum violation of Bell’s inequality and the correlation of $R$-matrix. The equivalence in two-qubit pure states is again a coincidence. We generalize the $R$-matrix and use it to show a successful diagnose of Quantum Entanglement. We show our conclusion in Fig. 1. To summarize our results:

- The characterization of 3-qubit Quantum Entanglement is from five entanglement measures. We only turn on one entanglement measure. Therefore, a product state has the vanishing Quantum Entanglement and quantumness. For a proper diagnose of Quantum Entanglement, one quantity must be monotonically increasing.
We show the loss of monotonically increasing for the maximum violation. Hence it implies “Violation≠Quantum”.

- We generalize the $R$-matrix and show that the two largest eigenvalues provide the upper bound of maximum violation of Merlin’s inequality. It implies that the correlation of the $R$-matrix is not equivalent to the maximum violation. Our analytical solution simultaneously depends on all necessary entanglement measures. Therefore, the correlation of the generalized $R$-matrix should generate all 3-qubit Quantum Entanglement.

- We turn on one entanglement measure. The correlation of the generalized $R$-matrix shows the monotonically increasing result. Hence this result concretely distinguishes maximum violation from the correlation of generalized $R$-matrix. Since a general 3-qubit state has two different entangled classes, finding a classification [16, 17, 18, 19, 20, 21] is unavoidable. We realize the classification and show the monotonically increasing result for each class in general.

The organization of this paper is as follows: We show “Violation≠Quantum” by considering all 3-qubit operators in Sec. 2. We then generalize the $R$-matrix to a 3-qubit state and show that it is a proper diagnosis of Quantum Entanglement [22] in Sec. 3. In the end, we discuss our results and conclude in Sec. 4. We put all numerical results
of 3-qubit operators for a single entanglement measure case in Appendix A. We show the detailed calculation of generalized $R$-matrix in Appendix B.

2 Violation $\neq$ Quantum

We first show all possible 3-qubit operators with a symmetric permutation. Exchanging the qubits does not change the maximum violation. We only turn on one entanglement measure for our numerical study. The result shows a loss of monotonic relation of maximum violation and the measure. Therefore, we show that the maximum degree of violation cannot quantify Quantum Entanglement. For convenient reading, we put figures or numerical results in Appendix A.

2.1 Three-Qubit Operators

We construct 3-qubit operators from a linear combination of the following operators:

\begin{align*}
A_1 \otimes A_2 \otimes A_3' + A_1 \otimes A_2' \otimes A_3 + A_1' \otimes A_2 \otimes A_3; \\
A_1' \otimes A_2' \otimes A_3 + A_1' \otimes A_2 \otimes A_3' + A_1 \otimes A_2' \otimes A_3'; \\
A_1' \otimes A_2' \otimes A_3'; \\
A_1 \otimes A_2 \otimes A_3,
\end{align*}

where

\begin{align*}
A_j &\equiv \vec{a}_j \cdot \vec{\sigma}; \\
A_j' &\equiv \vec{a}'_j \cdot \vec{\sigma}; \\
\vec{\sigma} &\equiv (\sigma_x, \sigma_y, \sigma_z).
\end{align*}

The $\vec{a}$ and $\vec{a}'$ are unit vectors:

\begin{align*}
\vec{a} \cdot \vec{a} = 1; \\
\vec{a}' \cdot \vec{a}' = 1.
\end{align*}

The notation of Pauli matrix is given by:

\begin{align*}
\sigma_x &\equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \\
\sigma_y &\equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \\
\sigma_z &\equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{align*}

Each operator is symmetric for exchanging qubits. This symmetry also implies invariance of the expectation value of the operators

\begin{align*}
\langle \mathcal{O} \rangle &\equiv \text{Tr}(\rho \mathcal{O}),
\end{align*}
where $\mathcal{O}$ is some operator, and the density matrix is given by

$$\rho \equiv |\psi\rangle \langle \psi|.$$  \hfill (6)

One can observe the maximum violation from considering all possible choices of operators (varying $\vec{a}$ and $\vec{a}'$)

$$\gamma \equiv \max_{\mathcal{O}} \langle \mathcal{O} \rangle.$$  \hfill (7)

Hence the maximum violation is invariant under a permutation for the following general 3-qubit operator

$$\mathcal{O}_0 \equiv \bar{\alpha}_1 (A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3)
+ \bar{\alpha}_2 (A'_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A'_3)
+ \bar{\alpha}_3 A'_1 \otimes A'_2 \otimes A'_3
+ \bar{\alpha}_4 A_1 \otimes A_2 \otimes A_3,$$  \hfill (8)

where

$$-\infty < \bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\alpha}_4 < \infty.$$  \hfill (9)

### 2.2 Three-Qubit State

A general 3-qubit state is given by [11]

$$|\psi\rangle = \lambda_0 |000\rangle + \lambda_1 e^{i\phi} |100\rangle + \lambda_2 |101\rangle + \lambda_3 |110\rangle + \lambda_4 |111\rangle,$$  \hfill (10)

up to a local unitary transformation. Since we normalized the density matrix

$$\text{Tr} \rho = 1,$$  \hfill (11)

it provides an spherical equation to constrain the coefficients

$$\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1.$$  \hfill (12)
Hence a general 3-qubit pure state only has five independent degrees of freedom on the variables. Later we will use the quantum state to calculate five necessary entanglement measures. Now we show some calculation results.

The density matrix is:

\[
\rho = |\psi\rangle \langle \psi| = \lambda_0^2|000\rangle \langle 000| + \lambda_0 \lambda_1 e^{-i\phi}|000\rangle \langle 100| + \lambda_0 \lambda_1 e^{i\phi}|100\rangle \langle 000| + \lambda_0 \lambda_2|000\rangle \langle 101| + \lambda_0 \lambda_2|101\rangle \langle 000| + \lambda_0 \lambda_3|000\rangle \langle 110| + \lambda_0 \lambda_3|110\rangle \langle 000| + \lambda_0 \lambda_4|000\rangle \langle 111| + \lambda_0 \lambda_4|111\rangle \langle 000| + \lambda_0^2|100\rangle \langle 100| + \lambda_1 \lambda_2 e^{i\phi}|100\rangle \langle 100| + \lambda_1 \lambda_2 e^{-i\phi}|100\rangle \langle 100| + \lambda_1 \lambda_3 e^{i\phi}|100\rangle \langle 110| + \lambda_1 \lambda_3 e^{-i\phi}|110\rangle \langle 100| + \lambda_1 \lambda_4 e^{i\phi}|100\rangle \langle 111| + \lambda_1 \lambda_4 e^{-i\phi}|111\rangle \langle 100| + \lambda_2 \lambda_3|101\rangle \langle 110| + \lambda_2 \lambda_3|110\rangle \langle 101| + \lambda_2 \lambda_4|101\rangle \langle 111| + \lambda_2 \lambda_4|111\rangle \langle 101| + \lambda_3^2|110\rangle \langle 110| + \lambda_3 \lambda_4|110\rangle \langle 111| + \lambda_3 \lambda_4|111\rangle \langle 110| + \lambda_4^2|111\rangle \langle 111|. \tag{13}
\]

