Attainable entanglement of unitary transformed thermal states in liquid-state nuclear magnetic resonance with the chemical shift

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Abstract
Yu, Brown and Chuang investigated the entanglement attainable from unitary transformed thermal states in liquid-state nuclear magnetic resonance (NMR). Their research gave insight into the role of entanglement in a liquid-state NMR quantum computer. However, they assumed that the Zeeman energy of each nuclear spin which corresponds to a qubit takes a common value for all; there is no chemical shift. In this paper, we research a model with chemical shifts and analytically derive the physical parameter region where unitary transformed thermal states are entangled, by employing the positive partial transposition (PPT) criterion with respect to any bipartition. The analysis taking account of the chemical shift reveals how the difference between quantum gates reflects on the physical parameter region where unitary transformed thermal states are entangled. In addition, we examine the distillability of unitary transformed thermal states and the effect of the chemical shifts on the boundary between the separability and the nonseparability.

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1. Introduction

Quantum mechanics has very different conceptual and mathematical characters from those of classical mechanics. The superposition and the entanglement (nonseparability) of quantum states make the difference clear. Recently, these characterizations have been utilized for a newly developing quantum technology. Actually, quantum entanglement is deeply related to quantum information processing (QIP) [1].

The role of entanglement in quantum computing has been researched from various viewpoints. In particular, the entanglement generation by quantum dynamics, or quantum algorithms, can give us useful information [2–4]. Recently, Yu, Brown and Chuang [4] investigated the entanglement of unitary transformed thermal states in a liquid-state nuclear magnetic resonance (NMR) quantum computer. Such states are defined as the density matrices transformed from the thermal state in a liquid-state NMR quantum computer by a specific class of unitary operators. Their definition will be explained in section 2.2. Furthermore, we call such states Bell-transformed thermal states. The thermal state in [4] is separable (i.e., there is no quantum correlation) [5] and characterized by two physical parameters: the one is the number of qubits and the other is a measure of the state's polarization. The authors in [4] studied two kinds of Bell transformations. One of their central interests is the difference between the Bell-transformed thermal states and effective pure states. The effective pure state is the convex sum of the identity operator and a pure state, and a typical one is used in the current liquid-state NMR quantum computer [6–8]. They concluded that the former should be more easily entangled than the latter; the Bell-transformed thermal states can be entangled even in the physical parameter region where effective pure states are separable.

Their research is very important for the following three reasons. First, they focused an elementary state in a liquid-state NMR quantum computer. Braunstein *et al* [9] pointed out that the effective pure states should be almost separable in the current liquid-state NMR experiments. After their study, various studies on the role of entanglement in liquid-state NMR quantum computing were done (see [4] for additional references). One should note that the most natural quantum state is the thermal one in liquid-state NMR and an effective pure state is constructed from it by a sequential operation of several quantum gates. Therefore, the authors in [4] investigated the entanglement of a more elementary state than effective pure states in liquid-state NMR quantum computers. Second, they attempted to reveal the role of mixed-state entanglement in quantum computing. Its evaluation and meaning will be more subtle than is the case with pure states. Nevertheless, they can be characterized from the viewpoint of quantum communication. In particular, distillability is important [10–12]. If a mixed state is distillable, it is useful for QIP (e.g., quantum teleportation); we can distill maximal entangled states by using a number of the copies, and local operations and classical communication (LOCC). Accordingly, their research could lead to an alternative understanding of mixed-state entanglement from the viewpoint of quantum computing. Finally, as mentioned in the beginning of this section, their work is related to the generation of entanglement by quantum dynamics. Actually, they found the difference of the entanglement generation between the two Bell transformations.

In this paper, we analytically derive, in a more general case, the physical parameter region where the Bell-transformed thermal states are entangled; specifically, the effect of the chemical shift [8, 13] is included in our Hamiltonian. The authors in [4] assumed that each nuclear spin which corresponds to a qubit has the common Zeeman energy. However, this implies that one cannot access the individual qubit; it is not a realistic model. Our interest is to understand the role of an important element for implementing quantum computation in the entanglement generation by quantum gates. The chemical shift is just such an important element in liquid-state NMR quantum computers. Moreover, the analysis taking account of the chemical shift will reveal how the difference between the Bell transformations reflects on the physical parameter region where the Bell-transformed thermal states are entangled. It will also be necessary if we are to evaluate the attainability of entanglement from the thermal state in the experiments. Our method of evaluating the entanglement is simple and straightforward: the positive partial transposition (PPT) criterion [14–16]. We analytically calculate the eigenvalues of the partial transposed Bell-transformed thermal states and find

the smallest ones. Here, we would like to emphasize that, in [4], the Dür–Cirac classification [17] has been applied to the evaluation of the entanglement with respect to two types of Bell-transformed thermal states, but it does not necessarily work.

This paper is organized as follows. In section 2, we introduce the Hamiltonian and the Bell transformations. As in [4], we concentrate on two unitary operators of the Bell transformations. In section 3, to begin, we explain how to specify an individual bipartition and briefly review the PPT criterion. Next, we explain the Bell-diagonal state [18, 19] in an N-qubit system, which plays a central role in this paper. Then, we show the main results in section 3.4: the sufficient conditions for the nonseparability of the Bell-transformed thermal states with respect to any bipartition. In section 4, we show the necessary conditions for the full separability and the full distillability. In particular, we show the necessary and sufficient conditions for full distillability when there is no chemical shift. In section 5, we examine the effect of the chemical shift on the boundary between the separability and the nonseparability determined by the PPT criterion. We summarize our results in section 6. Furthermore, in appendix, we briefly review the Dür–Cirac classification and show some examples in which this method does not work.

2. Model

2.1. Hamiltonian

In a liquid-state NMR quantum computer, the qubit is the nuclear spin in the molecule. We assume the number of qubits is N in one molecule. The dipole–dipole interaction between the molecules in solutions is negligible because they randomly collide with each other [8]. Therefore, we concentrate on the internal degrees of freedom (i.e., the nuclear spin) of one molecule. Let us define the computational bases as $|0\rangle_i$ and $|1\rangle_i$ ($_i\langle 0|0\rangle_i = 1, _i\langle 1|1\rangle_i = 1$ and $_i\langle 0|1\rangle_i = 0$). The subscription $i (=1, 2, \ldots, N)$ is the label of the qubit. Furthermore, we introduce the following standard operators: $I_i = |0\rangle_i\langle 0| + |1\rangle_i\langle 1|$, $Z_i = |0\rangle_i\langle 0| - |1\rangle_i\langle 1|$, $X_i = |0\rangle_i\langle 1| + |1\rangle_i\langle 0|$ and $H_i = (Z_i + X_i)/\sqrt{2}$. We analyze the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \frac{h\nu_i}{2} Z_i, \tag{1}$$

where $h\nu_i$ is the Zeeman energy of the ith qubit. Note that we neglect the J-coupling between the neighboring qubits because it is much smaller than the Zeeman energy in a liquid-state NMR [8, 13]. The model includes the important physical effect; every value of $h\nu_i$ is different from the others, due to the chemical shift. The difference allows us to access each qubit individually. In [4], every $h\nu_i$ is a common value. In this paper, we do not mention the relationship between the above computational basis and the physical spin state, and the Hamiltonian (1) is a mathematical model.

