In this paper, we show a direct method of deriving the Peres–Horodecki criterion for the two-qubit states from the Hill–Wootters formula for the entanglement of formation. Although the Peres–Horodecki criterion and the Hill–Wootters formula are established results in the field of quantum information theory, they are proved independently and connections between them are not discussed precisely. In this paper, we clarify these connections.

First, we replace the original Peres–Horodecki criterion with an equivalent statement found by Augusiak et al. [Augusiak, R.; Demianowicz, M.; Horodecki, M.; Horodecki, K. Rev. Mod. Phys. 2009, 81, 865–942]. Second, we obtain an analytical form of the concurrence of an arbitrary two-qubit state, using Ferrari’s method to solve a quartic equation for eigenvalues. Finally, with the above preparations, we accomplish the direct derivation of the Peres–Horodecki criterion from the Hill–Wootters formula.

Keywords: Peres–Horodecki criterion; Hill–Wootters formula; separability; entanglement of formation

1. Introduction

Since Einstein, Podolsky and Rosen pointed out the importance of entanglement that appears in the quantum state of the bipartite system, many researchers have investigated the nature of the entanglement [1]. Because it is understood that the entanglement can be a resource of quantum information processing, both classifying and quantifying the entanglement have become topics that attract a wide audience in the field of quantum information [2].

To investigate the entanglement theoretically, we can take two different approaches. One is the qualitative analysis, such as concentrating on how to distinguish entangled (inseparable) states of the bipartite system from separable states. The other is the quantitative analysis, such as finding an appropriate measure of entanglement to represent the entanglement as an amount numerically.

The Peres–Horodecki criterion belongs in the former approach [3,4]. It gives the necessary and sufficient conditions for separability of mixed states of two-qubit systems and qubit-qutrit systems. At first, Peres obtains this criterion as a conjecture and proves that it is a necessary condition of separability [3]. Next, Horodecki et al. [4] prove that this criterion is a sufficient condition of separability for two-qubit systems and qubit-qutrit systems. To follow the proof of [4], we have to utilize some results of pure mathematics, for example, the Hahn–Banach theorem in the functional analysis and Strømer and Woronowicz’s results about positive maps [5–7]. Thus, in spite of its simple form, the derivation of the Peres–Horodecki criterion is not accessible to physicists.

The Hill–Wootters formula for the entanglement of formation belongs in the latter approach [8,9]. It gives an explicit formula of the entanglement of formation of the two-qubit mixed states. (The entanglement of formation of a mixed state is defined as the minimum average entanglement of an ensemble of pure states that represents the original mixed state.) To obtain this formula, we use general properties of entropy, so that the derivation of the Hill–Wootters formula is accessible to physicists.

As mentioned above, the Peres–Horodecki criterion and the Hill–Wootters formula are derived independently with each other. However, deriving the Peres–Horodecki criterion from the Hill–Wootters formula in a direct manner has to be possible in principle, so that there must be connections between them. This is the motivation of this paper.

In this paper, we show a direct method of deriving the Peres–Horodecki criterion for the two-qubit mixed states from the Hill–Wootters formula. First, we replace the original Peres–Horodecki criterion with...
the following equivalent statement obtained by Augusiak et al. [10,11]: an arbitrary two-qubit mixed state is inseparable if and only if the determinant of the partial transpose of its density matrix is less than zero. Second, we obtain an analytical form of the concurrence of an arbitrary two-qubit state \( \rho \), using Ferrari’s method to solve a quartic equation for eigenvalues \( \rho \bar{\rho} \). Finally, with the above preparations, we accomplish the direct derivation of the Peres–Horodecki criterion from the Hill–Wootters formula.

In the middle of the above derivation, we show an alternative method of obtaining Augusiak et al.’s results [10,11]. Using the so-called Lewenstein–Sanpera decomposition and Weyl’s inequality [12,13], we show that an arbitrary two-qubit mixed state is inseparable if and only if the partial transpose of its density matrix has three positive eigenvalues and one negative eigenvalue. Thus, it never has zero eigenvalues. In contrast, the partial transpose of a density matrix of a separable two-qubit state is positive-semidefinite. Hence, we reach at Augusiak et al.’s two-qubit separability condition.

Here, we refer to previous works that relate to our results. Sanpera et al. show that the partial transpose of a density matrix of an arbitrary inseparable two-qubit state has at most one negative eigenvalue [14]. Hayden obtains similar results [15]. Vidal and Werner propose negativity, which is a sum of the absolute values of all negative eigenvalues of the partially transposed density matrix, as a measure of entanglement [16]. Augusiak et al. show that an arbitrary two-qubit mixed state is inseparable if and only if the determinant of the partial transpose of its density matrix is less than zero [10,11]. (Augusiak et al. pointed out that the partial transpose of an inseparable two-qubit density matrix never has zero eigenvalues.)

Recently, two-qubit X-states, whose non-zero elements of the density matrix are in an ‘X’ formation, are studied eagerly in relation to the investigation of the entanglement sudden death [17–19]. In these works, it is confirmed that the negativity is essentially equivalent to the concurrence on condition that the density matrix is in the two-qubit X-state. Because the Werner states are a subclass of the X-states, this result is interesting from the viewpoint of the quantum information theory.