The reduced density matrix of region one is:

\[
\rho_1 = \lambda_0^2|0\rangle \langle 0| + \lambda_0 \lambda_1 e^{-i\phi}|0\rangle \langle 1| + \lambda_0 \lambda_1 e^{i\phi}|1\rangle \langle 0| + \lambda_1^2|1\rangle \langle 1| + \lambda_2^2|1\rangle \langle 1| + \lambda_3^2|1\rangle \langle 1| + \lambda_4^2|1\rangle \langle 1| = \lambda_0^2|0\rangle \langle 0| + \lambda_0 \lambda_1 e^{-i\phi}|0\rangle \langle 1| + \lambda_0 \lambda_1 e^{i\phi}|1\rangle \langle 0| + (1 - \lambda_0^2)|1\rangle \langle 1|. \tag{14}
\]

The reduced density matrix of region two is given by:

\[
\rho_2 = \lambda_0^2|0\rangle \langle 0| + \lambda_1^2|0\rangle \langle 0| + \lambda_3 e^{i\phi}|0\rangle \langle 1| + \lambda_1 \lambda_3 e^{-i\phi}|1\rangle \langle 0| + \lambda_2 \lambda_4|0\rangle \langle 1| + \lambda_2 \lambda_4|1\rangle \langle 0| + \lambda_3^2|1\rangle \langle 1| + \lambda_4^2|1\rangle \langle 1| = (\lambda_0^2 + \lambda_1^2 + \lambda_3^2)|0\rangle \langle 0| + (\lambda_2 \lambda_4 + \lambda_1 \lambda_3 e^{i\phi})|0\rangle \langle 1| + (\lambda_2 \lambda_4 + \lambda_1 \lambda_3 e^{-i\phi})|1\rangle \langle 0| + (\lambda_3^2 + \lambda_4^2)|1\rangle \langle 1|. \tag{15}
\]
The reduced density matrix of region three is given by:

\[
\rho_3 = \lambda_0^2 |0\rangle \langle 0| + \lambda_1^2 |0\rangle \langle 0| + \lambda_1 \lambda_2 e^{i\phi} |0\rangle \langle 1| + \lambda_1 \lambda_2 e^{-i\phi} |1\rangle \langle 0| \\
+ \lambda_2^2 |1\rangle \langle 1| + \lambda_3^2 |0\rangle \langle 0| + \lambda_3 \lambda_4 |0\rangle \langle 1| + \lambda_3 \lambda_4 |1\rangle \langle 0| + \lambda_4^2 |1\rangle \langle 1| \\
= (\lambda_0^2 + \lambda_1^2 + \lambda_2^2) |0\rangle \langle 0| \\
+ (\lambda_3 \lambda_4 + \lambda_1 \lambda_2 e^{i\phi}) |0\rangle \langle 1| \\
+ (\lambda_3 \lambda_4 + \lambda_1 \lambda_2 e^{-i\phi}) |1\rangle \langle 0| \\
+ (\lambda_2^2 + \lambda_4^2) |1\rangle \langle 1|. 
\]

\(2.3\) Entanglement Measures

For a 3-qubit quantum state, all invariant quantities under a local unitary transformation are the following:

\[
I_1 = \text{Tr} \rho_1^2 = \lambda_0^4 + 2\lambda_0^2 \lambda_1^2 + (1 - \lambda_0^2)^2; \\
I_2 = \text{Tr} \rho_2^2 = (1 - \lambda_2^2 - \lambda_3^2)^2 + 2|\lambda_2 \lambda_4 + \lambda_1 \lambda_3 e^{i\phi}|^2 + (\lambda_3^2 + \lambda_4^2)^2; \\
I_3 = \text{Tr} \rho_3^2 = (1 - \lambda_2^2 - \lambda_3^2)^2 + 2|\lambda_3 \lambda_4 + \lambda_1 \lambda_2 e^{i\phi}|^2 + (\lambda_2^2 + \lambda_4^2)^2; \\
I_4 = \tau_{1|23} - \tau_{1|2} - \tau_{1|3}; \\
I_5 = \text{Tr}((\rho_1 \otimes \rho_2)\rho_{12}) - \frac{1}{3} \text{Tr}(\rho_1^3) - \frac{1}{3} \text{Tr}(\rho_2^3) \\
= \text{Tr}((\rho_2 \otimes \rho_3)\rho_{23}) - \frac{1}{3} \text{Tr}(\rho_2^3) - \frac{1}{3} \text{Tr}(\rho_3^3) \\
= \text{Tr}((\rho_3 \otimes \rho_1)\rho_{31}) - \frac{1}{3} \text{Tr}(\rho_3^3) - \frac{1}{3} \text{Tr}(\rho_1^3), 
\]

\text{(17)}

where

\[
\tau_{1|23} \equiv 2(1 - \text{Tr} \rho_1^2). \quad \text{(18)}
\]

The \(\rho_j\) is a reduced density matrix of the \(j\)-th qubit. The \(\sqrt{\tau_{i_1|i_2}}\) is the entanglement of formation of the \(i_1\) qubit and \(i_2\) qubit after tracing out a qubit \([7]\). The entanglement of formation is defined by a minimization of \(p_j\) and \(\psi_j\) as the following \([6, 7]\):

\[
C(\rho) \equiv \min_{p_j, \psi_j} \sum_j p_j C(\psi_j) = \max(0, Q_1 - Q_2 - Q_3 - Q_4), \\
Q_1 \geq Q_2 \geq Q_3 \geq Q_4; \\
\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|. 
\]

\text{(19)}
where $Q_j$ are the eigenvalues of $\sqrt{\rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)}$ \cite{8, 9}, and $C(\psi)$ is the concurrence

$$C(\psi) \equiv \sqrt{2(1 - \text{Tr}\rho^2)}.$$\hspace{1cm} (20)

