CHIN. PHYS. LETT. Vol. 29, No. 1 (2012) 010305

Randomly Generating Four Mixed Bell-Diagonal States with a Concurrences Sum to Unity

S. P. Toh[1**], Hishamuddin Zainuddin[2,3], Kim Eng Foo[2,4]

[1] *Faculty of Engineering, The University of Nottingham Malaysia Campus, Jalan Broga, 43500 Semenyih, Selangor Darul Ehsan, Malaysia*

[2] *Laboratory of Computational Sciences and Mathematical Physics, Institute for Mathematical Research, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia*

[3] *Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia*

[4] *Faculty of Health and Life Sciences, INTI International University, Persiaran Perdana BBN, Putra Nilai, 71800 Nilai, Negeri Sembilan, Malaysia*

(Received 23 September 2011)

A two-qubit system in quantum information theory is the simplest bipartite quantum system and its concurrence for pure and mixed states is well known. As a subset of two-qubit systems, Bell-diagonal states can be depicted by a very simple geometrical representation of a tetrahedron with sides of length $2\sqrt{2}$. Based on this geometric representation, we propose a simple approach to randomly generate four mixed Bell decomposable states in which the sum of their concurrence is equal to one.

PACS: 03.67.Mn DOI:10.1088/0256-307X/29/1/010305

It is well known that quantum entanglement is an important resource in quantum information processing.[1] It describes the phenomena of nonclassical correlations between two (or more) parts of a quantum system. A state of a composite quantum system factored into two subsystems can be described by a density matrix ρ in a Hilbert-Schmidt space $H\otimes H$ and it is called *entanglement* if it cannot be represented as a tensor product of states of its subsystems.[2] On the other hand, it will describe a *separable* state if it can be expressed mathematically as a statistical mixture of product states,

$$\rho=\sum_i p_i\rho_i^A\otimes\rho_i^B, \tag{1}$$

where p_i's is a positive real number with $\sum_i p_i=1$; ρ_i^A and ρ_i^B are density matrices of subsystem A and B, respectively. In the case of pure states of such a bipartite system, it is easy to check if a given state is entangled or separable, but in the case of mixed states the situation is more complicated. For a two-qubit system, a necessary criterion for separability is that the partial transpose ρ^{T_B} of the density matrix ρ is again a density matrix.[3] This criterion has also been shown to be sufficient for the separability of a two-qubit system.[4]

Fifteen parameters are required to fully describe the density matrix of a 2×2 system. However, Bell-diagonal states require only three and can be depicted by a simple three-dimensional geometrical picture called the Horodecki diagram.[5] This diagram represents the Bell-basis states as the vertices of a tetrahedron in which all other Bell-diagonal states lie. The tetrahedron can be further subdivided into five regions, namely, a central octahedron representing the separable states and four similar tetrads representing nonseparable states. Due to its ease of visualization and clear boundary between separable and non-separable states, the Horodecki diagram has been widely researched (e.g. Refs. [6,7]) and exploited in quantum information research (e.g. Refs. [8–10]). Practical applications of such Bell-diagonal states in the diagram can be found in quantum cryptography (e.g. Ref. [11]).

One of the fundamental aspects studied in quantum information theory is to quantify the amount of entanglement of a state and various measures have been proposed such as entanglement of formation,[12−14] relative entropy of entanglement,[15] negativity,[16,17] and so on. More recently, the idea of quantum discord was also introduced[18] to further study nonclassical correlations and comparison studies have been made.[19] Entanglement of formation is a monotonic function of Wootters concurrence,[13,14] which is the focus of this Letter. The maximum of the latter corresponds to the maximum of the former and thus for two-qubit systems, to compute entanglement of formation is equivalent to computing concurrence. For Bell-diagonal states, it has been shown[20] that its concurrence is related to the Euclidean distance between the point representing the state and the set of separable states in the Horodecki diagram.

Our aim is to exploit the simplicity of Horodecki diagram to provide a geometrical approach to generating four mixed Bell-diagonal states with the nice feature of its concurrences sum being to one. The

**Corresponding author. Email: SingPoh.Toh@nottingham.edu.my; singpoh@gmail.com

rational of the approach arises from the simple transformation of four small tetrahedra that represent the mixed entangled states in the Horodecki diagram.

