Entanglement and Discord of superposition of Greenberger-Horne-Zeilinger states

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We have calculated the analytic expression for geometric measure of entanglement for arbitrary superposition of two $N$-qubit canonical orthonormal GHZ states and the same for two $W$ states. Explicit formula for Quantum Discord for the former class of states has been presented. We conjecture that the discord for $N$-qubit $W$ states is $\log_2 N$.

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I. INTRODUCTION

Quantum entanglement has emerged as a key resource for quantum computing, quantum communication and information related processes. Characterization and quantification of multipartite entanglement is an interesting challenging problem in the field of quantum information and computation. There are several approaches to deal with the issue and various measures have been proposed (see e.g. [1], [2] for nice reviews). For multipartite pure states, a frequently used measure is the Geometric measure of entanglement (GME) [3–8]. GME is a distance measure and for an arbitrary pure state $|\psi\rangle$, it is usually defined as

$$GME(|\psi\rangle) = 1 - \Lambda_\psi$$  \hspace{1cm} (1)

where

$$\Lambda_\psi = \max_{|\phi\rangle \in \{\text{product states}\}} |\langle \phi | \psi \rangle|$$  \hspace{1cm} (2)

The notion of GME has also been extended to mixed states through the convex-roof construction. Another well-known measure, the Groverian measure of entanglement [9–11] is exactly the same as GME, up to a square operation. The Groverian measure originated from the modified quantum search algorithm [9] and is defined through the success probability in the search using the given state as the initial state:

$$G(|\psi\rangle) = \sqrt{1 - P_{\max}(|\psi\rangle)}$$  \hspace{1cm} (3)

where

$$P_{\max}(|\psi\rangle) = \max_{|\phi\rangle \in \{\text{product states}\}} |\langle \phi | \psi \rangle|^2$$  \hspace{1cm} (4)

Throughout this paper we shall consider the definition (3) for GME.

It is clear that analytic calculation of GME for an arbitrary state is reasonably difficult since it involves non-linear maximization process. However, recently it has been shown [5] that if a pure state is permutationally invariant, then the calculation of GME becomes greatly simplified. In this case, the optimal product state can be taken as tensor product of the same single system thereby drastically reducing the number of variables in the maximization process.

Like all other well-known entanglement measures (von Neumann Entropy for bipartite pure states [12], Negativity [13], Concurrence [14] etc.) there are some known bounds on the GME of superposition of pure states (see e.g.,[15, 16]). In this work, we will explicitly calculate the analytic expression of GME for arbitrary superposition of two $N$-qubit canonical orthonormal GHZ states and also for $W$ states. As we shall see later, these states do not saturate the bound obtained in [16]. Clearly, the former states are not permutationally invariant in general and hence the theorem given in [5] cannot be applied directly. However we will use it to derive our result.

There exist quantum correlations other than entanglement, and one such is the quantum discord which has been studied extensively [17]. Basically, it quantifies the total non-classical correlations in a quantum state. However, most of these investigations pertain to bipartite systems only. Here, our aim is to study multipartite states and hence we shall follow the approach of Modi et. al. [18] in quantifying discord. In this unified view of all kinds of correlations in a quantum state, the quantifications are done by the relative entropy, which makes this approach more challenging. Indeed optimization of relative entropy is known to be a difficult problem, e.g., there does not exist a formula for the relative entropy of entanglement (REE) even for the simplest case of arbitrary 2-qubit (mixed) states [19]. Very recently, the reverse problem of finding the set of entangled states for which the chosen separable state is the closest one, has been solved [20]. The necessary and sufficient condition given therein would help us in our analysis.

The organization of this article is as follows: In Sec II, we will calculate the explicit expressions for GME of superposition of two orthonormal $N$-qubit GHZ states and also of two $W$ states and compare the results. In Sec III, quantum discord is derived analytically for the former class of states. In Sec IV, we conjecture the discord for $N$-qubit $W$ states to be $\log_2 N$. Finally we discuss some possible extensions and related issues in Sec V.

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II. GME OF ARBITRARY SUPERPOSITION OF TWO GHZ AND W STATES

In this section we consider the superposition of two N-qubit GHZ states and derive its GME. An analogous analysis is done for W states and the results are compared.

A. GME of arbitrary superposition of two N-qubit GHZ states

The full set of canonical orthonormal N-qubit GHZ states is given by (up to an irrelevant global phase)

\[ |G^\pm_N(i)\rangle = \frac{|B_N(i)\rangle \pm |B_N(2^N - 1 - i)\rangle}{\sqrt{2}} \]

(5)

where \( i = 0, 1, \ldots, 2^N - 1 \) and \( |B_N(i)\rangle = |i_1 i_2 \ldots i_N\rangle \) is the ‘binary representation of the decimal number \( i \) in an N-bit string’. In a more convenient notation (5) can be written as

\[ |G^\pm_N\rangle = \sum_{i = 0}^{2^N - 1} \frac{|i_1 i_2 \ldots i_N\rangle}{\sqrt{2}} \]

(6)

where \( i_k = 0, 1 \) \( \forall k = 2, 3, \ldots, N \) and a bar over a bit value indicates its logical negation.

