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THREE-QUBIT GROVERIAN MEASURE

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The Groverian measures are analytically computed in various types of three-qubit states. The final results are also expressed in terms of local-unitary invariant quantities in each type. This fact reflects the manifest local-unitary invariance of the Groverian measure. It is also shown that the analytical expressions for various types have correct limits to other types. For some types (type 4 and type 5) we failed to compute the analytical expression of the Groverian measure in this paper. However, from the consideration of local-unitary invariants we have shown that the Groverian measure in type 4 should be independent of the phase factor φ, which appear in the three-qubit state $|\psi\rangle$. This fact with geometric interpretation on the Groverian measure may enable us to derive the analytical expressions for general arbitrary three-qubit states in near future.

Keywords: Groverian measure, Geometric measure, Three-qubit LU-invariants

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1. Introduction

Recently, much attention is paid to quantum entanglement[1]. It is believed in quantum information community that entanglement is the physical resource which makes quantum computer outperforms classical one[2]. Thus in order to exploit fully this physical resource for constructing and developing quantum algorithms it is important to quantify the entanglement. The quantity for the quantification is usually called entanglement measure.

About decade ago the axioms which entanglement measures should satisfy were studied[3]. The most important property for measure is monotonicity under local operation and classical communication (LOCC)[4]. Following the axioms, many entanglement measures were constructed such as relative entropy[5], entanglement of distillation[6] and formation[7, 8, 9, 10], geometric measure[11, 12, 13, 14], Schmidt measure[15] and Groverian measure[16]. Entanglement measures are used in various branches of quantum mechanics. Especially, recently, they are used to try to understand Zamolodchikov's c-theorem[17] more profoundly. It may be an important application of the quantum information techniques to understand the effect of renormalization group in field theories[18].

The purpose of this paper is to compute the Groverian measure for various three-qubit quantum states.The Groverian measure $G(\psi)$ for three-qubit state $|\psi\rangle$ is defined by $G(\psi) \equiv \sqrt{1 - P_{max}}$ where

$$P_{max} = \max_{|q_1\rangle, |q_2\rangle, |q_3\rangle} |\langle q_1|\langle q_2|\langle q_3|\psi\rangle|^2. \tag{1}$$

Thus P_{max} can be interpreted as a maximal overlap between the given state $|\psi\rangle$ and product states. Groverian measure is an operational treatment of a geometric measure. Thus, if one can compute $G(\psi)$, one can also compute the geometric measure of pure state by $G^2(\psi)$. Sometimes it is more convenient to re-express Eq.(1) in terms of the density matrix $\rho = |\psi\rangle\langle\psi|$. This can be easily accomplished by an expression

$$P_{max} = \max_{R^1, R^2, R^3} \mathrm{Tr}\left[\rho R^1 \otimes R^2 \otimes R^3\right] \tag{2}$$

where $R^i \equiv |q_i\rangle\langle q_i|$ is the density matrix for the product state. Eq.(1) and Eq.(2) manifestly show that P_{max} and $G(\psi)$ are local-unitary(LU) invariant quantities. Since it is well-known that three-qubit system has five independent LU-invariants[19, 20, 21], *say* $J_i (i = 1, \cdots, 5)$, we would like to focus on the relation of the Groverian measures to LU-invariants J_i's in this paper.

This paper is organized as follows. In section II we review simple case, *i.e.* two-qubit system. Using Bloch form of the density matrix it is shown in this section that two-qubit system has only one independent LU-invariant quantity, *say* J. It is also shown that Groverian measure and P_{max} for arbitrary two-qubit states can be expressed solely in terms of J. In section III we have discussed how to derive LU-invariants in higher-qubit systems. In fact, we have derived many LU-invariant quantities using Bloch form of the density matrix in three-qubit system. It is shown that all LU-invariants derived can be expressed in terms of J_i's discussed in Ref.[20]. Recently, it was shown in Ref.[22] that P_{max} for n-qubit state can be computed from $(n-1)$-qubit reduced mixed state. This theorem was used in Ref.[23] and Ref.[24] to compute analytically the geometric measures for various three-qubit states. In this section we have discussed the physical reason why this theorem is possible from the aspect of LU-invariance. In section IV we have computed the Groverian measures for various types of the three-qubit system. The five types we discussed in this section were originally developed in Ref.[20] for the classification of the three-qubit states. It has been shown that the Groverian measures for type 1, type 2, and type 3 can be analytically computed. We have expressed all analytical results in terms of LU-invariants J_i's. For type 4 and type 5 the analytical computation seems to be highly nontrivial and may need separate publications. Thus the analytical calculation for these types is not presented in this paper. The results of this section are summarized in Table I. In section V we have discussed the modified W-like state, which has three-independent real parameters. In fact, this state cannot be categorized in the five types discussed in section IV. The analytic expressions of the Groverian measure for this state was computed recently in Ref.[24]. It was shown that the measure has three different expressions depending on the domains of the parameter space. It turned out that each expression has its own geometrical meaning. In this section we have re-expressed all expressions of the Groverian measure in terms of LU-invariants. In section VI brief conclusion is given.

2. Two Qubit: Simple Case

In this section we consider P_{max} for the two-qubit system. The Groverian measure for two-qubit system is already well-known[25]. However, we revisit this issue here to explore how the measure is expressed in terms of the LU-invariant quantities. The Schmidt decomposition[26] makes the most general expression of the two-qubit state vector to be simple form

$$|\psi\rangle = \lambda_0|00\rangle + \lambda_1|11\rangle \tag{3}$$

with $\lambda_0, \lambda_1 \geq 0$ and $\lambda_0^2 + \lambda_1^2 = 1$. The density matrix for $|\psi\rangle$ can be expressed in the Bloch form as following:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{4}\left[\mathbb{1}\otimes\mathbb{1} + v_{1\alpha}\sigma_\alpha\otimes\mathbb{1} + v_{2\alpha}\mathbb{1}\otimes\sigma_\alpha + g_{\alpha\beta}\sigma_\alpha\otimes\sigma_\beta\right], \tag{4}$$

where

$$\vec{v}_1 = \vec{v}_2 = \begin{pmatrix} 0 \\ 0 \\ \lambda_0^2 - \lambda_1^2 \end{pmatrix}, \qquad g_{\alpha\beta} = \begin{pmatrix} 2\lambda_0\lambda_1 & 0 & 0 \\ 0 & -2\lambda_0\lambda_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

In order to discuss the LU transformation we consider first the quantity $U\sigma_\alpha U^\dagger$ where U is 2×2 unitary matrix. With direct calculation one can prove easily

$$U\sigma_\alpha U^\dagger = \mathcal{O}_{\alpha\beta}\sigma_\beta, \tag{6}$$

where the explicit expression of $\mathcal{O}_{\alpha\beta}$ is given in appendix A. Since $\mathcal{O}_{\alpha\beta}$ is a real matrix satisfying $\mathcal{O}\mathcal{O}^T = \mathcal{O}^T\mathcal{O} = \mathbb{1}$, it is an element of the rotation group O(3). Therefore, Eq.(6) implies that the LU-invariants in the density matrix (4) are $|\vec{v}_1|$, $|\vec{v}_2|$, Tr$[gg^T]$ etc.