2.2. Bell-transformed thermal states

Let us consider the separable state which is characterized by a set of physical parameters. Our interest is the parameter region in which the state transformed from a separable one by quantum gates is a nonseparable one. Therefore, we have to specify a suitable initial separable state and quantum gates which generate the entanglement in a liquid-state NMR quantum computer.

First, we refer to the initial separable state. The system in a liquid-state NMR experiment is a thermal equilibrium state with room temperature. Accordingly, the most natural choice for the initial state is the thermal state

$$\rho_{\text{th}} = \frac{1}{\mathcal{Z}} \, \mathrm{e}^{-\beta \mathcal{H}}. \tag{2}$$

In our model, the Hamiltonian $\mathcal{H}$ is given by (1). Here, β and $\mathcal{Z} = \mathrm{tr} \, \mathrm{e}^{-\beta \mathcal{H}}$ are the inverse temperature and the partition function, respectively. Note that state (2) is a separable state with respect to any bipartition of the system. The physical parameters in (2) are the number of the qubit N, the Zeeman energy of the ith qubit $h\nu_i$ and the inverse temperature β, which are regarded as the free parameters. Actually, the values of the parameters are restricted by the experiments for liquid-state NMR quantum computing. For the comparison with [4], we introduce the parameter $\alpha_i = \beta h \nu_i / 2$, which is called a measure of the state's polarization in the reference. Hereafter, we simply call it polarization. The physical meaning of α_i is quite clear. Let us consider the expectation value of the z-component of the total spin operator $J_z \left(\equiv \sum_{i=1}^N Z_i / 2 \right)$ with respect to ρ_{th}: $m_z \equiv \mathrm{tr}(J_z \rho_{\text{th}}) = - \sum_{i=1}^N (\tanh \alpha_i)/2$. We assume the value of N is fixed. The value of $|m_z|$ becomes larger as α_i increases; the system is strongly polarized in the direction of the z-axis. Summarizing the above argument, we can say that the initial thermal state (2) is characterized by the number of qubits N and the polarization α_i.

Next, we explain the unitary operators for generating entanglement. We will have to investigate all types of the quantum gates which are considered as the generator of entanglement and essential parts in a quantum algorithm. However, this task will be very difficult. In this paper, as in [4], we concentrate on the following two unitary operators: the controlled-NOT–Hadamard (CH) transformation, $U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I)$, and the CH-fanout transformation, $U_{\text{CF}} = U_{\text{CH}} U_{\text{fan}}$. The fanout gate U_{fan} is defined as follows: $U_{\text{fan}} = |0\rangle_1 \langle 0| \otimes I + |1\rangle_1 \langle 1| \otimes X$, where $I = \bigotimes_{i=2}^N I_i$, $X = \bigotimes_{i=2}^N X_i$. The above unitary operators are examples in quantum gates, but they include the essential quantum gates for the generation of entanglement: controlled-NOT gates and Hadamard gates. In this case, they generate the entanglement between the first qubit and the remaining qubits. Let us consider, for example, the case of $N = 3$. When the initial state is $|000\rangle = |0\rangle_1 \otimes |0\rangle_2 \otimes |0\rangle_3$, we obtain the following results: $U_{\text{CH}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ and $U_{\text{CF}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$.

In summary, we examine the entanglement of the states

$$\rho_{\text{CH}} = U_{\text{CH}} \rho_{\text{th}} U_{\text{CH}}^\dagger, \tag{3}$$

$$\rho_{\text{CF}} = U_{\text{CF}} \rho_{\text{th}} U_{\text{CF}}^\dagger. \tag{4}$$

The above states are called the Bell-transformed thermal states. The initial state ρ_{th} is separable with any bipartition of the system for the arbitrary values of N and $\{\alpha_i\}_{i=1}^N$.

3. Entanglement of Bell-transformed thermal states with chemical shift

3.1. Specification of a bipartition

In order to study the entanglement of a system, it is necessary to specify the way to divide it into two parts. We divide the N-qubit system into two subsystems, party A and party B, in the following [4]. First, let us consider a set of binary numbers, $\{k_i\}_{i=1}^N$ ($k_i = 0, 1$). When $k_i = 0$, let the ith qubit be in party A. On the other hand, when $k_i = 1$, it is in party B. We always set $k_1 = 0$; the first qubit is always in party A. For convenience, we introduce an integer $k = \sum_{i=2}^N k_i 2^{i-2}$. Therefore, a partition is specified if an integer $k (\in [1, 2^{N-1} - 1])$ is chosen; we call such a partition the bipartition k. Let us choose, for instance, $k = 4$ in the

case of $N = 4$ (i.e., $k_2 = 0$, $k_3 = 0$ and $k_4 = 1$). The elements of party A are the 1st, 2nd and 3rd qubit, and party B contains only the 4th qubit.

3.2. PPT criterion

The PPT criterion is the simple and computable way to investigate entanglement. We briefly recapitulate it. Let us consider a density matrix ρ in a quantum system with finite dimension d. The total system is divided into two subsystems, system A and system B. Introducing an orthonormal basis of the system A, $\{|u_i\rangle_A\}_{i=1}^{d_A}$ and the system B, $\{|v_k\rangle_B\}_{k=1}^{d_B}$, we can expand the density matrix ρ as follows:

$$\rho = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} C(ik|jl)|u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|, \tag{5}$$

where $C(ik|jl)$ is a complex number and $d = d_A d_B$. Next, using (5), we define the partial transposition of the density matrix with respect to the system B as

$$\rho^{T_B} = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} C(il|jk)|u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|. \tag{6}$$

Then, we calculate the eigenvalues of ρ^{T_B} and investigate their positivity. If all eigenvalues of (6) are positive (i.e., $\rho^{T_B} \geqslant 0$), it is called a density matrix with PPT. On the other hand, if at least one of its eigenvalues is negative, it is called a density matrix with the negative partial transposition (NPT). The most important thing to note here is the following criterion (i.e., the PPT criterion):

$$\rho: \text{separable} \quad \Rightarrow \quad \rho: \text{PPT}, \tag{7}$$

or, equivalently,

$$\rho: \text{NPT} \quad \Rightarrow \quad \rho: \text{entangled (nonseparable)}. \tag{8}$$

Moreover, the following statement is also known [11, 12]:

$$\rho: \text{distillable} \quad \Rightarrow \quad \rho: \text{NPT}. \tag{9}$$

3.3. Bell-diagonal states

Before showing our results, we explain the special class of a density matrix, the Bell-diagonal state [18, 19]. It plays a central role in later discussion.