Let us now consider an arbitrary superposition of two orthonormal GHZ states \( |G^\pm_N\rangle \) and \( |G^\pm_N\rangle \) (\( i \neq j \)) as follows

\[ |G_{ij}\rangle = \cos \alpha |G^+_N\rangle + \sin \alpha e^{i\gamma} |G^-_N\rangle \]

(7)

First of all we note that the state in (7) is not Schmidt decomposable (SD) [21]. From the definition, if \( |\psi\rangle \) is SD, then

\[ |\psi\rangle = \sum \sqrt{\lambda_i} |i_1 i_2 \ldots i_n\rangle := \text{Schmidt} \{\lambda_i\} \]

(8)

So, tracing out any subsystem would give a separable state and it is a necessary condition for SD. However, in this case, tracing out the third qubit from the 3-qubit state \( |G_{01}\rangle = \cos \alpha (|G^+_0\rangle + \sin \alpha e^{i\gamma} |G^-_0\rangle \) gives an entangled state, which can be easily checked by the PPT criterion.

We also note that (7) is not permutationally invariant and hence the theorem in [5] is not directly applicable to it. Though apparently it looks that the phase \( \gamma \) cannot be driven out, we will show that the GME is independent of \( \gamma \).

To calculate the GME, let us write the state (7) in the following convenient form

\[ |G_{ij}\rangle = c_1 |\psi_m\rangle |\phi_n\rangle + c_2 |\tilde{\psi}_m\rangle |\tilde{\phi}_n\rangle + c_3 |\hat{\psi}_m\rangle |\hat{\phi}_n\rangle + c_4 |\hat{\tilde{\psi}_m}\rangle |\hat{\tilde{\phi}_n}\rangle \]

(9)

where \( |\psi_m\rangle \) is the collection of (qu)bits when the two strings \( |B_N(i)\rangle \) and \( |B_N(j)\rangle \) agree and \( |\phi_n\rangle \) is the collection when they disagree, \( m + n = N \); \( c_1 = \frac{\cos \alpha}{\sqrt{2}} = \pm c_4 \), \( c_2 = \pm \frac{\sin \alpha}{\sqrt{2}} = \pm c_3 \).

Noting that the right hand side of (9) can be written as

\[ |\psi_m\rangle (c_1 |\phi_n\rangle + c_2 |\tilde{\phi}_n\rangle) + |\tilde{\psi}_m\rangle (c_3 |\tilde{\phi}_n\rangle + c_4 |\hat{\tilde{\phi}_n}\rangle) \]

(10)

it follows that [22]

\[ P_{\text{max}}(|G_{ij}\rangle) = \left\{ \begin{array}{ll} \max \left\{ \frac{\cos^2 \alpha}{2}, \frac{\sin^2 \alpha}{2} \right\} & \text{if } m, n \geq 2 \\ \frac{1}{2} & \text{if } m = 1 \text{ or } n = 1 \end{array} \right. \]

(11)

The only known bound for GME of superposition (Eq. (3) in [16]) gives \( P_{\text{max}} \leq \frac{1}{2} + cs \), where \( c = \cos \alpha \), \( s = \sin \alpha \). Since for \( cs \neq 0 \), \( \max \left\{ \frac{\cos^2 \alpha}{2}, \frac{\sin^2 \alpha}{2} \right\} < \frac{1}{2} \), therefore \( P_{\text{max}} \) can not saturate this bound.

B. Proof of the result (10)

By suitable local unitary (LU) operations the state (9) can be transformed to the following form

\[ |G_{ij}\rangle = \frac{c}{\sqrt{2}} (|0\rangle_m |0\rangle_n \pm |1\rangle_m |1\rangle_n) + \frac{s}{\sqrt{2}} e^{i\gamma} (|0\rangle_m |1\rangle_n \pm |1\rangle_m |0\rangle_n) \]

(12)

Clearly (11) remains invariant under permutation among the first m parties (and similarly for the rest n parties) and hence we can assume the optimal product state to be of the form [23]

\[ |\Phi\rangle = (\cos \theta_1 |0\rangle + e^{i\lambda_1} \sin \theta_1 |1\rangle) \otimes m \otimes (\cos \theta_2 |0\rangle + e^{i\lambda_2} \sin \theta_2 |1\rangle) \otimes n \]

(13)