All LU-invariant quantities can be written in terms of one quantity, *say* $J \equiv \lambda_0^2\lambda_1^2$. In fact, J can be expressed in terms of two-qubit concurrence[9] $\mathcal{C}$ by $\mathcal{C}^2/4$. Then it is easy to show

$$|\vec{v}_1|^2 = |\vec{v}_2|^2 = 1 - 4J, \tag{7}$$
$$g_{\alpha\beta}g_{\alpha\beta} = 1 + 8J.$$

It is well-known that P_{max} is simply square of larger Schmidt number in two-qubit case

$$P_{max} = \max\left(\lambda_0^2, \lambda_1^2\right). \tag{8}$$

It can be re-expressed in terms of reduced density operators

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4\det\rho^A}\right], \tag{9}$$

where $\rho^A = \mathrm{Tr}_B\rho = (1 + v_{1\alpha}\sigma_\alpha)/2$. Since P_{max} is invariant under LU-transformation, it should be expressed in terms of LU-invariant quantities. In fact, P_{max} in Eq.(9) can be re-written as

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4J}\right]. \tag{10}$$

Eq.(10) implies that P_{max} is manifestly LU-invariant.

3. Local Unitary Invariants

The Bloch representation of the 3-qubit density matrix can be written in the form

$$\rho = \frac{1}{8}\Big[\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + v_{1\alpha}\sigma_\alpha\otimes\mathbb{1}\otimes\mathbb{1} + v_{2\alpha}\mathbb{1}\otimes\sigma_\alpha\otimes\mathbb{1} + v_{3\alpha}\mathbb{1}\otimes\mathbb{1}\otimes\sigma_\alpha \tag{11}$$
$$+ h^{(1)}_{\alpha\beta}\mathbb{1}\otimes\sigma_\alpha\otimes\sigma_\beta + h^{(2)}_{\alpha\beta}\sigma_\alpha\otimes\mathbb{1}\otimes\sigma_\beta + h^{(3)}_{\alpha\beta}\sigma_\alpha\otimes\sigma_\beta\otimes\mathbb{1} + g_{\alpha\beta\gamma}\sigma_\alpha\otimes\sigma_\beta\otimes\sigma_\gamma\Big],$$

where σ_α is Pauli matrix. According to Eq.(6) and appendix A it is easy to show that the LU-invariants in the density matrix (11) are $|\vec{v}_1|$, $|\vec{v}_2|$, $|\vec{v}_3|$, Tr$[h^{(1)}h^{(1)T}]$, Tr$[h^{(2)}h^{(2)T}]$, Tr$[h^{(3)}h^{(3)T}]$, $g_{\alpha\beta\gamma}g_{\alpha\beta\gamma}$ etc.

Few years ago Acín et al[20] represented the three-qubit arbitrary states in a simple form using a generalized Schmidt decomposition[26] as following:

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{12}$$

with $\lambda_i \geq 0$, $0 \leq \varphi \leq \pi$, and $\sum_i \lambda_i^2 = 1$. The five algebraically independent polynomial LU-invariants were also constructed in Ref.[20]:

$$\begin{aligned} &J_1 = \lambda_1^2\lambda_4^2 + \lambda_2^2\lambda_3^2 - 2\lambda_1\lambda_2\lambda_3\lambda_4\cos\varphi, \\ &J_2 = \lambda_0^2\lambda_2^2, \qquad J_3 = \lambda_0^2\lambda_3^2, \qquad J_4 = \lambda_0^2\lambda_4^2, \\ &J_5 = \lambda_0^2(J_1 + \lambda_2^2\lambda_3^2 - \lambda_1^2\lambda_4^2). \end{aligned} \tag{13}$$

In order to determine how many states have the same values of the invariants $J_1, J_2, ...J_5$, and therefore how many further discrete-valued invariants are needed to specify uniquely a pure state of three qubits up to local transformations, one would need to find the number of different sets of parameters φ and $\lambda_i (i = 0, 1, ...4)$, yielding the same invariants. Once λ_0 is found, other parameters are determined uniquely and therefore we derive an equation defining λ_0 in terms of polynomial invariants

$$(J_1 + J_4)\lambda_0^4 - (J_5 + J_4)\lambda_0^2 + J_2J_3 + J_2J_4 + J_3J_4 + J_4^2 = 0. \tag{14}$$

This equation has at most two positive roots and consequently an additional discrete-valued invariant is required to specify uniquely a pure three qubit state. Generally 18 LU-invariants, nine of which may be taken to have only discrete values, are needed to determine a mixed 2-qubit state [27].

If one represents the density matrix $|\psi\rangle\langle\psi|$ as a Bloch form like Eq.(11), it is possible to construct $v_{1\alpha}$, $v_{2\alpha}$, $v_{3\alpha}$, $h^{(1)}_{\alpha\beta}$, $h^{(2)}_{\alpha\beta}$, $h^{(3)}_{\alpha\beta}$, and $g_{\alpha\beta\gamma}$ explicitly, which are summarized in appendix B. Using these explicit expressions one can show directly that all polynomial LU-invariant quantities of pure states are expressed in terms of J_i as following:

$$\begin{aligned} &|\vec{v}_1|^2 = 1 - 4(J_2 + J_3 + J_4), \qquad |\vec{v}_2|^2 = 1 - 4(J_1 + J_3 + J_4) \\ &|\vec{v}_3|^2 = 1 - 4(J_1 + J_2 + J_4), \qquad \mathrm{Tr}[h^{(1)}h^{(1)T}] = 1 + 4(2J_1 - J_2 - J_3) \\ &\mathrm{Tr}[h^{(2)}h^{(2)T}] = 1 - 4(J_1 - 2J_2 + J_3), \qquad \mathrm{Tr}[h^{(3)}h^{(3)T}] = 1 - 4(J_1 + J_2 - 2J_3) \\ &g_{\alpha\beta\gamma}g_{\alpha\beta\gamma} = 1 + 4(2J_1 + 2J_2 + 2J_3 + 3J_4) \\ &h^{(3)}_{\alpha\beta}v^{(1)}_\alpha v^{(2)}_\beta = 1 - 4(J_1 + J_2 + J_3 + J_4 - J_5). \end{aligned} \tag{15}$$

Recently, Ref.[22] has shown that P_{max} for n-qubit pure state can be computed from $(n-1)$-qubit reduced mixed state. This is followed from a fact

$$\max_{R^1, R^2 \cdots R^n} \mathrm{Tr}\left[\rho R^1 \otimes R^2 \otimes \cdots \otimes R^n\right] = \max_{R^1, R^2 \cdots R^{n-1}} \mathrm{Tr}\left[\rho R^1 \otimes R^2 \otimes \cdots \otimes R^{n-1} \otimes \mathbb{1}\right] \tag{16}$$

which is Theorem I of Ref.[22]. Here, we would like to discuss the physical meaning of Eq.(16) from the aspect of LU-invariance. Eq.(16) in 3-qubit system reduces to

$$P_{max} = \max_{R^1, R^2} \mathrm{Tr}\left[\rho^{AB} R^1 \otimes R^2\right] \tag{17}$$

where $\rho^{AB} = \mathrm{Tr}_C \rho$. From Eq.(11) ρ^{AB} simply reduces to

$$\rho = \frac{1}{4}\left[\mathbb{1}\otimes\mathbb{1} + v_{1\alpha}\sigma_\alpha \otimes \mathbb{1} + v_{2\alpha}\mathbb{1}\otimes\sigma_\alpha + h^{(3)}_{\alpha\beta}\sigma_\alpha\otimes\sigma_\beta\right] \tag{18}$$

where $v_{1\alpha}$, $v_{2\alpha}$ and $h^{(3)}_{\alpha\beta}$ are explicitly given in appendix B. Of course, the LU-invariant quantities of ρ^{AB} are $|\vec{v}_1|$, $|\vec{v}_2|$, $\mathrm{Tr}[h^{(3)}h^{(3)T}]$, $h^{(3)}_{\alpha\beta}v_{1\alpha}v_{2\beta}$ etc, all of which, of course, can be re-expressed in terms of J_1, J_2, J_3, J_4 and J_5. It is worthwhile noting that we need all J_i's to express the LU-invariant quantities of ρ^{AB}. This means that the reduced state ρ^{AB} does have full information on the LU-invariance of the original pure state ρ.