To begin, let us explain the generalized Greenberger–Horne–Zeilinger (GHZ) state [4, 17] in the N-qubit system

$$|\Psi_j^{\pm}\rangle = \frac{1}{\sqrt{2}}(|0j\rangle \pm |1\bar{j}\rangle) \qquad (0 \leqslant j \leqslant 2^{N-1} - 1), \tag{10}$$

where $j = \sum_{i=2}^{N} j_i 2^{i-2}$ for the binary number j_i ($=0, 1$), $|0j\rangle = |0\rangle_1 \bigotimes_{i=2}^{N} |j_i\rangle_i$ and $|1\bar{j}\rangle = |1\rangle_1 \bigotimes_{i=2}^{N} |1 - j_i\rangle_i$. The symbol $\bar{j}$ means a bit-flip of j: $\bar{j} = 2^{N-1} - 1 - j$. We can easily find the generalized GHZ states are the elements of an orthonormal basis of the Hilbert space corresponding to the N-qubit system.

We introduce the following density matrix:

$$\rho_{BD} = \sum_{j=0}^{2^{N-1}-1} \left(\omega_j^+ |\Psi_j^+\rangle\langle\Psi_j^+| + \omega_j^- |\Psi_j^-\rangle\langle\Psi_j^-| \right), \tag{11}$$

where $\omega_j^\pm = \langle \Psi_j^\pm | \rho_{BD} | \Psi_j^\pm \rangle$ and $\sum_{j=0}^{2^{N-1}-1} (\omega_j^+ + \omega_j^-) = 1$. Equation (11) is a Bell-diagonal state in an N-qubit system. We will show that ρ_{CH} and ρ_{CF} take the form of (11) in the following subsection.

We introduce the Bell-diagonal state so that we can easily obtain its partial transposition [19]. We confirm this in the following procedure. First, let us consider a bipartition k. Second, we represent $|\Psi_j^\pm\rangle\langle\Psi_j^\pm|$ in the computational basis: $|\Psi_j^\pm\rangle\langle\Psi_j^\pm| = (|0j\rangle\langle0j| \pm |0j\rangle\langle1\bar{j}| \pm |1\bar{j}\rangle\langle0j| + |1\bar{j}\rangle\langle1\bar{j}|)/2$. The diagonal parts of $|\Psi_j^\pm\rangle\langle\Psi_j^\pm|$ are $|0j\rangle\langle0j|$ and $|1\bar{j}\rangle\langle1\bar{j}|$, and they are invariant under the partial transposition with respect to party B. The off-diagonal ones are $|0j\rangle\langle1\bar{j}|$ and $|1\bar{j}\rangle\langle0j|$ because $j \neq \bar{j}$. If the ith qubit is in party B (i.e., $k_i = 1$), the binary number j of the off-diagonal parts is transformed into $j_i + 1(=j_i + k_i)$ modulo 2 (e.g., $0 + 1 = 1$ and $1 + 1 = 0$) by the partial transposition with respect to party B. On the other hand, if the ith qubit is in the party A (i.e., $k_i = 0$), the corresponding j_i is unchanged; $j_i = j_i + k_i$. As a result, we obtain the following expression: $(|\Psi_j^\pm\rangle\langle\Psi_j^\pm|)^{T_B} = (|\Psi_j^+\rangle\langle\Psi_j^+| + |\Psi_j^-\rangle\langle\Psi_j^-| \pm |\Psi_{j\oplus k}^+\rangle\langle\Psi_{j\oplus k}^+| \mp |\Psi_{j\oplus k}^-\rangle\langle\Psi_{j\oplus k}^-|)/2$, where $j \oplus k = \sum_{i=2}^{N} l_i 2^{i-2}$ ($l_i \equiv j_i + k_i$ mod 2). Accordingly, the Bell-diagonal state partially transposed with respect to party B is given by

$$\rho_{BD}^{T_B} = \sum_{j=0}^{2^{N-1}-1} \left(\mu_j^+ |\Psi_j^+\rangle\langle\Psi_j^+| + \mu_j^- |\Psi_j^-\rangle\langle\Psi_j^-|\right), \tag{12}$$

where

$$\mu_j^\pm = \frac{\omega_j^+ + \omega_j^-}{2} \pm \frac{\omega_{j\oplus k}^+ - \omega_{j\oplus k}^-}{2}. \tag{13}$$

3.4. Sufficient conditions for nonseparability

First of all, let us show (3) and (4) are just the Bell-diagonal state. Using the standard relations $(H_1 \otimes I)|0j\rangle = (|0j\rangle + |1j\rangle)/\sqrt{2}$, $(H_1 \otimes I)|1j\rangle = (|0j\rangle - |1j\rangle)/\sqrt{2}$, $U_{fan}|0j\rangle = |0j\rangle$, and $U_{fan}|1j\rangle = |1\bar{j}\rangle$, we obtain the following results:

$$\langle \Psi_j^\pm | \rho_{CH} | \Psi_{j'}^\pm \rangle = \frac{\delta_{jj'}}{\mathcal{Z}} e^{\mp\alpha_1} e^{-\sum_{i=2}^{N}(-1)^{j_i}\alpha_i}, \tag{14}$$

$$\langle \Psi_j^\pm | \rho_{CF} | \Psi_{j'}^\pm \rangle = \frac{\delta_{jj'}}{\mathcal{Z}} e^{\mp\alpha_1} e^{\mp\sum_{i=2}^{N}(-1)^{j_i}\alpha_i}, \tag{15}$$

$$\langle \Psi_j^\pm | \rho_{CH} | \Psi_{j'}^\mp \rangle = \langle \Psi_j^\pm | \rho_{CF} | \Psi_{j'}^\mp \rangle = 0, \tag{16}$$

where $0 \leqslant j, j' \leqslant 2^{N-1} - 1$. Consequently, both ρ_{CH} and ρ_{CF} are Bell-diagonal states.

Let us define the mean values of the polarization of party A, ξ and party B, η for given j and k as follows:

$$\xi = \frac{1}{N-w} \sum_{i \in A_k} (-1)^{j_i} \alpha_i, \qquad \eta = \frac{1}{w} \sum_{i \in B_k} (-1)^{j_i} \alpha_i, \tag{17}$$

where $A_k = \{i \in \mathbb{Z}; k_i = 0, 1 \leqslant i \leqslant N\}$, $B_k = \{i \in \mathbb{Z}; k_i = 1, 1 \leqslant i \leqslant N\}$. In (17), we conventionally assign zero to j_1. The number w is the total number of the elements of party B ($1 \leqslant w \leqslant N - 1$). In other words, it is the Hamming weight of k (i.e., the number of one in $\{k_i\}_{i=1}^{N}$). Each of ξ and η is a function of j if N, $\{\alpha_i\}_{i=1}^{N}$, and k are fixed.