This paper is organized as follows. In the remains of this section, we give brief reviews of the Peres–Horodecki criterion and the Hill–Wootters formula. In Section 2, we show that an arbitrary two-qubit mixed state is inseparable if and only if the partial transpose of its density matrix has three positive eigenvalues and one negative eigenvalue. In Section 3, we show a direct method of deriving the Peres–Horodecki criterion from the Hill–Wootters formula for general two-qubit mixed states. In Section 4, we consider an example of a convex combination of a separable pure state and an inseparable pure state. Assuming that the two-qubit system is in this state, we show that we can derive the Peres–Horodecki criterion from the Hill–Wootters formula without difficulty. In Section 5, we give brief discussions. In Appendix 1, we show some results of calculations obtained in Section 3.

In this paper, we define the separability of the two-qubit system \( AB \) as follows: if the density matrix \( \rho_{AB} \) can be written as a convex combination of product states,

\[
\rho_{AB} = \sum_i p_i \rho_{A,i} \otimes \rho_{B,i},
\]

where \( p_i \geq 0, \) tr\( \rho_{A,i} \) = 1, tr\( \rho_{B,i} \) = 1 \( \forall i \) and \( \sum_i p_i = 1 \), then \( \rho_{AB} \) is separable. If and only if \( \rho_{AB} \) is not separable, it is inseparable [20].

Here, we give exact descriptions of the Peres–Horodecki criterion and the Hill–Wootters formula.

The Peres–Horodecki criterion for the two-qubit states is described as follows. We let \( \rho_{AB} \) be a density matrix of an arbitrary mixed state of the two-qubit system \( AB \). \( \rho_{AB}^{PT} \) denotes the partial transpose of \( \rho_{AB} \) with respect to the qubit \( B \). The necessary and sufficient condition for separability of \( \rho_{AB} \) is the positivity of \( \rho_{AB}^{PT} \).

The Hill–Wootters formula for the entanglement formation of the two-qubit states is described as follows. We let \( \rho_{AB} \) be a density matrix of an arbitrary mixed state of the two-qubit system \( AB \). We write matrix elements of \( \rho_{AB} \) in the fixed basis \( \{|0\}_A |0\>_B, |0\>_A |1\>_B, |1\>_A |0\>_B, |1\>_A |1\>_B \} \). We describe \( \rho_{AB}^{PT} \) as the complex conjugate of \( \rho_{AB} \) in this fixed basis. Moreover, we define a new matrix \( \tilde{\rho}_{AB} = (\sigma_x A \otimes \sigma_x B) \rho_{AB}^{PT} \). Next, we write four eigenvalues of \( \rho_{AB}^{PT} \) as \( \lambda_1, \lambda_2, \lambda_3, \lambda_4 \) in decreasing order. Because of the definition of \( \tilde{\rho}_{AB} \), we have the relation \( \lambda_1 \geq 0 \) \( \forall \) \( \lambda_{AB} \). Hence, we can expect \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0 \).

After these preparations, we define the concurrence,

\[
C(\rho_{AB}) = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4} \}.
\]

If \( \rho_{AB} \) represents a pure state, we obtain \( C(\rho_{AB}) = \lambda_{AB} \). Therefore, we can obtain the relation \( 0 \leq C(\rho_{AB}) \leq 1 \) for an arbitrary mixed state \( \rho_{AB} \). The entanglement of formation is defined as \( E(\rho_{AB}) = \mathcal{E}(C(\rho_{AB})) \), where

\[
\mathcal{E}(C) = \frac{1 + \sqrt{1 - C^2}}{2} \log_2 \frac{1 + \sqrt{1 - C^2}}{2} - \frac{1 - \sqrt{1 - C^2}}{2} \log_2 \frac{1 - \sqrt{1 - C^2}}{2}.
\]

The function \( \mathcal{E}(C) \) increases monotonically and varies from zero to unity as \( C \) goes from zero to unity. Thus, if and only if \( C(\rho_{AB}) = 0, \rho_{AB} \) is separable.
2. The number of negative eigenvalues of the partially transposed inseparable density matrix

In this section, we show that the partial transpose of the density matrix of the inseparable mixed state for the two-qubit system always has three positive eigenvalues and one negative eigenvalue, so that it never has zero eigenvalues. We then obtain another expression which is equivalent to the Peres–Horodecki criterion for the two-qubit states as follows: the two-qubit mixed state is inseparable if and only if the determinant of the partial transpose of its density matrix is negative. (As mentioned in Section 1, we show a simple method of deriving Augusiak et al.’s results [10,11].)

First of all, we consider the separability and inseparability of an arbitrary two-qubit pure state $|\psi\rangle_{AB}$. We can describe $|\psi\rangle_{AB}$ as the following four-element ket vector without losing generality,

$$
|\psi\rangle_{AB} = \begin{pmatrix}
    a \\
    b \exp(i\theta_1) \\
    c \exp(i\theta_2) \\
    \sqrt{1-a^2-b^2-c^2} \exp(i\theta_3)
\end{pmatrix},
$$

(3)

where the basis is given by $\{|0\rangle_A|0\rangle_B, |0\rangle_A|1\rangle_B, |1\rangle_A|0\rangle_B, |1\rangle_A|1\rangle_B\}$ and we assume $a \geq 0$, $b \geq 0$, $c \geq 0$, $1-a^2-b^2-c^2 \geq 0$, $0 \leq \theta_i < 2\pi$ for $i \in \{1, 2, 3\}$.

