Bell’s Inequality, Generalized Concurrence and Entanglement in Qubits

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Abstract

We demonstrate an alternative evaluation of quantum entanglement by measuring maximum violation of Bell’s inequality without performing a partial trace operation in an \(n\)-qubit system by bridging maximum violation of Bell’s inequality and a generalized concurrence of a pure state. We show that this proposal is realized when one subsystem only contains one qubit and a quantum state is a linear combination of two product states. We also use a toric code model with smooth and rough boundary conditions on a cylinder manifold and a disk manifold with holes to show that a choice of a generalized concurrence of a pure state depends on boundary degrees of freedom of a Hilbert space. A relation of a generalized concurrence of a pure state and maximum violation of Bell’s inequality is also demonstrated in a \(2n\)-qubit state. Finally, we apply our theoretical studies to a two-qubit system with a non-uniform magnetic field at a finite temperature as well as a Wen-Plaquette model with four and six qubits at zero temperature.

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1 Introduction

Quantum mechanics is a fundamental theory in our nature and expected to be included in all fundamental theories. Especially at a low energy regime, atomic physics experiments provide abundant evidence supporting that counterintuitive quantum mechanics governs our microscopic world. This leads us to study entanglement, quantum information [1], quantum algorithm [2] and Bell’s inequality [3, 4].

Entanglement is a physical phenomenon, which can be contributed by quantum configurations and classical configurations. The quantum configuration of the entanglement is called quantum entanglement, which occurs when a quantum state of each particle cannot be factorized. Thus, the quantum entanglement is a physical phenomenon in a pure state. When we consider a mixed state, the mixed state is a liner combination of pure states with a probability distribution function. The probability distribution function provides the classical configurations of the entanglement.

Entanglement is one property to characterize the quantumness of a system. The most significant measure of entanglement is given by the entanglement entropy,

$$S_A = -\text{Tr} \rho_A \ln \rho_A$$  \hspace{1cm} (1)

with

$$\rho_A = \text{Tr}_B \rho$$  \hspace{1cm} (2)

being a reduced density matrix of a subsystem $A$ and $\rho$ being a density matrix of a Hilbert space

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B.$$  \hspace{1cm} (3)

In other words, entanglement entropy can characterize entanglement between two complementary subsystems $A$ and $B$. Entanglement entropy has been observed experimentally in a two-qubit system, but measuring entanglement entropy in a higher-qubit system is still under development.

One interesting study of entanglement entropy in an $n$-qubit system is topological entanglement entropy [5]. The topological entanglement entropy is a universal term of entanglement entropy. This universal term can show a number of distinct quasi-particles when subregions are contractible [5, 6] and the topological entanglement entropy is also demonstrated in ground states of a (2+1) dimensional toric code model [7, 8, 9] and ground states of a (2+1)-dimensional Wen-Plaquette model [10].
An experimental study of the lattice topological system has new progress. The ground states of the toric code model is already observed in [11] by using a $^{13}$C-labeled trichloroethylene molecule and the ground states in the Wen-Plaquette model with four sites were also measured in the Iodotrifluoroethylene ($C_2F_3I$) [12, 13] by using geometric algebra procedures [14], which can give a four-body interaction [12, 13] from a combination of two-body interactions and radio-frequency pulses [14, 15]. The topological entanglement entropy in (2+1)-dimensional lattice topological systems also plays a role of a topological order, which is also already measured in [13] by observing a modular matrix. Thus, a study of entanglement in an $n$-qubit system should be interesting for theoretical physics and experimental physics.

A qualitative detection of quantum entanglement can be performed experimentally by an observation of violation of Bell’s inequality [3], which is originally proposed by John S. Bell [4]. It was proven that correlations between different measurements of two separated particles must satisfy the inequality under local realism, which means that speed of transmitting of information cannot be faster than speed of light and any measurement should have a physical value before we measure. The violation of the constraints (the Bell’s inequality) also indicates quantum effect of correlations in a system, which can be presented in two-qubit systems theoretically [16]. Although violation of the Bell’s inequality may not present quantum entanglement in a generic quantum state, a relation between quantum entanglement, measured in terms of the concurrence [17], and violation of the Bell’s inequality was shown in two-qubit systems [18, 19]. An upper bound of Bell’s inequality for some three qubit quantum states is also studied in [20].

In this paper, we study relations between maximum violation of Bell’s inequality of an $n$-qubit Bell’s operator [21, 22] and a generalized concurrence of a pure state when the qubit operator on each site in a Bell’s operator is $\mathbf{n} \cdot \sigma$, where $\mathbf{n}$ is a unit vector and $\sigma$ is a vector of Pauli matrices. At first glance, a quantitative entanglement measure by Bell’s inequality is difficult because quantum entanglement depends on a partial trace operation in a system, but Bell’s inequality does not. Thus, a connection of maximum violation of Bell’s inequality and measures of quantum entanglement provides an interesting application of an entanglement measure without performing a partial trace operation to indirectly detect entanglement quantities.

To exhibit entanglement entropy from maximum violation of Bell’s inequality, we need to introduce a generalized concurrence for a pure state. We demonstrate this study in a toric code model [7] on a cylinder manifold [23] and find that a choice of a generalized concurrence of a pure state depends on boundary degrees of freedom of a
Hilbert space. The relation can be found because we consider that sub-regions can be non-contractible. On a disk manifold, we show that the relation cannot be found in a toric code model. To enhance our observed result, we also provide a 2n-qubit quantum state to compute maximum violation of Bell’s inequality to understand a choice of a generalized concurrence of a pure state, which should depend on degrees of freedom of a sub-Hilbert space.

We also apply our theoretical studies to a two-qubit system and a (2+1)-dimensional Wen-Plaquette model [10]. In a two-qubit system, we consider an XY-type interaction with a non-uniform magnetic field at a finite temperature. We find that the critical temperature, where the mixed state concurrence vanishes, does not depend on a magnetic field when the magnetic field is uniform. It is interesting to observe the dependence of the critical temperature on a non-uniform parameter of the magnetic field in an experiment. In a Wen-Plaquette model, we find that an upper bound of maximum violation of Bell’s inequality can indicate that ground states are maximally entangled [22] from a maximum generalized concurrence. The use of the maximally entangled property for six-qubit quantum states in a Wen-Plaquette model can give topological entanglement entropy through an upper bound of maximum violation of Bell’s inequality [22].

The structure of this paper is as follows. We first study a relation between quantum entanglement and maximum violation of Bell’s inequality when we only consider that each quantum state is just a linear combination of two product states in Sec. 2 and use a (2+1)-dimensional toric code model and a 2n-qubit quantum state to demonstrate how to choose a generalized concurrence of the pure state to obtain a relation between quantum entanglement and maximum violation of Bell’s inequality in Sec. 3 and Sec. 4. We also apply our theoretical result to a two-qubit system and a (2+1)-dimensional Wen-Plaquette model in Sec. 5 and Sec. 6. Finally, we discuss and conclude in Sec. 7.

2 Entanglement and Maximum Violation

A Bell’s operator of n qubits is defined iteratively as $B_n$ [21]:

$$B_n = B_{n-1} \otimes \frac{1}{2} \left( A_n + A'_n \right) + B'_{n-1} \otimes \frac{1}{2} \left( A_n - A'_n \right),$$

where

$$A_n = a_n \cdot \sigma, \quad A'_n = a'_n \cdot \sigma$$

are the operators in the n-th qubit with $a_n$ and $a'_n$ being unit vectors and

$$\sigma = (\sigma_x, \sigma_y, \sigma_z)$$

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being a vector of the Pauli matrices. The \((n-1)\)-qubit operators \(\frac{1}{2}B_{n-1}\) and \(\frac{1}{2}B'_{n-1}\) act on the rest of the qubits. Notice that we choose

\[
\frac{1}{2}B_1 = b \cdot \sigma, \quad \frac{1}{2}B'_1 = b' \cdot \sigma
\]

with \(b\) and \(b'\) being unit vectors. It is known that for an \(n\)-qubit system, the upper bound of the expectation value of the Bell’s operator \([21]\)

\[
\text{Tr}(\rho B_n) \leq 2^{\frac{n+1}{2}}
\]

leads to violation of the Bell-CHSH inequality \([3]\).

For a given density matrix \(\rho\), a maximum expectation value of a Bell’s operator is called maximum violation of Bell’s inequality. Here we prove a relation between maximum violation of the Bell’s inequality and a concurrence of a pure state (an entanglement quantity) in an \(n\)-qubit system \([22]\) when the all \(i\)-th operators in the Bell’s operator are \(A_i\) and \(A'_i\) for \(2 \leq i < n\):

\[
\tilde{B}_n = B_1 \otimes A_2 \otimes A_3 \cdots \otimes A_{n-2} \otimes A_{n-1} \otimes \frac{1}{2} \left( A_n + A'_n \right) + B'_1 \otimes A'_2 \otimes A'_3 \cdots \otimes A'_{n-2} \otimes A'_{n-1} \otimes \frac{1}{2} \left( A_n - A'_n \right).
\]

To proceed our derivation, we introduce a generalized \(R\)-matrix

\[
R_{i_1i_2\cdots i_n} = \text{Tr}(\rho \sigma_{i_1} \otimes \sigma_{i_2} \otimes \cdots \otimes \sigma_{i_n}) \equiv R_{Ii_n},
\]

where \(\rho\) is a density matrix, \(\sigma_{i_\alpha}\) is the Pauli matrix labeled by \(i_\alpha = x, y, z\) with site indices \(\alpha = 1, 2, \cdots, n\). We express the generalized \(R\)-matrix as a \(3^{n-1} \times 3\) matrix \(R_{Ii_n}\) with the first index being a multi-index \(I = i_1i_2\cdots i_{n-1}\) and the second index being \(i_n\).

In a two-qubit system, maximum violation of the Bell’s inequality is computed from a \(3 \times 3\) matrix \(R_{ij} \) \([19]\), which is a special case of the generalized \(R\)-matrix. Now we use the generalized \(R\)-matrix to generalize the maximum violation of the Bell’s inequality \((\tilde{B}_n)\) in an \(n\)-qubit system \([22]\).

