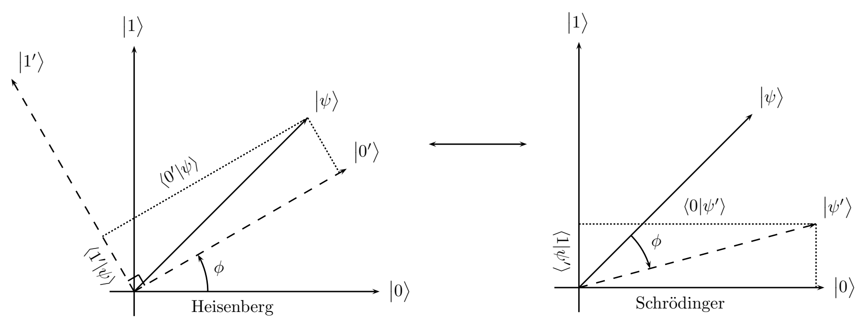
Entanglement, Bell States, EPR Paradox, Bell Inequalities.

1 One qubit:

Recall that the state of a single qubit can be written as a superposition over the possibilities 0 and 1: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. Measuring in the standard basis, then, there is probability $|\alpha|^2$ that we get 0 and the new state is $|\psi'\rangle = |0\rangle$, and probability $|\beta|^2$ that we get 1 and $|\psi'\rangle = |1\rangle$.

More generally, we can measure the qubit in any orthonormal basis simply by projecting $|\psi\rangle$ onto the two basis vectors. The new state of the system $|\psi'\rangle$ is the outcome of the measurement. This is known as the Heisenberg picture.

The Schrodinger picture is equivalent. Instead of measuring the system in a rotated basis, we rotate the system (in the opposite direction) and measure it in the original, standard basis.



Rotations over a complex vector space are called unitary transformations. For example, rotation by θ is unitary. Reflection about the line $\theta/2$ is also unitary.

Hadamard gate:

The Hadamard gate is a reflection about the line $\theta = \pi/8$. This reflection maps the x-axis to the 45° line, and the y-axis to the $-45°$ line. That is

$$|0\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \equiv |+\rangle \tag{1}$$

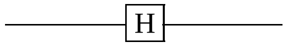
$$|1\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle \equiv |-\rangle \quad . \tag{2}$$

In matrix form, we write

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad .$$

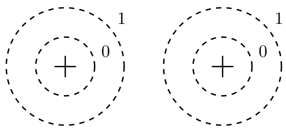
Notice that, starting in $|\psi\rangle$ either $|0\rangle$ or $|1\rangle$, $H|\psi\rangle$ when measured is equally likely to give 0 and 1. There is no longer any distinguishing information in the bit. This information has moved to the phase (in the computational basis).

In a quantum circuit diagram, we imagine the qubit travelling from left to right along the wire. The following diagram shows the application of a Hadamard gate.



2 Two qubits:

Now let us examine the case of two qubits. Consider the two electrons in two hydrogen atoms:



Since each electron can be in either of the ground or excited state, classically the two electrons are in one of four states – 00, 01, 10, or 11 – and represent 2 bits of classical information. Quantum mechanically, they are in a superposition of those four states:

$$\left|\psi\right\rangle = \alpha_{00}\left|00\right\rangle + \alpha_{01}\left|01\right\rangle + \alpha_{10}\left|10\right\rangle + \alpha_{11}\left|11\right\rangle \quad ,$$

where $\sum_{ij}|\alpha_{ij}|^2 = 1$. Again, this is just Dirac notation for the unit vector in $\mathscr{C}^4$:

$$\begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}$$

where $\alpha_{ij} \in \mathscr{C}$, $\sum |\alpha_{ij}|^2 = 1$.

Measurement:

If the two electrons (qubits) are in state $\left|\psi\right\rangle$ and we measure them, then the probability that the first qubit is in state i, and the second qubit is in state j is $P(i,j) = |\alpha_{ij}|^2$. Following the measurement, the state of the two qubits is $\left|\psi'\right\rangle = \left|ij\right\rangle$. What happens if we measure just the first qubit? What is the probability that the first qubit is 0? In that case, the outcome is the same as if we had measured both qubits: $\Pr\{\text{1st bit } = 0\} = |\alpha_{00}|^2 + |\alpha_{01}|^2$. The new state of the two qubit system now consists of those terms in the superposition that are consistent with the outcome of the measurement – but normalized to be a unit vector:

$$\left|\phi\right\rangle = \frac{\alpha_{00}\left|00\right\rangle + \alpha_{01}\left|01\right\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}}$$

.