By tracing out the freedom of the qubit B, we obtain the reduced density matrix of the qubit A as

$$
\rho_A = \text{tr}_B(|\psi\rangle_{AB}\langle\psi|) = \begin{pmatrix}
    \rho_{A,00} & \rho_{A,01} \\
    \rho_{A,10} & 1 - \rho_{A,00}
\end{pmatrix},
$$

(4)

where

$$
\rho_{A,00} = a^2 + b^2,
$$

$$
\rho_{A,01} = ac \exp(-i\theta_2) + b \sqrt{1-a^2-b^2-c^2} \exp[i(\theta_1 - \theta_3)].
$$

(5)

Then, the eigenvalues of $\rho_A$ are given by

$$
\lambda_{\pm} = \frac{1}{2} \left(1 \pm \sqrt{1-C^2}\right),
$$

(6)

where

$$
C = 2[a^2(1-a^2-b^2-c^2) + b^2 c^2 \\
-2abc \sqrt{1-a^2-b^2-c^2} \cos(\theta_1 + \theta_2 - \theta_3)]^{1/2}.
$$

(7)

The quantity $C$ in Equation (7) is equal to the concurrence of $|\psi\rangle_{AB}$ given by the Hill–Wootters formula. Because $\rho_A$ is positive-semidefinite and $\text{tr} \rho_A = 1$, we obtain $0 \leq \lambda_{\pm} \leq 1$. Thus, from Equation (6), we obtain $0 \leq C \leq 1$. If $C = 0$, $|\psi\rangle_{AB}$ is separable. In contrast, if $C > 0$, $|\psi\rangle_{AB}$ is inseparable. On the other hand, writing the density matrix as $\rho_{AB} = |\psi\rangle_{AB}\langle\psi|$, we obtain four eigenvalues of $\rho_{AB}^{PT}$ as follows:

$$
\eta_1 = (1/2)C,
$$

$$
\eta_2 = -(1/2)C,
$$

$$
\eta_3 = (1/2)(1 + \sqrt{1-C^2}),
$$

$$
\eta_4 = (1/2)(1 - \sqrt{1-C^2}).
$$

(8)

From the above results and the relation $0 \leq C \leq 1$, we can conclude that $\rho_{AB}^{PT}$ is positive-semidefinite if and only if $C(|\psi\rangle_{AB}) = 0$. At the same time, we find that $\rho_{AB}^{PT}$ has three positive eigenvalues and one negative eigenvalue if and only if $C(|\psi\rangle_{AB}) \neq 0$.

Hence, we obtain the following fact. If and only if an arbitrary pure state of the two-qubit system $|\psi\rangle_{AB}$ is inseparable, $\rho_{AB}^{PT} = (|\psi\rangle_{AB}\langle\psi|)^{PT}$ has three positive eigenvalues and one negative eigenvalue.

Next, we use the following result obtained by Lewenstein and Sanpera [12]. An arbitrary two-qubit mixed state $\rho$ has a decomposition in the form,

$$
\rho = p \rho_s + (1-p) \rho_c,
$$

(9)

where $0 \leq p \leq 1$, $\rho_s$ is a normalized separable mixed state and $\rho_c = |\psi_\rangle \langle \psi|$ is a normalized inseparable pure state. (Here, we pay attention to the following fact. The decomposition of Equation (9) is obtained with neither the Peres–Horodecki criterion nor the Hill–Wootters formula. Thus, the so-called Lewenstein–Sanpera decomposition is derived independently from the Peres–Horodecki criterion and the Hill–Wootters formula.)

Let us take the partial transpose of Equation (9),

$$
\rho^{PT} = p \rho_s^{PT} + (1-p) \rho_c^{PT}.
$$

(10)

According to the Peres–Horodecki criterion, all of the four eigenvalues of $\rho_s^{PT}$ are equal to or larger than zero. Thus, we write the eigenvalues of $p \rho_s^{PT}$ as

$$
\eta_1^j(p \rho_s^{PT}) \geq \eta_2^j(p \rho_s^{PT}) \geq \eta_3^j(p \rho_s^{PT}) \geq \eta_4^j(p \rho_s^{PT}) \geq 0,
$$

(11)

in decreasing order. In contrast, from the fact obtained before, $\rho_c^{PT} = (|\psi\rangle \langle \psi|)^{PT}$ has three positive eigenvalues and one negative eigenvalue. Thus, we write the eigenvalues of $(1-p) \rho_c^{PT}$ as

$$
\eta_1^j((1-p) \rho_c^{PT}) \geq \eta_2^j((1-p) \rho_c^{PT}) \geq \eta_3^j((1-p) \rho_c^{PT}) \geq \eta_4^j((1-p) \rho_c^{PT}) > 0 \quad \text{for } p \neq 1,
$$

(12)

in decreasing order.