**Lemma 1.** The maximum violation of the Bell’s inequalities has the following relation:

\[
\gamma \equiv \max_{\tilde{B}_n} \text{Tr}(\rho \tilde{B}_n) \leq 2\sqrt{u_1^2 + u_2^2},
\]

where \(u_1^2\) and \(u_2^2\) are the first two largest eigenvalues of the matrix \(R^\dagger R\) when \(n > 2\) and

\[
\gamma = 2\sqrt{u_1^2 + u_2^2}
\]

when \(n = 2\). Note that the matrix \(R^\dagger R\) is contracted over the multi-index \(I\).
Proof. We first introduce two three-dimensional orthonormal vectors \( \hat{c} \) and \( \hat{c}' \) such that:

\[
\hat{a} + \hat{a}' = 2\hat{c}\cos \theta, \quad \hat{a} - \hat{a}' = 2\hat{c}'\sin \theta,
\]

where \( \theta \in [0, \frac{1}{2}\pi] \), through three-dimensional unit vectors \( \hat{a} \) and \( \hat{a}' \). The maximum violation of the Bell’s inequality is defined as

\[
\gamma \equiv \max_{\tilde{B}_n} \text{Tr}(\rho \tilde{B}_n)
\]

with the Bell’s operator of \( n \)-qubit \( \tilde{B}_n \) defined in [9]. By using the generalized \( R \)-matrix and the unit vectors:

\[
\begin{align*}
\hat{B} & \equiv \hat{B}_I = \hat{B}_{i_1 i_2 \cdots i_{n-1}} \equiv \hat{a}_{1,i_1} \hat{a}_{2,i_2} \cdots \hat{a}_{n-1,i_{n-1}}, \\
\hat{B}' & \equiv \hat{B}'_I = \hat{B}'_{i_1 i_2 \cdots i_{n-1}} \equiv \hat{a}'_{1,i_1} \hat{a}'_{2,i_2} \cdots \hat{a}'_{n-1,i_{n-1}}, \\
\hat{a} & \equiv \hat{a}_{n,i_n}, \\
\hat{a}' & \equiv \hat{a}'_{n,i_n},
\end{align*}
\]

in which \( \hat{B} \) and \( \hat{B}' \) are unit vectors in \( 3^{n-1} \) dimensions, we have:

\[
\gamma = \max_{\hat{B}, \hat{B}', \hat{a}, \hat{a}'} \left( \langle \hat{B}, R(\hat{a} + \hat{a}') \rangle + \langle \hat{B}', R(\hat{a} - \hat{a}') \rangle \right)
\leq \max_{\hat{c}, \hat{c}', \theta} \left( 2||R\hat{c}|| \cos \theta + 2||R\hat{c}'|| \sin \theta \right) = 2\sqrt{u_1^2 + u_2^2},
\]

in which \( u_1^2 \) and \( u_2^2 \) are the first two largest eigenvalues of the matrix \( R^\dagger R \). The inner product and the norm are defined as:

\[
\langle P, Q \rangle \equiv P^\dagger Q, \quad ||U|| \equiv \sqrt{U^\dagger U}.
\]

Because \( R(\hat{a} + \hat{a}') \) and \( R(\hat{a} - \hat{a}') \) are defined in \( 3^{n-1} \) dimensions and each unit vector \( \hat{B} \) and \( \hat{B}' \) only contains \( 2(n-1) \) parameters, there is no guarantee that

\[
\hat{B} = k_1 R(\hat{a} + \hat{a}'), \quad \hat{B}' = k_2 R(\hat{a} - \hat{a}'),
\]

except for \( n = 2 \), where \( k_1 \) and \( k_2 \) are two arbitrary constants. \( \square \)

An earlier approach to relate the maximum violation of the Bell’s inequality and the concurrence of a pure state [17]

\[
C(\psi) \equiv \sqrt{2(1 - \text{Tr} \rho_A^2)}
\]

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in a two-qubit system is discussed in [18].

Now we generalize the relation of the maximum violation of the Bell’s inequality and the concurrence of a pure state in an $n$-qubit system, which still monotonically increases with respect to entanglement entropy, when a quantum state is a linear combination of two product states. The concurrence of the pure state is computed with respect to the bipartition with $(n - 1)$ qubits in a subsystem $B$ and one qubit in a subsystem $A$.

**Theorem 1.** We consider an $n$-qubit state

$$|\psi\rangle = |u\rangle_B \otimes (\lambda_+|v\rangle_B \otimes |1\rangle_A + \lambda_-|\bar{v}\rangle_B \otimes |0\rangle_A)$$

(20)

with $\lambda_+|v\rangle_B \otimes |1\rangle_A + \lambda_-|\bar{v}\rangle_B \otimes |0\rangle_A$ being a non-biseparable, $\alpha$-qubit state, $|u\rangle_B$, $|v\rangle_B$, $|\bar{v}\rangle_B$ being product states consisting of $|0\rangle$’s and $|1\rangle$’s. The state $|v\rangle_B$ is orthogonal to the state $|\bar{v}\rangle_B$ by choosing opposite bits on each site. Coefficients $\lambda_+$ and $\lambda_-$ are real numbers and $\lambda_+^2 + \lambda_-^2 = 1$. The maximum violation of the Bell’s inequality in an $n$-qubit system is

$$\gamma = 2f_\alpha(\psi),$$

(21)

in which the function $f_\alpha(\psi)$ is defined as:

(1) $\alpha$ is an even number:

$$f_\alpha(\psi) \equiv \sqrt{1 + 2^{\alpha-2}C^2(\psi)},$$

$$f_\alpha(\psi) \equiv 2^{\frac{\alpha-1}{2}}C(\psi),$$

(22)

(2) $\alpha$ is an odd number:

$$f_\alpha(\psi) \equiv \sqrt{1 + \left(2^{\alpha-2} - 1\right)C^2(\psi)},$$

$$f_\alpha(\psi) \equiv 2^{\frac{\alpha-1}{2}}C(\psi),$$

(23)

Here $C(\psi)$ is the concurrence of the pure state computed with respect to the bipartition that the subsystem $B$ contains $(n - 1)$ qubits and the subsystem $A$ contains one qubit.

**Proof.** The Hilbert space of an $n$-qubit system is bipartitioned as

$$\mathbb{H} = \mathbb{H}_B \otimes \mathbb{H}_A,$$

(24)

in which dimensions of the sub-Hilbert spaces are:

$$\dim(\mathbb{H}_A) = 2, \quad \dim(\mathbb{H}_B) = 2^{n-1}.$$
We consider a quantum state with respect to this bipartition
\[
|\psi\rangle = |u\rangle_B \otimes (\lambda_+|v\rangle_B \otimes |1\rangle_A + \lambda_-|\bar{v}\rangle_B \otimes |0\rangle_A),
\]
where \(|u\rangle_B \otimes |v\rangle_B\) and \(|u\rangle_B \otimes |\bar{v}\rangle_B\) are the product states in \(\mathbb{H}_B\) and \(|1\rangle_A\) and \(|0\rangle_A\) are the product states in \(\mathbb{H}_A\). By using the property:
\[
\text{Tr} \rho_A = \lambda_+^2 + \lambda_-^2 = 1, \quad C(\psi) = \sqrt{2(1 - \lambda_+^4 - \lambda_-^4)},
\]
the coefficients \(\lambda_\pm\) can be expressed in terms of the concurrence,
\[
\lambda_\pm^2 = \left(1 \pm \sqrt{1 - C^2(\psi)}\right)/2.
\]

The generalized \(R\)-matrix is:
\[
R_{Ix} = \lambda_+ \lambda_- \text{Tr} [\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} (|v\rangle \langle v| + |\bar{v}\rangle \langle v|)],
\]
\[
R_{Iy} = -i \lambda_+ \lambda_- \text{Tr} [\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} (|v\rangle \langle v| - |\bar{v}\rangle \langle v|)],
\]
\[
R_{Iz} = -\lambda_+^2 \text{Tr} [\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |v\rangle \langle v|] + \lambda_-^2 \text{Tr} [\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |\bar{v}\rangle \langle \bar{v}|],
\]
where \(I \equiv I_1 I_2\) concatenating two strings of indices:
\[
I_1 \equiv i_1 \cdots i_{n-\alpha-1}, \quad I_2 \equiv i_{n-\alpha} \cdots i_{n-1},
\]
and
\[
\sigma_{I_1} \equiv \sigma_1 \otimes \cdots \otimes \sigma_{i_{n-\alpha-1}}, \quad \sigma_{I_2} \equiv \sigma_{n-\alpha} \otimes \cdots \otimes \sigma_{i_{n-1}}.
\]

Here we choose the basis that \(|0\rangle \equiv (1, 0)^T\) and \(|1\rangle \equiv (0, 1)^T\). One should notice that the dimensions of \(|u\rangle\langle u|\) is \(2^{n-\alpha}\), and the dimensions of \(|v\rangle\langle v|\), \(|\bar{v}\rangle\langle \bar{v}|\), \(|v\rangle\langle \bar{v}|\), and \(|\bar{v}\rangle\langle v|\) are \(2^{\alpha-1}\). The non-vanishing matrix elements of \(R_{I\alpha}\), \(\alpha = x, y, z\), come from the diagonal matrix elements of \(\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |v\rangle \langle v|\), \(\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |\bar{v}\rangle \langle \bar{v}|\), \(\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |\bar{v}\rangle \langle \bar{v}|\), and \(\sigma_{I_1} |u\rangle \langle u| \otimes \sigma_{I_2} |v\rangle \langle v|\). Then the conditions of non-vanishing matrix elements of \(R_{I\alpha}\), where \(\alpha = x, y, z\), require that \(\sigma_{I_1} |u\rangle \rightarrow |u\rangle\), \(\sigma_{I_2} |\bar{v}\rangle \rightarrow |v\rangle\), and \(\sigma_{I_2} |v\rangle \rightarrow |\bar{v}\rangle\) for \(R_{Ix}\) and \(\sigma_{I_2} |u\rangle \rightarrow |u\rangle\), \(\sigma_{I_2} |v\rangle \rightarrow |v\rangle\), and \(\sigma_{I_2} |\bar{v}\rangle \rightarrow |\bar{v}\rangle\) for \(R_{Iz}\).

The conditions of the non-vanishing matrix elements \(R_{Iz}\) are \((n - \alpha)\) number of \(\sigma_z\) matrices in indices \(I_1\), \((\alpha - 1 - i)\) number of \(\sigma_x\) matrices and \(i\) number of \(\sigma_y\) matrices in indices \(I_2\) with \(i\) being an even integer. The conditions of the non-vanishing matrix elements \(R_{Iy}\) are \((n - \alpha)\) number of \(\sigma_z\) matrices in indices \(I_1\), \((\alpha - 1 - j)\) number of \(\sigma_x\) matrices and \(j\) number of \(\sigma_y\) matrices in indices \(I_2\) with \(j\) being an odd integer. The
conditions of the non-vanishing matrix elements $R_{Iz}$ are $(n-\alpha)$ number of $\sigma_z$ matrices in indices $I_1$, $(\alpha-1)$ number of $\sigma_z$ matrices in indices $I_2$.

The above conditions lead to a diagonal form of a matrix $R^\dagger R$. In the case that $\alpha$ is an even integer, the eigenvalues of the matrix $R^\dagger R$ are:

\[
(1 + C_2^{-m} + C_4^{-m} + \cdots + C_{n-1}^{-m})C^2(\psi) = 2^{n-2}C^2(\psi),
\]

\[
(1 + C_2^{-m} + C_4^{-m} + \cdots + C_{n-1}^{-m})C^2(\psi) = 2^{n-2}C^2(\psi),
\]

\[
1.
\]

In the case that the integer $\alpha$ is an odd integer, the eigenvalues of the matrix $R^\dagger R$ are:

\[
(1 + C_2^{-m} + C_4^{-m} + \cdots + C_{n-1}^{-m})C^2(\psi) = 2^{n-2}C^2(\psi),
\]

\[
(1 + C_2^{-m} + C_4^{-m} + \cdots + C_{n-1}^{-m})C^2(\psi) = 2^{n-2}C^2(\psi),
\]

\[
1 - C^2(\psi).
\]

We used $C_n = C_{k-1}^{-m} + C_{k-2}^{-m}$, which comes from each coefficient of $(1 + x)^n = (1 + x)^{n-1}(1 + x)$, to compute $(R^\dagger R)_{xx}$ and $(R^\dagger R)_{yy}$.