We denote the complex conjugate as $\ast$. The $I_4$ or 3-tangle controls the 3-body entanglement \cite{13}. The appearance of 3-body entanglement quantity implies that the 2-body entanglement quantities are not enough \cite{13}. Now we calculate $I_4$ as in the following:

$$\tau_{1|23} = 2(1 - \text{Tr}\rho_{11}^2) = 2(1 - \lambda_0^4 - 2\lambda_0^2\lambda_1^2 - (1 - \lambda_0^2)^2);$$\hspace{1cm} (21)

\begin{align*}
\rho_{12}(\sigma_y \otimes \sigma_y)\rho_{12}^*(\sigma_y \otimes \sigma_y) \\
= 2\lambda_0^3\lambda_3|00\rangle\langle 11| - \lambda_0^2(2\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4)|00\rangle\langle 01| + \lambda_0^2(2\lambda_3^2 + \lambda_4^2)|00\rangle\langle 00| \\
+ \lambda_0^2(2\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4)|10\rangle\langle 11| - 2\lambda_0\lambda_1e^{i\phi}(\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4)|10\rangle\langle 01| \\
+ (\lambda_0\lambda_1e^{i\phi}(\lambda_3^2 + \lambda_1^2) + \lambda_0\lambda_3(\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4))|10\rangle\langle 00| + \lambda_0^2(2\lambda_3^2 + \lambda_4^2)|11\rangle\langle 11| \\
- (\lambda_0\lambda_3(\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4) + \lambda_0\lambda_1e^{i\phi}(\lambda_3^2 + \lambda_4^2))|11\rangle\langle 01| + 2\lambda_0\lambda_3(\lambda_3^2 + \lambda_4^2)|11\rangle\langle 00|; \hspace{1cm} (22)
\end{align*}

\begin{align*}
\rho_{13}(\sigma_y \otimes \sigma_y)\rho_{13}^*(\sigma_y \otimes \sigma_y) \\
= 2\lambda_0^3\lambda_2|00\rangle\langle 11| - \lambda_0^2(2\lambda_1\lambda_2e^{i\phi} + \lambda_3\lambda_4)|00\rangle\langle 01| + \lambda_0^2(2\lambda_2^2 + \lambda_4^2)|00\rangle\langle 00| \\
+ \lambda_0^2(2\lambda_1\lambda_2e^{i\phi} + \lambda_3\lambda_4)|10\rangle\langle 11| - 2\lambda_0\lambda_1e^{i\phi}(\lambda_1\lambda_2e^{i\phi} + \lambda_3\lambda_4)|10\rangle\langle 01| \\
+ (\lambda_0\lambda_1e^{i\phi}(\lambda_2^2 + \lambda_1^2) + \lambda_0\lambda_2(\lambda_1\lambda_2e^{i\phi} + \lambda_3\lambda_4))|10\rangle\langle 00| + \lambda_0^2(2\lambda_2^2 + \lambda_4^2)|11\rangle\langle 11| \\
- (\lambda_0\lambda_2(\lambda_1\lambda_2e^{i\phi} + \lambda_3\lambda_4) + \lambda_0\lambda_1e^{i\phi}(\lambda_2^2 + \lambda_4^2))|11\rangle\langle 01| + 2\lambda_0\lambda_2(\lambda_2^2 + \lambda_4^2)|11\rangle\langle 00|; \hspace{1cm} (23)
\end{align*}

\begin{align*}
\tau_{1|23} &= 2(1 - \lambda_0^4 - 2\lambda_0^2\lambda_1^2 - (1 - \lambda_0^2)^2) = 4\lambda_0^2(1 - \lambda_0^2 - \lambda_1^2); \\
\tau_{1|2} &= 4\lambda_0^2\lambda_3^2; \\
\tau_{1|3} &= 4\lambda_0^2\lambda_2^2. \hspace{1cm} (24)
\end{align*}

Hence we obtain:

$$I_4 = 4\lambda_0^2(1 - \lambda_0^2 - \lambda_1^2 - \lambda_2^2 - \lambda_3^2) = 4\lambda_0^2\lambda_4^2. \hspace{1cm} (25)$$

Here we use the following convenient identities:

$$\sigma_y = -i|0\rangle\langle 1| + i|1\rangle\langle 0|;$$
$$\sigma_y \otimes \sigma_y = -|00\rangle\langle 11| + |01\rangle\langle 10| + |10\rangle\langle 01| - |11\rangle\langle 00|, \hspace{1cm} (26)$$

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In the end, we calculate $I_5$ as in the following:

$$
\text{Tr}(\rho_1^2) = \lambda_0^6 + 3\lambda_0^4\lambda_4^2 + (1 - \lambda_0^2)^3 = 3\lambda_0^2\lambda_4^2 + 3\lambda_0^4 - 3\lambda_0^2 + 1;
\quad \text{Tr}(\rho_2^3) = (1 - \lambda_3^2 - \lambda_4^2)^3 + 3|\lambda_2\lambda_4 + \lambda_1\lambda_3 e^{i\phi}|^2 + (\lambda_3^2 + \lambda_4^2)^3; \quad (27)
$$

\[
\rho_{12} = \lambda_0^2|00\rangle\langle 00| + \lambda_0\lambda_1 e^{-i\phi}|00\rangle\langle 10| + \lambda_0\lambda_1 e^{i\phi}|10\rangle\langle 00|
+ \lambda_0\lambda_3|00\rangle\langle 11| + \lambda_0\lambda_3|11\rangle\langle 00| + \lambda_1^2|10\rangle\langle 10|
+ \lambda_1\lambda_3 e^{i\phi}|10\rangle\langle 11| + \lambda_1\lambda_3 e^{-i\phi}|11\rangle\langle 10| + \lambda_2^2|10\rangle\langle 10|
+ \lambda_2\lambda_4|10\rangle\langle 11| + \lambda_2\lambda_4|11\rangle\langle 10| + \lambda_3^2|11\rangle\langle 11| + \lambda_4^2|11\rangle\langle 11|;
\]