Indeed, any reduced state resulting from a partial trace over a single qubit uniquely determines any entanglement measure of original system, given that the initial state is pure. Consider an (n-1)-qubit reduced density matrix that can be purified by a single qubit reference system. Let $|\psi'\rangle$ be any joint pure state. All other purifications can be obtained from the state $|\psi'\rangle$ by LU-transformations $U\otimes\mathbb{1}^{\otimes(n-1)}$, where U is a local unitary matrix acting on single qubit. Since any entanglement measure must be invariant under LU-transformations, it must be the same for all purifications independently of U. Hence the reduced density matrix determines any entanglement measure on the initial pure state. That is why we can compute P_{max} of n-qubit pure state from the $(n-1)$-qubit reduced mixed state.

Generally, the information on the LU-invariance of the original n-qubit state is partly lost if we take partial trace twice. In order to show this explicitly let us consider $\rho^A \equiv \mathrm{Tr}_B\rho^{AB}$ and $\rho^B \equiv \mathrm{Tr}_A\rho^{AB}$:

$$\rho^A = \frac{1}{2}\left[\mathbb{1} + v_{1\alpha}\sigma_\alpha\right], \quad \rho^B = \frac{1}{2}\left[\mathbb{1} + v_{2\alpha}\sigma_\alpha\right]. \tag{19}$$

Eq.(6) and appendix A imply that their LU-invariant quantities are only $|\vec{v}_1|$ and $|\vec{v}_2|$ respectively. Thus, we do not need J_5 to express the LU-invariant quantities of ρ^A and ρ^B. This fact indicates that the mixed states ρ^A and ρ^B partly lose the information of the LU-invariance of the original pure state ρ. This is why $(n-2)$-qubit reduced state cannot be used to compute P_{max} of n-qubit pure state.

4. Calculation of P_{max}

4.1. *General Feature*

If we insert the Bloch representation

$$R^1 = \frac{\mathbb{1} + \vec{s}_1\cdot\vec{\sigma}}{2} \qquad R^2 = \frac{\mathbb{1} + \vec{s}_2\cdot\vec{\sigma}}{2} \tag{20}$$

with $|\vec{s}_1| = |\vec{s}_2| = 1$ into Eq.(17), P_{max} for 3-qubit state becomes

$$P_{max} = \frac{1}{4}\max_{|\vec{s}_1|=|\vec{s}_2|=1}\left[1 + \vec{r}_1\cdot\vec{s}_1 + \vec{r}_2\cdot\vec{s}_2 + g_{ij}s_{1i}s_{2j}\right] \tag{21}$$

where

$$\vec{r}_1 = \mathrm{Tr}\left[\rho^A\vec{\sigma}\right], \quad \vec{r}_2 = \mathrm{Tr}\left[\rho^B\vec{\sigma}\right], \quad g_{ij} = \mathrm{Tr}\left[\rho^{AB}\sigma_i\otimes\sigma_j\right]. \tag{22}$$

Since in Eq.(21) P_{max} is maximization with constraint $|\vec{s}_1| = |\vec{s}_2| = 1$, we should use the Lagrange multiplier method, which yields a pair of equations

$$\begin{aligned} \vec{r}_1 + g\vec{s}_2 &= \Lambda_1\vec{s}_1 \\ \vec{r}_2 + g^T\vec{s}_1 &= \Lambda_2\vec{s}_2, \end{aligned} \tag{23}$$

where the symbol g represents the matrix g_{ij} in Eq.(22). Thus we should solve $\vec{s}_1$, $\vec{s}_2$, Λ_1 and Λ_2 by eq.(23) and the constraint $|\vec{s}_1| = |\vec{s}_2| = 1$. Although it is highly nontrivial to solve Eq.(23), sometimes it is not difficult if the given 3-qubit state $|\psi\rangle$ has rich symmetries. Now, we would like to compute P_{max} for various types of 3-qubit system.

4.2. *Type 1 (Product States):* $J_1 = J_2 = J_3 = J_4 = J_5 = 0$

In order for all J_i's to be zero we have two cases $\lambda_0 = J_1 = 0$ or $\lambda_2 = \lambda_3 = \lambda_4 = 0$.

4.2.1. $\lambda_0 = J_1 = 0$

If $\lambda_0 = 0$, $|\psi\rangle$ in Eq.(12) becomes $|\psi\rangle = |1\rangle \otimes |BC\rangle$ where

$$|BC\rangle = \lambda_1 e^{i\varphi}|00\rangle + \lambda_2|01\rangle + \lambda_3|10\rangle + \lambda_4|11\rangle. \tag{24}$$

Thus P_{max} for $|\psi\rangle$ equals to that for $|BC\rangle$. Since $|BC\rangle$ is two-qubit state, one can easily compute P_{max} using Eq.(9), which is

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4\mathrm{det}\left(\mathrm{Tr}_B|BC\rangle\langle BC|\right)}\right] = \frac{1}{2}\left[1 + \sqrt{1 - 4J_1}\right]. \tag{25}$$

If, therefore, $\lambda_0 = J_1 = 0$, we have $P_{max} = 1$, which gives a vanishing Groverian measure.

4.2.2. $\lambda_2 = \lambda_3 = \lambda_4 = 0$

In this case $|\psi\rangle$ in Eq.(12) becomes

$$|\psi\rangle = \left(\lambda_0|0\rangle + \lambda_1 e^{i\varphi}|1\rangle\right) \otimes |0\rangle \otimes |0\rangle. \tag{26}$$

Since $|\psi\rangle$ is completely product state, P_{max} becomes one.

4.3. *Type2a (biseparable states)*

In this type we have following three cases.

4.3.1. $J_1 \neq 0$ *and* $J_2 = J_3 = J_4 = J_5 = 0$

In this case we have $\lambda_0 = 0$. Thus P_{max} for this case is exactly same with Eq.(25).