From the eigenvalues of the matrix $R^\dagger R$, we can obtain:

\[
f_\alpha(\psi) \equiv \sqrt{1 + 2^{n-2}C^2(\psi)}, \quad 2^{2-\alpha} \geq C^2(\psi),
\]

\[
f_\alpha(\psi) \equiv 2^{\frac{\alpha-1}{2}}C(\psi), \quad 2^{2-\alpha} \leq C^2(\psi). \quad (34)
\]

when $\alpha$ is an even number,

\[
f_\alpha(\psi) \equiv \sqrt{1 + \left(2^{n-2} - 1\right)C^2(\psi)}, \quad \frac{1}{1 + 2^{a-2}} \geq C^2(\psi),
\]

\[
f_\alpha(\psi) \equiv 2^{\frac{\alpha-1}{2}}C(\psi), \quad \frac{1}{1 + 2^{a-2}} \leq C^2(\psi). \quad (35)
\]

when $n$ is an odd number and

\[
\gamma \leq 2f_\alpha(\psi). \quad (36)
\]

Now we want to show

\[
\gamma = \max_{\hat{B},\hat{B}',\hat{a},\hat{a}'} \langle \hat{B}, R(\hat{a} + \hat{a}') \rangle + \langle \hat{B}', R(\hat{a} - \hat{a}') \rangle = 2\sqrt{u_1^2 + u_2^2}, \quad (37)
\]

in which $u_1^2$ and $u_2^2$ are the first two largest eigenvalues of the matrix $R^\dagger R$, and

\[
\hat{B} \equiv \hat{a}_{1,i_1,1,i_2} \cdots \hat{a}_{n-1,i_{n-1},1},
\]

\[
\hat{B}' \equiv \hat{a}'_{1,i_1,1,i_2} \cdots \hat{a}'_{n-1,i_{n-1},1},
\]

\[
\hat{a} \equiv \hat{a}_{n,i_n}
\]

\[
\hat{a}' \equiv \hat{a}'_{n,i_n}, \quad (38)
\]

\[\]
where

\[ \hat{a}_{n,i} + \hat{a}'_{n,i} \equiv 2\hat{c}_{n,i} \cos \theta, \quad \hat{a}_{n,i} - \hat{a}'_{n,i} \equiv 2\hat{c}'_{n,i} \sin \theta, \quad \theta \in [0, \pi/2]. \] (39)

This equality holds when

\[ \hat{B} = k_1 R(\hat{a} + \hat{a}'), \quad \hat{B}' = k_2 R(\hat{a} - \hat{a}'), \] (40)

where \( k_1 \) and \( k_2 \) are constants. One natural choice of \( a_{\alpha,i} \) and \( a'_{\alpha,i} \) can be obtained by equating two ratios:

\[ \left| \frac{R_{Ix}(\hat{a}_x + \hat{a}'_x)}{R_{Iy}(\hat{a}_y + \hat{a}'_y)} \right| = \left| \frac{B_I}{B'_I} \right|, \quad \left| \frac{R_{Ix}(\hat{a}_x - \hat{a}'_x)}{R_{Iy}(\hat{a}_y - \hat{a}'_y)} \right| = \left| \frac{B'_I}{B''_I} \right|, \] (41)

where \( I \) and \( I' \) are chosen in a way that one site of the multi-index \( I_2 \) in indices \( I \) is labeled by \( x \) and in indices \( I' \) is labeled by \( y \), and other sites of the indices \( I_2 \) in indices \( I \) and indices \( I' \) are labeled by the same symbols. This leads to:

\[ \left| \frac{\hat{a}_{I,x}}{\hat{a}'_{I',y}} \right| = \left| \frac{\hat{c}_{n,x}}{\hat{c}_{n,y}} \right|, \quad \left| \frac{\hat{a}'_{I,x}}{\hat{a}'_{I',y}} \right| = \left| \frac{\hat{c}'_{n,x}}{\hat{c}'_{n,y}} \right|. \] (42)

When

\[ u_1^2 = (R^t R)_{xx}, \quad u_2^2 = (R^t R)_{yy}, \] (43)

we can choose:

\[ (\hat{c}_{n,x}, \hat{c}_{n,y}, \hat{c}_{n,z})^T = \frac{1}{\sqrt{2}} (1, 1, 0)^T, \quad (\hat{c}'_{n,x}, \hat{c}'_{n,y}, \hat{c}'_{n,z})^T = \frac{1}{\sqrt{2}} (1, -1, 0)^T, \]

\[ \cos(\theta) = \sin(\theta) = \frac{\sqrt{2}}{2} \] (44)

to show

\[ \gamma = 2 \sqrt{u_1^2 + u_2^2}. \] (45)

For the other case,

\[ u_1^2 = (R^t R)_{zz}, \quad u_2^2 = (R^t R)_{xx}, \] (46)

we can choose:

\[ (\hat{c}_{n,x}, \hat{c}_{n,y}, \hat{c}_{n,z})^T = (0, 0, 1)^T, \quad (\hat{c}'_{n,x}, \hat{c}'_{n,y}, \hat{c}'_{n,z})^T = \frac{1}{\sqrt{2}} (1, 1, 0)^T, \]

\[ \cos(\theta) = \frac{u_1}{\sqrt{u_1^2 + u_2^2}}, \quad \sin(\theta) = \frac{u_2}{\sqrt{u_1^2 + u_2^2}} \] (47)
to prove
\[ \gamma = 2 \sqrt{u_1^2 + u_2^2}. \] 
(48)

We prove that the maximum violation of the Bell’s inequality (\( \tilde{B}_n \)) is directly related to the concurrence of the pure state when the subsystem A only contains one qubit and the quantum state is a linear combination of two product states. Because the concurrence of the pure state also monotonically increases with respect to entanglement entropy, the maximum violation of the Bell’s inequality is also related to entanglement entropy directly. For the maximally entangled state with the maximum concurrence of the pure state
\[ C(\psi) = 1, \] 
(49)
the maximum violation of the Bell’s inequality:
\[ \gamma = 2^{n+1} \leq 2^{n+1} \] 
(50)
satisfies the upper bound of the Bell’s operator in an \( n \)-qubit system. Although we do not use the most generic form of the Bell’s operator, information of the quantum state is already contained in the \( n \)-th qubit operators. Thus, the computing of the generalized \( R \)-matrix can give the maximum violation of the Bell’s inequality (\( \tilde{B}_n \)) directly when a quantum state is a linear superposition of two product states.

Now we discuss the maximum violation of the Bell’s inequality of a mixed state. The mixed state of a density matrix is
\[ \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|, \] 
(51)
in which the sum of \( p_i \) is one. Because we have:
\[
\max_{\mathcal{B}_n} \text{Tr}(\rho \mathcal{B}_n) = \max_{\mathcal{B}_n} \text{Tr} \left( \sum_i p_i |\psi_i\rangle \langle \psi_i| \mathcal{B}_n \right) = \max_{\mathcal{B}_n} \sum_i p_i \langle \psi_i| \mathcal{B}_n |\psi_i\rangle \leq \sum_i p_i \cdot \max_{\mathcal{B}_n} \langle \psi_i| \mathcal{B}_n |\psi_i\rangle,
\] 
(52)
we can find that the maximum value of the maximum violation of the pure state should be an upper bound of the maximum violation of the mixed state, which is a linear
superposition of the pure states. The result is not surprising because the maximum value of the maximum violation of the Bell’s inequality is reached by choosing a Bell’s operator. When we consider a larger number of a linear combination of pure states, maximum violation of Bell’s inequality should be lower than or equal to maximum violation of Bell’s inequality of a lower number of a linear combination of pure states because a choice of the Bell’s operator depends on a choice of the pure states.

When we compute the maximum violation of the Bell’s inequality in a mixed state, we are interested in considering the minimum value of $2 \sum_i p_i f_\alpha (C(\psi_i))$ with respect to the probability distribution of the decomposition of the quantum states $p_i$ and the quantum states $\psi_i$:

$$2 \min_{p_i, \psi_i} \sum_i p_i f_\alpha (C(\psi_i)) \geq 2f_\alpha \left[ \min_{p_i, \psi_i} \left( \sum_i p_i C(\psi_i) \right) \right] \equiv 2f_\alpha (C(\rho_{AB})), \quad (53)$$

in which $C(\rho_{AB})$ is the concurrence of the mixed state:

$$C(\rho_{AB}) \equiv \min_{p_i, \psi_i} \sum_i p_i C(\psi_i), \quad \rho_{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (54)$$

to obtain maximum violation of Bell’s inequality in a particular decomposition of each pure state, which has the minimum concurrence of the pure state among the quantum states ($\psi_i$). Here we remind that the lower bound of $2 \min_{p_i, \psi_i} \sum_i p_i f_\alpha (C(\psi_i))$ can become

$$2 \min_{p_i, \psi_i} \sum_i p_i f_\alpha (C(\psi_i)) = 2f_\alpha (C(\rho_{AB})), \quad (55)$$

when we choose the partition. Thus, we could use the concurrence of the mixed state to obtain the upper bound of the maximum violation of the Bell’s inequality for the particular decomposition of the mixed state:

$$\max_{\mathcal{B}_n} \text{Tr}(\rho_{\mathcal{B}_n}) \leq 2f_\alpha (\rho_{AB}). \quad (56)$$

3 Generalized Concurrence, Entanglement Entropy and the Toric Code Model

We compute Rényi entropy [9, 8] in a toric code model [7] on a disk manifold, which can have an arbitrary number of holes, and a cylinder manifold [23] with boundary conditions. From our result of Rényi entropy, we can obtain a relation between a
generalized concurrence of a pure state and entanglement entropy. For the case of a disk manifold, we find that Rényi entropy always equals to entanglement entropy for any bipartition. For the case of a cylinder manifold, we consider a non-contractible region. Rényi entropy can be different from entanglement entropy [23]. The result is interesting because we can find that a choice of a "generalized concurrence" depends on boundary degrees of freedom of a Hilbert space in a toric code model. We first review a toric code model on a torus manifold, then compute Rényi entropy in a toric code model on a disk manifold and on a cylinder manifold. The generalized concurrence is useful for us to demonstrate a relation between the maximum violation of the Bell’s inequality and entanglement entropy in the next section or a 2\(n\)-qubit quantum state.

3.1 Review of a Toric Code on a Torus Manifold

We consider a lattice, which can be embedded in an arbitrary two dimensional surface. The simplest case is an \(L \times L\) square lattice with a periodic boundary condition which forms a torus. The Hilbert space of each site \(\mathcal{H}_i\) consists of a spin one-half degree of freedom and the total Hilbert space of a toric code model is a tensor product of the Hilbert space of each site as \(\mathcal{H} = \bigotimes_i \mathcal{H}_i\). The lattice model on a torus has \(L^2\) vertices and \(L^2\) plaquettes. Since the dimensions of the Hilbert space of each spin is two and the number of links on a square lattice is \(2L^2\), the total dimensions of the Hilbert space is \(2^{2L^2}\). The Hamiltonian of the toric code model is

\[
H = -\sum_v U_v A_v - \sum_p J_p B_p
\]

with \(U_v \geq 0\) and \(J_p \geq 0\), where

\[
A_v = \bigotimes_{i \in \text{star}(v)} \sigma^z_i = \sigma^z_{i_1} \otimes \sigma^z_{i_2} \otimes \sigma^z_{i_3} \otimes \sigma^z_{i_4}, \quad B_p = \bigotimes_{j \in \partial p} \sigma^x_j = \sigma^x_{j_1} \otimes \sigma^x_{j_2} \otimes \sigma^x_{j_3} \otimes \sigma^x_{j_4},
\]

in which the index \(i \in \text{star}(v)\) runs over all four edges around an vertex \(v\) and \(j \in \partial p\) goes around four edges on a boundary of a plaquette \(p\). We also remind that the operators \(A_v\) (vertex operators), and \(B_p\) (plaquette operators) act on the Hilbert space \(\mathcal{H}\) rather than acting on some local Hilbert spaces so the operators are trivial operators or identity operators for the sites, which are not in the vertex \(v\) and the plaquette \(p\).