\[
\rho_{13} = \lambda_0^2|00\rangle\langle 00| + \lambda_0\lambda_1 e^{-i\phi}|00\rangle\langle 10| + \lambda_0\lambda_1 e^{i\phi}|10\rangle\langle 00|
+ \lambda_0\lambda_2|00\rangle\langle 11| + \lambda_0\lambda_2|11\rangle\langle 00| + \lambda_1^2|10\rangle\langle 10|
+ \lambda_1\lambda_2 e^{i\phi}|10\rangle\langle 11| + \lambda_1\lambda_2 e^{-i\phi}|11\rangle\langle 10| + \lambda_2^2|11\rangle\langle 11|
+ \lambda_3^2|10\rangle\langle 10| + \lambda_3\lambda_4|10\rangle\langle 11| + \lambda_3\lambda_4|11\rangle\langle 10| + \lambda_4^2|11\rangle\langle 11|
= \lambda_0^2|00\rangle\langle 00| + \lambda_0\lambda_1 e^{-i\phi}|00\rangle\langle 10| + \lambda_0\lambda_1 e^{i\phi}|10\rangle\langle 00|
+ \lambda_0\lambda_2|00\rangle\langle 11| + \lambda_0\lambda_2|11\rangle\langle 00| + \lambda_1^2 + \lambda_3^2|10\rangle\langle 10|
+ \lambda_1\lambda_2 e^{i\phi} + \lambda_3\lambda_4|10\rangle\langle 11| + \lambda_1\lambda_2 e^{-i\phi} + \lambda_3\lambda_4|11\rangle\langle 10| + (\lambda_2^2 + \lambda_4^2)|11\rangle\langle 11|;
\quad (28)
\]
\[ \text{Tr}((\rho_1 \otimes \rho_2)\rho_{12}) = \lambda_0^4 + 2\lambda_1^2\lambda_0^2 + (\lambda_1^2 + \lambda_1^2)(1 - \lambda_0^2) \\
+ (-\lambda_0^4 + (-\lambda_1^2 + \lambda_2^2 - \lambda_3^2 - \lambda_4^2)\lambda_0^2 + (-\lambda_1^2 - \lambda_2^2 + \lambda_3^2 + \lambda_4^2)(\lambda_3^2 + \lambda_4^2) \\
+ 2|\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4|^2(1 - \lambda_0^2) \\
+ \lambda_0^2\lambda_1\lambda_3e^{i\phi}(\lambda_2\lambda_4 + \lambda_1\lambda_3e^{-i\phi}) + \lambda_0^2\lambda_1\lambda_3e^{-i\phi}(\lambda_2\lambda_4 + \lambda_1\lambda_3e^{i\phi}) \\
= \lambda_0^4 + 2\lambda_1^2\lambda_0^2 + (\lambda_1^2 + \lambda_2^2)(1 - \lambda_0^2) \\
+ (2(\lambda_1^2 - 1)\lambda_0^2 - 2(\lambda_1^2 + \lambda_2^2) + 1)(\lambda_3^2 + \lambda_4^2) \\
+ 2|\lambda_1\lambda_3e^{i\phi} + \lambda_2\lambda_4|^2(1 - \lambda_0^2) \\
+ \lambda_0^2\lambda_1\lambda_3e^{i\phi}(\lambda_2\lambda_4 + \lambda_1\lambda_3e^{-i\phi}) + \lambda_0^2\lambda_1\lambda_3e^{-i\phi}(\lambda_2\lambda_4 + \lambda_1\lambda_3e^{i\phi}). \] (29)

Therefore, we obtain

\[ I_5 \]
\[ = 1 + 3\lambda_0^2(\lambda_0^2 - 1 + \lambda_1^2 - \lambda_2^2\lambda_4^2 + \lambda_2^2\lambda_3^2) - 3(1 - \lambda_0^2)|\lambda_1\lambda_4e^{i\phi} - \lambda_2\lambda_3|^2. \] (30)

Now we introduce different invariant quantities as in the following:

\[ E_1 \equiv \tau_{1|2} = 2\lambda_0\lambda_3; \]
\[ E_2 \equiv \tau_{1|3} = 2\lambda_0\lambda_2; \]
\[ E_3 \equiv \tau_{2|3} = 2|\lambda_1\lambda_4e^{i\phi} - \lambda_2\lambda_3|; \]
\[ E_4 \equiv \tau = 2\lambda_0\lambda_4; \]
\[ E_5 \equiv \text{Tr}((\rho_1 \otimes \rho_2)\rho_{12}) - \frac{1}{3}\text{Tr}(\rho_1^3) - \frac{1}{3}\text{Tr}(\rho_2^3) + \frac{1}{4}(E_1^2 + E_2^2 + E_4^2) + E_3^2 \\
= \lambda_0^2(\lambda_2^2\lambda_3^2 - \lambda_1^2\lambda_4^2 + |\lambda_1\lambda_4e^{i\phi} - \lambda_2\lambda_3|^2). \] (31)

We then can find the correlation of reduced density matrices is relevant to \( E_5 \):

\[ \text{Tr}((\rho_1 \otimes \rho_2)\rho_{12}) - \text{Tr}(\rho_1^2) - \text{Tr}(\rho_2^2) \]
\[ = E_5 - 1 + \frac{E_1^2 + E_4^2}{4}; \] (32)

\[ \text{Tr}((\rho_2 \otimes \rho_3)\rho_{23}) - \text{Tr}(\rho_2^2) - \text{Tr}(\rho_3^2) \]
\[ = E_5 - 1 - \frac{E_1^2 + E_2^2 + E_3^2 + 2E_4^2}{4}; \] (33)
\[
\begin{align*}
\text{Tr}(\rho_3 \otimes \rho_1) - \text{Tr}(\rho_3^2) - \text{Tr}(\rho_1^3) & = E_5 - 1 + \frac{E_2^2 + E_4^2}{4}. \\
\end{align*}
\]

Hence the necessity of \( I_5 \) is due to the correlation of reduced density matrices. The invariant quantities \( E_1, E_2, E_3, E_4, E_5 \) will be helpful in the next section or the generalized \( R \)-matrix.

### 2.4 Optimization

We do a numerical optimization for obtaining the maximum violation. In the numerical study, we separate the general case from the following eight operators:

\[ O_1 \equiv A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3; \quad (35) \]

\[ O_2 \equiv |\tilde{\alpha}_1|(A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3) \\
+ |\tilde{\alpha}_2|(A'_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A'_3); \quad (36) \]

\[ O_3 \equiv \tilde{\alpha}_1(A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3) \\
+ \tilde{\alpha}_2 A'_1 \otimes A'_2 \otimes A'_3; \quad (37) \]

\[ O_4 \equiv |\tilde{\alpha}_1|(A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3) \\
+ |\tilde{\alpha}_2|A_1 \otimes A_2 \otimes A_3; \quad (38) \]

\[ O_5 \equiv \tilde{\alpha}_1 A'_1 \otimes A'_2 \otimes A'_3 + \tilde{\alpha}_2 A_1 \otimes A_2 \otimes A_3; \quad (39) \]

\[ O_6 \equiv \tilde{\alpha}_1(A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3) \\
+ \tilde{\alpha}_2(A'_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A'_3) \\
+ \tilde{\alpha}_3 A'_1 \otimes A'_2 \otimes A'_3; \quad (40) \]
\[ O_7 \equiv \tilde{\alpha}_1 (A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A_3) + \tilde{\alpha}_2 A'_1 \otimes A_2 \otimes A'_3 + \tilde{\alpha}_3 A_1 \otimes A_2 \otimes A_3; \] (41)

\[ O_8 \equiv \tilde{\alpha}_1 (A_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A'_3) + \tilde{\alpha}_2 (A'_1 \otimes A'_2 \otimes A_3 + A'_1 \otimes A_2 \otimes A'_3 + A_1 \otimes A'_2 \otimes A'_3) + \tilde{\alpha}_3 A'_1 \otimes A'_2 \otimes A_3 + \tilde{\alpha}_4 A_1 \otimes A_2 \otimes A_3. \] (42)