4.3.2. $J_2 \neq 0$ *and* $J_1 = J_3 = J_4 = J_5 = 0$

In this case we have $\lambda_2 = \lambda_4 = 0$. Thus P_{max} for $|\psi\rangle$ equals to that for $|AC\rangle$, where

$$|AC\rangle = \lambda_0|00\rangle + \lambda_1 e^{i\varphi}|10\rangle + \lambda_2|11\rangle. \tag{27}$$

Using Eq.(9), therefore, one can easily compute P_{max}, which is

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4J_2}\right]. \tag{28}$$

4.3.3. $J_3 \neq 0$ *and* $J_1 = J_2 = J_4 = J_5 = 0$

In this case P_{max} for $|\psi\rangle$ equals to that for $|AB\rangle$, where

$$|AB\rangle = \lambda_0|00\rangle + \lambda_1 e^{i\varphi}|10\rangle + \lambda_3|11\rangle. \tag{29}$$

Thus P_{max} for $|\psi\rangle$ is

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4J_3}\right]. \tag{30}$$

4.4. *Type2b (generalized GHZ states):* $J_4 \neq 0$, $J_1 = J_2 = J_3 = J_5 = 0$

In this case we have $\lambda_1 = \lambda_2 = \lambda_3 = 0$ and $|\psi\rangle$ becomes

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_4|111\rangle \tag{31}$$

with $\lambda_0^2 + \lambda_4^2 = 1$. Then it is easy to show

$$\begin{aligned} \vec{r}_1 &= \text{Tr}\left[\rho^A \vec{\sigma}\right] = (0, 0, \lambda_0^2 - \lambda_4^2) \\ \vec{r}_2 &= \text{Tr}\left[\rho^B \vec{\sigma}\right] = (0, 0, \lambda_0^2 - \lambda_4^2) \\ g_{ij} &= \text{Tr}\left[\rho^{AB} \sigma_i \otimes \sigma_j\right] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{32}$$

Thus P_{max} reduces to

$$P_{max} = \frac{1}{4} \max_{|\vec{s}_1|=|\vec{s}_2|=1} \left[1 + (\lambda_0^2 - \lambda_4^2)(s_{1z} + s_{2z}) + s_{1z}s_{2z}\right]. \tag{33}$$

Since Eq.(33) is simple, we do not need to solve Eq.(23) for the maximization. If $\lambda_0 > \lambda_4$, the maximization can be achieved by simply choosing $\vec{s}_1 = \vec{s}_2 = (0, 0, 1)$. If $\lambda_0 < \lambda_4$, we choose $\vec{s}_1 = \vec{s}_2 = (0, 0, -1)$. Thus we have

$$P_{max} = \max(\lambda_0^2, \lambda_4^2). \tag{34}$$

In order to express P_{max} in Eq.(34) in terms of LU-invariants we follow the following procedure. First we note

$$P_{max} = \frac{1}{2}\left[(\lambda_0^2 + \lambda_4^2) + |\lambda_0^2 - \lambda_4^2|\right]. \tag{35}$$

Since $|\lambda_0^2 - \lambda_4^2| = \sqrt{(\lambda_0^2 + \lambda_4^2)^2 - 4\lambda_0^2\lambda_4^2} = \sqrt{1 - 4J_4}$, we get finally

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4J_4}\right]. \tag{36}$$

4.5. *Type3a (tri-Bell states)*

In this case we have $\lambda_1 = \lambda_4 = 0$ and $|\psi\rangle$ becomes

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle \tag{37}$$

with $\lambda_0^2 + \lambda_2^2 + \lambda_3^2 = 1$. If we take LU-transformation σ_x in the first-qubit, $|\psi\rangle$ is changed into $|\psi'\rangle$ which is usual W-type state[28] as follows:

$$|\psi'\rangle = \lambda_0|100\rangle + \lambda_3|010\rangle + \lambda_2|001\rangle. \tag{38}$$

The LU-invariants in this type are

$$J_1 = \lambda_2^2 \lambda_3^2 \qquad J_2 = \lambda_0^2 \lambda_2^2 \tag{39}$$
$$J_3 = \lambda_0^2 \lambda_3^2 \qquad J_5 = 2\lambda_0^2 \lambda_2^2 \lambda_3^2.$$

Then it is easy to derive a relation

$$J_1 J_2 + J_1 J_3 + J_2 J_3 = \sqrt{J_1 J_2 J_3} = \frac{1}{2} J_5. \tag{40}$$

Recently, P_{max} for $|\psi'\rangle$ is computed analytically in Ref.[23] by solving the Lagrange multiplier equations (23) explicitly. In order to express P_{max} explicitly we first define

$$\begin{aligned} r_1 &= \lambda_3^2 + \lambda_2^2 - \lambda_0^2 \\ r_2 &= \lambda_0^2 + \lambda_2^2 - \lambda_3^2 \\ r_3 &= \lambda_0^2 + \lambda_3^2 - \lambda_2^2 \\ \omega &= 2\lambda_0 \lambda_3. \end{aligned} \tag{41}$$

Also we define

$$\begin{aligned} a &= \max(\lambda_0, \lambda_2, \lambda_3) \\ b &= \mathrm{mid}(\lambda_0, \lambda_2, \lambda_3) \\ c &= \min(\lambda_0, \lambda_2, \lambda_3). \end{aligned} \tag{42}$$

Then P_{max} is expressed differently in two different regions as follows. If $a^2 \geq b^2 + c^2$, P_{max} becomes

$$P_{max}^{>} = a^2 = \max(\lambda_0^2, \lambda_2^2, \lambda_3^2). \tag{43}$$

In order to express P_{max} in terms of LU-invariants we express Eq.(43) differently as

$$P_{max}^{>} = \frac{1}{4} \left[(\lambda_0^2 + \lambda_3^2 + \lambda_2^2) + |\lambda_0^2 + \lambda_3^2 - \lambda_2^2| + |\lambda_0^2 - \lambda_3^2 + \lambda_2^2| + |\lambda_0^2 - \lambda_3^2 - \lambda_2^2| \right]. \tag{44}$$

Using equalities

$$\begin{aligned} |\lambda_0^2 + \lambda_3^2 - \lambda_2^2| &= \sqrt{1 - 4\lambda_0^2\lambda_2^2 - 4\lambda_2^2\lambda_3^2} = \sqrt{1 - 4(J_1 + J_2)} \\ |\lambda_0^2 - \lambda_3^2 + \lambda_2^2| &= \sqrt{1 - 4\lambda_0^2\lambda_3^2 - 4\lambda_2^2\lambda_3^2} = \sqrt{1 - 4(J_1 + J_3)} \\ |\lambda_0^2 - \lambda_3^2 - \lambda_2^2| &= \sqrt{1 - 4\lambda_0^2\lambda_2^2 - 4\lambda_0^2\lambda_3^2} = \sqrt{1 - 4(J_2 + J_3)}, \end{aligned} \tag{45}$$

we can express P_{max} in Eq.(43) as follows:

$$P_{max}^{>} = \frac{1}{4} \left[1 + \sqrt{1 - 4(J_1 + J_2)} + \sqrt{1 - 4(J_1 + J_3)} + \sqrt{1 - 4(J_2 + J_3)} \right]. \tag{46}$$

If $a^2 \leq b^2 + c^2$, P_{max} becomes

$$P_{max}^{<} = \frac{1}{4} \left[1 + \frac{\omega\sqrt{(\omega^2 + r_1^2 - r_3^2)(\omega^2 + r_2^2 - r_3^2)} - r_1 r_2 r_3}{\omega^2 - r_3^2} \right]. \tag{47}$$

It was shown in Ref.[23] that $P_{max} = 4R^2$, where R is a circumradius of the triangle λ_0, λ_2 and λ_3. When $a^2 \leq b^2 + c^2$, one can show easily $r_1 = \sqrt{1 - 4(J_2 + J_3)}$, $r_2 = \sqrt{1 - 4(J_1 + J_3)}$, $r_3 = \sqrt{1 - 4(J_1 + J_2)}$, and $\omega = 2\sqrt{J_3}$. Using $\omega^2 - r_3^2 - r_1 r_2 r_3 = 8\lambda_0^2\lambda_2^2\lambda_3^2$, One can show easily that P_{max} in Eq.(47) in terms of LU-invariants becomes

$$P_{max}^{<} = \frac{4\sqrt{J_1 J_2 J_3}}{4(J_1 + J_2 + J_3) - 1}. \tag{48}$$

Let us consider $\lambda_0 = 0$ limit in this type. Then we have $J_2 = J_3 = 0$. Thus $P_{max}^{>}$ reduces to $(1/2)(1 + \sqrt{1 - 4J_1})$ which exactly coincides with Eq.(25). By same way one can prove that Eq.(46) has correct limits to various other types.