To have a complete set of observables on a torus, it turns out that we also need two loop operators of two non-contractible cycles on a torus:

\[
Z(C_1) \equiv \bigotimes_{i \in C_1} \sigma^z_i, \quad X(C_2) = \bigotimes_{j \in C_2} \sigma^x_j,
\]

in which \(C_1\) and \(C_2\) are loops.
3.2 A Disk Manifold with Holes

We compute entanglement entropy in the toric code model on a disk manifold with an arbitrary number of holes. A non-zero number of holes on a disk manifold can increase ground state energy of the toric code model compared to ground state energy of the toric code model on the disk manifold without holes. This could be seen as a generation of anyons on a disk manifold through increasing a number of holes. Note that we pick boundary conditions, where an upper edge of the disk manifold and a right edge of the disk manifold are smooth boundary conditions and a lower edge of the disk manifold and the left edge of the disk manifold are rough boundary conditions. A vertex operator at a smooth boundary only acts on three qubits on the three links meeting at a vertex. A plaquette operator at a rough boundary lacks a qubit so it only acts on three qubits on the three links nearby.

When we do a bipartition, there are $(n_{L,v}, n_{L,c}, n_{R,v}, n_{R,c})$ anyons, where $L$ stands for a left region in the system and $R$ stands for a right region in the system, $v$ represents vortex particles, $c$ represents charge particles. In our convention, the vortex particles are created by $X$ operators acting on links and the charge particles are created by $Z$ operators acting on a dual lattice. For the convenience, we remove the vertex operators and plaquette operators corresponding to a position of the anyons so that the quantum state is in fact a ground state of the Hamiltonian. We also find that entanglement entropy of the disk manifold with a number of holes is independent of cutting because we can use vertex or the plaquette operators to deform $X$ and $Z$ operators, as shown in Fig. 1 and Fig. 2. The other decomposition method can be implemented by putting boundary conditions on the entangling surface. We can set the rough boundary on the left side of an entangling surface and set the smooth boundary condition on the right side of the entangling surface. A form of entanglement entropy is not modified.

We define a group $G$ as the group generated by all the plaquette operators, including those sitting at an edge and those at a position of anyons. Hence, the quantum state $|\Omega\rangle$, the ground state of the Hamiltonian without quasiparticles, can be written as:

$$|\Omega\rangle \equiv \frac{1}{\sqrt{|G|}} \sum_{g \in G} g|0\rangle = \frac{1}{\sqrt{|G|}} \sum_{g \in G} g|0_L\rangle \otimes |0_R\rangle,$$

where $|0_L\rangle$ and $|0_R\rangle$ are just shorthand expressions representing qubits live in a left

\footnote{It is also referred to a surface code model if a manifold is not a torus.}

\footnote{Now quantum states with the presence and the absence of anyons are all ground states of the Hamiltonian, we have a larger ground state degeneracy than a toric code model on a disk manifold without any hole.}
Figure 1: We can move the line operator creating charge anyons by applying plaquette operators on the edge as shown in Figure (a) or in the bulk as shown in Figure (b).

Figure 2: We can move the line operator creating vortex anyons by applying vertex operators on the edge as shown in Figure (a) or in the bulk as shown in Figure (b).
region and a right region. Therefore, the quantum state $|\psi\rangle$ on a disk manifold with holes can be written as:

$$|\psi\rangle = \prod_{i} X_{i,v}^{L} \prod_{i} Z_{i,c}^{L} \prod_{i} X_{i,v}^{R} \prod_{i} Z_{i,c}^{R} |\Omega\rangle$$

$$= \frac{1}{\sqrt{|G|}} \prod_{i} X_{i,v}^{L} \prod_{i} Z_{i,c}^{L} \prod_{i} X_{i,v}^{R} \prod_{i} Z_{i,c}^{R} \sum_{g \in G} g |0_{L}\rangle \otimes |0_{R}\rangle.$$

For convenience, we define:

$$E_{L} \equiv \prod_{i} X_{i,v}^{L} \prod_{i} Z_{i,c}^{L}, \quad E_{R} \equiv \prod_{i} X_{i,v}^{R} \prod_{i} Z_{i,c}^{R}, \quad E_{L}^{2} = 1, \quad E_{R}^{2} = 1, \quad (60)$$

and write $g \equiv g_{L} \otimes g_{R}$ and

$$|\psi\rangle = \frac{1}{\sqrt{|G|}} \sum_{g \in G} E_{L} g_{L} |0_{L}\rangle \otimes E_{R} g_{R} |0_{R}\rangle.$$

The operator $g_{L}$ and the operator $g_{R}$ do not contain a complete plaquette operators on an entangling surface. The operator $g_{L}$ only acts on one qubit for each plaquette operator and the action acts on three qubits for each plaquette operator on the entangling surface.

Each $X$ and $Z$ operator has one ending point attached to an edge and the other ending point fixed at where the corresponding anyon sits as in Fig. 3.

Now we have the reduced density matrix of the $L$ system (the notations we use here are summarized in the Table. 1 and the Table. 2):

$$\rho_{L} = \text{Tr}_{R} |\psi\rangle \langle \psi| = \frac{1}{|G|} \sum_{g,g' \in G} E_{L} g_{L} |0_{L}\rangle \langle 0_{L}| g_{L}' E_{L} \cdot \langle 0_{R}| g_{R}' E_{R} g_{R} |0_{R}\rangle$$

$$= \frac{1}{|G|} \sum_{g,g' \in G} E_{L} g_{L} |0_{L}\rangle \langle 0_{L}| g_{L}' E_{L} \cdot \langle 0_{R}| g_{R}' g_{R} |0_{R}\rangle$$

$$= \frac{1}{|G|} \sum_{g \in G} E_{L} g_{L} |0_{L}\rangle \langle 0_{L}| g_{L} \tilde{g}_{L} E_{L} \cdot \langle 0_{R}| \tilde{g}_{R} |0_{R}\rangle$$

$$= \frac{|G_{R}|}{|G|} \sum_{h \in G/G_{R}, \tilde{g} \in G_{L}} E_{L} h_{L} |0_{L}\rangle \langle 0_{L}| h_{L} \tilde{g}_{L} E_{L}, \quad (61)$$

where

$$\tilde{g}_{L} \equiv g_{L}' g_{L}, \quad \tilde{g}_{R} \equiv g_{R}' g_{R}. \quad (62)$$

Because the operator $g_{L}$ and the operator $g_{R}$ do not contain complete plaquette operators on the entangling surface, we remind our reader: $g_{L} \notin G_{L}$ and $g_{R} \notin G_{R}$, in which
Figure 3: Condensation of each type of anyons is created on the corresponding boundary, costing no energy to produce anyon at the boundary. An anyon in the bulk can be created by a string operator with one end attached to a suitable edge. Each blue line consists of a string of $X$ operators, which create vortex particle pairs. The orange lines are strings of $Z$ operators, which create charge particle pairs. Vortex particles condense at the rough boundary while charge particles condensed at the smooth boundary. By using the operation in Fig. 1 and Fig. 2 we can move any configuration of blue lines and orange lines with bulk ends fixed and boundary ends at their proper boundary to the configuration shown in this Figure. Note that qubits live on links.
$G_L$ is a group generated by all the plaquette operators fully supported on a left region and $G_R$ is a group generated by all the plaquette operators fully supported on a right region. We also remind that the operator $\tilde{g}_L$ and the operator $\tilde{g}_R$ do not contain any plaquette operator on an entangling surface.

| Notation   | Comment                                                                 |
|------------|-------------------------------------------------------------------------|
| $G_L$      | The group generated by all the plaquette operators fully supported on the left region, as illustrated in Fig. 4 (a). We also remind $g_L \notin G_L$. |
| $G_R$      | The group generated by all the plaquette operators fully supported on the right region, as illustrated in Fig. 4 (b). We also remind $g_R \notin G_R$. |
| $G$        | The group generated by all the plaquette operators, as illustrated in Fig. 4 (c). |
| $G/G_R$    | A quotient group. Each element is an equivalence class of elements of the group $G$ which have the same action on the left region, as illustrated in Fig. 5. |
| $G/(G_R \times G_L)$ | A quotient group. The representative of this quotient group are generated by the plaquette operators on a border. The size of this group is $2^{n_L}$, where $n_L$ is a number of plaquette operators on a border. This is illustrated by Fig. 6. |

Table 1: List of notations of the groups.

We used

$$\langle 0_R|\tilde{g}_R|0_R \rangle = \delta_{\tilde{g}_R,1}$$  \hspace{1cm} (63)
Figure 4: Illustration of groups $G$, $G_L$, and $G_R$. (a) The group $G_L$ is generated by plaquette operators supported on the left region. (b) The group $G_R$ is generated by plaquette operators supported on the left region. (c) The group $G$ is generated by plaquette operators on the whole region.

Figure 5: The illustration of $G/G_R$. Two group elements in $G$ colored by red and blue having the same action on the left region are in the same equivalence class $h$ colored by the purple.
| Notation | Comment |
|----------|---------|
| $g$      | An element of the group $G$. The element of the group $G$, $g = g_L \otimes g_R$, the operator $g_L$ is supported on the left region and the operator $g_R$ is supported on the right region. The operator $g$ is related to the operator $g'$ by $g' = g\tilde{g}$. We remind that the operator $g_L$ and the operator $g_R$ contain non-complete plaquette operators. |
| $g'$     | An element of the group $G$. The operator $g' = g_L' \otimes g_R'$, $g_L'$ is supported on the left region and the operator $g_R'$ is supported on the right region. The operator $g$ is related to the operator $g'$ by $g' = g\tilde{g}$. We remind that the operator $g_L'$ and the operator $g_R'$ contain non-complete plaquette operators. |
| $\tilde{g}$ | An element of the group $G$. The operator $\tilde{g} = \tilde{g}_L \otimes \tilde{g}_R$, the operator $\tilde{g}_L$ is supported on the left region, while the operator $\tilde{g}_R$ is supported on the right region. After the requirement that the operator is an identity operator on the right region, $\tilde{g}_R = \mathbb{I}$, the operator $\tilde{g}$ becomes an element of $G_L$. |
| $h$      | An element of the quotient group $G/G_R$. We also define the operator $h \equiv h_L \otimes h_R$. |

Table 2: List of notations of the operators.

In the third equality. Then we can obtain:

\[
\rho_L^2 = \frac{|G_R|^2}{|G|^2} \sum_{h, h' \in G/G_R, \tilde{g}, \tilde{g}' \in G_L} E_L h |0_L\rangle \langle 0_L| h\tilde{g}_L h'|0_L\rangle \langle 0_L|h'\tilde{g}'_LE_L \\
= \frac{|G_R|^2}{|G|^2} \sum_{h \in G/G_R, \tilde{g}, \tilde{g}' \in G_L} E_L h |0_L\rangle \langle 0_L| h\tilde{g}_L \tilde{g}'_LE_L \\
= \frac{|G_R|^2|G_L|}{|G|^2} \sum_{h \in G/G_R, \tilde{g} \in G_L} E_L h |0_L\rangle \langle 0_L| h\tilde{g}_L E_L \\
= \frac{|G_L||G_R|}{|G|^2} \rho_L \\
\equiv \lambda \rho_L, \tag{64}
\]

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Figure 6: Illustration of the group $G/(G_L \times G_R)$. The group is generated by plaquette operators living on the border.

where

$$\lambda \equiv \frac{|G_L||G_R|}{|G|} = 2^{-n_L}. \quad (65)$$

We used

$$\langle 0_L | h \tilde{g}_L h' | 0_L \rangle = \delta_{h', h \tilde{g}_L} \quad (66)$$

in the second equality. Thus, it is also easy to use the same way to obtain

$$\rho^n_L = \lambda^n \left( \frac{\rho_L}{\lambda} \right). \quad (67)$$

The Rényi entropy in the toric code model on a disk manifold with any number of holes is

$$S_\alpha \equiv \frac{1}{1 - \alpha} \ln \text{Tr} \rho^n_L = n_L \ln 2, \quad (68)$$

where $n_L$ is a number of plaquettes on the entangling surface between the region $L$ and the region $R$. In summary, entanglement entropy of the system with an arbitrary number of holes is

$$S_{EE,L} = S_\alpha = n_L \ln 2. \quad (69)$$

Note that at each hole, we can have two possibilities: presence and absence of an anyon. In this section, we consider the case where anyons are present at each hole. It turns out that all the other cases actually give the same Rényi entropy expression.
3.3 A Cylinder Manifold

We consider the toric code model on a cylinder manifold, cutting it into two non-contractible sub-cylinders, region $A$ and region $B$. The operators on a boundary of the cylinder manifold satisfy the periodic boundary conditions for the upper and lower sides of the cylinder manifold. We also set the rough (smooth) boundary conditions for other two sides. We can put boundary conditions on an entangling surface to decompose a region [9]. When we cut the cylinder manifold into two sub-cylinder manifolds, the operators on an entangling surface between the region $A$ and the region $B$ in the sub-cylinder manifolds satisfy the rough (smooth) boundary condition.