Here, we use Weyl’s inequality given by the following form [13]. We let $X$ and $Y$ be arbitrary
Thus, from Equations (11), (12) and (13), we obtain
\[
\lambda_i^1(X + Y) \leq \lambda_i^1(X) + \lambda_{i+j-1}^1(Y) \quad \text{for } i \leq j,
\]
\[
\lambda_i^1(X + Y) \geq \lambda_i^1(X) + \lambda_{i+j+n}^1(Y) \quad \text{for } i \geq j.
\]
(13)

Thus, from Equations (11), (12) and (13), we obtain
\[
\eta_j^1(\rho^\text{PT}) \geq \eta_j^1(p \rho^\text{PT}_x) + \eta_j^1((1-p)\rho^\text{PT}_y) > 0 \quad \text{for } p \neq 1.
\]
(14)

Hence, if \( \rho \) is inseparable, \( \rho^\text{PT} \) has three positive eigenvalues.

On the other hand, the Peres–Horodecki criterion tells us that \( \rho^\text{PT} \) has negative eigenvalues if and only if \( \rho \) is inseparable. Therefore, if the two-qubit mixed state \( \rho \) is inseparable, its partial transpose has only one negative eigenvalue. Moreover, the other eigenvalues are positive and \( \rho^\text{PT} \) never has zero eigenvalues, when \( \rho \) is inseparable.

From the above discussions, we obtain another expression, which is equivalent to the Peres–Horodecki criterion for two-qubit mixed states, as follows: a two-qubit mixed state is inseparable if and only if the determinant of the partial transpose of its density matrix is negative. Because we obtain this statement, we change the purpose of this paper. From the next section, we replace the original Peres–Horodecki criterion with this new expression and we try to derive this new expression from the Hill–Wootters formula in a direct manner.

3. Direct derivation of the Peres–Horodecki criterion from the Hill–Wootters formula for the general two-qubit mixed states

In this section, we show the direct derivation of the Peres–Horodecki criterion from the Hill–Wootters formula for general two-qubit mixed states.

First of all, we give a density matrix of an arbitrary two-qubit mixed state as
\[
\rho_{AB} = \begin{pmatrix}
 r_0 & u_0 e^{i\theta_0} & u_1 e^{i\theta_1} & u_2 e^{i\theta_2} \\
u_0 e^{-i\theta_0} & r_1 & u_3 e^{i\theta_3} & u_4 e^{i\theta_4} \\
u_1 e^{-i\theta_1} & u_3 e^{-i\theta_3} & r_2 & u_5 e^{i\theta_5} \\
u_2 e^{-i\theta_2} & u_4 e^{-i\theta_4} & u_5 e^{-i\theta_5} & 1 - r_0 - r_1 - r_2
\end{pmatrix},
\]
(15)

where the basis is given by \([0]_A [0]_B, [0]_A [1]_B, [1]_A [0]_B, [1]_A [1]_B\), \(r_i \geq 0 \) for \( i \in \{0, 1, 2\}, 1 - r_0 - r_1 - r_2 \geq 0, u_j \geq 0 \) for \( j \in \{0, 1, \ldots, 5\} \) and \( 0 \leq \theta_k < 2\pi \) for \( k \in \{0, 1, \ldots, 5\} \).

Next, we remove some real parameters, which describe the local freedom of each qubit, from the expression of Equation (15). We think about the following submatrix, which is obtained by setting a basis vector of the qubit \( A \) on \([0]_A\),
\[
\begin{pmatrix}
 r_0 & u_0 e^{i\theta_0} \\
u_0 e^{-i\theta_0} & r_1 \\
u_1 e^{-i\theta_1} & u_3 e^{-i\theta_3} \\
u_2 e^{-i\theta_2} & u_4 e^{-i\theta_4}
\end{pmatrix}.
\]
(16)

We can always diagonalize this submatrix by applying a certain SU(2) rotation to the basis of the qubit \( B \), \([0]_B, [1]_B\). In a similar way, we think about the following submatrix, which is obtained by setting a basis vector of the qubit \( B \) on \([0]_B\),
\[
\begin{pmatrix}
 r_0 & u_1 e^{i\theta_1} \\
u_1 e^{-i\theta_1} & r_1 \\
u_2 e^{-i\theta_2} & u_3 e^{-i\theta_3} \\
u_3 e^{-i\theta_3} & u_4 e^{-i\theta_4} \\
u_4 e^{-i\theta_4} & u_5 e^{-i\theta_5} \\
u_5 e^{-i\theta_5} & 1 - r_0 - r_1 - r_2
\end{pmatrix}.
\]
(17)

We can always diagonalize this submatrix by applying a certain SU(2) rotation to the basis of the qubit \( A \), \([0]_A, [1]_A\), as well. We can take these two local SU(2) rotations independently of each other, and these transformations never cause the effects on the entanglement between qubits \( A \) and \( B \). Thus, these local transformations never give rise to the effects on both the Peres–Horodecki criterion and the Hill–Wootters formula.

From these discussions, we can replace the form of \( \rho_{AB} \) written in Equation (15) with the following form,
\[
\rho_{AB} = \begin{pmatrix}
 r_0 & u_0 e^{i\theta_0} & u_1 e^{i\theta_1} & u_2 e^{i\theta_2} \\
0 & r_1 & u_3 e^{i\theta_3} & u_4 e^{i\theta_4} \\
u_1 e^{-i\theta_1} & u_3 e^{-i\theta_3} & r_2 & u_5 e^{i\theta_5} \\
u_2 e^{-i\theta_2} & u_4 e^{-i\theta_4} & u_5 e^{-i\theta_5} & 1 - r_0 - r_1 - r_2
\end{pmatrix},
\]
(18)

where \( r_i, |u_i|, |\theta_i| \) given in Equation (18) do not need to be equal to \( r_i, |u_i|, |\theta_i| \) given in Equation (15).