4.6. *Type3b (extended GHZ states)*

This type consists of 3 types, *i.e.* $\lambda_1 = \lambda_2 = 0$, $\lambda_1 = \lambda_3 = 0$ and $\lambda_2 = \lambda_3 = 0$.

4.6.1. $\lambda_1 = \lambda_2 = 0$

In this case the state (12) becomes

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{49}$$

with $\lambda_0^2 + \lambda_3^2 + \lambda_4^2 = 1$. The non-vanishing LU-invariants are

$$J_3 = \lambda_0^2\lambda_3^2, \qquad J_4 = \lambda_0^2\lambda_4^2. \tag{50}$$

Note that $J_3 + J_4$ is expressed in terms of solely λ_0 as

$$J_3 + J_4 = \lambda_0^2(1 - \lambda_0^2). \tag{51}$$

Eq.(49) can be re-written as

$$|\psi\rangle = \lambda_0|00q_1\rangle + \sqrt{1 - \lambda_0^2}|11q_2\rangle \tag{52}$$

where $|q_1\rangle = |0\rangle$ and $|q_2\rangle = (1/\sqrt{1 - \lambda_0^2})(\lambda_3|0\rangle + \lambda_4|1\rangle)$ are normalized one qubit states. Thus, from Ref.[23], P_{max} for $|\psi\rangle$ is

$$P_{max} = \max\left(\lambda_0^2, 1 - \lambda_0^2\right) = \frac{1}{2}\left[1 + \sqrt{(1 - 2\lambda_0^2)^2}\right]. \tag{53}$$

With an aid of Eq.(51) P_{max} in Eq.(53) can be easily expressed in terms of LU-invariants as following:

$$P_{max} = \frac{1}{2}\left[1 + \sqrt{1 - 4(J_3 + J_4)}\right]. \tag{54}$$

If we take $\lambda_3 = 0$ limit in this type, we have $J_3 = 0$, which makes Eq.(54) to be $(1/2)(1 + \sqrt{1 - 4J_4})$. This exactly coincides with Eq.(36).

4.6.2. $\lambda_1 = \lambda_3 = 0$

In this case $|\psi\rangle$ and LU-invariants are

$$|\psi\rangle = \lambda_0|0q_10\rangle + \sqrt{1-\lambda_0^2}|1q_21\rangle \tag{55}$$

and

$$J_2 = \lambda_0^2\lambda_2^2, \qquad J_4 = \lambda_0^2\lambda_4^2 \tag{56}$$

where $|q_1\rangle = |0\rangle$, $|q_2\rangle = (1/\sqrt{1-\lambda_0^2})(\lambda_2|0\rangle + \lambda_4|1\rangle)$, and $\lambda_0^2+\lambda_2^2+\lambda_4^2 = 1$. The same method used in the previous subsection easily yields

$$P_{max} = \frac{1}{2}\left[1+\sqrt{1-4(J_2+J_4)}\right]. \tag{57}$$

One can show that Eq.(57) has correct limits to other types.

4.6.3. $\lambda_2 = \lambda_3 = 0$

In this case $|\psi\rangle$ and LU-invariants are

$$|\psi\rangle = \sqrt{1-\lambda_4^2}|q_100\rangle + \lambda_4|q_211\rangle \tag{58}$$

and

$$J_1 = \lambda_1^2\lambda_4^2, \qquad J_4 = \lambda_0^2\lambda_4^2 \tag{59}$$

where $|q_1\rangle = (1/\sqrt{1-\lambda_4^2})(\lambda_0|0\rangle + \lambda_1 e^{i\varphi}|1\rangle)$, $|q_2\rangle = |1\rangle$, and $\lambda_0^2+\lambda_1^2+\lambda_4^2 = 1$. It is easy to show

$$P_{max} = \frac{1}{2}\left[1+\sqrt{1-4(J_1+J_4)}\right]. \tag{60}$$

One can show that Eq.(60) has correct limits to other types.

4.7. *Type4a* ($\lambda_4 = 0$)

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle \tag{61}$$

with $\lambda_0^2+\lambda_1^2+\lambda_2^2+\lambda_3^2 = 1$. The non-vanishing LU-invariants are

$$\begin{aligned} J_1 &= \lambda_2^2\lambda_3^2 & J_2 &= \lambda_0^2\lambda_2^2 \\ J_3 &= \lambda_0^2\lambda_3^2 & J_5 &= 2\lambda_0^2\lambda_2^2\lambda_3^2. \end{aligned} \tag{62}$$

From Eq.(62) it is easy to show

$$\sqrt{J_1J_2J_3} = \frac{1}{2}J_5. \tag{63}$$

The remarkable fact deduced from Eq.(62) is that the non-vanishing LU-invariants are independent of the phase factor φ. This indicates that the Groverian measure for Eq.(61) is also independent of φ

In order to compute P_{max} analytically in this type, we should solve the Lagrange multiplier equations (23) with

$$\begin{aligned} \vec{r}_1 &= \mathrm{Tr}[\rho^A\vec{\sigma}] = (2\lambda_0\lambda_1\cos\varphi, 2\lambda_0\lambda_1\sin\varphi, 2\lambda_0^2-1) \\ \vec{r}_2 &= \mathrm{Tr}[\rho^B\vec{\sigma}] = (2\lambda_1\lambda_3\cos\varphi, -2\lambda_1\lambda_3\sin\varphi, 1-2\lambda_3^2) \\ g_{ij} &= \mathrm{Tr}[\rho^{AB}\sigma_i\otimes\sigma_j] = \begin{pmatrix} 2\lambda_0\lambda_3 & 0 & 2\lambda_0\lambda_1\cos\varphi \\ 0 & -2\lambda_0\lambda_3 & 2\lambda_0\lambda_1\sin\varphi \\ -2\lambda_1\lambda_3\cos\varphi & 2\lambda_1\lambda_3\sin\varphi & \lambda_0^2-\lambda_1^2-\lambda_2^2+\lambda_3^2 \end{pmatrix}. \end{aligned} \tag{64}$$

Although we have freedom to choose the phase factor φ, it is impossible to find singular values of the matrix g, which makes it formidable task to solve Eq.(23). Based on Ref.[23] and Ref.[24], furthermore, we can conjecture that P_{max} for this type may have several different expressions depending on the domains in parameter space. Therefore, it may need long calculation to compute P_{max} analytically. We would like to leave this issue for our future research work and the explicit expressions of P_{max} are not presented in this paper.

4.8. *Type4b*

This type consists of the 2 cases, *i.e.* $\lambda_2 = 0$ and $\lambda_3 = 0$.

4.8.1. $\lambda_2 = 0$

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{65}$$

with $\lambda_0^2 + \lambda_1^2 + \lambda_3^2 + \lambda_4^2 = 1$. The LU-invariants are

$$J_1 = \lambda_1^2\lambda_4^2 \qquad J_3 = \lambda_0^2\lambda_3^2 \qquad J_4 = \lambda_0^2\lambda_4^2. \tag{66}$$

Eq.(66) implies that the Groverian measure for Eq.(65) is independent of the phase factor φ like type 4a. This fact may drastically reduce the calculation procedure for solving the Lagrange multiplier equation (23). In spite of this fact, however, solving Eq.(23) is highly non-trivial as we commented in the previous type. The explicit expressions of the Groverian measure are not presented in this paper and we hope to present them elsewhere in the near future.