The toric code model on a cylinder manifold has two ground states [23]:

\[
|\psi_{00}\rangle = \frac{1}{\sqrt{2N_q}} \sum_{l=1}^{N_q} \left( |q_l = 0, 0_A\rangle |q_l = 0, 0_B\rangle + |q_l = 0, 1_A\rangle |q_l = 0, 1_B\rangle \right),
\]

\[
|\psi_{01}\rangle = \frac{1}{\sqrt{2N_q}} \sum_{l=1}^{N_q} \left( |q_l = 0, 0_A\rangle |q_l = 0, 1_B\rangle + |q_l = 0, 1_A\rangle |q_l = 0, 0_B\rangle \right),
\]

in which a crossing number to an entangling surface is always an even number, which is labeled by 0 at the first index of $q_l$, a winding number around the sub-cylinders $A$ or $B$ can be an even number, which is labeled by 0 at the second index of $q_l$, or an odd number, which is labeled by 0 at the second index of $q_l$, and $N_q = 2^{n_L-1}$, where $n_L$ is a number of plaquettes on an entangling surface. A generic ground state is

\[
|\psi\rangle = \alpha_{00} |\psi_{00}\rangle + \alpha_{01} |\psi_{01}\rangle.
\]

Thus, the reduced density matrix in the region $A$ is

\[
\rho_A = \frac{1}{2N_q} \sum_{l=1}^{N_q} \left( |\alpha_{00}|^2 + |\alpha_{01}|^2 \right) \left( |q_l = 0, 0_A\rangle \langle q_l = 0, 0_A| + |q_l = 0, 1_A\rangle \langle q_l = 0, 1_A| \right) \\
+ \left( \alpha_{00}^* \alpha_{01} + \alpha_{00} \alpha_{01}^* \right) \left( |q_l = 0, 0_A\rangle \langle q_l = 0, 1_A| + |q_l = 0, 1_A\rangle \langle q_l = 0, 0_A| \right).
\]

We can diagonalize the reduced density matrix of the region $A$ to obtain the eigenvalues of the reduced density matrix of the region $A$:

\[
\frac{1}{2N_q} |\alpha_{00} + \alpha_{01}|^2, \quad \frac{1}{2N_q} |\alpha_{00} - \alpha_{01}|^2,
\]

(73)
and the Rényi entropy is:

\[ S_n = \frac{1}{1-n} \ln \left( \left( \frac{1}{2N_q^n} \right)^n N_q \left( \sum_{i=1}^{2} (2p_i^n) \right) \right) = \ln N_q + \frac{1}{1-n} \ln \left( \sum_{i=1}^{2} p_i^n \right) \]

\[ = n_L \ln 2 - \left( \ln 2 - \frac{1}{1-n} \ln \left( \sum_{i=1}^{2} p_i^n \right) \right), \tag{74} \]

where

\[ p_1 \equiv \frac{1}{2}|a_{00} + a_{01}|^2, \quad p_2 \equiv \frac{1}{2}|a_{00} - a_{01}|^2, \quad p_1 + p_2 = 1. \tag{75} \]

Topological entanglement entropy is defined as a boundary independent part of entanglement entropy and from (74), it is \( \ln 2 + \sum_{i=1}^{2} p_i \ln p_i \). The maximum topological entanglement entropy is \( \ln 2 \). When \( p_i = 1/2 \) for each \( i \) we can get vanishing topological entanglement entropy:

\[ \ln 2 - \sum_{i} p_i \ln p_i = \ln 2 - \frac{1}{2} \ln 2 - \frac{1}{2} \ln 2 = \ln 2 - \ln 2 = 0. \tag{76} \]

Since we only have one independent parameter for \( p_i \) from the second Renyi entropy in (74), we have:

\[ (n_L - 1) \ln 2 + \ln \text{Tr} \rho_A^2 = \ln \left( 2p_1^2 - 2p_1 + 1 \right), \quad 2p_1^2 - 2p_1 + \left( 1 - 2^{n_L-1} \text{Tr} \rho_A^2 \right) = 0, \tag{77} \]

\[ p_1 = \frac{1 \pm \sqrt{1 - 2(1 - 2^{n_L-1} \text{Tr} \rho_A^2)}}{2}, \quad p_2 = \frac{1 \mp \sqrt{1 - 2(1 - 2^{n_L-1} \text{Tr} \rho_A^2)}}{2}. \tag{78} \]

By comparing (78) and (28), we find the entanglement entropy is quite similar to the entanglement entropy of the two qubits [17]. We can know that the entanglement entropy should monotonically increase by decreasing \( \text{Tr} \rho_A^2 \) and also find that the generalized concurrence of the pure state in a toric code model on a cylinder manifold is defined by

\[ C(n_A, \psi) \equiv \sqrt{2 \left( 1 - 2^{n_A-1} \text{Tr} \rho_A^2 \right)}. \tag{79} \]

If \( n_A = 1 \), a definition of the generalized concurrence of the pure state goes back to the concurrence of two qubits [17]. Even if \( n_A = 1 \), the entanglement entropy of the toric model on the cylinder manifold does not vanish, and has the contribution from classical
Shannon entropy because the region $A$ is non-contractible. Hence, it is interesting to obtain the generalized concurrence of the pure state between different regions in the toric code model. We also find that the factor $2^{n_A-1}$ in the concurrence of the pure state depend on boundary degrees of freedom of the Hilbert space. Thus, a relation between maximum violation of Bell’s inequality and entanglement entropy possibly be expressed in terms of the generalized concurrence $C(n_A, \psi)$ with corresponding boundary degrees of freedom of the Hilbert space in the toric code model.

4 Generalized Concurrence, Entanglement Entropy and $2n$ Qubits

Unlike entanglement entropy and generalized concurrence depending on a reduced density matrix, a measure of Bell’s inequality does not involve in the reduced density matrix and is not sensitive to a bipartition of a system. To relate the maximum violation of Bell’s inequality to entanglement entropy/generalized concurrence with respect to a different bipartition, we demonstrate a solvable case of $2n$ qubits example that the maximum violation of Bell’s inequality is bounded by a function of generalized concurrence depending on a bipartition.

We want to consider a solvable case for an arbitrary number of qubits so we choose a quantum state of $2n$ qubits:

$$|\psi\rangle = \frac{1}{\sqrt{2^n}}(\alpha_0 + \alpha_1) \left( |00 \cdots 00_A \rangle |00 \cdots 00_B\rangle + |00 \cdots 010_A \rangle |00 \cdots 010_B\rangle + \cdots + |11 \cdots 110_A \rangle |11 \cdots 110_B\rangle \right)$$

$$+ \frac{1}{\sqrt{2^n}}(\alpha_0 - \alpha_1) \left( |00 \cdots 01_A \rangle |00 \cdots 01_B\rangle + |00 \cdots 011_A \rangle |00 \cdots 011_B\rangle + \cdots + |11 \cdots 111_A \rangle |11 \cdots 111_B\rangle \right),$$

(80)

where each region $A$ and region $B$ contains $n$ qubits. For each region, apart from the last qubit, we consider a linear superposition of all possible configurations in the first $n-1$ qubits.

We also define the generalized concurrence of the pure state

$$C(m, \psi) = \sqrt{2 \left( 1 - 2^{m-1} \text{Tr} \rho_A^2 \right)}.$$  

(81)
The entanglement entropy of the region $A$ is

$$S_{EE,A} = (n - 1) \ln 2 - \frac{1}{2}(\alpha_0 + \alpha_1)^2 \ln \left( \frac{1}{2}(\alpha_0 + \alpha_1)^2 \right) - \frac{1}{2}(\alpha_0 - \alpha_1)^2 \ln \left( \frac{1}{2}(\alpha_0 - \alpha_1)^2 \right).$$

(82)

The coefficients $\alpha_0$ and $\alpha_1$ for $2n$ qubits also satisfy:

$$\frac{1}{2}(\alpha_0 + \alpha_1)^2 = \frac{1 \pm \sqrt{1 - C(n, \psi)^2}}{2}, \quad \frac{1}{2}(\alpha_0 - \alpha_1)^2 = \frac{1 \mp \sqrt{1 - C(n, \psi)^2}}{2}. \quad (83)$$

The entanglement entropy of the region $A$ also monotonically increases with respect to concurrence of the pure state $C(n, \psi)$.

To compute the upper bound of the maximum violation of the Bell’s inequality, we
need to compute:

\[
\begin{align*}
\text{Tr} & \left( (a_1 \otimes a_2 \otimes \cdots \otimes a_n) \otimes (a_1 \otimes a_2 \otimes \cdots \otimes a_n) \right) \\
& \times ((b_1^T \otimes b_2^T \otimes \cdots \otimes b_n^T) \otimes (b_1^T \otimes b_2^T \otimes \cdots \otimes b_n^T)) \\
& \times (\sigma_{i_1} \otimes \sigma_{i_2}) \otimes (\sigma_{i_3} \otimes \sigma_{i_4}) \otimes \cdots \otimes (\sigma_{i_{2n-1}} \otimes \sigma_{i_{2n}}) \\
& = \text{Tr} \left( (a_1 \otimes a_2 \otimes \cdots \otimes a_n) \cdot (b_1^T \otimes b_2^T \otimes \cdots \otimes b_n^T) \right) \\
& \otimes ((a_1 \otimes a_2 \otimes \cdots \otimes a_n) \cdot (b_1^T \otimes b_2^T \otimes \cdots \otimes b_n^T)) \\
& \times (\sigma_{i_1} \otimes \sigma_{i_2}) \otimes (\sigma_{i_3} \otimes \sigma_{i_4}) \otimes \cdots \otimes (\sigma_{i_{2n-1}} \otimes \sigma_{i_{2n}}) \\
& = \text{Tr} \left( ((a_1 b_1^T) \otimes (a_2 b_2^T)) \otimes \cdots \otimes ((a_n b_n^T)) \right) \otimes ((a_1 b_1^T) \otimes (a_2 b_2^T)) \otimes \cdots \otimes ((a_n b_n^T)) \\
& \times (\sigma_{i_1} \otimes \sigma_{i_2}) \otimes (\sigma_{i_3} \otimes \sigma_{i_4}) \otimes \cdots \otimes (\sigma_{i_{2n-1}} \otimes \sigma_{i_{2n}}) \\
& = \text{Tr} \left( ((a_1 b_1^T) \otimes (a_2 b_2^T)) \otimes \cdots \otimes ((a_n b_n^T)) \right) \times \text{Tr} \left( ((a_1 b_1^T) \otimes (a_2 b_2^T)) \otimes \cdots \otimes ((a_n b_n^T)) \right) \times \cdots \\
& \times \text{Tr} \left( ((a_1 b_1^T) \otimes (a_2 b_2^T)) \otimes \cdots \otimes ((a_n b_n^T)) \right) \\
& = \text{Tr} \left( (\sigma_{i_1} \otimes \sigma_{i_2}) \cdot ((a_1 b_1^T) \otimes (a_2 b_2^T)) \right) \times \text{Tr} \left( (\sigma_{i_3} \otimes \sigma_{i_4}) \cdot ((a_3 b_3^T) \otimes (a_4 b_4^T)) \right) \times \cdots \\
& \times \text{Tr} \left( (\sigma_{i_{2n-1}} \otimes \sigma_{i_{2n}}) \cdot ((a_n b_n^T)) \right) \\
& = \text{Tr} \left( (\sigma_{i_1} a_1 b_1^T) \otimes (\sigma_{i_2} a_2 b_2^T) \right) \times \text{Tr} \left( (\sigma_{i_3} a_3 b_3^T) \otimes (\sigma_{i_4} a_4 b_4^T) \right) \times \cdots \\
& \times \text{Tr} \left( (\sigma_{i_{2n-1}} a_{n-1} b_{n-1}^T) \otimes (\sigma_{i_{2n}} a_n b_n^T) \right) \\
& = \text{Tr} \left( (\sigma_{i_1} a_1 b_1^T) \right) \times \text{Tr} \left( (\sigma_{i_2} a_2 b_2^T) \right) \times \cdots \times \text{Tr} \left( (\sigma_{i_n} a_n b_n^T) \right) \times \text{Tr} \left( (\sigma_{i_{n+1}} a_{n+1} b_{n+1}^T) \right) \times \text{Tr} \left( (\sigma_{i_{n+2}} a_{n+2} b_{n+2}^T) \right) \times \cdots \\
& \times \text{Tr} \left( (\sigma_{i_{2n}} a_{2n} b_{2n}^T) \right). 
\end{align*}
\]
where the notation $\otimes$ represents a tensor product of matrices while $\times$ and $\cdot$ stand for a matrix multiplication, a scalar multiplication or a dyad product, depending on the context. The two-component vectors $a_i$ and $b_j$ can be
\begin{equation}
\begin{pmatrix}
1 \\
0
\end{pmatrix}
\quad \text{or} \quad
\begin{pmatrix}
0 \\
1
\end{pmatrix}.
\end{equation}
(85)

To obtain the eigenvalues of the matrix $R^\dagger R$, we list the following useful identities:
\begin{align*}
\text{Tr} \left[ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] &= 1, \\
\text{Tr} \left[ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \right] &= 1, \\
\text{Tr} \left[ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \right] &= i, \\
\text{Tr} \left[ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \right] &= -i, \\
\text{Tr} \left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \right] &= 1, \\
\text{Tr} \left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \right] &= -1.
\end{align*}
(86)

Now we first compute and discuss the maximum violation of the Bell’s inequality for $n = 2$. The non-vanishing elements of the generalized $R$-matrix are:
\begin{align*}
R_{xxxx} &= R_{yxyx} = R_{zxxz} = \frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1) + \frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1), \\
R_{xyxy} &= R_{zyzy} = -\frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1) - \frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1), \\
R_{yyzy} &= \frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1) + \frac{1}{2}(\alpha_0 + \alpha_1)(\alpha_0 - \alpha_1), \\
R_{xxxx} &= R_{zxxz} = \frac{1}{2}(\alpha_0 + \alpha_1)^2 + \frac{1}{2}(\alpha_0 - \alpha_1)^2 = 1, \\
R_{yzyz} &= -\frac{1}{2}(\alpha_0 + \alpha_1)^2 - \frac{1}{2}(\alpha_0 - \alpha_1)^2 = -1.
\end{align*}
(87)

Thus, the eigenvalues of the matrix $R^\dagger R$ are:
\begin{align*}
3C^2(\psi), \quad 3C^2(\psi), \quad 3.
\end{align*}
(88)

Now we can obtain the upper bound of the maximum violation of the Bell’s inequality:
\begin{equation}
\gamma \leq 2\sqrt{3}\sqrt{1 + C^2(\psi)}.
\end{equation}
(89)

Now we consider different bipartitions, the quantum state can be rewritten as
\begin{equation}
|\psi\rangle = \frac{1}{2}(\alpha_0 + \alpha_1)(|000\rangle + |101\rangle)|0_B\rangle + \frac{1}{2}(\alpha_0 - \alpha_1)(|010\rangle + |111\rangle)|1_B\rangle.
\end{equation}
(90)
Then we can find:
\[
\frac{1}{2}(\alpha_0 + \alpha_1)^2 = \frac{1 \pm \sqrt{1 - C(1, \psi)^2}}{2},
\]
the entanglement entropy of the region \(A\) is
\[
S_{EE,A} = -\frac{1}{2}(\alpha_0 + \alpha_1)^2 \ln \left( \frac{1}{2}(\alpha_0 + \alpha_1)^2 \right) - \frac{1}{2}(\alpha_0 - \alpha_1)^2 \ln \left( \frac{1}{2}(\alpha_0 - \alpha_1)^2 \right),
\]
and the upper bound of the maximum violation of the Bell’s inequality is
\[
\gamma \leq 2\sqrt{3}\sqrt{1 + C^2(1, \psi)}.
\]
The entanglement entropy of the region \(A\) also monotonically increases with respect to the concurrence of the pure state \(C(1, \psi)\). Although the bipartition does not affect the maximum violation of the Bell’s inequality, we can use the concurrence of the pure state to express intensity of entanglement entropy or how large of entanglement entropy for the corresponding bipartition from the upper bound of the maximum violation of the Bell’s inequality.

This example also shows that even if a quantum state is not just a linear combination of two product states, the upper bound of the maximum violation of the Bell’s inequality still directly exhibit intensity of entanglement entropy.

For a generalization of an arbitrary number of \(n\), it is easy to obtain the upper bound of the maximum violation of the Bell’s inequality:
\[
\gamma \leq 2\sqrt{3^{n-1}}\sqrt{1 + C^2(n, \psi)}.
\]
When we consider \(\alpha_0 = 1\) and \(\alpha_1 = 0\), entanglement entropy reaches the maximum, but the maximum violation of Bell’s inequality does not reach \(2^{n+1}\). In other words, entanglement entropy should not contain all entanglement information. It is interesting to note that the upper bound of the maximum violation of the Bell’s inequality is expressed in terms of a corresponding generalized concurrence of the pure state to obtain meaning of quantum entanglement. For each \(n\), we can find that the quantum state of the region \(A\) contains \(2^n\) different quantum states. Thus, a choice of the generalized concurrence of the pure state also matches the degrees of freedom of the Hilbert space.

5 Applications to a Two-Qubit System

We apply our theoretical results to a two qubits system at zero temperature and a finite temperature and use the concurrence to obtain the maximum violation of the Bell’s inequality.
5.1 Zero Temperature

We consider the 2-qubit XY model with the non-uniform magnetic field:

\[ H_{2\text{qubits}} = -\frac{J}{2}(1 + \gamma)\sigma_x \otimes \sigma_x - \frac{J}{2}(1 - \gamma)\sigma_y \otimes \sigma_y - B(1 + \delta)\sigma_z \otimes I - B(1 - \delta)I \otimes \sigma_z, \]  

where \( 0 \leq \gamma \leq 1, \quad 0 \leq \delta \leq 1, \quad J \geq 0, \quad B \geq 0. \)  

Thus, the Hamiltonian is:

\[ H_{2\text{qubits}} = -\frac{J}{2}(1 + \gamma)\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} - \frac{J}{2}(1 - \gamma)\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} - B(1 + \delta)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} - B(1 - \delta)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -2B & 0 & 0 & -J\gamma \\ 0 & 2B\delta & -J & 0 \\ 0 & -J & -2B\delta & 0 \\ -J\gamma & 0 & 0 & 2B \end{pmatrix}. \]  

To obtain eigenvalues \( \{\lambda_i\} \) of the Hamiltonian easily, we first choose:

\[ |\Psi_1\rangle = \begin{pmatrix} a \\ 0 \\ 0 \\ b \end{pmatrix}, \quad H_{2\text{qubits}}|\Psi_1\rangle = \lambda_1|\Psi_1\rangle. \]  

We can find the eigenvalues and its eigenstates:

\[ \lambda_{1,\pm} = \pm\sqrt{4B^2 + J^2\gamma^2}, \]  

\[ |\Psi_{1,\pm}\rangle = \begin{pmatrix} \sqrt{\frac{|\lambda_{1,\pm}| \pm 2B}{2|\lambda_{1,\pm}|}} \\ 0 \\ 0 \\ \sqrt{\frac{|\lambda_{1,\pm}| \mp 2B}{2|\lambda_{1,\pm}|}} \end{pmatrix} = \pm\sqrt{\frac{|\lambda_{1,\pm}| \mp 2B}{2|\lambda_{1,\pm}|}}|00\rangle + \sqrt{\frac{|\lambda_{1,\pm}| \pm 2B}{2|\lambda_{1,\pm}|}}|11\rangle, \]
where $|00\rangle = (1, 0, 0, 0)^T$ and $|11\rangle = (0, 0, 0, 1)^T$. Other eigenvalues and eigenstates can also be found by choosing:

$$|\Psi_2\rangle = \begin{pmatrix} 0 \\ c \\ d \\ 0 \end{pmatrix}, \quad H_{2\text{qubits}}|\Psi_2\rangle = \lambda_2|\Psi_2\rangle.$$  \hfill (100)

The eigenvalues and the eigenstates can be solved:

$$\lambda_{2,\pm} = \pm \sqrt{J^2 + 4B^2\delta^2},$$

$$|\Psi_{2,\pm}\rangle = \begin{pmatrix} 0 \\ \mp \sqrt{\frac{|\lambda_{2,\pm}| \pm 2B\delta}{2|\lambda_{2,\pm}|}} \\ \sqrt{\frac{|\lambda_{2,\pm}| \pm 2B\delta}{2|\lambda_{2,\pm}|}} \\ 0 \end{pmatrix} = \mp \sqrt{\frac{|\lambda_{2,\pm}| \pm 2B\delta}{2|\lambda_{2,\pm}|}}|10\rangle + \sqrt{\frac{|\lambda_{2,\pm}| \pm 2B\delta}{2|\lambda_{2,\pm}|}}|01\rangle,$$  \hfill (101)

where $|10\rangle = (0, 1, 0, 0)^T$ and $|01\rangle = (0, 0, 1, 0)^T$. The concurrences of the pure state for all ground states are:

$$C(\Psi_{1,\pm}) = \sqrt{\frac{\theta^2}{4 + \theta^2}}, \quad C(\Psi_{2,\pm}) = \sqrt{\frac{\tilde{\theta}^2}{4 + \tilde{\theta}^2}},$$  \hfill (102)

where

$$\theta \equiv \frac{J\gamma}{B}, \quad \tilde{\theta} \equiv \frac{J}{B\delta}.$$  \hfill (103)

Thus, it is easy to find that increasing the concurrence of the pure state or the maximum violation of the Bell’s inequality by increasing the value of $J$, and decreasing the value of $B$ or $\delta$. One interesting observation is that the concurrence of the pure state does not depend on $\gamma$. Although $\gamma$ and $\delta$ play the same role of the degree of the anisotropy, they can offer different effects to affect the concurrence of the pure state. Because the system is a two-qubit system, a larger concurrence of a generic pure state should give larger maximum violation of the Bell’s inequality for the generic pure state.
5.2 Finite Temperature