Then, we calculate the eigenvalues of $\rho_{CH}^{T_B}$ and $\rho_{CF}^{T_B}$ with respect to the bipartition k. Now that we know the general expression (13) for the partially transposed Bell-diagonal state, we

easily obtain the desired results of Bell-transformed thermal states with the chemical shift. For a given bipartition k, the eigenvalue of $\rho_{\text{CH}}^{\text{T}_\text{B}}$ is given by

$$\mu_{\text{CH},j}^\pm = \frac{1}{\mathcal{Z}} e^{\alpha_1} \cosh \alpha_1 e^{-(N-w)\xi} n_{\text{CH}}^\pm(\eta), \tag{18}$$

where $n_{\text{CH}}^\pm(\eta) = e^{-w\eta} \mp \tanh \alpha_1 e^{w\eta}$. Similarly, the eigenvalue of $\rho_{\text{CF}}^{\text{T}_\text{B}}$ is given by

$$\mu_{\text{CF},j}^\pm = \frac{1}{\mathcal{Z}} n_{\text{CF}}^\pm(\xi, \eta), \tag{19}$$

where $n_{\text{CF}}^\pm(\xi, \eta) = e^{\mp(N-w)\xi} \cosh(w\eta) \pm e^{\pm(N-w)\xi} \sinh(w\eta)$.

In general, the relative signs between α_i's can be different. For the latter discussion, we evaluate the range of ξ and η for the given $\{\alpha_i\}_{i=1}^N$ and k. We rewrite (17) as

$$\xi = \frac{1}{N-w} \sum_{i \in A_k} (-1)^{j_i+s_i} |\alpha_i|, \qquad \eta = \frac{1}{w} \sum_{i \in B_k} (-1)^{j_i+s_i} |\alpha_i|,$$

where $s_i = 0$ for $\alpha_i \geqslant 0$ and $s_i = 1$ for $\alpha_i < 0$. We readily obtain the inequalities

$$|\xi| \leqslant \frac{1}{N-w} \sum_{i \in A_k} |\alpha_i| \equiv \xi_*, \qquad |\eta| \leqslant \frac{1}{w} \sum_{i \in B_k} |\alpha_i| \equiv \eta_*. \tag{20}$$

The condition for $\xi = \xi_* (\equiv \xi_{\max})$ is easily found: $j_i + s_i = 0 \pmod 2$ for any $i \in A_k$. Similarly, the conditions for $\eta = \eta_* (\equiv \eta_{\max})$ and $\eta = -\eta_* (\equiv \eta_{\min})$ are given by $j_i + s_i = 0 \pmod 2$ and $j_i + s_i = 1 \pmod 2$ for any $i \in B_k$, respectively. Note that the minimum value of ξ is not always $-\xi_*$ because $j_1 = 0$; it is $-\xi_* + [1 + (-1)^{s_1}]|\alpha_1|/(N-w) \equiv \xi_{\min}$.

Now, we analytically derive the sufficient conditions for the nonseparability of ρ_{CH} and ρ_{CF}. What is needed is that we search for the minimum values of the eigenvalues which can be negative.

First, we examine (18). In order to discuss definitely, we assume α_1 is positive for a while. We find that the eigenvalue $\mu_{\text{CH},j}^-$ is always positive because all factors of the right-hand side are positive. Then we focus on $\mu_{\text{CH},j}^+$. The positivity is determined by the value of $n_{\text{CH}}^+(\eta)$. Note that it is a monotonic decreasing function of η, because $\partial n_{\text{CH}}^+(\eta)/\partial \eta < 0$. Therefore, the minimum value of $n_{\text{CH}}^+(\eta)$ is given by $n_{\text{CH}}^+(\eta_{\max}) = n_{\text{CH}}^+(\eta_*) = e^{-w\eta_*} - \tanh \alpha_1 e^{w\eta_*}$. We examine the case of negative α_1 in turn. In the case, the value of $n_{\text{CH}}^-(\eta)$ is important for the examination of the positivity of ρ_{CH}. We can readily check that the minimum value of $n_{\text{CH}}^-(\eta)$ is given by $n_{\text{CH}}^-(\eta_{\max}) = n_{\text{CH}}^-(\eta_*) = e^{-w\eta_*} - \tanh |\alpha_1| e^{w\eta_*}$. Summarizing the above argument, we can say that ρ_{CH} is NPT with respect to the bipartition k if and only if

$$n_{\text{CH}}^+(\eta_*) < 0 \qquad \Longleftrightarrow \qquad e^{-2w\eta_*} < \tanh |\alpha_1|. \tag{21}$$

Second, let us consider (19). We concentrate on the behavior of $n_{\text{CF}}^\pm(\xi, \eta)$ because $\mathcal{Z} > 0$. First, we investigate $n_{\text{CF}}^+(\xi, \eta)$. Note that the value is always positive for $\eta \geqslant 0$ or $\xi, \eta \leqslant 0$. Hereafter, we consider the case of $\xi > 0$ and $\eta < 0$. In this case, we find $\partial n_{\text{CF}}^+(\xi, \eta)/\partial \xi < 0$ and $\partial n_{\text{CF}}^+(\xi, \eta)/\partial \eta > 0$. Therefore, the minimum value of $n_{\text{CF}}^+(\xi, \eta)$ is given by $n_{\text{CF}}^+(\xi_{\max}, \eta_{\min}) = n_{\text{CF}}^+(\xi_*, -\eta_*) = e^{-(N-w)\xi_*} \cosh(w\eta_*) - e^{(N-w)\xi_*} \sinh(w\eta_*)$. Next, we consider $n_{\text{CF}}^-(\xi, \eta)$. It should be noted that the following relation is fulfilled: $n_{\text{CF}}^+(\xi, \eta) = n_{\text{CF}}^-(-\xi, -\eta)$. Therefore, we readily obtain the information on $n_{\text{CF}}^-(\xi, \eta)$. Through the above arguments, the minimum value of $n_{\text{CF}}^-(\xi, \eta)$ is given by $n_{\text{CF}}^-(\xi_{\min}, \eta_{\max}) = n_{\text{CF}}^-(\xi_{\min}, \eta_*) = e^{-(N-w)\xi_* + [1+(-1)^{s_1}]|\alpha_1|} \cosh(w\eta_*) - e^{(N-w)\xi_* - [1+(-1)^{s_1}]|\alpha_1|} \sinh(w\eta_*)$. On the other hand, $n_{\text{CF}}^-(\xi_{\min}, \eta_*)$ is clearly greater than or equal to $n_{\text{CF}}^+(\xi_*, -\eta_*)$. Consequently, ρ_{CF} is NPT with respect to the bipartition k if and only if

$$n_{\text{CF}}^+(\xi_*, -\eta_*) < 0 \qquad \Longleftrightarrow \qquad \cosh[(N-w)\xi_* - w\eta_*] < \sinh(N\bar{\alpha}), \tag{22}$$

where $N\bar{\alpha} \equiv \sum_{i=1}^N |\alpha_i| = (N-w)\xi_* + w\eta_*$.