4.8.2. $\lambda_3 = 0$

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1 e^{i\varphi}|100\rangle + \lambda_2|101\rangle + \lambda_4|111\rangle \tag{67}$$

with $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_4^2 = 1$. The LU-invariants are

$$J_1 = \lambda_1^2\lambda_4^2 \qquad J_2 = \lambda_0^2\lambda_2^2 \qquad J_4 = \lambda_0^2\lambda_4^2. \tag{68}$$

Eq.(68) implies that the Groverian measure for Eq.(67) is independent of the phase factor φ like type 4a.

4.9. *Type4c* *($\lambda_1 = 0$)*

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{69}$$

with $\lambda_0^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1$. The LU-invariants in this type are

$$\begin{aligned} &J_1 = \lambda_2^2\lambda_3^2 \qquad J_2 = \lambda_0^2\lambda_2^2 \qquad J_3 = \lambda_0^2\lambda_3^2 \\ &J_4 = \lambda_0^2\lambda_4^2 \qquad J_5 = 2\lambda_0^2\lambda_2^2\lambda_3^2. \end{aligned} \tag{70}$$

From Eq.(70) it is easy to show

$$J_1(J_2 + J_3 + J_4) + J_2 J_3 = \sqrt{J_1 J_2 J_3} = \frac{1}{2} J_5. \tag{71}$$

In this type $\vec{r}_1$, $\vec{r}_2$ and g_{ij} defined in Eq.(22) are

$$\begin{aligned}
\vec{r}_1 &= (0, 0, 2\lambda_0^2 - 1) \\
\vec{r}_2 &= (2\lambda_2\lambda_4, 0, \lambda_0^2 + \lambda_2^2 - \lambda_3^3 - \lambda_4^2) \\
g_{ij} &= \left(\begin{array}{ccc} 2\lambda_0\lambda_3 & 0 & 0 \\ 0 & -2\lambda_0\lambda_3 & 0 \\ -2\lambda_2\lambda_4 & 0 & 1 - 2\lambda_2^2 \end{array} \right).
\end{aligned} \tag{72}$$

Like type 4a and type 4b solving Eq.(23) is highly non-trivial mainly due to non-diagonalization of g_{ij}. Of course, the fact that the first component of $\vec{r}_2$ is non-zero makes hard to solve Eq.(23) too. The explicit expressions of the Groverian measure in this type are not given in this paper.

4.10. *Type5 (real states):* $\varphi = 0$, π

4.10.1. $\varphi = 0$

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle + \lambda_1|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{73}$$

with $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1$. The LU-invariants in this case are

$$\begin{aligned}
&J_1 = (\lambda_2\lambda_3 - \lambda_1\lambda_4)^2 \qquad J_2 = \lambda_0^2\lambda_2^2 \qquad J_3 = \lambda_0^2\lambda_3^2 \\
&J_4 = \lambda_0^2\lambda_4^2 \qquad J_5 = 2\lambda_0^2\lambda_2\lambda_3(\lambda_2\lambda_3 - \lambda_1\lambda_4).
\end{aligned} \tag{74}$$

It is easy to show $\sqrt{J_1 J_2 J_3} = J_5/2$.

4.10.2. $\varphi = \pi$

In this case the state vector $|\psi\rangle$ in Eq.(12) reduces to

$$|\psi\rangle = \lambda_0|000\rangle - \lambda_1|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \tag{75}$$

with $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1$. The LU-invariants in this case are

$$\begin{aligned}
&J_1 = (\lambda_2\lambda_3 + \lambda_1\lambda_4)^2 \qquad J_2 = \lambda_0^2\lambda_2^2 \qquad J_3 = \lambda_0^2\lambda_3^2 \\
&J_4 = \lambda_0^2\lambda_4^2 \qquad J_5 = 2\lambda_0^2\lambda_2\lambda_3(\lambda_2\lambda_3 + \lambda_1\lambda_4).
\end{aligned} \tag{76}$$

It is easy to show $\sqrt{J_1 J_2 J_3} = J_5/2$ in this type.

The analytic calculation of P_{max} in type 5 is most difficult problem. In addition, we don't know whether it is mathematically possible or not. However, the geometric interpretation of P_{max} presented in Ref.[23] and Ref.[24] may provide us valuable insight. We hope to leave this issue for our future research work too. The results in this section is summarized in Table I.

Type		conditions	P_{max}
Type I		$J_i = 0$	1
Type II	a	$J_i = 0$ except J_1	$\frac{1}{2}\left(1+\sqrt{1-4J_1}\right)$
		$J_i = 0$ except J_2	$\frac{1}{2}\left(1+\sqrt{1-4J_2}\right)$
		$J_i = 0$ except J_3	$\frac{1}{2}\left(1+\sqrt{1-4J_3}\right)$
	b	$J_i = 0$ except J_4	$\frac{1}{2}\left(1+\sqrt{1-4J_4}\right)$
Type III	a	$\lambda_1 = \lambda_4 = 0$	$\frac{1}{4}\left(1+\sqrt{1-4(J_1+J_2)}+\sqrt{1-4(J_1+J_3)}+\sqrt{1-4(J_2+J_3)}\right)$ if $a^2 \geq b^2+c^2$
			$4\sqrt{J_1J_2J_3}/\left(4(J_1+J_2+J_3)-1\right)$ if $a^2 \leq b^2+c^2$
	b	$\lambda_1 = \lambda_2 = 0$	$\frac{1}{2}\left(1+\sqrt{1-4(J_3+J_4)}\right)$
		$\lambda_1 = \lambda_3 = 0$	$\frac{1}{2}\left(1+\sqrt{1-4(J_2+J_4)}\right)$
		$\lambda_2 = \lambda_3 = 0$	$\frac{1}{2}\left(1+\sqrt{1-4(J_1+J_4)}\right)$
Type IV	a	$\lambda_4 = 0$	independent of φ: not presented
	b	$\lambda_2 = 0$	independent of φ: not presented
		$\lambda_3 = 0$	independent of φ: not presented
	c	$\lambda_1 = 0$	not presented
Type V		$\varphi = 0$	not presented
		$\varphi = \pi$	not presented

Table I: Summary of P_{max} in various types.

5. New Type

5.1. *standard form*

In this section we consider new type in 3-qubit states. The type we consider is

$$|\Phi\rangle = a|100\rangle + b|010\rangle + c|001\rangle + q|111\rangle, \quad a^2+b^2+c^2+q^2 = 1. \tag{77}$$

First, we would like to derive the standard form like Eq.(12) from $|\Phi\rangle$. This can be achieved as following. First, we consider LU-transformation of $|\Phi\rangle$, *i.e.* $(U \otimes \mathbb{1} \otimes \mathbb{1})|\Phi\rangle$, where

$$U = \frac{1}{\sqrt{aq+bc}} \begin{pmatrix} \sqrt{aq}e^{i\theta} & \sqrt{bc}e^{i\theta} \\ -\sqrt{bc} & \sqrt{aq} \end{pmatrix}. \tag{78}$$