Here we consider the non-zero coefficients

\[ 0 < |\tilde{\alpha}_1|, |\tilde{\alpha}_2|, |\tilde{\alpha}_3|, |\tilde{\alpha}_4| < \infty. \] (43)

We do not have a mixed term of \( A_j \) and \( A'_j \) in \( O_5 \). Therefore, it is easy to show that

\[ \gamma \propto \tilde{\alpha}_1 + \tilde{\alpha}_2. \] (44)

The choice of coefficients does not change the conclusion in \( O_5 \).

Without an ambiguity of interpretation, we only turn on one entanglement measure. The entanglement diagnosis must be monotonic increasing for the measure. Now we discuss the one entanglement measure. Turning off \( \lambda_2 \) and \( \lambda_4 \) provides the only non-vanishing \( E_1 \). When turning off \( \lambda_3 \) and \( \lambda_4 \), the only non-vanishing measure is \( E_2 \). For the case of \( E_3 \), one only needs to turn off \( \lambda_0 \). In the end, we choose

\[ \lambda_1 = \lambda_2 = \lambda_3 = 0 \] (45)

to leave the only non-vanishing \( E_4 \) or 3-tangle.

Now we study the numerical solution for \( \langle O_j \rangle \) for the single measure case. For a convenient reading of the main context, we put the numerical results or figures in Appendix [A]. For a proper presentation, we present our result for a part of the \( \tilde{\alpha}_j \) parameter space. Our physical conclusion and result presented also holds for other
parameter spaces. Because all operators are symmetric in the permutation of the three qubits, the result of \( \langle O_j \rangle \) has the same behavior for \( E_1, E_2, \) and \( E_3 \). One can observe the above phenomenon in Figs. 3, 4, 5, 6, and 7. Without showing too much same information, we only calculate \( E_2 \) and \( E_4 \) for \( \langle O_6 \rangle, \langle O_7 \rangle, \) and \( \langle O_8 \rangle \) in Figs. 8, 9, and 10. Because all results show the loss of monotonically increasing, we conclude that the violation is not equivalent to quantumness.

3 Generalized \( R \)-Matrix

We introduce an alternative diagnosis, generalized \( R \)-matrix. We then show the monotonic result for one entanglement measure. The analytical solution generates one classification of all 3-qubit quantum states. In each class, the monotonically increasing result also holds. The details of the generalized \( R \)-Matrix is in Appendix B.

3.1 Generalized \( R \)-Matrix and Merlin’s Operator

The Merlin’s operator \( M \) is \( O_3 \) with the choice of coefficients:

\[
\tilde{\alpha}_1 = -\tilde{\alpha}_2 = 1.
\]  

(46)

We can rewrite the expectation value of \( M \) in terms of the generalized \( R \)-matrix:

\[
\langle M \rangle = \sum_{i_1,i_2,i_3} \left( a_{1,i_1}a_{2,i_2}a'_{3,i_3} + a_{1,i_1}a'_{2,i_2}a_{3,i_3} + a'_{1,i_1}a_{2,i_2}a_{3,i_3} - a'_{1,i_1}a'_{2,i_2}a'_{3,i_3} \right) R_{i_1i_2i_3}
\]

\[
= \left( a_1, a_2^T R a'_{3} \right) + \left( a_1, a_2^T R a_3 \right) + \left( a'_{1}, a_2^T R a_3 \right) - \left( a'_{1}, a_2^T R a'_3 \right),
\]  

(47)

where

\[
a_j \equiv \begin{pmatrix} a_{j,x} \\ a_{j,y} \\ a_{j,z} \end{pmatrix}; \quad a'_j \equiv \begin{pmatrix} a'_{j,x} \\ a'_{j,y} \\ a'_{j,z} \end{pmatrix},
\]

\[
R_{i_1i_2i_3} \equiv \text{Tr}(\rho \sigma_{i_1} \otimes \sigma_{i_2} \otimes \sigma_{i_3}).
\]  

(48)
We indicate a transpose operation as the superscript $T$. The generalized $R$-matrix is given by:

\[
R \equiv (R_x, R_y, R_z), \quad R_x \equiv \begin{pmatrix}
R_{xxx} & R_{xxy} & R_{xxz} \\
R_{xyx} & R_{xyy} & R_{xyz} \\
R_{xzx} & R_{xzy} & R_{xzz}
\end{pmatrix},
\]

\[
R_y \equiv \begin{pmatrix}
R_{yxx} & R_{yxy} & R_{yxz} \\
R_{yyx} & R_{yyy} & R_{yyz} \\
R_{yzx} & R_{yzy} & R_{yzz}
\end{pmatrix},
\]

\[
R_z \equiv \begin{pmatrix}
R_{zxx} & R_{zxy} & R_{zxz} \\
R_{zyx} & R_{zyy} & R_{zyz} \\
R_{zzx} & R_{zzy} & R_{zzz}
\end{pmatrix}.
\]

We define the inner product as:

\[
\left( a_1, a_2^T R a_3' \right) \equiv \left( (a_1, a_2^T R_x a_3'), (a_1, a_2^T R_y a_3'), (a_1, a_2^T R_x a_3') \right) = \sum_{i_1, i_2, i_3} a_{1, i_1} a_{2, i_2} a_{3, i_3} R_{i_1, i_2, i_3}. \tag{50}
\]

Now we show that the generalized $R$-matrix can provide an upper bound to $\langle M \rangle$. We first observe that the following vectors are orthogonal:

\[
V \equiv V_{j,k} = (a_{2,j} a_{3,k} + a'_{2,j} a_{3,k}); \quad V' \equiv V'_{j,k} = (a_{2,j} a_{3,k} - a'_{2,j} a_{3,k}),
\]

\[
\sum_{j,k=1}^3 V_{j,k} V'_{j,k} = 0. \tag{51}
\]