Table 1. Necessary and sufficient conditions for NPT with respect to the bipartition k for each Bell transformation, where $\xi_* = \sum_{i \in A_k} |\alpha_i|/(N-w)$, $\eta_* = \sum_{i \in B_k} |\alpha_i|/w$ and $\bar{\alpha} = \sum_{i=1}^{N} |\alpha_i|/N$.

Bell transformation	Condition for NPT
CH	$e^{-2w\eta_*} < \tanh |\alpha_1|$
CH-fanout	$\cosh[(N-w)\xi_* - w\eta_*] < \sinh(N\bar{\alpha})$

We summarize the sufficient conditions for the nonseparability of ρ_{CH} and ρ_{CF} with respect to the bipartition k in table 1. Note that the information of the bipartition k is included in ξ_* and η_* through A_k and B_k. The definitions of A_k and B_k are explained below (17). With respect to the bipartition k, ρ_{CH} is an entangled state if the inequality (21) is fulfilled, and ρ_{CF} is an entangled one if the inequality (22) is fulfilled. The sufficient condition for the nonseparability of ρ_{CH} is given by α_1 and the mean value of the magnitude of polarization for party B, η_*; it does not depend on α_i ($i \in A_k$) in party A, except for α_1. On the other hand, the sufficient condition of ρ_{CF} is determined by ξ_* and η_*; it depends on the mean values of the magnitude of polarization for party A and party B. It should be noted that if every α_i is a common value and positive, we can readily check whether both sufficient conditions (21) and (22) are equivalent to the corresponding results in [4].

3.5. Characterization of the Bell transformations

It is important for the deep understanding of the quantum algorithm to characterize the property of quantum dynamics in terms of entanglement. Let us therefore consider the ability and mechanism of the Bell transformations U_{CH} and U_{CF} to generate entanglement from the thermal state.

The authors in [4] discussed this ability without taking account of the chemical shift. They concluded that U_{CF} is a more effective Bell transformation than U_{CH}, because the parameter region, in which ρ_{CF} is entangled with respect to a given bipartition, is wider than the corresponding one of ρ_{CH}. Such a result is quite natural because the number of the controlled-NOT gates in U_{CF} is twice as many as in U_{CH}.

The analysis of the sufficient conditions for the nonseparability of the Bell-transformed thermal states with the chemical shift reveals the difference between U_{CH} and U_{CF} from another point of view. We assume that the maximum value of η, η_* is given with respect to a bipartition k. In this case, let us consider the necessary information of party A needed to examine the entanglement of the Bell-transformed thermal states by the PPT criterion. As for ρ_{CH}, from (21), we find that only the value of α_1 is needed; in other words, the local information of party A is required. On the other hand, we have to know the maximum value of ξ, ξ_* to investigate whether ρ_{CF} is entangled or not, according to (22); in other words, the global information of party A is required. These observations can lead to understanding how the Bell transformations entangle party A and party B.

4. Full separability and full distillability

Let us consider an N-particle system. A state of this system is called fully separable (or N-separable) if the corresponding density matrix ρ can be written as a convex combination of direct product states:

$$\rho = \sum_i p_i \bigotimes_{j=1}^{N} \rho_i^{(j)} \qquad \left(\sum_i p_i = 1, \, p_i \geqslant 0 \right), \tag{23}$$

where $\rho_i^{(j)}$ is the density matrix on the partial Hilbert space corresponding to the jth particle [17, 20]. One can easily check that a density matrix has PPT with respect to any bipartition of the system if it is fully separable. On the other hand, we call ρ fully distillable if it is distillable with respect to any bipartition (i.e., we can create a maximal entangled pair between qubits in party A and party B by a number of the copies and LOCC), according to [4]. Through statement (9), we can readily show that a density matrix has NPT with respect to any bipartition, if it is fully distillable.

As in [4], we examine the full separability and the full distillability of ρ_{CH} and ρ_{CF}. We summarize the necessary condition for the separability of ρ_{CH} and ρ_{CF}. According to (21) and (22), the necessary conditions for the separability of ρ_{CH} and ρ_{CF}, respectively, with respect to the bipartition k are given by

$$e^{-2w\eta_*} \geqslant \tanh|\alpha_1|, \tag{24}$$

$$\cosh[(N-w)\xi_* - w\eta_*] \geqslant \sinh(N\bar{\alpha}). \tag{25}$$

Moreover, from (9), we find that the necessary conditions for the distillability of ρ_{CH} and ρ_{CF} with respect to the bipartition k are given by (21) and (22), respectively. Note that the equalities of (24) and (25) give the boundaries between the separability and the distillability.

Let us consider the full separability and the full distillability of ρ_{CH}. The necessary condition for the full separability and the full distillability is given by $\min_k \left(e^{-2w\eta_*}\right) \geqslant \tanh|\alpha_1|$ and $\max_k \left(e^{-2w\eta_*}\right) < \tanh|\alpha_1|$, respectively. In conclusion, we obtain the necessary conditions for the full separability and the full distillability of ρ_{CH} as follows:

$$\rho_{CH}: \text{fully separable} \quad \Rightarrow \quad e^{-2b_{\max}} \geqslant \tanh|\alpha_1|, \tag{26}$$

$$\rho_{CH}: \text{fully distillable} \quad \Rightarrow \quad e^{-2b_{\min}} < \tanh|\alpha_1|, \tag{27}$$

where $b_{\max} = \max_k(w\eta_*) = N\bar{\alpha} - |\alpha_1|$ and $b_{\min} = \min_k(w\eta_*) = \min_{i \neq 1}(|\alpha_i|)$. The value of $w\eta_*$ takes the maximum value $b_{\max}$ when $k = 2^{N-1} - 1$ (i.e., $w = N - 1$). On the other hand, it takes the minimum value $b_{\min}$ when k_i corresponding to the minimum value of α_i's is 1 and the remainders are 0 (i.e., $w = 1$).