Now, applying \( |z_1 + z_2| \leq |z_1| + |z_2| \) successively, we have

\[ |\cos^m \theta_1 (c \cos \theta_2 + s e^{i(\gamma - \lambda_2)} \sin \theta_2) + e^{-im\lambda_1} \sin^m \theta_1 (\pm ce^{im\lambda_2} \sin^m \theta_2 + se^{i\gamma} \cos^m \theta_2)| \]

\[ \leq \cos^m \theta_1 |(c \cos \theta_2 + s e^{i(\gamma - \lambda_2)} \sin \theta_2)| \]

\[ + \sin^m \theta_1 |(\pm ce^{im\lambda_2} \sin^m \theta_2 + se^{i\gamma} \cos^m \theta_2)| \]

\[ \leq \cos^m \theta_1 |(c \cos \theta_2 + s \sin \theta_2)| \]

\[ + \sin^m \theta_1 |(c \sin \theta_2 + s \cos \theta_2) | \]

(14)

Note that

\[ \max_{0 \leq \theta_1, \theta_2 \leq \frac{\pi}{2}} \left\{ \cos^2 \theta_1 (c \cos \theta_2 + s \sin \theta_2) \right\} \]

\[ + \sin^2 \theta_1 (c \sin \theta_2 + s \cos \theta_2) \right\} = 1 \]

(15)

which occurs at \((\theta_1, \theta_2) = (0, \alpha), (\frac{\pi}{2}, \frac{\pi}{2} - \alpha)\); additionally at \((\text{arbitrary} \theta_1, \frac{\pi}{2})\) if \(\alpha = \frac{\pi}{4}\).

So taking \( n = 1 \) (the case \( m = 1 \) is similar by symmetry) in (14),

\[ \cos^m \theta_1 (c \cos \theta_2 + s \sin \theta_2) + \sin^m \theta_1 (c \sin \theta_2 + s \cos \theta_2) \]

\[ \leq \cos^2 \theta_1 (c \cos \theta_2 + s \sin \theta_2) + \sin^2 \theta_1 (c \sin \theta_2 + s \cos \theta_2) \]

\[ \leq 1 \]

(16)
where, in the second line, we have used \( \cos^n \theta \leq \cos^2 \theta, \ \sin^m \theta \leq \sin^2 \theta \ \forall m \geq 2 \). Thus, if \( n = 1 \) or \( m = 1 \), we have from (13), (15) and (16), \( P_{\text{max}}(|G_{ij}|) = \frac{1}{2} \).

Similarly using
\[
\max_{0 \leq \theta, t \leq \frac{\pi}{2}} \left[ \cos^2 \theta_1 (c \cos^2 \theta_2 + s \sin^2 \theta_2) + \sin^2 \theta_1 \right]
= \max \{c, s\}, \tag{17}
\]
it follows that \( P_{\text{max}}(|G_{ij}|) = \max \{c^2, s^2\} \), if \( m, n \geq 2 \).

C. GME of arbitrary superposition of two \( N \)-qubit \( W \) states

The GME of superposition of two 3-qubit \( W \) states has been presented in [3]. Although the generalization to \( N \)-qubit case is quite straightforward, still we wish to derive it for completeness and it will help us to compare with the case of GHZ states. Interestingly, it is shown that the 4-qubit case is the easiest one (easier than even the 3-qubit case) and an explicit formula of GME has been derived.

Let us consider an arbitrary superposition of the two \( N \)-qubit \( W \) states namely \(|W\rangle = \frac{1}{\sqrt{N}}(|00\ldots 1\rangle + \ldots + |10\ldots 0\rangle)\) and \(|\tilde{W}\rangle = \frac{1}{\sqrt{N}}(|01\ldots 1\rangle + \ldots + |11\ldots 0\rangle)\) as follows
\[
|W\tilde{W}\rangle = \cos \alpha |W\rangle + e^{i\gamma} \sin \alpha |\tilde{W}\rangle, \quad 0 \leq \alpha \leq \frac{\pi}{2} \tag{19}
\]

Since the state \(|W\tilde{W}\rangle\) is permutationally invariant (with positive coefficients), we can assume the nearest product state as [5]
\[
|\phi\rangle = (\cos \theta |0\rangle + \sin \theta |1\rangle) \otimes |\omega\rangle, \quad 0 \leq \theta \leq \frac{\pi}{2} \tag{20}
\]
The overlap is given by
\[
|\langle \phi |W\tilde{W}\rangle|^2 = Q = N|s C^{N-1} S + cC S^{N-1}|^2 \tag{21}
\]
where \( C = \cos \theta, \quad S = \sin \theta, \quad c = \cos \alpha, \quad s = \sin \alpha \).