After LU-transformation, we perform Schmidt decomposition following Ref.[20]. Finally we choose θ to make all λ_i to be positive. Then we can derive the standard form (12) from $|\Phi\rangle$ with $\varphi = 0$ or π, and

$$\lambda_0 = \sqrt{\frac{(ac+bq)(ab+cq)}{aq+bc}} \tag{79}$$

$$\lambda_1 = \frac{\sqrt{abcq}}{\sqrt{(ab+cq)(ac+bq)(aq+bc)}}|a^2+q^2-b^2-c^2|$$

$$\lambda_2 = \frac{1}{\lambda_0}|ac-bq| \qquad \lambda_3 = \frac{1}{\lambda_0}|ab-cq| \qquad \lambda_4 = \frac{2\sqrt{abcq}}{\lambda_0}.$$

It is easy to prove that the normalization condition $a^2+b^2+c^2+q^2 = 1$ guarantees the normalization

$$\lambda_0^2+\lambda_1^2+\lambda_2^2+\lambda_3^2+\lambda_4^2 = 1. \tag{80}$$

Since $|\Phi\rangle$ has three free parameters, we need one more constraint between λ_i's. This additional constraint can be derived by trial and error. The explicit expression for this additional relation is

$$\lambda_0^2(\lambda_2^2+\lambda_3^2+\lambda_4^2)=\frac{1}{4}-\frac{\lambda_1^2}{\lambda_4^2}(\lambda_2^2+\lambda_4^2)(\lambda_3^2+\lambda_4^2). \tag{81}$$

Since all λ_i's are not vanishing but there are only three free parameters, $|\Phi\rangle$ is not involved in the types discussed in the previous section.

5.2. *LU-invariants*

Using Eq.(79) it is easy to derive LU-invariants which are

$$\begin{aligned}
J_1 &= (\lambda_1\lambda_4-\lambda_2\lambda_3)^2=\frac{1}{(ab+cq)^2(ac+bq)^2} \\
&\quad\times\left[2abcq|a^2+q^2-b^2-c^2|-(aq+bc)|(ab-cq)(ac-bq)|\right]^2 \\
J_2 &= \lambda_0^2\lambda_2^2=(ac-bq)^2 \\
J_3 &= \lambda_0^2\lambda_3^2=(ab-cq)^2 \\
J_4 &= \lambda_0^2\lambda_4^2=4abcq \\
J_5 &= \lambda_0^2\left(J_1+\lambda_2^2\lambda_3^2-\lambda_1^2\lambda_4^2\right).
\end{aligned} \tag{82}$$

One can show directly that $J_5 = 2\sqrt{J_1J_2J_3}$. Since $|\Phi\rangle$ has three free parameters, there should exist additional relation between J_i's. However, the explicit expression may be hardly derived. In principle, this constraint can be derived as following. First, we express the coefficients a, b, c, and q in terms of J_1, J_2, J_3 and J_4 using first four equations of Eq.(82). Then the normalization condition $a^2+b^2+c^2+q^2=1$ gives explicit expression of this additional constraint. Since, however, this procedure requires the solutions of quartic equation, it seems to be hard to derive it explicitly.

Since J_1 contains absolute value, it is dependent on the regions in the parameter space. Direct calculation shows that J_1 is

$$J_1=\begin{cases}(aq-bc)^2 & \text{when } (a^2+q^2-b^2-c^2)(ab-cq)(ac-bq)\geq 0\\ (aq-bc)^2\left[1+2(ab-cq)(ac-bq)(aq+bc)/(ab+cq)(ac+bq)(aq-bc)\right]^2 & \\ \qquad\qquad \text{when } (a^2+q^2-b^2-c^2)(ab-cq)(ac-bq)<0. & \end{cases} \tag{83}$$

Since P_{max} is manifestly LU-invariant quantity, it is obvious that it also depends on the regions on the parameter space.

5.3. *calculation of* P_{max}

P_{max} for state $|\Phi\rangle$ in Eq.(77) has been analytically computed recently in Ref.[24]. It turns out that P_{max} is differently expressed in three distinct ranges of definition in parameter space. The final expressions can be interpreted geometrically as discussed in Ref.[24]. To express P_{max} explicitly we define

$$\begin{aligned}
&r_1\equiv b^2+c^2-a^2-q^2 \qquad r_2\equiv a^2+c^2-b^2-q^2 \\
&r_3\equiv a^2+b^2-c^2-q^2 \qquad \omega\equiv ab+qc \qquad \mu\equiv ab-qc.
\end{aligned} \tag{84}$$

The first expression of P_{max}, which can be expressed in terms of circumradius of convex quadrangle is

$$P_{max}^{(Q)} = \frac{4(ab+qc)(ac+qb)(aq+bc)}{4\omega^2 - r_3^2}. \tag{85}$$

The second expression of P_{max}, which can be expressed in terms of circumradius of crossed-quadrangle is

$$P_{max}^{(CQ)} = \frac{(ab-cq)(ac-bq)(bc-aq)}{4S_x^2} \tag{86}$$

where

$$S_x^2 = \frac{1}{16}(a+b+c+q)(a+b-c-q)(a-b+c-q)(-a+b+c-q). \tag{87}$$

The final expression of P_{max} corresponds to the largest coefficient:

$$P_{max}^{(L)} = \max(a^2, b^2, c^2, q^2) = \frac{1}{4}\left(1 + |r_1| + |r_2| + |r_3|\right). \tag{88}$$

The applicable domain for each P_{max} is fully discussed in Ref.[24].

Now we would like to express all expressions of P_{max} in terms of LU-invariants. For the simplicity we choose a simplified case, that is $(a^2+q^2-b^2-c^2)(ab-cq)(ac-bq) \geq 0$. Then it is easy to derive

$$\begin{aligned} r_1^2 &= 1 - 4(J_2+J_3+J_4) \qquad & r_2^2 &= 1 - 4(J_1+J_3+J_4) \\ r_3^2 &= 1 - 4(J_1+J_2+J_4) \qquad & \omega^2 &= J_3 + J_4. \end{aligned} \tag{89}$$

Then it is simple to express $P_{max}^{(Q)}$ and $P_{max}^{(CQ)}$ as following:

$$\begin{aligned} P_{max}^{(Q)} &= \frac{4\sqrt{(J_1+J_4)(J_2+J_4)(J_3+J_4)}}{4(J_1+J_2+J_3+2J_4)-1} \\ P_{max}^{(CQ)} &= \frac{4\sqrt{J_1J_2J_3}}{4(J_1+J_2+J_3+J_4)-1}. \end{aligned} \tag{90}$$

If we take $q=0$ limit, we have $\lambda_4 = J_4 = 0$. Thus $P_{max}^{(Q)}$ and $P_{max}^{(CQ)}$ reduce to $4\sqrt{J_1J_2J_3}/(4(J_1+J_2+J_3)-1)$, which exactly coincides with $P_{max}^{<}$ in Eq.(48). Finally Eq.(89) makes $P_{max}^{(L)}$ to be

$$P_{max}^{(L)} = \frac{1}{4}\left(1 + \sqrt{1-4(J_2+J_3+J_4)} + \sqrt{1-4(J_1+J_3+J_4)} + \sqrt{1-4(J_1+J_2+J_4)}\right). \tag{91}$$

One can show that $P_{max}^{(L)}$ equals to $P_{max}^{>}$ in Eq.(46) when $q=0$. This indicates that our results (90) and (91) have correct limits to other types of three-qubit system.

6. Conclusion

We tried to compute the Groverian measure analytically in the various types of three-qubit system. The types we considered in this paper are given in Ref.[20] for the classification of the three-qubit system.

For type 1, type 2 and type 3 the Groverian measures are analytically computed. All results, furthermore, can be represented in terms of LU-invariant quantities. This reflects the manifest LU-invariance of the Groverian measure.