Similarly, we obtain the following results for ρ_{CF}:

$$\rho_{CF}: \text{fully separable} \quad \Rightarrow \quad \cosh d_{\min} \geqslant \sinh(N\bar{\alpha}), \tag{28}$$

$$\rho_{CF}: \text{fully distillable} \quad \Rightarrow \quad \cosh d_{\max} < \sinh(N\bar{\alpha}), \tag{29}$$

where $d_{\max} = \max_k |(N-w)\xi_* - w\eta_*|$ and $d_{\min} = \min_k |(N-w)\xi_* - w\eta_*|$. The value of $|(N-w)\xi_* - w\eta_*|$ takes the maximum value, $d_{\max}$, when the difference between $(N-w)\xi_*$ and $w\eta_*$ is the largest. When $\alpha_i = \alpha(>0)$ for any i, the condition for $d_{\max}$ is quite simple. The value of $d_{\max}$ is $(N-2)\alpha$, where $k = 2^{N-1} - 1$ (i.e., $w = N - 1$) or $k = 1$ (i.e., $w = N - 1$). On the other hand, it takes the minimum value, $d_{\min}$ when $(N-w)\xi_*$ is the closest value to $w\eta_*$. If every α_i is a common value, the value of $d_{\min}$ is 0, where $w = \lfloor N/2 \rfloor$. Here, the symbol $\lfloor x \rfloor$ means the greatest integer that is less than or equal to $x \in \mathbb{R}$.

Our results (26)–(29) are the necessary conditions for the full separability or the full distillability. When $\alpha_i = \alpha(>0)$ for any i, the authors in [4] showed the sufficient condition for the full distillability, through the statements proved in [17]. In this case, combining our results (27) and (29) with theirs, we can obtain the following necessary and sufficient conditions:

$$\rho_{CH}: \text{fully distillable} \quad \Longleftrightarrow \quad e^{-2\alpha} < \tanh\alpha, \tag{30}$$
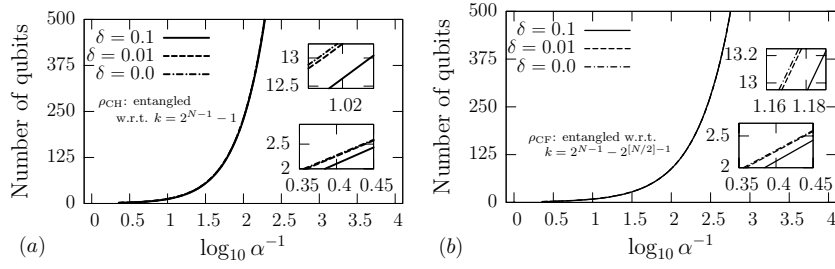
Figure 1. Boundary between the separability and the nonseparability in term of the PPT criterion. The solid line is for $\delta = 0.1$, the broken line is for $\delta = 0.01$ and the broken dotted line is for $\delta = 0$; actually, the difference between these is very small (see the insets). (*a*) The CH transformation ($k = 2^{N-1} - 1$). (*b*) The CH-fanout transformation ($k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$).

$$\rho_{CF}: \text{fully distillable} \quad \Longleftrightarrow \quad \tanh \alpha > e^{-2(N-1)\alpha}. \tag{31}$$

(We can find that the necessary condition for the full distillability of ρ_{CF} is $\cosh[(N-2)\alpha] < \sinh(N\alpha)$ from (29) and this inequality is equal to the corresponding expression in (31) after a short calculation.) Therefore, we obtain the complete physical parameter regions in which ρ_{CH} and ρ_{CF} can be useful for QIP.

5. Boundary between separability and nonseparability

The equalities in the inequalities (24) and (25) imply the boundary between the separability and the nonseparability in term of the PPT criterion. We investigate the effect of the chemical shift on such boundaries. Hereafter, we assume all α_i's are positive, for the sake of simplicity.

Through the above argument, we easily obtain the following expression of the boundary for ρ_{CH}:

$$e^{-2w\eta_*} = \tanh \alpha_1. \tag{32}$$

Similarly, the boundary for ρ_{CF} is given by

$$\cosh[(N-w)\xi_* - w\eta_*] = \sinh(N\bar{\alpha}). \tag{33}$$

To compare the boundaries with the chemical shift to those without it, we try a toy model for α_i. The polarization α_i divides into a reference value $\alpha(>0)$ and the deviation $\delta\alpha_i$ from it: $\alpha_i = \alpha + \delta\alpha_i$. Here, we regard $x_i \equiv \delta\alpha_i/\alpha$ as a uniform random variable in $[-\delta, \delta]$ ($0 \leqslant \delta < 1$). Therefore, in our toy model, the polarization of the ith qubit is given by $\alpha_i = \alpha(1 + x_i)$. Furthermore, the value of α is regarded as the mean value of polarization.

Let us explain how to calculate the boundaries. In the first, we choose the value of δ; actually, $\delta = 0.1, 0.01$ and 0. Then, a sequence of random numbers in $[-\delta, \delta]$ is generated by the Mersenne Twister [21]. Next, we specify a bipartition. For the sake of simplicity, we assume the first $N - w$ qubits are in party A and the latter w qubits are in party B. Finally, we numerically calculate the value of α satisfying (32) or (33) for a given N by the bisection method.

In figures 1(*a*) and (*b*), we show the boundaries on an (α, N) plan for a specific sequence of x_i. The horizontal axis is the common logarithm of the inverse of α. The larger value of $\log_{10} \alpha^{-1}$ corresponds to the case of the higher temperature. The longitudinal axis is the number of qubits. The solid line, the broken line and the broken dotted line correspond to the boundaries for $\delta = 0.1$, $\delta = 0.01$ and $\delta = 0$, respectively. We show the results for ρ_{CH} with

respect to a bipartition $k = 2^{N-1} - 1$ (i.e., $w = N - 1$) in figure 1(a), and the case of ρ_{CF} with respect to a bipartition $k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$ (i.e., $w = \lfloor N/2 \rfloor$) in figure 1(b). The left sides of those lines are the parameter regions where ρ_{CH} and ρ_{CF} are nonseparable with respect to the corresponding bipartition. We find that the clear distinction among the different values of δ is invisible in both figures 1(a) and (b); for example, denoting the value of α on the boundary as $\alpha_b(\delta)$ for a given δ, we can find that $|\log_{10}[\alpha_b(0)/\alpha_b(\delta)]| \leqslant 10^{-2}$ for $\delta = 0.1$ and 0.01, as N is large. In addition, we can find a similar behavior even if we change the sequence of random variables and the kind of bipartitions. Consequently, the effect of the chemical shift on the boundary between the separability and the nonseparability is negligible in our model for $\{\alpha_i\}_{i=1}^N$. This result implies that one has only to examine the number of qubits N and the mean value of polarization α for the determination of the entanglement of the Bell-transformed thermal states (3) and (4).

Let us consider why the effect of the chemical shift is negligible. The boundaries for both ρ_{CH} and ρ_{CF} between the separability and the nonseparability are given by (32) and (33), respectively. Those equations are mainly determined by the mean values of the polarization of party A, ξ_* and party B, η_*. Therefore, the deviation from the mean value of α_i's is not important for the determination of the boundaries. However, the model for α_i is quite simple; the distribution of α_i is uniform and random. We have also assumed that α_i's are positive in this section. Therefore, it is necessary to investigate a more general and realistic model for α_i.