To compute the density matrix at finite temperature, we first compute

$$\rho_{AB} = \exp\left(-\frac{1}{T}H_{2qubits}\right) \sum_{i=1,2;\alpha=\pm} |\Psi_{i,\alpha}\rangle \langle \Psi_{i,\alpha}|$$

$$= \left( \cosh\left(\frac{1}{T}\right) + 2 \frac{B}{|\lambda_{1,\pm}|} \sinh\left(\frac{1}{T}\right) \right) |00\rangle\langle 00|$$

$$+ \left( \cosh\left(\frac{1}{T}\right) - 2 \frac{B}{|\lambda_{1,\pm}|} \sinh\left(\frac{1}{T}\right) \right) |11\rangle\langle 11|$$

$$+ \sinh\left(\frac{1}{T}\right) \sqrt{1 - \frac{4B^2}{\lambda_{1,\pm}^2}} \left( |00\rangle\langle 11| + |11\rangle\langle 00| \right)$$

$$+ \left( \cosh\left(\frac{1}{T}\right) - 2 \frac{B\delta}{|\lambda_{2,\pm}|} \sinh\left(\frac{1}{T}\right) \right) |10\rangle\langle 10|$$

$$+ \left( \cosh\left(\frac{1}{T}\right) + 2 \frac{B\delta}{|\lambda_{2,\pm}|} \sinh\left(\frac{1}{T}\right) \right) |01\rangle\langle 01|$$

$$+ \sinh\left(\frac{1}{T}\right) \sqrt{1 - \frac{4B^2\delta^2}{\lambda_{2,\pm}^2}} \left( |10\rangle\langle 01| + |01\rangle\langle 10| \right).$$

(104)

where $T$ is a temperature. We can use the density matrix at a finite temperature to compute the concurrence of the mixed state. When the concurrences of the mixed state vanish, we can determine a critical temperature. When a temperature of a system beyond the critical temperature, entanglement entropy or the concurrence of the mixed state vanishes.

The concurrence defined for a mixed state is determined by $C(\rho_{AB}) = \max(0, \xi_1 - \xi_2 - \xi_3 - \xi_4)$, where $\xi_i$ are the eigenvalues, in decreasing order, of $\sqrt{\rho_{AB}(\sigma_y \otimes \sigma_y)\rho_{AB}^*(\sigma_y \otimes \sigma_y)}$:

$$\left\{ \xi_i \right\} = \left\{ \sqrt{\cosh^2\left(\frac{1}{T}\right) - \frac{4B^2}{|\lambda_{1,\pm}|^2} \sinh^2\left(\frac{1}{T}\right)} \pm \sinh\left(\frac{1}{T}\right) \sqrt{1 - \frac{4B^2}{|\lambda_{1,\pm}|^2}} \right\}$$

$$\left\{ \sqrt{\cosh^2\left(\frac{1}{T}\right) - \frac{4B^2\delta^2}{|\lambda_{2,\pm}|^2} \sinh^2\left(\frac{1}{T}\right)} \pm \sinh\left(\frac{1}{T}\right) \sqrt{1 - \frac{4B^2\delta^2}{|\lambda_{2,\pm}|^2}} \right\}. $$

(105)
The concurrence of the mixed state is

\[
\max \left( 2 \sinh \left( \frac{|\lambda_{1, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2}{|\lambda_{1, \pm}|^2}}, -2 \sqrt{\cosh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right) - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right)} , 0 \right)
\]

(106)

when

\[
\sqrt{\cosh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right) - \frac{4B^2}{|\lambda_{1, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right)} + \sinh \left( \frac{|\lambda_{1, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2}{|\lambda_{1, \pm}|^2}} \geq \sqrt{\cosh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right) - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right)} + \sinh \left( \frac{|\lambda_{2, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}},
\]

and the concurrence of the mixed state is

\[
\max \left( 2 \sinh \left( \frac{|\lambda_{2, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}}, -2 \sqrt{\cosh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right) - \frac{4B^2}{|\lambda_{1, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right)} , 0 \right)
\]

(108)

when

\[
\sqrt{\cosh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right) - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{2, \pm}|}{T} \right)} + \sinh \left( \frac{|\lambda_{2, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2\delta^2}{|\lambda_{2, \pm}|^2}} \leq \sqrt{\cosh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right) - \frac{4B^2}{|\lambda_{1, \pm}|^2}\sinh^2 \left( \frac{|\lambda_{1, \pm}|}{T} \right)} + \sinh \left( \frac{|\lambda_{1, \pm}|}{T} \right) \sqrt{1 - \frac{4B^2}{|\lambda_{1, \pm}|^2}}.
\]

(109)

Thus, we have two cases for the concurrence of the mixed state. We refer these two cases to Scenario A (first case) and Scenario B (second case). To understand physical meaning of the concurrence of the mixed state in the two qubits system, we consider special cases in the parameter space \((B, J, \gamma, \delta)\). We first discuss the case where the magnetic field vanishes, \(B = 0\). We obtain

\[
C(\rho_{AB}) = \max \left( 2 \sinh \left( \frac{|\lambda_{2, \pm}|}{T} \right) - 2 \cosh \left( \frac{|\lambda_{1, \pm}|}{T} \right), 0 \right),
\]

(110)
and the case is the Scenario B. The critical temperature $T_c$, where the concurrence vanishes, is

$$\sinh \left( \frac{J}{T_c} \right) = \cosh \left( \frac{J\gamma}{T_c} \right).$$

(111)

For this case, we cannot understand the behavior of the critical temperature analytically. Thus, we consider $\gamma = 0$. In this case, it is also the Scenario B and the concurrence of the mixed state is

$$C(\rho_{AB}) = \max \left( 2 \sinh \left( \frac{\sqrt{J^2 + 4B^2\delta^2}}{T} \right) \sqrt{1 - \frac{4B^2\delta^2}{J^2 + 4B^2\delta^2} - 2}, 0 \right).$$

(112)

The critical temperature is

$$T_c = \frac{\sqrt{J^2 + 4B^2\delta^2}}{\sinh^{-1} \left( \frac{\sqrt{J^2 + 4B^2\delta^2}}{J} \right)}.$$  

(113)

The Scenario B shows that the critical temperature depends on the magnetic field, except for $\delta = 0$. Thus, it is interesting to compare our analytical result to the experiments with the non-uniform magnetic field. The preparation of the uniform magnetic field should be difficult in an experiment so our analytical results of non-uniform magnetic field should be easier to study than the case of a uniform magnetic field in an experiment. When $J \to \infty$, the critical temperature $T_c$ also approaches infinity. Hence, this means that the mixed state should be entangled for each temperature under the limit. When we consider the limit $B/J \to \infty$, the critical temperature approximately equals to $J$. Then we take one additional limit $J \to 0$, the concurrence of the mixed state approaches zero. Thus, the mixed state should approach to a product state for each temperature. These two limits show useful and interesting applications to entanglement from the concurrence of the mixed state at a finite temperature.

If each pure state has the same concurrence of the pure state and the concurrence of the pure state has the minimal value when we choose a particular decomposition, the concurrence of the mixed state can be related to the upper bound of the maximum violation of the Bell’s inequality as we discussed.

6 Applications to the Wen-Plaquette Model

The Wen-Plaquette model [10] is defined by the Hamiltonian on a two-dimensional periodic square lattice (torus) as

$$H = \sum_i \sigma^+_x \sigma^+_y \sigma^+_{x+\hat{x}} \sigma^+_{y+\hat{y}} \sigma^+_{y+\hat{y}}.$$

(114)
in which qubits live on vertices with a four-spin interaction on each plaquette. A quantum state of the Hamiltonian is an \( n \)-qubit quantum state with \( n \) being a number of vertices. We apply our Theorem to a four-qubit quantum state, with geometry of the system containing four vertices, eight edges, and four faces, in which the Euler number of the torus is zero,

\[
\chi = V - E + F = 0 \tag{115}
\]

with \( V \), \( E \), and \( F \) being a number of vertices, edges, and faces, respectively. There are four degenerate ground states \( |G\rangle_{4\text{-qubit}} \):

\[
\frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle), \quad \frac{1}{\sqrt{2}}(|1010\rangle + |0101\rangle), \quad \frac{1}{\sqrt{2}}(|0011\rangle - |1100\rangle), \quad \frac{1}{\sqrt{2}}(|1001\rangle - |0110\rangle). \tag{116}
\]

We define the order of each site in these four-qubit states in the Fig. 7 (a). Since the maximum violation of the Bell’s inequality for these ground states is \( \gamma = 4\sqrt{2} \), the ground states have the maximum concurrence of the pure state

\[
C(\psi) = 1. \tag{117}
\]

According to the Theorem, the ground states are maximally entangled.

Before computing the upper bound of the maximum violation of the Bell’s inequality of ground states of the six-qubit in the Wen-Plaquette model, we give six-qubit quantum

Figure 7: (a) A four-qubit quantum state in the Wen-Plaquette model and (b) A six-qubit quantum state of the Wen-Plaquette model on a torus. The right dashed line is identified as the left solid line and the top dashed line is identified as the bottom solid line in (a) and (b). The numbers are the site indices. The gray colored number is identified with the corresponding black colored number.
states, $|G\rangle_{6\text{-qubit}}$:

$$|G_1\rangle_{6\text{-qubit}} = \frac{\lambda_+}{\sqrt{2}}(-|111000\rangle + |001110\rangle) + \frac{\lambda_-}{\sqrt{2}}(|100011\rangle + |010101\rangle),$$  \hspace{1cm} (118)  

$$|G_2\rangle_{6\text{-qubit}} = \frac{\lambda_+}{\sqrt{2}}(-|000111\rangle + |110001\rangle) + \frac{\lambda_-}{\sqrt{2}}(|011100\rangle + |101010\rangle),$$  \hspace{1cm} (119)  

with the site labels shown in Fig. 7 (b). We can relate the upper bound of the maximum violation of the Bell’s inequality to the generalized concurrence of the pure states. Two different bipartitions are considered: (1) subsystem $A$ contains a site number six, and (2) subsystem $A$ contains a site number five and a site number six. Here we use $\delta = 1$ or 2 as an indicator for the case one and the case two. According to the Lemma, we find that the upper bound of the maximum violation of the Bell’s inequality can be expressed as a function of the concurrence of the pure state when we exchange the final site with the first site of the Bell’s operator ($\tilde{B}_n$) \hspace{0.5cm} (We define  

$$C(\delta) \equiv \sqrt{2 \left(1 - 2^{\delta-1} \text{Tr} \rho^2_{A(\delta)}\right)}$$  \hspace{1cm} (120)  

as the generalized concurrence of the six-qubit pure state with respect to two different bipartitions).  