The condition for maximum of \( Q \) \( (\frac{\partial Q}{\partial \theta} = 0) \) becomes
\[
s[t^N - (N - 1)t^{N-2}] + c[(N - 1)t^2 - 1] = 0 \quad \tag{22}
\]
and hence we have
\[
P_{\text{max}}(|W\tilde{W}\rangle) = \frac{Nt^2}{(1 + t^2)^N} |c + st^{N-2}|^2 \quad \tag{23}
\]
where \( t = \tan \theta \geq 0 \) will be determined from the polynomial equation (22). We note that Eq.(22) has only one positive root for \( N = 3, 4 \) and has at most three positive roots for \( N \geq 5 \). Hence the GME can be calculated using numerical techniques of root finding.

Particularly, for \( N = 4 \), we have
\[
t^2 = 3(c - s) + \sqrt{9 - 14cs} \tag{24}
\]

which readily gives the expression for GME. The graph of GME vs. \( s \) for 4-qubit case is exactly analogous to the 3-qubit case (Fig.-1 in [3]) and hence we are not reproducing it here.

It is worth mentioning that if we consider the superposition of two other (even LU equivalent) \( W \) states, the GME will not be the same.

D. Comparison between GME of superposition of GHZ and \( W \) states (with respect to the results presented here)

1. For \( N = 3 \), either \( m = 1 \), or \( n = 1 \) and hence
\[
P_{\text{max}}(|G_{ij}|) = \frac{1}{2} = P_{\text{max}}(|G_{ij}^\pm\rangle) \tag{25}
\]

Thus for the three-qubit GHZ states, the GME of the superposition is independent of the superposition parameter \( \alpha \) and the phase \( \gamma \) whereas for the \( W \) states, it is dependent on \( \alpha \). Of course, the GME of superposition of \(|G_{ij}^+\rangle\) and \(|G_{ij}^-\rangle\) (which is \( \min\{|\cos \alpha + \sin \alpha e^{i\gamma}|, |\cos \alpha - \sin \alpha e^{i\gamma}|\} \) depends on both \( \alpha \) and \( \gamma \).

For arbitrary \( N \), if \( m = 1 \) or \( n = 1 \) (i.e., if the Hamming distance between \(|B_N(i)\rangle\) and \(|B_N(j)\rangle\) be 1 or \( N - 1 \)), then \( G(|G_{ij}|) = \frac{1}{\sqrt{2}} \).

2. For \( N = 3 \), we note that by superposing two orthonormal \( W \) states, we can get the resultant entanglement equal to that of a GHZ state. For example, \( G(|W_1\rangle + |W_2\rangle) = \frac{1}{\sqrt{2}} = G(|G_{ij}^\pm\rangle) \), where \(|W_1\rangle = \frac{1}{\sqrt{3}}(|001\rangle - \omega|010\rangle + \omega^2|100\rangle), |W_2\rangle = \frac{1}{\sqrt{3}}(|001\rangle + \omega|010\rangle - \omega^2|100\rangle) \); \( \omega \) being a complex cubic root of unity. If we consider the superposition of \( W \) and \( \tilde{W} \), it follows from Fig-1 in [3] that we can choose a specific value of \( s \) to get \( G(|W\tilde{W}\rangle) = \frac{1}{\sqrt{2}} = G(|GHZ\rangle) \).

On the other hand we can not get the entanglement of a \( W \) state by superposing any two orthonormal GHZ states from the canonical set (5) since \( G(|G_{ij}|) \leq \frac{1}{\sqrt{2}} < G(|W\rangle) \).

However, for \( N = 4 \) the situation is different. By superposing two \( W \) states, we can get the entanglement of a GHZ state and vice-versa. For example, \( G(|W_1\rangle + |W_2\rangle) = \frac{1}{\sqrt{2}} = G(|G_{ij}^\pm\rangle) \), where \(|W_1\rangle = \frac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle) \) and
\[ |W_2\rangle = \frac{1}{2}(|0001\rangle + |0010\rangle - |0100\rangle - |1000\rangle) \]

It can be checked that by superposing \( |G_0\rangle \) and \( |G_4\rangle \) we can get the entanglement of the W state:

\[ G(|G_{03}\rangle) = \sqrt{\frac{3}{4}} = G(|W\rangle), \]

where \( |G_{03}\rangle \) is given by (7) with \( \alpha \) given by \( \sin \alpha = \sqrt{\frac{3}{2}} \).

For large \( N \), the situation is somehow opposite to the 3-qubit case. Here we can always get the entanglement of a W state by superposing two GHZ state, but we don’t know if the converse is also true. This requires further investigation.