Moreover, we apply the following local SU(2) transformation to \( \rho_{AB} \) defined in Equation (18),
\[
\begin{align*}
[0]_A & \to [0]_A, \\
[1]_A & \to \exp(-i\theta_3)[1]_A.
\end{align*}
\]
(19)

By this transformation, we can change the complex numbers of the \([01]_{10}\)- and \([10]_{01}\)-entries of \( \rho_{AB} \) defined in Equation (18) into real numbers as \( u_{3X} \exp(\pm i\theta_3) \to u_3 \). Thus, we obtain the final form of the general \( \rho_{AB} \) as
\[
\rho_{AB} = \begin{pmatrix}
 r & 0 & 0 & u \exp(i\tau_1) \\
0 & s & v & w \exp(i\tau_2) \\
0 & v & t & q \exp(i\tau_3) \\
u \exp(-i\tau_1) & w \exp(-i\tau_2) & q \exp(-i\tau_3) & 1 - r - s - t
\end{pmatrix},
\]
(20)

where \( r \geq 0, s \geq 0, t \geq 0, 1 - r - s - t \geq 0, u \geq 0, v \geq 0, w \geq 0, q \geq 0, 0 \leq \tau_i < 2\pi \) for \( i \in \{1, 2, 3\} \).
Because \( \rho_{AB} \) defined in Equation (20) is a density matrix, \( \rho_{AB} \) has to be positive-semidefinite. In particular, its determinant is always equal to or larger than zero, so that we obtain
\[
\det(\rho_{AB}) = -tsw^2 - tw^2 + \left[r(1 - r - s - t) - u^2\right](st - v^2) + 2wtwq\cos(\tau_2 - \tau_3) \geq 0.
\] (21)
This relation is used in the latter half of this section.

Here, we pay attention to the fact that \( \rho_{AB} \) defined in Equation (20) includes ten real parameters. General two-qubit mixed states include 15 real parameters because of the degree of freedom of SU(4). However, each local qubit has three real parameters that come from the degree of freedom of SU(2). Thus, to describe the entanglement of the two-qubit system, we need nine real parameters. In fact, Luo suggests the following form for \( \rho_{AB} \) to investigate the entanglement [21],
\[
\rho_{AB} = \frac{1}{4} \left( I_{1,AB} + \sum_{i=1}^{3} \sigma_{i,A} \otimes I_{2,B} + \sum_{i=1}^{3} b_i I_{2,A} \otimes \sigma_{i,B} \right.
+ \left. \sum_{i=1}^{3} c_i \sigma_{i,A} \otimes \sigma_{i,B} \right).
\] (22)
However, we dare to choose Equation (20) rather than Equation (22). The reason why we do not choose Equation (22) as the expression of the general density matrix is as follows. \( \rho_{AB} \) defined in Equation (22) does not include zero elements, so that it is very difficult to calculate a determinant of \( \rho_{AB}^\text{PT} \) and eigenvalues of \( \rho_{AB} \rho_{AB}^\text{PT} \) explicitly. By contrast, if we choose Equation (20) as the expression of \( \rho_{AB} \), it includes some zero elements in the matrix form and explicit calculations of determinants and eigenvalues are not so difficult. Thus, although it has one extra real parameter, we choose Equation (20).

We now construct \( \rho_{AB} \rho_{AB}^\text{PT} \) from \( \rho_{AB} \) given by Equation (20), and calculate its eigenvalues \( \{\lambda_i: i \in \{1, 2, 3, 4\}\} \). The eigenvalues are solutions of the following quartic equation,
\[
\det(\rho_{AB} \rho_{AB}^\text{PT} - \lambda I) = 0.
\] (23)
Writing down Equation (23) as a polynomial in \( \lambda \), we obtain
\[
\lambda^4 + f_1(|r|)\lambda^3 + f_2(|r|)\lambda^2 + f_3(|r|)\lambda + f_4(|r|) = 0,
\] (24)
where \( f_i(|r|) \) for \( i \in \{1, 2, 3, 4\} \) is a short form of \( f_i(r, s, t, u, v, w, q, \tau_1, \tau_2, \tau_3) \). An explicit form of \( f_i(|r|) \) is given by
\[
f_i(|r|) = -2[r(1 - r - s - t) + st + u^2 + v^2].
\] (25)
It is obvious that \( f_1(|r|) \leq 0 \). Because explicit forms of \( f_2(|r|), f_3(|r|) \) and \( f_4(|r|) \) are too complicated, we give them in Appendix 1.

Next, we use Ferrari’s method for solving the quartic Equation (24) [22,23]. We introduce a new variable \( x \) as
\[
x = \lambda - \frac{\Delta}{4}.
\] (26)
where
\[
\Delta = -f_1(|r|)(\geq 0).
\] (27)
Then, we rewrite the quartic equation given by Equation (24) as follows:
\[
x^4 + a(|r|)x^3 + b(|r|)x + c(|r|) = 0.
\] (28)
We pay attention to the fact that Equation (28) does not include the third-order term \( x^3 \). We give explicit forms of \( a(|r|), b(|r|) \) and \( c(|r|) \) in Appendix 1.