A more formal way of describing this partial measurement is that the state vector is projected onto the subspace spanned by $\left|00\right\rangle$ and $\left|01\right\rangle$ with probability equal to the square of the norm of the projection, or onto the orthogonal subspace spanned by $\left|10\right\rangle$ and $\left|11\right\rangle$ with the remaining probability. In each case, the new state is given by the (normalized) projection onto the respective subspace.

Tensor products (informal):

Suppose the first qubit is in the state $\left|\phi_1\right\rangle = \alpha_1\left|0\right\rangle + \beta_1\left|1\right\rangle$ and the second qubit is in the state $\left|\phi_2\right\rangle = \alpha_2\left|0\right\rangle + \beta_2\left|1\right\rangle$. How do we describe the joint state of the two qubits?

$$\begin{aligned} \left|\phi\right\rangle &= \left|\phi_1\right\rangle \otimes \left|\phi_2\right\rangle \\ &= \alpha_1\alpha_2\left|00\right\rangle + \alpha_1\beta_2\left|01\right\rangle + \beta_1\alpha_2\left|10\right\rangle + \beta_1\beta_2\left|11\right\rangle \quad . \end{aligned}$$

We have simply multiplied together the amplitudes of $|0\rangle_1$ and $|0\rangle_2$ to determine the amplitude of $|00\rangle_{12}$, and so on. The two qubits are not entangled with each other and measurements of the two qubits will be distrbuted independently.

Given a general state of two qubits can we say what the state of each of the individual qubits is? The answer is usually no. For a random state of two qubits is entangled — it cannot be decomposed into state of each of two qubits. In next section we will study the Bell states, which are maximally entangled states of two qubits.

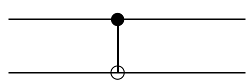
CNOT gate: The controlled-not (CNOT) gate exors the first qubit into the second qubit ($|a,b\rangle \rightarrow |a,a\oplus b\rangle = |a,a+b \bmod 2\rangle$). Thus it permutes the four basis states as follows:

$$\begin{array}{ll} 00 \rightarrow 00 & 01 \rightarrow 01 \\ 10 \rightarrow 11 & 11 \rightarrow 10 \ . \end{array}$$

As a unitary 4×4 matrix, the CNOT gate is

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

In a quantum circuit diagram, the CNOT gate has the following representation. The upper wire is called the control bit, and the lower wire the target bit.



It turns out that this is the only two qubit gate we need to think about ...

3 Spooky Action at a Distance

Consider a state known as a EPR pair (also called a Bell state)

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

Measuring the first bit of $|\Psi^-\rangle$ in the standard basis yields a 0 with probability 1/2, and 1 with probability 1/2. Likewise, measuring the second bit of $|\Psi^-\rangle$ yields the same outcomes with the same probabilities. Measuring one bit of this state yields a perfectly random outcome.

However, determining either bit exactly determines the other.

Furthermore, measurement of $|\Psi^-\rangle$ in any basis will yield opposite outcomes for the two qubits. To see this, check that $|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|vv^\perp\rangle - |v^\perp v\rangle\right)$, for any $|v\rangle = \alpha|0\rangle + \beta|1\rangle$, $|v^\perp\rangle = \bar{\alpha}|1\rangle - \bar{\beta}|0\rangle$.

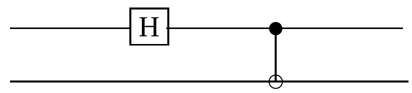
Bell states:

Including $|\Psi^-\rangle$, there are four Bell states:

$$\begin{aligned} |\Phi^\pm\rangle &= \tfrac{1}{\sqrt{2}}\left(|00\rangle \pm |11\rangle\right) \\ |\Psi^\pm\rangle &= \tfrac{1}{\sqrt{2}}\left(|01\rangle \pm |10\rangle\right) \ . \end{aligned}$$

These are maximally entangled states on two qubits. They cannot be product states because there are no cross terms.

We can generate the Bell states with a Hadamard gate and a CNOT gate. Consider the following diagram:



The first qubit is passed through a Hadamard gate and then both qubits are entangled by a CNOT gate.