3. For \( N = 3 \), even if we consider equal superposition \( (\alpha = \frac{\pi}{2}, \gamma = 0) \), the state \( |G_{ij}\rangle \) is not invariant under permutation. The corresponding product state would also not be permutationally invariant. As an example, the state \( \alpha \) may lead to the intuition that the optimal product state may still be permutationally invariant. As an example, the state \( |G_{01}\rangle = \frac{1}{2}(|000\rangle + |111\rangle + |001\rangle + |110\rangle) \), is not permutationally invariant. But we can choose the nearest product state as \( \left| \frac{1}{2}(|010\rangle + |101\rangle + |110\rangle + |011\rangle) \right\rangle \). Of course, there exist other optimal product states which are not permutationally invariant e.g., \( |q\rangle|q\rangle + |\rangle \rangle \) where \( q = 0, 1, - \) and \( |\rangle = \frac{1}{\sqrt{2}}(|011\rangle + |101\rangle) \). This may lead to the intuition that the optimal product state may be permutationally invariant even if the state itself is not. However, in [5], the authors have proved the stronger result that this is not the case if the state is genuinely entangled (or we look into those parties for which this state is entangled and symmetric, e.g., \( |G_{01}\rangle = |\phi^+\rangle + |\rangle \rangle \), so we have to consider only the first two particles. Being symmetric and entangled, the combined state of these two particles have the necessarily symmetric closest product states \( |q\rangle|q\rangle \).

III. QUANTUM DISCORD FOR THE CLASS OF STATES (7)

As mentioned earlier, we will follow the approach of [18] to characterize and quantify all kinds of correlations in a quantum state. The definitions of relevant quantities are:

\[
\begin{align*}
\text{Entanglement} \ E &= \min_{\sigma \in \mathcal{D}} S(\rho||\sigma) \\
\text{Discord} \ D &= \min_{\chi \in \mathcal{E}} S(\rho||\chi) \\
\text{Dissonance} \ Q &= \min_{\chi \in \mathcal{E}} S(\sigma||\chi) \\
\text{Classical correlations} \ C &= \min_{\pi \in \mathcal{P}} S(\rho||\pi)
\end{align*}
\]

where \( \mathcal{P} \) is the set of all product states (i.e., states of the form \( \pi = \pi_1 \otimes \pi_2 \otimes \ldots \otimes \pi_N \)), \( \mathcal{E} \) is the set of all classical states (i.e., states of the form \( \chi = \sum_k \pi_k |k\rangle \langle k| \)), with the local states \( |k_n\rangle \) spanning an orthonormal basis, \( \mathcal{D} \) is the set of all separable states (i.e., states of the form \( \sigma = \sum_k \mu_k |k\rangle \langle k| \otimes \ldots \otimes |\pi_N\rangle \langle \pi_N| \) and \( S(x||y) = \text{Tr}[x \log x - x \log y] \) is the relative entropy of \( x \) with respect to \( y \). We shall first find out the closest separable state (CSS) to the class of states (7). Fortunately it turns out that the CSS is also a classical state thereby implying \( D = E = R_{\text{C}}(|G_{ij}\rangle) \), \( Q = 0 \).

Before proceeding to calculations, we recall that finding out the CSS is a challenging problem [19, 24]. To obtain the CSS to a multiparty state, two interesting tools are available in the literature. The first one is a lower bound through the generalization of Plenio-Vedral formula [25]:

\[
S(\rho_N||\sigma_N) \geq S(\rho_{N-1}||\sigma_{N-1}) + S(\rho_{N-1}) - S(\rho_N),
\]

where \( \rho_N \) is any \( N \)-partite state and \( \sigma_N \) is an \( N \)-separable state. So, for any \( N \)-qubit pure state \( \rho_N \), we have the lower bound

\[
E(\rho_N) \geq \max \{ E(\rho_{N-1}) + S(\rho_{N-1}) \}
\]

where the maximum is taken over all possible bipartition of \( N - 1 \) versus single qubit.

The second tool is due to Wei et. al. [4]. For any \( N \)-partite pure state \( |\psi\rangle \), it gives a lower bound on \( E \) through \( P_{\text{max}}(|\psi\rangle) \):

\[
E(|\psi\rangle\langle\psi|) \geq - \log_2 P_{\text{max}}(|\psi\rangle).
\]

Since \( E \) is defined through minimization, if we can find a separable state \( \sigma \) which saturates either of the bounds in (31) and (32), then \( \sigma \) will be the required CSS. In fact the later bound has been extensively used to derive REE of symmetric Dicke states [4] and even mixtures of them [26]. But unfortunately, these bounds are not saturated for the states in (7). Indeed, the bound (32) is not saturated even for the simplest 2-qubit non-maximally Bell states (e.g., for \( |\phi\rangle = a|00\rangle + b|11\rangle \) with \( |a|^2 + |b|^2 = 1 \), one has \( P_{\text{max}} = \max \{|a|^2, |b|^2\} \) whereas \( E(|\phi\rangle) = -|a|^2 \log |a|^2 - |b|^2 \log |b|^2 = H(|a|^2) \). It is thus quite challenging to derive the CSS. The reverse problem (i.e., starting from a \( \sigma \) on the boundary of \( \mathcal{D} \), determining all entangled state \( \rho \) for which \( \sigma \) is the CSS) is also interesting and has been solved for the 2-qubit case [28], very recently for multiparty states [20]. We shall apply this multi-party criteria to derive the CSS. The criteria reads:

**Necessary and sufficient criteria for CSS [20]:**

\[
\sigma \in \mathcal{D} \text{ is a CSS for an entangled state } \rho \text{ if and only if } \\
\max_{\chi \in \mathcal{E}} \text{Tr} \sigma' L_{\alpha}(\rho) = 1,
\]

where the linear operator \( L_{\alpha} \) is defined in the following way. Let the eigendecomposition of hermitian positive operator \( \alpha \) be \( \alpha = \text{diag}(a_1, a_2, \ldots, a_n) \). Then for any \( \beta = [b_{ij}]_{i,j=1}^{n} \), \( L_{\alpha}(\beta) \) is defined by

\[
[L_{\alpha}(\beta)]_{ij} = \begin{cases} 
\frac{b_{ij} \ln a_i - \ln a_j}{a_k - a_i}, & \text{if } a_k \neq a_i \\
\frac{b_{ij} \ln a_i - \ln a_j}{a_k - a_i}, & \text{if } a_k = a_i = a
\end{cases}
\]

We shall now derive the CSS of our states. Since REE is invariant under LU and (7) can be transformed to (11)
by LU, we can consider REE of this state, without loss of generality. The state (11) has GME similar to the non-maximal Bell state. So we assume that it will have a similar REE also. Hence we take the CSS as

$$\sigma = \frac{c^2}{2}(|00\rangle\langle00| + |11\rangle\langle11|) + \frac{s^2}{2}(|01\rangle\langle01| + |10\rangle\langle10|),$$

(35)

where (and hereafter) we have dropped the suffixes \(m\) and \(n\).

**Proof:**

$$\sigma = \text{diag}(\frac{c^2}{2}, \frac{s^2}{2}, \frac{s^2}{2})$$

and \(\rho = \frac{1}{2} \begin{pmatrix} c^2 & \text{cse}^{-\gamma} & \text{cse}^{-\gamma} & \pm c^2 \\ \text{cse}^{\gamma} & s^2 & s^2 & \pm \text{cse}^{\gamma} \\ \text{cse}^{\gamma} & s^2 & s^2 & \pm \text{cse}^{\gamma} \\ \pm c^2 & \pm \text{cse}^{-\gamma} & \pm \text{cse}^{-\gamma} & c^2 \end{pmatrix}.$$  

Hence from the definition of \(L_\sigma(\rho)\),

$$L_\sigma(\rho) = \begin{pmatrix} 1 & qe^{-\gamma} & qe^{-\gamma} & \pm 1 \\ qe^{\gamma} & 1 & 1 & \pm qe^{\gamma} \\ \pm 1 & \pm qe^{-\gamma} & \pm qe^{-\gamma} & 1 \end{pmatrix}$$

where \(q = \frac{c^2 \log 2}{c^2 - s^2} \). Note that \(|q| \leq 1\).

Now let \(\sigma' = \sum p_k|\phi_k\rangle\langle\phi_k|\). Then

$$\text{Tr} \sigma'L_\sigma(\rho) = \sum p_k\langle\phi_k|L_\sigma(\rho)|\phi_k\rangle$$

$$= \sum p_k[||\phi_k\rangle\langle00||^2 + ||\phi_k\rangle\langle01||^2 + ||\phi_k\rangle\langle10||^2 + ||\phi_k\rangle\langle11||^2$$

$$+ 2\text{Real}(qe^{-\gamma}\langle\phi_k|00\rangle\langle01|\phi_k + \langle10|\phi_k\rangle)| + 2\text{Real}(\langle\phi_k|00\rangle\langle11|\phi_k + \langle01|\phi_k\rangle)|$$

$$\pm 2\text{Real}(q^{-\gamma}\langle\phi_k|11\rangle\langle00|\phi_k + \langle01|\phi_k\rangle)|$$

$$\pm 2\text{Real}(q^{-\gamma}\langle\phi_k|11\rangle\langle00|\phi_k + \langle01|\phi_k\rangle)|$$

$$\leq \sum p_k[||\phi_k\rangle\langle00||^2 + ||\phi_k\rangle\langle01||^2 + ||\phi_k\rangle\langle10||^2 + ||\phi_k\rangle\langle11||^2$$

$$+ ||\phi_k\rangle\langle00|| + ... + ||\phi_k\rangle\langle11||]$$

$$= \sum p_k[||\phi_k\rangle\langle00|| + ||\phi_k\rangle\langle01|| + ||\phi_k\rangle\langle10|| + ||\phi_k\rangle\langle11||]^2$$

Since each \(|\phi_k\rangle\) is a product state, we have \(|\phi_k\rangle = |\phi_k\rangle\langle\psi_k|\psi_k\rangle\). So the last expression above can be written as

$$\sum p_k[||\phi_k\rangle\langle00|| + ||\phi_k\rangle\langle01|| + ||\phi_k\rangle\langle10|| + ||\phi_k\rangle\langle11||] \leq 1,$$

since for any normalized product state \(|\phi\rangle\) of \(q\) 2-qubits, \(|\phi\rangle\langle00|| + ... + ||\phi\rangle\langle11|| \leq 1\) (which can be seen from (17)).