Arbitrary two spin-1/2 particles can be completely described by the following 4×4 density matrix:[5]

$$\rho = \frac{1}{4}(I\otimes I + \boldsymbol{r}\cdot\boldsymbol{\sigma}\otimes I + I\otimes\boldsymbol{s}\cdot\boldsymbol{\sigma} + \sum_{m,n=1}^{3} t_{nm}\sigma_n\otimes\sigma_m), \quad (2)$$

with I and $\boldsymbol{\sigma}$ standing for identity and Pauli matrices. For the subsystem A and B, one can obtain two reduced density matrices

$$\rho_A = tr_B(\rho_{AB}) = \frac{1}{2}(I+\boldsymbol{r}\cdot\boldsymbol{\sigma}),$$
$$\rho_B = tr_A(\rho_{AB}) = \frac{1}{2}(I+\boldsymbol{s}\cdot\boldsymbol{\sigma}), \quad (3)$$

where $\boldsymbol{r}$ and $\boldsymbol{s}$ are Bloch vectors for particles A and B, respectively. The T matrix describes the correlations between the particles and is given as $t_{nm} = Tr(\rho\sigma_n\otimes\sigma_m)$.

Aravind[7] has shown that by using the twirl operation introduced by Bennett *et al.*,[12] an arbitrary two-state mixture can be transformed such that $\boldsymbol{r}=\boldsymbol{s}=0$ and only t_{mn} is non-vanishing, by executing four elements of the finite group of rotation in three dimensions, D_2 bilaterally on both particles.

The states with $\boldsymbol{r}=\boldsymbol{s}=0$ are also called T states by Horodecki *et al.*,[5] with the density matrix

$$\rho = \frac{1}{4}\begin{pmatrix} 1+r_z & 0 & 0 & r_x-r_y \\ 0 & 1-r_z & r_x+r_y & 0 \\ 0 & r_x+r_y & 1-r_z & 0 \\ r_x-r_y & 0 & 0 & 1+r_z \end{pmatrix}, \quad (4)$$

and the T matrix becomes diagonal with r_x, r_y and r_z as elements. Straightforward calculation gives the eigenvalues of ρ as

$$\lambda_1 = \frac{1}{4}(1-r_x-r_y-r_z),$$
$$\lambda_2 = \frac{1}{4}(1-r_x+r_y+r_z),$$
$$\lambda_3 = \frac{1}{4}(1+r_x-r_y+r_z),$$
$$\lambda_4 = \frac{1}{4}(1+r_x+r_y-r_z). \quad (5)$$

When $r_x=r_y=r_z=-1$, it gives $\lambda_1=1$ and $\lambda_2=\lambda_3=\lambda_4=0$, and the ρ gives rise density matrix for Bell state Ψ^-. Similarly, $r_y=r_z=1=-r_x$, $r_x=r_z=1=-r_y$ and $r_x=r_y=1=-r_z$ corresponding to Bell states Φ^-, Φ^+ and Ψ^+, respectively. For other values of r_x, r_y and r_z, ρ results density matrices of mixture of Bell states. Thus ρ is parameterized by the diagonal elements of T matrix and can be represented by 3 dimensional vector (r_x, r_y, r_z). The space spanned by these vectors is called T-space.[5] The four Bell states vectors depicted as points in T-space form vertices of a regular tetrahedron with length $2\sqrt{2}$ and they are labeled as A, B, C and D, respectively. All the other points in the tetrahedron or on the surfaces represent mixture states while the origin represents the completely random state $I/4$. We will call the tetrahedron that represents the Bell-diagonal states as physical tetrahedron and denote it as PT.

According to Peres–Horodecki's criterion,[3,4] a 2×2 quantum state is separable if and only if the partially transposed matrix is again a density matrix. Applying partial transposition to ρ gives

$$\rho^{T_B} = \frac{1}{4}\begin{pmatrix} 1+r_z & 0 & 0 & r_x+r_y \\ 0 & 1-r_z & r_x-r_y & 0 \\ 0 & r_x-r_y & 1-r_z & 0 \\ r_x+r_y & 0 & 0 & 1+r_z \end{pmatrix}. \quad (6)$$

By calculating the eigenvalues of ρ^{T_B} and following the analysis outlined above, we will obtain another regular tetrahedron with the vertices $rA=(-1,1,-1)$, $rB=(-1,-1,1)$, $rC=(1,1,1)$ and $rD=(1,-1,-1)$. The partial transpose executed in the Peres-Horodecki criterion reflects the PT in the x–z plane, thus rA can be obtained from A by multiplying r_y of A by -1, and so on. We thus label the latter tetrahedron as rt (reflected tetrahedron).

The portion of the rt that lies outside of PT does not represent any physical states. To find the intersection sector of PT and rt we calculate the points of the intersection between any two planes of PT and each plane of rt. The results we obtained are $a=(1,0,0)$, $b=(-1,0,0)$, $c=(0,1,0)$, $d=(0,-1,0)$, $e=(0,0,1)$ and $f=(0,0,-1)$ which are vertices of a octahedron. As the octahedron are produced from taking partial transposition, and all the states in it must have positive eigenvalues due to the Peres–Horodecki criterion, the octahedron thus represents all the separable Bell-diagonal states.