Because the result and the computation method are the same, we only show the computation for one quantum state ($|G_1\rangle_{6\text{-qubit}}$). To obtain the upper bound of the maximum violation of the Bell’s inequality, we first compute the density matrix:

$$\rho_{6\text{-qubit},1} = \frac{\lambda_+^2}{2}(|111000\rangle\langle111000| + |001110\rangle\langle001110|$$
$$\quad - |111000\rangle\langle001110| - |001110\rangle\langle111000|)$$
$$\quad + \frac{\lambda_+^2}{2}(|100011\rangle\langle100011| + |010101\rangle\langle010101|$$
$$\quad + |100011\rangle\langle010101| + |010101\rangle\langle100011|)$$
$$\quad + \frac{\lambda_+\lambda_-}{2}(-|111000\rangle\langle100011| - |111000\rangle\langle010101|$$
$$\quad + |001110\rangle\langle100011| + |001110\rangle\langle010101|$$
$$\quad - |100011\rangle\langle100011| - |010101\rangle\langle111000|$$
$$\quad + |100011\rangle\langle100011| + |010101\rangle\langle001110|).$$  \hspace{1cm} (121)
The non-vanishing matrix elements of the generalized $R$-matrix are:

\[
R_{zzzzzz} = R_{yyzxx} = R_{xxzxx} = -1, \\
R_{xxxzzz} = R_{zyzxyz} = R_{xyzxyz} = \lambda_+^2 - \lambda_-^2 \\
R_{yxyxyz} = R_{xyzxyz} = 1, \\
R_{zxyyzz} = -2\lambda_+\lambda_- \\
R_{zzyyzz} = -2\lambda_+\lambda_- \\
R_{zxyzyz} = 2\lambda_+\lambda_- \\
R_{zxxyyz} = 2\lambda_+\lambda_- \\
R_{zxxzzz} = R_{yyzyyz} = \lambda_+^2 - \lambda_-^2. \\
\]

The eigenvalues of the matrix $R^\dagger R$ are:

\[
5 + 4(\lambda_+^2 - \lambda_-^2)^2, \\ 16\lambda_+^2\lambda_-^2, \\ 16\lambda_+^2\lambda_-^2. \\
\]

If we denote the last qubit as the region $A$ and the complementary region as the region $B$, the entanglement entropy of the region $A$ is

\[
S_{EE,A} = -\lambda_+^2 \ln \lambda_+^2 - \lambda_-^2 \ln \lambda_-^2. \\
\]

We also obtain:

\[
\text{Tr}\rho_A^2 = \lambda_+^4 + \lambda_-^4 = 1 - 2\lambda_+^2\lambda_-^2. \\
\]

Therefore, this can imply:

\[
\lambda_+^2 = \frac{1 \pm \sqrt{1 - C^2(1, \psi)}}{2}, \\
\lambda_-^2 = \frac{1 \mp \sqrt{1 - C^2(1, \psi)}}{2}. \\
\]

It is easy to find that the entanglement entropy of the region $A$ can increase by increasing the concurrence of the pure state $C(1, \psi)$. Therefore, the eigenvalues of the matrix $R^\dagger R$ are:

\[
9 - 4C^2(1, \psi), \\ 4C^2(1, \psi), \\ 4C^2(1, \psi). \\
\]

The maximum violation of the Bell’s inequality is

\[
\gamma \leq 6. \\
\]

If we denote the last two qubits as the region $A$ and the complementary region as the region $B$, entanglement entropy of the region $A$ is

\[
S_{EE,A} = \ln 2 - \lambda_+^2 \ln \lambda_+^2 - \lambda_-^2 \ln \lambda_-^2. \\
\]

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We also have:

\[ \text{Tr} \rho_A^2 = \frac{\lambda^4}{2} + \frac{\lambda^4}{2} = \frac{1}{2} - \lambda^2 \lambda^2. \]  

(130)

Thus, we can show:

\[ \lambda^2 = \frac{1 \pm \sqrt{1 - C^2(2, \psi)}}{2}, \quad \lambda^2 = \frac{1 \mp \sqrt{1 - C^2(2, \psi)}}{2}. \]  

(131)

It is easy to find that entanglement entropy of the region \( A \) can monotonically increase by increasing the generalized concurrence \( C(2, \psi) \).

Therefore, the eigenvalues of the matrix \( R^\dagger R \) are:

\[ 9 - 4C^2(2, \psi), \quad 4C^2(2, \psi), \quad 4C^2(2, \psi). \]  

(132)

The maximum violation of the Bell’s inequality is

\[ \gamma \leq 6. \]  

(133)

The above result shows that the upper bound of the maximum violation of the Bell’s inequality does not depend on a choice of the generalized concurrence of the pure state. This result is due to the specific wavefunction. In general, the upper bound of the maximum violation of the Bell’s inequality depends on the generalized concurrence and we demonstrate the relation by exchanging the final site with the first site of the Bell’s operator \( (\tilde{B}) \).

We find that the eigenvalues of the matrix \( R^\dagger R \) are:

\[ 1 + 4C^2(1, \psi) = 1 + 4C^2(2, \psi), \quad 4, \quad 4. \]  

(134)

When

\[ C^2(1, \psi) = C^2(2, \psi) \geq \frac{3}{4}, \]  

(135)

the maximum violation of the Bell’s inequality is:

\[ \gamma \leq 2\sqrt{5 + 4C^2(1, \psi)} = 2\sqrt{5 + 4C^2(2, \psi)}. \]  

(136)

When

\[ C^2(1, \psi) = C^2(2, \psi) < \frac{3}{4}, \]  

(137)
the maximum violation of the Bell’s inequality is:

\[ \gamma \leq 4\sqrt{2}. \]  

(138)

Now we consider the ground state with six sites in the Wen-Plaquette model. This ground state is expressed in (118) when the coefficients \( \lambda_+ \) and \( \lambda_- \) are

\[ \lambda_+ = \lambda_- = \frac{1}{\sqrt{2}} \]  

(139)

and the corresponding concurrence is

\[ C(\delta) = 1, \]  

(140)

which indicates that the ground state is a maximally entangled state. The entanglement entropy with respect to the two bipartitions are:

\[ S_{A(\delta=1)} = \ln 2, \quad S_{A(\delta=2)} = 2 \ln 2, \]  

(141)

which can be obtained from the generalized \( R \)-matrix through the inverse mapping:

\[ \gamma \leq 6 = 2\sqrt{13 - 2^{\delta+2}e^{-S_A(\delta)}}. \]  

(142)

In general, the entanglement entropy has the form

\[ S_{EE,A(L)} = \alpha L - S_{TEE}, \]  

(143)

in which the first term indicates the area law with \( L \) being the length of an entangling boundary, \( \alpha \) being a constant, and \( S_{TEE} \) is called topological entanglement entropy \( [5] \).

In the Wen-Plaquette model, the length of an entangling boundary \( L \) is a number of bonds that connect the subsystem \( A \) and the subsystem \( B \). We consider:

\[ L(\delta = 1) = 4, \quad L(\delta = 2) = 6 \]  

(144)

to extract the area law of entanglement entropy and obtain the topological entanglement entropy

\[ S_{TEE} = \ln 2 = \ln \sqrt{D}, \]  

(145)

where

\[ D = 4 \]  

(146)
is the number of distinct quasiparticles \[5, 6\]. We remind the reader that \( m \) is a number of bonds connecting the subsystem \( A \) and the subsystem \( B \). In the case that the subsystem \( A \) contains one site, \( m = 4 \). In the case that subsystem \( A \) contains two adjacent sites along a vertical direction, \( m = 4 \). In the case that the subsystem \( A \) contains two adjacent sites along a horizontal direction, \( m = 6 \). In the case that the subsystem \( A \) contains two disjointed sites, \( m = 6 \). In the case that the subsystem \( A \) contains three adjacent sites, \( m = 6 \). In the case that the subsystem \( A \) contains two adjacent sites and one disjointed site, \( m = 6 \). Thus, we use the generalized \( R \)-matrix to demonstrate an indirect measure of the topological entanglement entropy.

7 Discussion and Outlook

We demonstrated the relations between the maximum violation of the Bell’s inequality and the generalized concurrence of \( n \)-qubit pure states and also demonstrated its applications to the various models. The maximum violation of the Bell’s inequality is operated in a full system while the generalized concurrence is defined by taking a partial trace operation. The relation provides an alternative way to observe quantum entanglement through the measurement of the Bell’s operator and the generalized \( R \)-matrix. We first discussed a linear combination of two product states and showed that the maximum violation of the Bell’s inequality can be directly related to the concurrence of the pure state, which also monotonically increases with respect to entanglement entropy.

To understand a relation between the generalized concurrence, a bipartition of a system and the maximum violation of the Bell’s inequality, we studied the toric code model on a disk manifold and a cylinder manifold with boundary conditions. Our result showed that information of a bipartition depends on a choice of the generalized concurrence and boundary degrees of the Hilbert space in the toric code model. We also provided the \( 2n \)-qubit quantum state to explicitly express the upper bound of the maximum violation of the Bell’s inequality in terms of the generalized concurrence of the pure state. A choice of the generalized concurrence of the pure state also depends on the degrees of the Hilbert space in the \( 2n \)-qubit quantum state.

Finally, we applied our theoretical studies to the various models. We first considered the two-qubit system with the non-uniform magnetic field at a finite temperature. The most interesting observation is that the critical temperature in the \( XY \)-model depends on the non-uniformity of the magnetic field. When the magnetic field is uniform, the critical temperature does not depend on the magnetic field. On an experimental side, it is hard to control the magnetic field uniformly. Hence, our theoretical and analytical
studies can give more accurate comparison to the experiments. We also studied the maximum violation of the Bell’s inequality in the Wen-Plaquette model \cite{10} for four sites and six sites on a torus manifold. Our computation of the generalized $R$-matrix in the Wen-Plaquette model reveals that the ground states are maximally entangled or the generalized concurrence of the pure state is one. We also provide a possible detection of topological entanglement entropy \cite{5} through the maximum violation of the Bell’s inequality by using different bipartitions of the concurrence of the pure state.

The studies of the maximum violation of the Bell’s inequality should shed the light to understand a detection of entanglement quantities from a density matrix. The motivation is that the current experimental techniques is not mature enough to perform a partial trace operation in an $n$-qubit system. When $n$ approaches to infinity, the difficulties of a detection of entanglement quantities should be similar to a detection of the entanglement quantities in quantum field theory because the degrees of the freedom of the Hilbert space should be infinite. When $n$ approaches infinite, the first problem is that the upper bound of the maximum violation of the Bell’s inequality should go to infinity. Thus, the maximum violation of the Bell’s inequality should not be an observable quantity. We also find that the maximum violation of the Bell’s inequality is always related to the Rényi-2 entropy. Entanglement quantities in quantum field theory are always related to a regularization parameter. Thus, it is usually problematic to give an observable quantity in quantum field theory. If we directly apply a result of a universal term of Rényi-2 entropy of two dimensional conformal field theory to the upper bound of the maximum violation of the Bell’s inequality that we found, the upper bound of the maximum violation of the Bell’s inequality should vanish when a regularization parameter goes to zero. Hence, we expect that the Rényi-2 entropy does not offer additional divergences to the maximum violation of the Bell’s inequality in two dimensional conformal field theory. Therefore, we think that the maximum violation of the Bell’s inequality is divergent in quantum field theory due to a number of observables are infinite. One simple way to solve this problem is to divide the maximum violation of the Bell’s inequality to degrees of the freedom of a Hilbert space. Then we can find a finite quantity in an $n$-qubit system when $n$ goes to infinity. We can consider a two dimensional $CP^{N-1}$ model to demonstrate because the fields are constrained. Thus, a bounded Bell’s operator in the two dimensional $CP^{N-1}$ model is easily constructed. When a Bell’s operator is not bounded or a number of level is infinite, we can use the same way to obtain the Bell’s operator from a basis of an $n$-qubit system. Thus, we expect that our suggestion can also be applied to generic quantum field theory.

Our theoretical studies also showed that a region only has one-qubit and a state is a
linear combination of two product states, the maximum violation of the Bell’s inequality can be approximately proportional to the concurrence of the pure state when \( n \) is large enough. It is interesting to find the relation between entanglement quantities and the maximum violation of the Bell’s inequality. This may shed in light for finding a suitable quantity to measure or estimate intensity of quantum entanglement in quantum field theory.

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