Thus \(\sigma\) is indeed the CSS. Being a classical state as well, \(\sigma\) is also the CSS, thereby yielding \(D = E = -c^2 \log \frac{q}{2} - (1 - c^2) \log \sqrt{\frac{q}{2}} = 1 + H(\gamma)\) and \(Q = 0\). We have depicted all the known bounds and our exact results for this state in Fig. 1.

**IV. CONJECTURE FOR DISCORD OF N-QUBIT W STATE**

From the discussion of the previous section, it is clear that determining CSS is a non trivial task. Determining the CSS is even more complicated because the set \(C\) is not a convex set and hence the standard tools of convex optimization theory is not directly applicable. However, to calculate the discord \(D\) and dissonance \(Q\), the authors of [18] have simplified the task of minimizing over \(C\). They have shown that for any given \(\rho\), the CSS \(\chi_\rho\) is given by \(\chi_\rho = \sum_k |k\rangle\langle k|\rho|k\rangle\langle k|\), where \(|\{k\}\rangle\) forms the eigenbasis of \(\chi_\rho\). This simplifies expressions for \(D\) and \(Q\) as the minimization of the relative entropy over \(C\) reduces to minimization of the von Neumann entropy \(S(\chi_x)\) over the choice of local basis \(|\{k\}\rangle\).

$$D = S(\chi_x) - S(\rho), \quad Q = S(\chi_x) - S(\sigma),$$

(36)

where \(S(\chi_x) = \min_k S(\frac{1}{N}\sum |k\rangle\langle k|\chi_x|k\rangle\langle k|)\). Therefore, for numerical computation of \(D\), one can choose arbitrary local bases and find the minimum of the corresponding entropies. An even finer approach is to generate a vector (with equal spacing) and using Gram-Schmidt method construct a complete orthonormal basis and obtain the minimum entropy. This technique is useful mostly in low dimensional cases [29].

The CSS to the \(N\)-qubit W-state is known to be [4]

$$\sigma_W = \sum_{k=0}^{N} C_k \left(\frac{k}{N}\right)^k \left(\frac{N-k}{N}\right)^{N-k} |S(N,k)\rangle\langle S(N,k)|,$$

with \(|S(N,k)\rangle\) being the \(k\)-th symmetric (Dicke) state. For \(N \geq 3\), the above separable state is not a classical state. Therefore \(D \neq E \) and \(Q \neq 0\) for W states (contrary to the GHZ case, where the CSS was a classical state).

Since the \(W\) state is symmetric, we assume that the CSS can be chosen to be symmetric [30]. So we choose each of the local orthonormal basis of the classical state \(\chi_w\) as

$$|0\rangle' = \sqrt{p}|0\rangle + \sqrt{1-p}|1\rangle$$

$$|1\rangle' = \sqrt{1-p}|0\rangle - \sqrt{p}|1\rangle$$
so that \( \langle x'|x \rangle = (-1)^x \sqrt{p}, \langle x'|y \rangle = \sqrt{1-p}, x \neq y = 0, 1. \) Therefore we have

\[
\langle x'|x \rangle = (-1)^x \sqrt{p}, \langle x'|y \rangle = \sqrt{1-p}, x \neq y = 0, 1.
\]

Therefore we have

\[
\langle x'|y \rangle = (-1)^{m_1} (\sqrt{p})^{m_1} (\sqrt{1-p})^{N-m_1},
\]

where \( m \) is the number of positions where the two binary strings \( x \) and \( y \) agree and \( m_1 \) is the number of positions where they both have 1. Since for the \( W \) state each \( y \) has exactly one 1, the inner product \( \langle x'|W \rangle \) will just depend on the number of 1’s in \( x \). So, if a basis \( |x_k \rangle \) has \( k \) number of 1s, we have

\[
\langle x_k'|W \rangle = \frac{1}{\sqrt{N}} \left[ -k C_1 (\sqrt{p})^{N-k+1} (\sqrt{1-p})^{k-1} + N^{-k} C_1 (\sqrt{p})^{N-k-1} (\sqrt{1-p})^{k+1} \right] = \frac{1}{\sqrt{N}} (\sqrt{p})^{N-k-1} (\sqrt{1-p})^{k-1} |N(1-p) - k| \tag{37}
\]