If we let \( \{x_i: i \in \{1, 2, 3, 4\}\} \) be solutions of Equation (28), we obtain the following relations:
\[
\sum_i x_i = 0,
\]
\[
\sum_{i<j} x_i x_j = a(|r|),
\]
\[
\sum_{i<j<k} x_i x_j x_k = -b(|r|),
\]
\[
x_1 x_2 x_3 x_4 = c(|r|).
\] (29)
The solutions of Equation (28) \( \{x_i: i \in \{1, 2, 3, 4\}\} \) are given by
\[
x_1 = P - \frac{1}{2} \sqrt{-\frac{b}{P} + Q},
\]
\[
x_2 = P + \frac{1}{2} \sqrt{-\frac{b}{P} + Q},
\]
\[
x_3 = -P - \frac{1}{2} \sqrt{-\frac{b}{P} + Q},
\]
\[
x_4 = -P + \frac{1}{2} \sqrt{-\frac{b}{P} + Q},
\] (30)
where \( P, Q \) and \( b \) are short forms of \( P(|r|), Q(|r|) \) and \( b(|r|) \). Moreover, \( P(|r|) \) and \( Q(|r|) \) are given by
\[
P(|r|) = \frac{1}{2\sqrt{6}} \left[ -4a(|r|) + \frac{2\sqrt{2}R(|r|)}{S^{1/3}(|r|)} + \frac{1}{\sqrt{2}} S^{1/3}(|r|) \right]^{1/2},
\]
\[
Q(|r|) = \frac{1}{3} \left[ -4a(|r|) - \frac{\sqrt{2}R(|r|)}{S^{1/3}(|r|)} - \frac{1}{\sqrt{2}} S^{1/3}(|r|) \right],
\]
\[
R(|r|) = a^2(|r|) + 12c(|r|),
\]
\[
S(|r|) = T(|r|) + \sqrt{-4R^2(|r|) + T^2(|r|)},
\]
\[
T(|r|) = 2a^2(|r|) + 27b^2(|r|) - 72a(|r|)c(|r|).
\] (31)
Here, we remember
\[ \lambda_i = x_i + \frac{\Delta}{4} \quad \text{for } i \in \{1, 2, 3, 4\}, \]  
where we do not put \{\lambda_i\} in decreasing order. The relations \( \lambda_i \geq 0 \) for \( i \in \{1, 2, 3, 4\} \) and \( \Delta \geq 0 \) are always valid. Thus, \( x_i \) for \( i \in \{1, 2, 3, 4\} \) has to be real. Hence, we find that \( P \) is real and \( \pm(b/P) + Q \) are equal to or larger than zero.

From the above relations, we obtain
\[ x_2 \geq x_1, \quad x_4 \geq x_3. \]  
(33)

Thus, the maximum number of \{\lambda_i\} is \( x_2 \) or \( x_4 \). Hence, from now on, we assume \( x_2 \geq x_4 \). We consider the case where \( x_2 < x_4 \) later.

Assuming \( x_2 \geq x_4 \), we can describe the concurrence of \( \rho_{AB} \) defined in Equation (20) as
\[ C(\rho_{AB}) = \sqrt{x_2} - \sqrt{x_1} - \sqrt{x_3} - \sqrt{x_4}. \]  
(34)

Here, we think around the following relations, which are valid because of Equations (30) and (33),
\[ \sqrt{x_2} - \sqrt{x_1} \geq 0, \quad \sqrt{x_3} + \sqrt{x_4} \geq 0. \]  
(35)

Thus, we can rewrite \( C(\rho_{AB}) \) given by Equation (34) as
\[
\begin{align*}
C(\rho_{AB}) &= \sqrt{(\sqrt{x_2} - \sqrt{x_1})^2 - (\sqrt{x_3} + \sqrt{x_4})^2} \\
&= \sqrt{(\Delta/2) + x_1 + x_2 - 2\sqrt{[(\Delta/4) + x_1][(\Delta/4) + x_2]} \\
&\quad - \sqrt{(\Delta/2) + x_3 + x_4 + 2\sqrt{[(\Delta/4) + x_3][(\Delta/4) + x_4]}}.
\end{align*}
\]  
(36)

The necessary and sufficient condition for inseparability of \( \rho_{AB} \) is given by \( C(\rho_{AB}) > 0 \). Thus, from Equation (36), the necessary and sufficient condition for inseparability of \( \rho_{AB} \) can be rewritten as
\[ x_1 + x_2 - 2\sqrt{[(\Delta/4) + x_1][(\Delta/4) + x_2]} > x_3 + x_4 + 2\sqrt{[(\Delta/4) + x_3][(\Delta/4) + x_4]}. \]  
(37)

Moreover, from Equation (30), we rewrite Equation (37) as follows:
\[ 2P > \sqrt{[(\Delta/4) + x_1][(\Delta/4) + x_2]} + \sqrt{[(\Delta/4) + x_3][(\Delta/4) + x_4]} \geq 0. \]  
(38)