For type 4 and type 5 we could not derive the analytical expressions of the measures because the Lagrange multiplier equations (23) is highly difficult to solve. However, the consideration of LU-invariants indicates that the Groverian measure in type 4 should be independent of the phase factor φ. We expect that this fact may drastically simplify the calculational procedure for obtaining the analytical results of the measure in type 4. The derivation in type 5 is most difficult problem. However, it might be possible to get valuable insight from the geometric interpretation of P_{max}, presented in Ref.[23] and Ref.[24]. We would like to revisit type 4 and type 5 in the near future.

We think that the most important problem in the research of entanglement is to understand the general properties of entanglement measures in arbitrary qubit systems. In order to explore this issue we would like to extend, as a next step, our calculation to four-qubit states. In addition, the Groverian measure for four-qubit pure state is related to that for two-qubit mixed state via purification[29]. Although general theory for entanglement is far from complete understanding at present stage, we would like to go toward this direction in the future.

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Appendix A

One can easily show that the elements of $\mathcal{O}$ defined in Eq.(6) are given by

$$\begin{aligned}
\mathcal{O}_{11} &= \frac{1}{2}\left(u_{11}u_{22}^* + u_{11}^*u_{22} + u_{12}u_{21}^* + u_{12}^*u_{21}\right) \\
\mathcal{O}_{22} &= \frac{1}{2}\left(u_{11}u_{22}^* + u_{11}^*u_{22} - u_{12}u_{21}^* - u_{12}^*u_{21}\right) \\
\mathcal{O}_{33} &= |u_{11}|^2 - |u_{12}|^2 \\
\mathcal{O}_{12} &= \frac{i}{2}\left(u_{12}u_{21}^* + u_{11}u_{22}^* - u_{12}^*u_{21} - u_{11}^*u_{22}\right) \\
\mathcal{O}_{21} &= \frac{i}{2}\left(u_{12}u_{21}^* + u_{11}^*u_{22} - u_{12}^*u_{21} - u_{11}u_{22}^*\right) \\
\mathcal{O}_{13} &= u_{11}u_{12}^* + u_{11}^*u_{12} \\
\mathcal{O}_{31} &= u_{11}u_{21}^* + u_{11}^*u_{21} \\
\mathcal{O}_{23} &= -i\left(u_{11}u_{12}^* + u_{21}^*u_{22}\right) \\
\mathcal{O}_{32} &= i\left(u_{11}u_{21}^* + u_{12}^*u_{22}\right)
\end{aligned} \tag{A.1}$$

where u_{ij} is element of the unitary matrix defined in Eq.(6). It is easy to prove $\mathcal{O}\mathcal{O}^T = \mathcal{O}^T\mathcal{O} = \mathbb{1}$, which indicates that $\mathcal{O}_{\alpha\beta}$ is an element of O(3).

Appendix B

If the density matrix associated from the pure state $|\psi\rangle$ in Eq.(12) is represented by Bloch form like Eq.(11), the explicit expressions for $\vec{v}_i$ are

$$\vec{v}_1 = \begin{pmatrix} 2\lambda_0\lambda_1\cos\varphi \\ 2\lambda_0\lambda_1\sin\varphi \\ \lambda_0^2-\lambda_1^2-\lambda_2^2-\lambda_3^2-\lambda_4^2 \end{pmatrix} \qquad \vec{v}_2 = \begin{pmatrix} 2\lambda_1\lambda_3\cos\varphi+2\lambda_2\lambda_4 \\ -2\lambda_1\lambda_3\sin\varphi \\ \lambda_0^2+\lambda_1^2+\lambda_2^2-\lambda_3^2-\lambda_4^2 \end{pmatrix} \tag{B.1}$$
$$\vec{v}_3 = \begin{pmatrix} 2\lambda_1\lambda_2\cos\varphi+2\lambda_3\lambda_4 \\ -2\lambda_1\lambda_2\sin\varphi \\ \lambda_0^2+\lambda_1^2-\lambda_2^2+\lambda_3^2-\lambda_4^2 \end{pmatrix}$$

and the components of $h^{(i)}$ are

$$\begin{aligned}
&h^{(1)}_{11} = 2\lambda_2\lambda_3+2\lambda_1\lambda_4\cos\varphi, \qquad h^{(1)}_{22} = 2\lambda_2\lambda_3-2\lambda_1\lambda_4\cos\varphi \\
&h^{(1)}_{33} = \lambda_0^2+\lambda_1^2-\lambda_2^2-\lambda_3^2+\lambda_4^2, \qquad h^{(1)}_{12} = h^{(1)}_{21} = -2\lambda_1\lambda_4\sin\varphi \\
&h^{(1)}_{13} = -2\lambda_2\lambda_4+2\lambda_1\lambda_3\cos\varphi, \qquad h^{(1)}_{31} = -2\lambda_3\lambda_4+2\lambda_1\lambda_2\cos\varphi \\
&h^{(1)}_{23} = -2\lambda_1\lambda_3\sin\varphi, \qquad h^{(1)}_{32} = -2\lambda_1\lambda_2\sin\varphi \\
&h^{(2)}_{11} = -h^{(2)}_{22} = 2\lambda_0\lambda_2, \qquad h^{(2)}_{33} = \lambda_0^2-\lambda_1^2+\lambda_2^2-\lambda_3^2+\lambda_4^2 \\
&h^{(2)}_{12} = h^{(2)}_{21} = 0, \qquad h^{(2)}_{13} = 2\lambda_0\lambda_1\cos\varphi \\
&h^{(2)}_{31} = -2\lambda_3\lambda_4-2\lambda_1\lambda_2\cos\varphi, \qquad h^{(2)}_{23} = 2\lambda_0\lambda_1\sin\varphi \\
&h^{(2)}_{32} = 2\lambda_1\lambda_2\sin\varphi.
\end{aligned} \tag{B.2}$$

The matrix $h^{(3)}_{\alpha\beta}$ is obtained from $h^{(2)}_{\alpha\beta}$ by exchanging λ_2 with λ_3. The non-vanishing components of $g_{\alpha\beta\gamma}$ are

$$\begin{aligned}
&g_{111} = -g_{122} = -g_{212} = -g_{221} = 2\lambda_0\lambda_4 \\
&g_{113} = -g_{223} = 2\lambda_0\lambda_3, \qquad g_{131} = -g_{232} = 2\lambda_0\lambda_2 \\
&g_{133} = 2\lambda_0\lambda_1\cos\varphi, \qquad g_{233} = 2\lambda_0\lambda_1\sin\varphi \\
&g_{312} = g_{321} = 2\lambda_1\lambda_4\sin\varphi, \qquad g_{311} = -2\lambda_2\lambda_3-2\lambda_1\lambda_4\cos\varphi \\
&g_{313} = 2\lambda_2\lambda_4-2\lambda_1\lambda_3\cos\varphi, \qquad g_{322} = -2\lambda_2\lambda_3+2\lambda_1\lambda_4\cos\varphi \\
&g_{323} = 2\lambda_1\lambda_3\sin\varphi, \qquad g_{331} = 2\lambda_3\lambda_4-2\lambda_1\lambda_2\cos\varphi \\
&g_{332} = 2\lambda_1\lambda_2\sin\varphi, \qquad g_{333} = \lambda_0^2-\lambda_1^2+\lambda_2^2+\lambda_3^2-\lambda_4^2.
\end{aligned} \tag{B.3}$$