The geometrical object constructed above can be drawn into what is known as Horodecki diagram.[5] Readers can refer to Refs. [7,9,10] for its illustration.

Planes ace, adf, bcf and bde of the octahedron are the same as planes BCD, ACD, ABD and ABC of PT. The remaining four planes of the octahedron, i.e. bdf, bce, ade and acf together with four vertices of PT, i.e. A, B, C, D form four small regular tetrahedra and we label them as ptA, ptB, ptC and ptD, respectively. For ptA, the base is bdf, and the apex is A, and similarly for the other small tetrahedra. Figure 4 in Ref. [9] shows clearly some of the small tetrahedra. Therefore PT is divided into five sectors with octahedron representing separable states, and four small tetrahedra representing entangled mixed states, except for the apexes representing pure Bell states.

The side length and the height of the four small regular tetrahedra are $\sqrt{2}$ and $2/\sqrt{3}$, respectively. The centroids of ptA, ptB, ptC and ptD are $cI = (-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$, $cII = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $cIII = (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$, and $cIV = (\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, respectively.

The centroids of pt can be easily transformed to the centroid of PT, i.e. origin of the coordinated system for T-space. For example, adding $\frac{1}{2}$ to each element moves cI to $(0, 0, 0)$. The transformations translate the apexes of pt to their own centroids, and the four bases of pt meet to form a regular tetrahedron (again side length $\sqrt{2}$) with the origin as the centroid and cI–cIV as vertices, see Fig. 1. We call this tetrahedron a generator tetrahedron gt.

Now, by picking any point (x, y, z) located inside or on the surfaces of gt, and transform it to pt via

$$\begin{aligned}
ptA:\ & r_x \to x - \frac{1}{2},\ r_y \to y - \frac{1}{2},\ r_z \to z - \frac{1}{2},\\
ptB:\ & r_x \to x - \frac{1}{2},\ r_y \to y + \frac{1}{2},\ r_z \to z + \frac{1}{2},\\
ptC:\ & r_x \to x + \frac{1}{2},\ r_y \to y - \frac{1}{2},\ r_z \to z + \frac{1}{2},\\
ptD:\ & r_x \to x + \frac{1}{2},\ r_y \to y + \frac{1}{2},\ r_z \to z - \frac{1}{2},
\end{aligned} \tag{7}$$

we can generate four points that are located in pt. By substituting (r_x, r_y, r_z) into Eq. (4), four mixed Bell-diagonal states will be generated. The generated mixed states have the nice property of its sum of concurrence being equal to 1 (see the following).

One way to characterize entanglement is to calculate the concurrence. For a mixed state of two-qubit system, concurrence can be expressed as[13,14]

$$C(\rho) = \max\{\sqrt{r_1} - \sqrt{r_2} - \sqrt{r_3} - \sqrt{r_4}, 0\}, \tag{8}$$

where $r_1 \geq r_2 \geq r_3 \geq r_4$ are the eigenvalues of the operator

$$R = \rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{9}$$

with the asterisk denoting the complex conjugation in the computational basis.

For Bell-diagonal state, $R = \rho^2$ and square roots of its eigenvalues are the same as the eigenvalues of ρ given in Eq. (5). Since the maximum values of λ's of a state depend on which pt of the state is represented, we can rewrite the concurrence as

$$C(\rho) = \max\{2\lambda_{\max} - \sum_{i=1}^{4} \lambda_i, 0\}, \tag{10}$$

where

$$\lambda_{\max} = \max\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}. \tag{11}$$

For ptB, $r_x < 0$, $r_y > 0$ and $r_z > 0$, so by inspection of Eq. (5) we know that $\lambda_2 = \lambda_{\max}$, so

$$C(\rho_B) = 2\lambda_2 - 1 = \frac{1}{2}(-1 - r_x + r_y + r_z), \tag{12}$$

where we have used $\sum_{i=1}^{4} \lambda_i = 1$. Similar argument gives

$$\begin{aligned}
C(\rho_A) &= \frac{1}{2}(-1 - r_x - r_y - r_z),\\
C(\rho_C) &= \frac{1}{2}(-1 + r_x - r_y + r_z),\\
C(\rho_D) &= \frac{1}{2}(-1 + r_x + r_y - r_z).
\end{aligned} \tag{13}$$

Now let us pick a point (x, y, z) from gt at random, inverse transform it as shown in Eq. (7), and substitute the obtained coordinates (r_x, r_y, r_z) into the respective concurrence expressions of Eqs. (12) and (13); their sum gives

$$C(\rho_A) + C(\rho_B) + C(\rho_C) + C(\rho_D) = 1. \tag{14}$$

We can also prove Eq. (14) via the relationship between concurrence and the Euclidean distance between the points representing mixed states and the set of separable states. The equations of planes for the base of ptA, ptB, ptC, and ptD are

$$\begin{aligned}
&x + y + z + 1 = 0,\\
&x - y - z + 1 = 0,\\
&-x + y - z + 1 = 0,\\
&-x - y + z + 1 = 0.
\end{aligned} \tag{15}$$