(In the above derivation, we use \( \lambda_i = x_i + (\Delta/4) \geq 0 \ \forall i \). Because both the right-hand and the left-hand sides of inequality (38) are equal to or larger than zero, we can square both sides of inequality (38), respectively, and we obtain
\[
4P^2 > [(\Delta/4) + x_1][(\Delta/4) + x_2] + [(\Delta/4) + x_3][(\Delta/4) + x_4] \\
+ 2\sqrt{[(\Delta/4) + x_1][(\Delta/4) + x_2][(\Delta/4) + x_3][(\Delta/4) + x_4]}.
\]  
(39)

Looking at Equations (29) and (30), we notice that we can rewrite inequality (39) as
\[ 2P^2 > \frac{\Delta^2}{8} - \frac{Q}{2} + 2\sqrt{(\Delta/4)^4 + a(\Delta/4)^2 - b(\Delta/4) + c}. \]  
(40)

Substituting Equation (31) into inequality (40), we obtain
\[ -a - \frac{\Delta^2}{8} - 2\sqrt{(\Delta/4)^4 + a(\Delta/4)^2 - b(\Delta/4) + c} > 0. \]  
(41)

Here, we pay attention to the following relation, which is obtained from Equations (21), (25), (27), (56) and (57),
\[ (\Delta/4)^4 + a(\Delta/4)^2 - b(\Delta/4) + c = [\det(\rho_{AB})]^2. \]  
(42)

Thus, from Equation (21), we obtain
\[ \sqrt{(\Delta/4)^4 + a(\Delta/4)^2 - b(\Delta/4) + c} = \det(\rho_{AB}) \geq 0. \]  
(43)

Then, using Equation (43), we can rewrite Equation (41) as
\[
\begin{align*}
D(|\psi\rangle) &= rsq^2 + rtw^2 + (st - u^2)v^2 - r(1 - r - s - t) \\
&\quad - 2ruvw \cos(t_1 - t_2 - t_3)
\end{align*}
\]  
\[ > 0. \]  
(44)

Hence, we find that inequality (44) is the necessary and sufficient condition for inseparability of \( \rho_{AB} \) defined in Equation (20).

In the discussions given above, we assume \( x_2 \geq x_4 \). If \( x_2 < x_4 \), we can give similar discussions and we obtain inequality (44) as the necessary and sufficient condition for inseparability of \( \rho_{AB} \), as well. Therefore, we conclude that the necessary and sufficient condition for inseparability of \( \rho_{AB} \) derived from Hill–Wootters formula is given by inequality (44).

On the other hand, according to the Peres–Horodecki criterion, the necessary and sufficient condition for inseparability of \( \rho_{AB} \), which is defined in Equation (20), is given by
\[ \det(\rho^{'\text{PT}}_{AB}) < 0. \]  
(45)

Writing Equation (45) in an explicit form, we obtain
\[ \det(\rho^{'\text{PT}}_{AB}) = -D(|\psi\rangle) < 0. \]  
(46)

Inequality (46) is equivalent to inequality (44).
Therefore, we succeed in deriving the Peres–Horodecki criterion for two-qubit mixed states from the Hill–Wootters formula in a direct manner.

4. Separability for a convex combination of a separable pure state and an inseparable pure state

In this section, we consider an example of a convex combination of a separable pure state and an inseparable pure state,

\[ \rho_{AB} = p|\phi_1\rangle_{AB}|\phi_1\rangle + (1-p)|\psi_e\rangle_{AB}|\psi_e\rangle, \]

where \( 0 \leq p \leq 1 \), \( |\phi_1\rangle_{AB} \) is a normalized separable ket vector and \( |\psi_e\rangle_{AB} \) is a normalized inseparable ket vector. Under the assumption of Equation (47), we can derive the Peres–Horodecki criterion from the Hill–Wootters formula in a direct manner without difficulty, so that this can be a concrete example of the results obtained in Section 3.

At first, we consider a couple of SU(2) transformations \( U_{1,A} \) and \( U_{2,B} \), which cause the following transformation to the separable pure state given in Equation (47),

\[ |\phi_1\rangle_{AB} = |\phi_1\rangle_A \otimes |\phi_2\rangle_B \]
\[ \rightarrow (U_{1,A} \otimes U_{2,B}|\phi_1\rangle_{AB}) = U_{1,A}|\phi_1\rangle_A \otimes U_{2,B}|\phi_2\rangle_B = |0\rangle_A \otimes |0\rangle_B. \]

The couple of the unitary transformations \( U_{1,A} \) and \( U_{2,B} \) that satisfy Equation (48) always exists and we can choose \( U_{1,A} \) and \( U_{2,B} \) independently of each other. Moreover, applying \( U_{1,A} \otimes U_{2,B} \) to the system AB neither increases nor decreases the entanglement between the qubits A and B, because it is a local operation. Thus, applying \( U_{1,A} \otimes U_{2,B} \) never gives the actual effects on both the Peres–Horodecki criterion and the Hill–Wootters formula.