The chemical shifts of qubits are necessary for the realization of quantum computation in a liquid-state NMR system. What we want to know is the role of such an important effect for implementing quantum computation in the entanglement generation by quantum gates. Through our examinations, we find the effect of the chemical shift on the boundary between the separability and nonseparability is fortunately negligible. The presence of the chemical shift is attributed to the difference of the Zeeman energy between the nuclear spins; it is related to the individual and local property of the qubits. Therefore, such local information on the qubits is not so important for examining roughly whether the state transformed from the thermal state by quantum gates is entangled in liquid-state NMR. On the other hand, we expect the chemical shift will have a considerable effect on the quantitative evaluation of entanglement generation by quantum gates. We will study this issue in future.

6. Summary

We have analytically derived the physical parameter region where the Bell-transformed thermal states are entangled in the presence of the chemical shift, by employing the PPT criterion with respect to any bipartition. The chemical shifts of qubits are necessary for the realization of quantum computation in a liquid-state NMR system, because their difference allows us to control the individual qubits. The role of such an important element in liquid-state NMR on the entanglement generation has been studied. Two kinds of Bell transformations, the CH transformation U_{CH} and the CH-fanout transformation U_{CF}, have been examined, as in [4]. With respect to the bipartition k, ρ_{CH} is an entangled state if the inequality (21) is fulfilled and ρ_{CF} is an entangled one if the inequality (22) is fulfilled. We summarize our results in table 1. If the every α_i is a common value, our results are equal to the corresponding ones in [4]. There exists an obvious difference between (21) and (22) with respect to their dependence on α_i. The sufficient condition for the nonseparability of ρ_{CH} is given by α_1 and the mean value of $|\alpha_i|$ for party B, η_*; it does not depend on α_i ($i \in A_k$) in party A, except for α_1. On the other hand, the sufficient condition of ρ_{CF} is determined by ξ_* and η_*, the mean values of $|\alpha_i|$ for party A and party B, respectively.

Next, we have derived the necessary conditions for the full separability and the full distillability through the above analytical results. On the other hand, the authors in [4] obtained the sufficient conditions when all α_i's are equal. We have obtained the necessary and sufficient conditions for the full distillability of ρ_{CH} and ρ_{CF} in this case, combining our results with theirs. Accordingly, we can completely characterize the physical parameter regions in which those unitary transformed thermal states can be useful for QIP, if there is no chemical shift. When the chemical shift exists, we will have to examine the sufficiency of our results.

Finally, we have investigated the effect of the chemical shift on the boundary between the separability and the nonseparability determined by the PPT criterion. We have shown such an effect on the boundaries should be negligible. Actually, one has only to know the number of qubits N and the mean value of the magnitude of polarization $|\alpha_i|$ to evaluate the entanglement of the Bell-transformed thermal states (3) and (4). This result is quite natural, because the boundaries for both ρ_{CH} and ρ_{CF} between separability and nonseparability dominantly depend on the mean values of $|\alpha_i|$ for party A, ξ_* and party B, η_*. We will have to research a more general and realistic model for α_i for examining the effect of the chemical shifts on the boundary between the separability and the nonseparability.

It is also important to examine the difference between ρ_{CH} and ρ_{CF} (i.e., U_{CH} and U_{CF}) in terms of the entanglement generation. The authors in [4] concluded that U_{CF} is a more effective Bell transformation than U_{CH} because the parameter region in which ρ_{CF} is fully distillable is wider than the corresponding one of ρ_{CH}. The analysis taking account of the chemical shift has revealed the difference between U_{CH} and U_{CF} from another point of view. When the value of η_* is given with respect to a fixed bipartition k, the value of α_1 is necessary to examine the entanglement of ρ_{CH}; the local information of party A is required. On the other hand, for ρ_{CF}, the mean value of $|\alpha_i|$ for party A, ξ_* is essential; the global information of party A is required. In this paper, we have obtained the analytical expressions of the eigenvalues of $\rho_{\mathrm{CH}}^{\mathrm{T_B}}$ and $\rho_{\mathrm{CF}}^{\mathrm{T_B}}$. Therefore, the results allow us to characterize U_{CH} and U_{CF} in more detail; for instance, we can evaluate the negativity, which is an entanglement measure [22–24]. We will show the results in the near future.

Research on entanglement in liquid-state NMR involves various aspects of quantum information theory, for example, the role of mixed states in quantum computing and the classification of entanglement. One should note that the achievable range of the physical parameters N and α_i's is limited in a current liquid-state NMR experiment. Actually, it may be difficult to compare the theoretical results with the experiments. However, several experimental developments have been reported in liquid-state NMR, for example, the highly polarized initial states [25, 26] and the number of qubits greater than ten [27, 28]. Furthermore, research on a solid-state NMR quantum computer [29, 30], which can relax the limitation of liquid-state NMR, has been developed steadily. Consequently, we expect that theoretical research on the entanglement in liquid-state NMR could be connected with these experiments in the future.

Acknowledgments

Appendix

The Dür–Cirac classification [17] is a very effective way to evaluate the separability or the distillability of density matrices, of either pure or mixed states, in a multiqubit system, and it is widely used [4, 20, 31]. However, we have to take care of using it; we do not always obtain information on their entanglement from the method proposed in [17]. In the appendix, we show several examples in which the method does not work. Unfortunately, we do not know what kind of density matrices have the problem. Nevertheless, at the end of the appendix, we propose a prescription for solving this problem in specific examples.

First of all, we summarize the strategy of the Dür–Cirac classification. In order to evaluate the entanglement of a quantum state by the PPT criterion, one must examine the positivity of the partial transposed density matrices. In general, such tasks will be difficult as the number of qubits becomes large and many choices of bipartitions exist. On the other hand, if one uses the Dür–Cirac classification, it is only necessary to calculate some specific matrix elements of the state concerned. The main idea is that, using a sequence of local operations, one can transform an arbitrary density matrix ρ in a N–qubit system into the following state whose property of entanglement is easily examined:

$$\rho_N = \lambda_0^+ |\Psi_0^+\rangle\langle\Psi_0^+| + \lambda_0^- |\Psi_0^-\rangle\langle\Psi_0^-| + \sum_{j=1}^{2^{N-1}-1} \lambda_j \left(|\Psi_j^+\rangle\langle\Psi_j^+| + |\Psi_j^-\rangle\langle\Psi_j^-| \right). \quad (A.1)$$

The original density matrix ρ is related to ρ_N by the following expressions: $\lambda_0^{\pm} = \langle\Psi_0^{\pm}|\rho|\Psi_0^{\pm}\rangle$ and $2\lambda_j = \langle\Psi_j^+|\rho|\Psi_j^+\rangle + \langle\Psi_j^-|\rho|\Psi_j^-\rangle$. The property of ρ_N is characterized as follows:

$$\rho_N: \text{PPT with respect to a bipartition } k \quad \Longleftrightarrow \quad \Delta \leqslant 2\lambda_k \quad (A.2)$$

or

$$\rho_N: \text{NPT with respect to a bipartition } k \quad \Longleftrightarrow \quad \Delta > 2\lambda_k, \quad (A.3)$$

where $\Delta = |\lambda_0^+ - \lambda_0^-|$. The most important key idea is that the entanglement does not increase through local operations. Accordingly, if ρ_N is a nonseparable state with a bipartition, ρ is also such a state. It should be noted that we obtain information on the entanglement of ρ only if ρ_N is a nonseparable state.