The perpendicular distances from arbitrary point (r_x, r_y, r_z) in pt to the respective bases are then

$$\begin{aligned}
d_A &= \frac{1}{\sqrt{3}}(r_x + r_y + r_z + 1),\\
d_B &= \frac{1}{\sqrt{3}}(r_x - r_y - r_z + 1),\\
d_C &= \frac{1}{\sqrt{3}}(-r_x + r_y - r_z + 1),\\
d_D &= \frac{1}{\sqrt{3}}(-r_x - r_y + r_z + 1).
\end{aligned} \tag{16}$$

Comparing the magnitude of Eq. (16) with Eqs. (12) and (13), we can deduce that

$$C(\rho) = \frac{\sqrt{3}}{2} d. \tag{17}$$

By substituting (r_x, r_y, r_z) in terms of (x, y, z) picked from gt into Eq. (16) and taking the summation, we obtain

$$\sum d = \frac{2}{\sqrt{3}}, \tag{18}$$

which is the height of pt. Thus $\sum C(\rho) = 1$.

Figure 1 shows the vertices of gt formed by transforming the vertices of pt via the inverse translations given in Eq. (7). Vertices of ptA, which are denoted as the first letter in the four brackets, will be transformed to the vertices of gt. The base of ptA, namely bdf, thus forms the surface (cII, $cIII$, cIV) of gt. By using Fig. 1, the third alternative of explaining why the unit sum of concurrence for the four generated mixed states is as follows. Measuring the distance between arbitrary point (x, y, z) (represented as a dot in Fig. 1) in gt to its surfaces is equivalent to measuring the distance between the transformed (via Eq. (7)) point (r_x, r_y, r_z) to the respective bases of pt. In Fig. 1, it is clear that the length of blue line iv is the Euclidean distance between the point (x, y, z) and the surface (cII, $cIII$, cIV) of gt, and it is also the Euclidean distance between the point (r_x, r_y, r_z) and the base bdf of ptA. The sum of the distance for point (x, y, z) to the surfaces of gt, given by the sum of lengths of lines i-iv in Fig. 1, is always equal to the height of gt, which is $\frac{2}{\sqrt{3}}$, thus the sum of distance between (r_x, r_y, r_z) to the respective bases of pt must always be the same as the height of pt, because the transformation (7) will preserve the length of lines i–iv. Again, due to Eq. (17), it guarantees that $\sum C(\rho) = 1$.

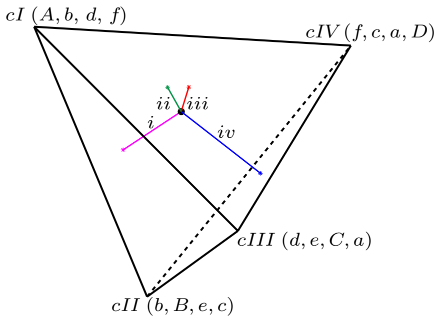

Fig. 1. Diagram showing the relationship between the surfaces of gt and the bases of pt. The first, second, third and fourth letters in each bracket denote the vertices of ptA, ptB, ptC and ptD, respectively. After being transformed through the inverse of translations (7), the bases of pt form the surfaces of gt. As one of the cases, via the inverse of translation given by the first equation of (7), A transformed to cI, b transformed to cII, d transformed to $cIII$ and f transformed to cIV, it means that the base bdf of ptA is transformed to surface (cII, $cIII$, cIV) of gt. The length of line iv in the diagram shows the Euclidean distance from the arbitrary point (x, y, z) in gt to the base (cII, $cIII$, cIV) and also the Euclidean distance from the transformed point (r_x, r_y, r_z) in ptA to the base bdf. The meaning of lines i, ii and iii can be interpreted in a similar way.

In summary, based on the geometrical properties of the Horodecki diagram representing Bell-diagonal states, we have constructed a simple approach to generating four mixed states with its sum of concurrence equal to 1. The unity summation is proved by using the direct calculation of concurrence and can be explained via the relationship between concurrence and the Euclidean distance between entangled states and the set of separable states. The transformations of bases of the four small tetrahedra to form surfaces of the generator tetrahedron also provide a geometrical picture of why the sum of concurrence is equal to 1.

It is interesting to note that most recently,[21] Ramsak showed that the concurrence can be expressed as the expectation values of trigonometric functions of the azimuthal angle between the two angular momenta of the entangled qubits. This will lay the foundations of the unit sum of concurrence discussed in the present study.

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