The norm of two vectors is:

\[
|V|^2 \equiv V_{j,k} V'_{j,k} = 2 + 2 \cos(\theta_2) \cos(\theta_3); \quad |V'|^2 \equiv V'_{j,k} V'_{j,k} = 2 - 2 \cos(\theta_2) \cos(\theta_3), \tag{52}
\]

where

\[
\vec{a}_2 \cdot \vec{a}_2' \equiv \cos(\theta_2); \quad \vec{a}_3 \cdot \vec{a}_3' \equiv \cos(\theta_3); \quad 0 \leq \theta_2, \theta_3 \leq \pi. \tag{53}
\]

We then introduce the orthogonal unit vectors ($c$ and $c'$) as in the following:

\[
V \equiv 2 c \cos(\theta); \quad V' \equiv 2 c' \sin(\theta), \quad \tag{54}
\]
where
\[ \cos(2\theta) \equiv \cos(\theta_2) \cos(\theta_3), \; 0 \leq \theta \leq \frac{\pi}{2}. \] (55)

Therefore, \( \langle M \rangle \) becomes
\[ \langle M \rangle = 2 \cos(\theta)(a_1, Rc) + 2 \sin(\theta)(a'_1, Rc'). \] (56)

Because \( c \) and \( c' \) are not independent, we only obtain an upper bound of maximum violation:
\[ \gamma \leq 2 \sqrt{u_1^2 + u_2^2}, \] (57)

where \( u_1^2 \) and \( u_2^2 \) are two largest eigenvalues of \( RR^T \). The generalized \( R \)-matrix now has one 3d index and one 9d index. Therefore, we can have three possible choices:
\[ R^{(1)}_{j_1,j_1} \equiv R_{j_1,j_2,j_3} |_{J_1=(j_2,j_3)}; \; \quad R^{(2)}_{j_2,j_2} \equiv R_{j_1,j_2,j_3} |_{J_2=(j_1,j_3)}; \; \quad R^{(3)}_{j_3,j_3} \equiv R_{j_1,j_2,j_3} |_{J_3=(j_1,j_2)}, \] (58)

where \( j_1, j_2, j_3 = x, y, z \). To obtain a tight bound of maximum violation, we define a new quantity \( \gamma_R \) as that:
\[ \gamma \leq \gamma_R = 2 \min_{R^{(1)}, R^{(2)}, R^{(3)}} \sqrt{u_1^2 + u_2^2}. \] (59)

Later we will rewrite \( \gamma_R \) from five entanglement quantities \( (E_{1,2,3,4,5}) \). This result implies that 3-qubit Quantum Entanglement is encoded by \( \gamma_R \).

### 3.2 Eigenvalues of Generalized \( R \)-Matrix

We solve the eigenvalues \( (x^{(j)}) \) of \( R^{(j)T} \equiv M^{(j)} \) from the following equation:
\[ x^{(j)3} + (-M_{xx}^{(j)} - M_{yy}^{(j)} - M_{zz}^{(j)})x^{(j)2} + (M_{xx}^{(j)} M_{yy}^{(j)} + M_{xx}^{(j)} M_{zz}^{(j)} + M_{yy}^{(j)} M_{zz}^{(j)} - M_{xy}^{(j)2} - M_{xz}^{(j)2} - M_{yz}^{(j)2})x^{(j)} + (-M_{xx}^{(j)} M_{yy}^{(j)} M_{zz}^{(j)} + M_{xx}^{(j)} M_{yz}^{(j)} + M_{yy}^{(j)} M_{xz}^{(j)} + M_{zz}^{(j)} M_{xy}^{(j)} + M_{xy}^{(j)} M_{yz}^{(j)} M_{xz}^{(j)} - 2 M_{xy}^{(j)} M_{yz}^{(j)} M_{xz}^{(j)})x^{(j)0} = 0. \] (61)
Therefore, we can obtain an analytical solution by solving the cubic equation. Because the eigenvalues are real-valued, the discriminant is non-positive

\[ \Delta^{(j)} \equiv -\frac{\alpha_1^{(j)}}{27} - \frac{\alpha_3^{(j)}}{2} + \frac{\alpha_1^{(j)} \alpha_2^{(j)}}{6} + \left( \frac{\alpha_2^{(j)}}{3} - \frac{\alpha_1^{(j)} \alpha_2^{(j)}}{9} \right)^3 \leq 0, \]  

(62)

where

\[ \gamma_1^{(j)} \equiv -\frac{\alpha_1^{(j)} \alpha_2^{(j)}}{27} - \frac{\alpha_3^{(j)} \alpha_2^{(j)}}{2} + \frac{\alpha_1^{(j)} \alpha_2^{(j)} \alpha_3^{(j)}}{6} ; \quad \gamma_2^{(j)} \equiv \frac{\alpha_2^{(j)}}{3} - \frac{\alpha_1^{(j)} \alpha_2^{(j)}}{9} \leq 0, \]  

(63)

\[ \alpha_1^{(j)} = -M_{xx}^{(j)} - M_{yy}^{(j)} - M_{zz}^{(j)} \leq 0; \]
\[ \alpha_2^{(j)} = M_{xx}^{(j)} M_{yy}^{(j)} + M_{xx}^{(j)} M_{zz}^{(j)} + M_{yy}^{(j)} M_{zz}^{(j)} - M_{xy}^{(j)^2} - M_{xz}^{(j)^2} - M_{yz}^{(j)^2}; \]
\[ \alpha_3^{(j)} = -2M_{xy}^{(j)} M_{yz}^{(j)} M_{xz}^{(j)}. \]  

(64)

The analytical solution of eigenvalues is:

\[ x_1^{(j)} = -\frac{\alpha_1^{(j)}}{3} + 2\sqrt{-\gamma_2^{(j)}} \cos \left[ \frac{1}{3} \arccos \left( \frac{\gamma_1^{(j)} \gamma_2^{(j)}}{(-\gamma_2^{(j)})^2} \right) \right]; \]
\[ x_2^{(j)} = -\frac{\alpha_1^{(j)}}{3} + 2\sqrt{-\gamma_2^{(j)}} \cos \left[ \frac{1}{3} \arccos \left( \frac{\gamma_1^{(j)} \gamma_2^{(j)}}{(-\gamma_2^{(j)})^2} + \frac{2\pi}{3} \right) \right]; \]
\[ x_3^{(j)} = -\frac{\alpha_1^{(j)}}{3} + 2\sqrt{-\gamma_2^{(j)}} \cos \left[ \frac{1}{3} \arccos \left( \frac{\gamma_1^{(j)} \gamma_2^{(j)}}{(-\gamma_2^{(j)})^2} - \frac{2\pi}{3} \right) \right]. \]  

(65)