If the input to the system is $|0\rangle \otimes |0\rangle$, then the Hadamard gate changes the state to

$$\tfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle = \tfrac{1}{\sqrt{2}}|00\rangle + \tfrac{1}{\sqrt{2}}|10\rangle \ ,$$

and after the CNOT gate the state becomes $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, the Bell state $|\Phi^+\rangle$. In fact, one can verify that the four possible inputs produce the four Bell states:

$$|00\rangle \mapsto \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = |\Phi^+\rangle; \qquad |01\rangle \mapsto \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = |\Psi^+\rangle;$$
$$|10\rangle \mapsto \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) = |\Phi^-\rangle; \qquad |11\rangle \mapsto \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) = |\Psi^-\rangle.$$

3.1 EPR Paradox:

In 1935, Einstein, Podolsky and Rosen (EPR) wrote a paper ”Can quantum mechanics be complete?” [Phys. Rev. 47, 777, Available online via PROLA: `http://prola.aps.org/abstract/PR/v47/i10/p777_1`]

For example, consider coin-flipping. We can model coin-flipping as a random process giving heads 50% of the time, and tails 50% of the time. This model is perfectly predictive, but incomplete. With a more accurate experimental setup, we could determine precisely the range of initial parameters for which the coin ends up heads, and the range for which it ends up tails.

For Bell state, when you measure first qubit, the second qubit is determined. However, if two qubits are far apart, then the second qubit must have had a determined state in some time interval before measurement, since the speed of light is finite. Moreover this holds in any basis. This appears analogous to the coin flipping example. EPR therefore suggested that there is a more complete theory where “God does not throw dice.”

What would such a theory look like? Here is the most extravagant framework... When the entangled state is created, the two particles each make up a (very long!) list of all possible experiments that they might be subjected to, and decide how they will behave under each such experiment. When the two particles separate and can no longer communicate, they consult their respective lists to coordinate their actions.

But in 1964, almost three decades later, Bell showed that properties of EPR states were not merely fodder for a philosophical discussion, but had verifiable consequences: local hidden variables are not the answer.

4 Bell’s Inequality

Bell’s inequality states: There does not exist any local hidden variable theory consistent with these outcomes of quantum physics.

Consider the following communication protocol in the classical world: Alice (A) and Bob (B) are two parties who share a common string S. They receive independent, random bits X_A, X_B, and try to output bits a, b respectively, such that $X_A \wedge X_B = a \oplus b$. (The notation $x \wedge y$ takes the AND of two binary variables x and y, i.e., is one if $x = y = 1$ and zero otherwise. $x \oplus y \equiv x + y \bmod 2$, the XOR.)

In the quantum mechanical analogue of this protocol, A and B share the EPR pair $\left|\Psi^-\right\rangle$. As before, they receive bits X_A, X_B, and try to output bits a, b respectively, such that $X_A \wedge X_B = a \oplus b$.

If the odd behavior of $\left|\Psi^-\right\rangle$ can be explained using some hidden variable theory, then the two protocols give above should be equivalent.

However, Alice and Bob's best protocol for the classical game, as you will prove in the homework, is to output $a = 0$ and $b = 0$, respectively. Then $a \oplus b = 0$, so as long as the inputs $(X_A, X_B) \neq (1,1)$, they are successful: $a \oplus b = 0 = X_A \wedge X_B$. If $X_A = X_B = 1$, then they fail. Therefore they are successful with probability exactly $3/4$.

We will show that the quantum mechanical system can do better. Specifically, if Alice and Bob share an EPR pair, we will describe a protocol for which the probability $\Pr\{X_A \wedge X_B = a \oplus b\}$ is greater than 3/4.

We can setup the following protocol:

- if $X_A = 0$, then Alice measures in the standard basis, and outputs the result.
- if $X_A = 1$, then Alice rotates by $\pi/8$, then measures, and outputs the result.
- if $X_B = 0$, then Bob measures in the standard basis, and outputs the complement of the result.
- if $X_B = 1$, then Bob rotates by $-\pi/8$, then measures, and outputs the complement of the result.

Now we calculate $\Pr\{a \oplus b \neq X_A \wedge X_B\}$. (Recall that if measurement in the standard basis yields $\left|0\right\rangle$ with probability 1, then if a state is rotated by θ, measurement yields $\left|0\right\rangle$ with probability $\cos^2(\theta)$.) There are four cases:

$$\Pr\{a \oplus b \neq X_A \wedge X_B\} = \sum_{X_A, X_B} \tfrac{1}{4} \Pr\{a \oplus b \neq X_A \wedge X_B | X_A, X_B\}$$

Now we claim

$$\begin{aligned}
\Pr\{a \oplus b \neq X_A \wedge X_B | X_A = 0, X_B = 0\} &= 0 \\
\Pr\{a \oplus b \neq X_A \wedge X_B | X_A = 0, X_B = 1\} &= \sin^2(\pi/8) \\
\Pr\{a \oplus b \neq X_A \wedge X_B | X_A = 1, X_B = 0\} &= \sin^2(\pi/8) \\
\Pr\{a \oplus b \neq X_A \wedge X_B | X_A = 1, X_B = 1\} &= \sin^2(\pi/4) = 1/2 \ .
\end{aligned}$$