Now, we show three examples. The first one is the case in which the Dür–Cirac classification works well. The remaining two are not such cases. Hereafter, we concentrate on a two-qubit system. Therefore, the value of k in (A.2) and (A.3) is always 1. In the first, let us consider the following state:

$$\rho_{\text{iso}} = (1 - f)\tfrac{1}{4}(I_1 \otimes I_2) + f|\Psi_0^+\rangle\langle\Psi_0^+|, \quad (A.4)$$

where $-\tfrac{1}{3} \leqslant f \leqslant 1$. The above density matrix is called an isotropic state [12]. Directly using the PPT criterion [14–16], we readily find ρ_{iso} is an entangled state if $f > \tfrac{1}{3}$. On the other hand, we apply the Dür–Cirac method to ρ_{iso}. We obtain the following results: $\langle\Psi_0^+|\rho_{\text{iso}}|\Psi_0^+\rangle = (1 + 3f)/4$, $\langle\Psi_0^-|\rho_{\text{iso}}|\Psi_0^-\rangle = (1 - f)/4$ and $\langle\Psi_1^+|\rho_{\text{iso}}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho_{\text{iso}}|\Psi_1^-\rangle = (1 - f)/2$. Accordingly, using (A.3), we also find ρ_{iso} is an entangled one if $f > \tfrac{1}{3}$.

Next, we consider a slightly different state from ρ_{iso},

$$\rho'_{\text{iso}} = (1 - f)\tfrac{1}{4}(I_1 \otimes I_2) + f|\Psi_1^+\rangle\langle\Psi_1^+|, \quad (A.5)$$

where $-\tfrac{1}{3} \leqslant f \leqslant 1$. Note that the condition for the nonseparability of ρ'_{iso} is the same one as ρ_{iso}; ρ'_{iso} is an entangled state if $f > \tfrac{1}{3}$. This result is quite natural, because the state ρ_{iso} is transformed into ρ'_{iso} by a local unitary operator; $\rho'_{\text{iso}} = (I_1 \otimes X_2)\rho_{\text{iso}}(I_1 \otimes X_2)^{\dagger}$. On

the other hand, we obtain the eigenvalues in the form of (A.1) as follows: $\langle\Psi_0^+|\rho'_{\mathrm{iso}}|\Psi_0^+\rangle = (1-f)/4$, $\langle\Psi_0^-|\rho'_{\mathrm{iso}}|\Psi_0^-\rangle = (1-f)/4$ and $\langle\Psi_1^+|\rho'_{\mathrm{iso}}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho'_{\mathrm{iso}}|\Psi_1^-\rangle = (1+f)/2$. Therefore, the value of Δ is less than $2\lambda_1$ for the arbitrary value of f and condition (A.2) is satisfied. This might imply that ρ'_{iso} is always separable. However, ρ'_{iso} is local unitary equivalent to the entangled state $\rho_{\mathrm{iso}}\,\left(f > \frac{1}{3}\right)$. In conclusion, we cannot obtain information on the entanglement of ρ'_{iso} by the method in [17], because the entangled state ρ'_{iso} is transformed into a separable state by LOCC.

The third example is related to the task in this paper. We consider the case of $N = 2$ and $\alpha_1 = \alpha_2 = \alpha$ in (3). We have known the condition for the nonseparability of ρ_{CH}; ρ_{CH} is an entangled state if $\mathrm{e}^{-2\alpha} > \tanh\alpha$. However, the value of Δ is less than $2\lambda_1$ for any α because $\langle\Psi_0^+|\rho_{\mathrm{CH}}|\Psi_0^+\rangle = \mathrm{e}^{-2\alpha}/\mathcal{Z}$, $\langle\Psi_0^-|\rho_{\mathrm{CH}}|\Psi_0^-\rangle = \mathcal{Z}^{-1}$ and $\langle\Psi_1^+|\rho_{\mathrm{CH}}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho_{\mathrm{CH}}|\Psi_1^-\rangle = (1+\mathrm{e}^{2\alpha})/\mathcal{Z}$. Accordingly, we cannot also obtain information on the entanglement of ρ_{CH} by the method in [17].

The authors in [4] pointed out that the local operations can decrease the entanglement of the state concerned and an alternative method is necessary. In particular, they discussed a more effective procedure for evaluating entanglement than the local operations in the Dür–Cirac classification in terms of the mathematical theory of majorization. Finally, we comment on a loop hole in the Dür–Cirac classification from another point view: we attempt to construct a prescription for solving the problem. As has been mentioned, the isotropic state ρ_{iso} is transformed into ρ'_{iso} by the local unitary operator $I_1 \otimes X_2$. The method in [17] works for the former but not for the latter. This suggests that, by suitable local unitary operators, the state for which the Dür–Cirac classification does not work, could be transformed into a proper one to which their method is applicable. Let us consider the above third example. When we use the local unitary operator $I_1 \otimes X_2$, the state concerned is transformed into $\rho'_{\mathrm{CH}} = (I_1 \otimes X_2)\rho_{\mathrm{CH}}(I_1 \otimes X_2)^\dagger$, where $\langle\Psi_0^+|\rho'_{\mathrm{CH}}|\Psi_0^+\rangle = \mathcal{Z}^{-1}$, $\langle\Psi_0^-|\rho'_{\mathrm{CH}}|\Psi_0^-\rangle = \mathrm{e}^{2\alpha}/\mathcal{Z}$ and $\langle\Psi_1^+|\rho'_{\mathrm{CH}}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho'_{\mathrm{CH}}|\Psi_1^-\rangle = (\mathrm{e}^{-2\alpha}+1)/\mathcal{Z}$. Calculating Δ and $2\lambda_1$, we can obtain the non-trivial expression for ρ'_{CH}; for example, ρ'_{CH} is NPT if and only if $\sinh(2\alpha) > 1$. If ρ'_{CH} is entangled, the corresponding state ρ_{CH} is also considered to be entangled. Therefore, we obtain the sufficient condition of the nonseparability for ρ_{CH} by using the Dür–Cirac classification; such a condition is just $\sinh(2\alpha) > 1$. This condition is equal to the one which is derived by the use of (21). It is necessary to examine whether such a prescription is generalized or not.

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