Now from (36), to determine \( D \), we have to find the minimum of

\[
S = S \left( \sum_{x=x_1x_2\ldots x_N : x_j = 0, 1} \langle x'|x \rangle \langle x'|W \rangle \langle W|x \rangle \langle x' | \rangle \right) = - \sum_{x'=x_1x_2\ldots x_N : x_j = 0, 1} |\langle x'|W \rangle|^2 \log_2 |\langle x'|W \rangle|^2
\]

\[
= - \sum_{k=0}^N C_k \lambda_k \log_2 \lambda_k, \tag{38}
\]

where \( \lambda_k = |\langle x_k'|W \rangle|^2 \) with \( x_k \) being any binary string of length \( N \) having \( k \) 1s, is given by (37). It can easily be checked that \( S \) has (global) minimum at \( p = 0, 1 \) (see Fig.-2). Therefore the CCS to \( W \) state is the dephased state in computational basis and consequently we have \( D = \log_2 N \).

Employing the method of [29], we have also numerically verified (independent of the assumption that the CCS is symmetric) that up to \( N = 5 \), this indeed is the minimum. We thus conjecture that discord of \( N \)-qubit \( W \) state is \( \log_2 N \).

V. DISCUSSION

First of all, we note that both the results (10) and (35) can straightforwardly be extended to the case of non-maximal GHZ states (i.e., \( a|1i_2\ldots i_N + b|i_1i_2\ldots i_N \rangle \), \( |a|^2 + |b|^2 = 1 \). However, calculation of GME for superposition of two arbitrary GHZ states is more involved. In fact, even for a single non-maximal (generalized) \( W \) state, obtaining the GME is quite nontrivial. Recently, the three qubit case has been studied in [6] which has been further generalized to \( N \)-qubits [7]. From a broader perspective, a generalization of GME in which the maximum distance would be calculated from the set of all states which are equivalent under stochastic local operations and classical communications (instead of just product states), has been introduced in [31]. It would be interesting to see how the GME of superposition behaves in this context.

Another basic question related to the measure of correlations is the additivity of the proposed measure. It is known that GME is in general not additive [32]; precisely, for \( N \geq 3 \), GME is not additive for any two \( N \)-partite antisymmetric states [33]. However, this is still not known for the case of total correlations \( T_p \) (defined as \( S(\rho||\pi_p) \)) in a quantum state. It has been conjectured [18] that \( T_p \) is subadditive: \( T_p > E + Q + C_\sigma \), where \( C_\sigma \) is the classical correlation \( S(\chi_\sigma||\sigma) \).

A further direction along our line of study would be to explore the correlations in \( N \)-qubit \( GHZ \)-diagonal states (an arbitrary mixture of the states \( |G_{(i)}^{+}\rangle \rangle |G_{(j)}^{+}\rangle \)). Because of the simple structure (both algebraic and geometric), the two qubit case allows easy computation of all the measures and has been studied extensively. But, beyond this, even the criteria for entanglement is unknown till date. We hope that the lower bound in (31) may provide some insight in determining the structure of the CSS which then can be verified using the necessary and sufficient condition given in [20].

To conclude, we have derived analytically the GME and discord (via REE) for superposition of some orthonormal \( GHZ \) states. We have also conjectured the discord for \( W \) states. Perhaps a similar approach could be applied to other permutationally invariant states.

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[21] It is obvious that for |ψ⟩ = Schmidt {λi}, Pmax(|ψ⟩) = \max\{λi\} and E(|ψ⟩) = −\sum \lambda_i \log \lambda_i.

[22] If \( m = 1 \), then one possible optimal product state is \( \Phi = \sqrt{2}(c_1|\psi_m\rangle + c_2|\psi_m\rangle)|\phi_n\rangle \) and it produces \( P_{max} = \frac{1}{2} \). The case \( n = 1 \) is similar. If \( m, n \geq 2 \), the possible optimal product states are \( |\psi_m\rangle|\phi_n\rangle, |\psi_m\rangle|\phi_n\rangle \) etc.

[23] This can be easily seen by defining a new state involving only the first \( m \) parties via projecting out the rest. This state is symmetric under permutation and hence the assertion follows from [5].

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[30] We assume it in the spirit of [5]. We note that in case of GME, the overlap function (which has to be maximized) is a multilinear function of complex variables and so the optimization was easier because of availability of mathematical results. In case of REE, however, the entropy function is highly non linear and so far (to our knowledge) there is no such result for its optimization. If it can be proved true, the calculation of REE will be greatly simplified. However, even if it is not the case, still we hope our conjecture on W states will hold, as it is supported by extensive numerical examples (this is why we make no comments on other permutationally invariant states). We note that the CSS is also symmetric.