Now we use the details of Appendix B to rewrite \( \alpha_1^{(1)} \), \( \alpha_2^{(1)} \), and \( \alpha_3^{(1)} \) in terms of entan-
glement quantities:
\[
\alpha^{(1)}_1 = -1 - (2E_1^2 + 2E_2^2 + 2E_3^2 + 3E_4^2) \\
\equiv -1 - C_T^2; \\
\alpha^{(1)}_2 = 2(E_1^2 + E_2^2)(E_3^2 + 2E_4^2)(E_4^2 + 1) + E_1^4 + E_2^4 + 4E_2^4 + 16E_5; \\
\alpha^{(1)}_3 = (E_1^2 + E_2^2 + 2E_3^2)(2E_4^4 + 2E_2^2E_4^2 + E_2^2E_4^2 - (E_1^2 + 2E_2^2 + 8E_3^2)^2). \\
\]  

The non-negative total concurrence
\[
C_T^2 = C_1^2 + C_2^2 + C_3^2, \\
\]
where
\[
C_1(\psi) \equiv \sqrt{2(1 - \text{Tr}\rho_1)} = \sqrt{E_1^2 + E_2^2 + E_4^2}; \\
C_2(\psi) \equiv \sqrt{2(1 - \text{Tr}\rho_2)} = \sqrt{E_1^2 + E_3^2 + E_4^2}; \\
C_3(\psi) \equiv \sqrt{2(1 - \text{Tr}\rho_3)} = \sqrt{E_2^2 + E_3^2 + E_4^2}; \\
\]
implies that
\[
\alpha^{(1)}_1 < 0. \\
\]
For \(\alpha^{(1)}_2\), the only negative contribution, \(-\lambda_0^2\lambda_1^2\lambda_4^2\) is in \(E_5\). We can combine \(4E_4^2\) with \(16E_5\) to cancel the negative contribution as that:
\[
4E_4^2 - 16\lambda_0^2\lambda_1^2\lambda_4^2 = 16(\lambda_0^2\lambda_4^2 - \lambda_0^2\lambda_1^2\lambda_4^2) = 16\lambda_0^2\lambda_4^2(1 - \lambda_1^2) \geq 0. \\
\]
Hence \(\alpha^{(1)}_2\) is not negative. We can use the following exchange to obtain other cases:
\[
E_2 \leftrightarrow E_3, \quad \alpha^{(1)}_1 \leftrightarrow \alpha^{(2)}_1, \alpha^{(1)}_2 \leftrightarrow \alpha^{(2)}_2, \alpha^{(1)}_3 \leftrightarrow \alpha^{(2)}_3; \\
E_1 \leftrightarrow E_3, \quad \alpha^{(1)}_1 \leftrightarrow \alpha^{(3)}_1, \alpha^{(1)}_2 \leftrightarrow \alpha^{(3)}_2, \alpha^{(1)}_3 \leftrightarrow \alpha^{(3)}_3. \\
\]
Because \(E_4\) is invariant for a different choice of generalized \(R\)-matrix, \(\alpha^{(j)}_1\) is independent of the index \(j\). One non-trivial fact is that \(E_5\) is also invariant because it depends on
Therefore, using $E_5$ is more convenient than $I_5$. Due to the invariance property of $E_4$ and $E_5$, we can show that

$$\alpha_2^{(2)}, \alpha_2^{(3)} \geq 0. \quad (72)$$

The eigenvalues of $RR^T$ are functions of $\alpha_{1,2,3}$. Therefore, it implies that 3-qubit entanglement information is all in $\gamma_R$.

Now we show an analytical solution of $\gamma_R$. Indeed, we know that $x_2^{(j)}$ is always negative, $x_1^{(j)}$ is always positive, and

$$x_3^{(j)} \geq x_2^{(j)}, \quad (73)$$

which is due to the following ranges:

$$0 \leq \theta^{(j)} \equiv \frac{1}{3} \arccos\left(\frac{\gamma_1^{(j)}}{(\gamma_2^{(j)})^\frac{2}{3}}\right) \leq \frac{\pi}{3}. \quad (74)$$

Therefore, two largest eigenvalues of $R^{(j)}R^{(j)T}$ are $x_1^{(j)}$ and $x_3^{(j)}$. Indeed, one can also show that the maximum eigenvalue is $x_1^{(j)}$. Hence the analytical solution is

$$\gamma_R = 2 \min_j \sqrt{-\frac{2\alpha_1^{(j)}}{3} + 2\sqrt{-\gamma_2^{(j)}} \cos\left(\theta^{(j)} - \frac{\pi}{3}\right)}. \quad (75)$$

Now we show the monotonic increasing result in Fig 2. The analytical solution also, in general, shows the monotonic increasing result for $-\alpha_1$ with a fixed $\gamma_2^{(j)}$ and $\theta^{(j)}$ in general. The LOCC showed that a general 3-qubit state has W-type and GHZ-type entanglement [12]. Therefore, we need to fix two parameters to indicate a choice of entanglement. The remaining parameter or total concurrence is to diagnose Quantum Entanglement. Therefore, Quantum Entanglement should be a source of $\gamma_R$ rather than the maximum violation $\gamma$.

4 Discussion and Conclusion

We showed that violating a constraint of correlations does not imply quantumness. For our goal, we require a symmetric permutation of qubits. The 3-qubit operators are just a combination of four kinds of operators. Therefore, we can consider all cases
Figure 2: We show that $\gamma_R$ restores the monotonically increasing behavior for $E_1^2$, $E_2^2$, $E_3^2$, and $E_4^2$. 
without losing generically. Hence we then see how the maximum violation varies for entanglement measures. Our results showed a loss of monotonically increasing. Here we only turn on one entanglement measure. In this case, the characterization of Quantum Entanglement does not have an ambiguity. In other words, the monotonically increasing result holds when Quantum Entanglement is a necessary and sufficient condition for the violation. Our results showed that Quantum Entanglement is only a necessary condition. Hence we need to find an alternative measure to replace the violation.

The two largest eigenvalues of $R$-matrix provides the maximum violation of Bell’s inequality \[2\]. We generalized the $R$-matrix and provided an upper bound to maximum violation of Merlin’s inequality. We then showed that the generalized $R$-matrix restores the loss behavior (monotonically increasing). Hence our result distinguishes the correlation of $R$-matrix and maximum violation. The equivalence only holds in 2-qubit. The correlation of the generalized $R$-matrix is more proper to diagnose quantumness than a violation. We also rewrite the analytical solution ($\gamma_R$) in terms of five entanglement measures. This non-trivial fact shows the expectation that $\gamma_R$ contains all entanglement information.