From the above discussions, we can use the following density matrix as a general form, instead of the density matrix given by Equation (47),

\[ \rho_{AB} = p \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + (1-p)|\psi_e\rangle_{AB}|\psi_e\rangle, \]

where \( 0 \leq p \leq 1 \),

\[ |\psi_e\rangle_{AB} = \begin{pmatrix} a \\ b \exp(i\theta_1) \\ c \exp(i\theta_2) \\ \sqrt{1-a^2-b^2-c^2} \exp(i\theta_3) \end{pmatrix}, \]

and \( a \geq 0, b \geq 0, c \geq 0, 1-a^2-b^2-c^2 \geq 0, 0 \leq \theta_i < 2\pi \) for \( i \in \{1, 2, 3\} \). Moreover, because \( |\psi_e\rangle_{AB} \) is an entangled state, we assume its concurrence to be positive as follows:

\[ C(|\psi_e\rangle_{AB}) = 2[a^2(1-a^2-b^2-c^2) + b^2c^2 - 2abc\sqrt{1-a^2-b^2-c^2}\cos(\theta_1 + \theta_2 - \theta_3)]^{1/2} > 0. \]

From the density matrix given by Equation (49), we calculate eigenvalues of \( \rho_{AB}^{\text{PT}} \). We write them as \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0 \), where

\[ \lambda_1 = X + \frac{1}{2}\sqrt{Y}, \quad \lambda_2 = X - \frac{1}{2}\sqrt{Y}, \quad \lambda_3 = \lambda_4 = 0, \]

\[ X = \frac{1}{4}(1-p)[(1-p)C^2(|\psi_e\rangle_{AB}) + 2p(1-a^2-b^2-c^2)], \]
\[ Y = (1-p)^2 C^2(|\psi_e\rangle_{AB})[(1-p)C^2(|\psi_e\rangle_{AB}) + 4p(1-a^2-b^2-c^2)]. \]

From the above equations, we can obtain \( X \geq 0 \) and \( Y \geq 0 \) at ease.

Thus, we can write the concurrence of \( \rho_{AB} \) as

\[ C(\rho_{AB}) = \sqrt{\lambda_1 - \lambda_2}. \]

Hence, we find that the necessary and sufficient condition of \( C(\rho_{AB}) > 0 \) (\( \rho_{AB} \) is inseparable) is \( Y > 0 \).

On the other hand, defining the density matrix \( \rho_{AB}^{\text{PT}} \) as Equation (49), we can obtain the determinant of \( \rho_{AB}^{\text{PT}} \) in the form,

\[ \det(\rho_{AB}^{\text{PT}}) = -\frac{Y}{16}. \]

Thus, the determinant of \( \rho_{AB}^{\text{PT}} \) is negative if and only if \( \rho_{AB} \) is inseparable, where we assume that \( \rho_{AB} \) is given by Equation (47). Hence, we derive the Peres–Horodecki criterion from the Hill–Wootters formula in a direct manner on condition that the density matrix is given by a convex combination of a separable pure state and an inseparable pure state.

5. Discussion

In this paper, we investigate connections between the Peres–Horodecki criterion for the two-qubit states and the Hill–Wootters formula for the entanglement of formation. In this study, the following expression being equivalent to the Peres–Horodecki criterion plays an important role: the two-qubit mixed state is inseparable if and only if the determinant of the partial transpose of its density matrix is less than zero. In [10], Augusiak et al. show that an entanglement measure for a two-qubit state can be constructed from \( \max\{0, -\det(\rho_{AB}^{\text{PT}})\} \). The authors suppose that there
are an infinite number of entanglement measures for two-qubit systems.

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Appendix 1
Explicit forms of $f_i(r)$ for $i \in \{2, 3, 4\}$ defined in Equation (24) are given by

\[
f_2(r) = -r^4 - 2r^2(1 - r - s - t) + s^2 r^2 + 2u^2 r^2 + 2st(2u^2 - v^2) + (u^2 + v^2)^2 + r^2[1 + (s - t)^2 - 2(s + t) + 2(2u^2 - v^2)] - 2r[2(q^2 - s(u^2 - 2v^2) + (1 - t)(u^2 - 2v^2 - 2st) + t(2u^2 + v^2)] + 4qrw[2wcos(t_1 - t_2 - t_3) - rcos(t_2 - t_3)],
\]

\[
f_3(r) = 2[-stu^4 - v^4[u^2 + r\eta([r])] + rs[st + r\eta([r])]\{q^2 - t\eta([r])\} - st^2(rq^2 + [st - 2r\eta([r])] - v^2[2rq^2 + 4[u^2 + v^2 - st - r\eta([r])] - v^2(rsq^2 + [u^2 - r\eta([r])] - 2qs[u^2 + r\eta([r])])] + 4ru[tvw^2 cos(t_1 - 2t_2) + qsvwcos(t_1 - t_2)] - (st + v^2)\eta \cos(t_1 - t_2 - t_3)],
\]

\[
f_4(r) = [rsq^2 + [u^2 - r(1 - r - s - t)](st - v^2) + rtw^2 - 2rsqwcos(t_2 - t_3)].
\]

The explicit forms of $a([r]), b([r])$ and $c([r])$ defined in Equation (28) are given by

\[
a([r]) = f_2([r]) - (3/8)\Delta^2,
\]

\[
b([r]) = f_3([r]) - (1/8)\Delta\Delta^2 - 4f_2([r])],
\]

\[
c([r]) = f_4([r]) - (1/256)\Delta\Delta^2 - 16f_2([r]) - 64f_3([r]).
\]