When one considers a 2-qubit mixed state, the non-vanishing entanglement entropy does not lead to the violation of Bell’s inequality. Therefore, entanglement (including mixed states) is a necessary but not sufficient condition for the violation. Performing a partial trace operation on a 3-qubit state generates a 2-qubit mixed density matrix. We expect that the origin of “Violation≠Quantum” may hide in a study of mixed states. One can use a partial trace operation to extend our analytical solution of generalized $R$-matrix to a 2-qubit mixed state. It should be interesting.

We proposed that the generalized $R$-matrix is a proper diagnosis of Quantum Entanglement. Our result rules out that the violation is a possible diagnosis of pure state entanglement. Therefore, it also reflects that the non-triviality of our proposal. The extension of $n$-qubits is simple in our proposal. Because measurement of $\gamma_R$ is unnecessary relevant to a partial trace operation, it simplifies an experimental study. Hence our proposal sheds light on exploring the mystery of many-body Quantum Entanglement.
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A Numerical Results of Maximum Violation

We show all numerical results of maximum violation here without affecting a reading of the main context. The results shows a loss of monotonic increasing for the single entanglement measure case.
Figure 3: We show $\langle O_1 \rangle$ for $E_1^2$, $E_2^2$, $E_3^2$, and $E_4^2$. 
Figure 4: We show \( \langle O_2 \rangle \) for \( E_2^1, E_2^2, E_2^3, \) and \( E_2^4. \)
Figure 5: We show $\langle \mathcal{O}_3 \rangle$ for $E_1^2$, $E_2^2$, $E_3^2$, and $E_4^2$. 
Figure 6: We show $\langle O_4 \rangle$ for $E_1^2$, $E_2^2$, $E_3^2$, and $E_4^2$.
Figure 7: We show $\langle O_5 \rangle$ for $E_1^2$, $E_2^2$, $E_3^2$, and $E_4^2$. 
Figure 8: We show $\langle O_6 \rangle$ for $E_1^2$ and $E_4^2$.
Figure 9: We show $\langle \mathcal{O}_T \rangle$ for $E_1^2$ and $E_4^2$. 
Figure 10: We show $\langle \mathcal{O}_8 \rangle$ for $E_1^2$ and $E_4^2$. 
B Calculation of $RR^T$

We first show the elements of $R_x$:

\[
\begin{align*}
R_{xxx} &= 2\lambda_0\lambda_4; \\
R_{xxy} &= 0; \\
R_{xxz} &= 2\lambda_0\lambda_3; \\
R_{xyx} &= 0; \\
R_{xyy} &= -2\lambda_0\lambda_4; \\
R_{xyz} &= 0; \\
R_{xzx} &= 2\lambda_0\lambda_2; \\
R_{xzy} &= 0; \\
R_{xzz} &= 2\lambda_0\lambda_1\cos(\phi). \\
\end{align*}
\]

(76)

We then show the elements of $R_y$:

\[
\begin{align*}
R_{yxx} &= 0; \\
R_{yxy} &= -2\lambda_0\lambda_4; \\
R_{yxz} &= 0; \\
R_{yyx} &= -2\lambda_0\lambda_4; \\
R_{yyy} &= 0; \\
R_{yyz} &= -2\lambda_0\lambda_3; \\
R_{yzx} &= 0; \\
R_{yzy} &= -2\lambda_0\lambda_2; \\
R_{yzz} &= 2\lambda_0\lambda_1\sin(\phi). \\
\end{align*}
\]

(77)
We finally show the elements of $R_z$:

\[
R_{zxx} = -2\lambda_1\lambda_4 \cos(\phi) - 2\lambda_2\lambda_3;
\]

\[
R_{zxy} = 2\lambda_1\lambda_4 \sin(\phi);
\]

\[
R_{zxz} = -2\lambda_1\lambda_3 \cos(\phi) + 2\lambda_2\lambda_4;
\]

\[
R_{zyx} = 2\lambda_1\lambda_4 \sin(\phi);
\]

\[
R_{zyz} = 2\lambda_1\lambda_3 \sin(\phi);
\]

\[
R_{zzy} = -2\lambda_1\lambda_2 \cos(\phi) + 2\lambda_3\lambda_4;
\]

\[
R_{zzz} = \lambda_0^2 - \lambda_1^2 + \lambda_2^2 + \lambda_3^2 - \lambda_4^2 = 1 - 2\lambda_1^2 - 2\lambda_4^2. \tag{78}
\]

Now we calculate

\[
(R^{(1)} R^{(1)T})_{jk} \equiv \sum_j R^{(1)}_{j,j} R^{(1)T}_{k,j}. \tag{79}
\]
The result is:

\[
\begin{align*}
(R^{(1)}R^{(1)T})_{xx} &= 4\lambda_0^2(\lambda_2^2 + \lambda_3^2 + 2\lambda_4^2) + 4\lambda_0^2\lambda_1^2 \cos^2(\phi); \\
(R^{(1)}R^{(1)T})_{xy} &= (R^{(1)}R^{(1)T})_{yx} = 4\lambda_0^2\lambda_1^2 \cos(\phi) \sin(\phi); \\
(R^{(1)}R^{(1)T})_{xz} &= (R^{(1)}R^{(1)T})_{zx} = 2\lambda_0\lambda_1(2\lambda_2^2 + 2\lambda_4^2 - 1) - 8\lambda_0\lambda_2\lambda_3\lambda_4 + 4\lambda_0\lambda_1(\lambda_2^2 + \lambda_3^2 + 2\lambda_4^2) \cos(\phi); \\
(R^{(1)}R^{(1)T})_{yy} &= 4\lambda_0^2(\lambda_2^2 + \lambda_3^2 + 2\lambda_4^2) + 4\lambda_0^2\lambda_1^2 \sin^2(\phi); \\
(R^{(1)}R^{(1)T})_{yz} &= (R^{(1)}R^{(1)T})_{zy} = 2\lambda_0\lambda_1 \sin(\phi)(1 - 2\lambda_0^2 + 4\lambda_4^2); \\
(R^{(1)}R^{(1)T})_{zz} &= (R^{(1)}R^{(1)T})_{zz} = (1 - 2\lambda_1^2 - 2\lambda_3^2)^2 + 4(\lambda_3\lambda_4 - \lambda_1\lambda_2 \cos(\phi))^2 + 4(\lambda_2\lambda_4 - \lambda_1\lambda_3 \cos(\phi))^2 + 4(\lambda_2\lambda_3 - \lambda_1\lambda_4 \cos(\phi))^2 + 4\lambda_1^2\lambda_2^2 \sin^2(\phi) + 4\lambda_1^2\lambda_3^2 \sin^2(\phi) + 8\lambda_1^2\lambda_4^2 \sin^2(\phi). 
\end{align*}
\]

(80)

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