Indeed, for the first case, $X_A = X_B = 0$ (so $X_A \wedge X_B = 0$), Alice and Bob each measure in the computational basis, without any rotation. If Alice measures $a = 0$, then Bob's measurement is the opposite, and Bob outputs the complement, $b = 0$. Therefore $a \oplus b = 0 = X_A \wedge X_B$, a success. Similarly if Alice measures $a = 1$, they are always successful.

In the second case, $X_A = 0$, $X_B = 1$ ($X_A \wedge X_B = 0$). If Alice measures $a = 0$, then the new state of the system is $\left|01\right\rangle$; Bob's qubit is in the state $\left|1\right\rangle$. In the rotated basis, Bob measures a 1 (and outputs its complement, 0) with probability $\cos^2(\pi/8)$. The probability of *failure* is therefore $1 - \cos^2(\pi/8) = \sin^2(\pi/8)$. Similarly if Alice measures $a = 1$. The third case, $X_A = 1$, $X_B = 0$ is symmetrical.

In the final case, $X_A = X_B = 1$ (so $X_A \wedge X_B = 1$), Alice and Bob are measuring in bases rotated 45 degrees from each other, so their measurements are independent. The probability of failure is $1/2$.

Averaging over the four cases, we find

$$\begin{aligned}
\Pr\{a \oplus b \neq X_A \wedge X_B\} &= 1/4\left(2\sin^2(\pi/8) + 1/2\right) \\
&= 1/4\left(1 - \cos(2 * \pi/8) + 1/2\right) \\
&= 1/4\left(3/2 - \sqrt{2}/2\right) \\
&\approx 1/8\,(3 - 1.4) \\
&= 1.6/8 = .2 \ \ .
\end{aligned}$$

The probability of success with this protocal is therefore around .8, better than any protocol could achieve in the classical, hidden variable model.

Exercise: Consider the GHZ (Greenberger-Horne-Zeilinger) state, of 3 qubits:

$$\frac{1}{2}\left(|000\rangle - |011\rangle - |101\rangle - |110\rangle\right)$$

Suppose three parties, A, B and C with experiments X_A, X_B, X_C respectively, with the constraint $X_A \oplus X_B \oplus X_C = 0$. Output a, b, c s.t. $X_A \vee X_B \vee X_C = a \oplus b \oplus c$. Show that this can be done with certainty. Hint: you'll need the Hadamard matrix,

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

which takes

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|1\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$$

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A complete basis of generalized Bell states

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A complete basis of generalized Bell states

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Abstract. A generalization of the Bell states and Pauli matrices to dimensions which are powers of 2 is considered. A basis of maximally entangled multidimensional bipartite states (MEMBS) is chosen very similar to the standard Bell states and constructed of only symmetric and antisymmetric states. This special basis of MEMBS preserves all basic properties of the standard Bell states. We present a recursive and non-recursive method for the construction of MEMBS and discuss their properties. The antisymmetric MEMBS possess the property of rotationally invariant exclusive correlations which is a generalization of the rotational invariance of the antisymmetric singlet Bell state.

Contents

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1. Introduction

Entanglement is one of the most astonishing and most exploited effects in the quantum world. Although this astonishing aspect was already noticed in the early stages of quantum theory [1]–[3], it was not until much later that it attracted appreciable attention, with the theoretical and experimental development of quantum information science.

The simplest example of entanglement is represented by the four maximally entangled two-qubit states, or *Bell states* $|\Phi^{\pm}\rangle_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A|0\rangle_B \pm |1\rangle_A|1\rangle_B)$, $|\Psi^{\pm}\rangle_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A|1\rangle_B \pm |1\rangle_A|0\rangle_B)$ [4]. Their properties are well known and can be found in various books on quantum information [5]–[7]. Here we mention only the following:

1. the Bell states form an orthonormal basis in two-qubit Hilbert space, i.e. each pure two-qubit state can be written as a superposition of the Bell states;
2. the Bell states are of only two types—symmetric and antisymmetric with respect to permutation of the subsystems, i.e. if one exchanges indices of subsystems $A \leftrightarrow B$, the symmetric Bell states remain the same $|\Phi^{\pm}\rangle_{BA} = |\Phi^{\pm}\rangle_{AB}$, $|\Psi^{+}\rangle_{BA} = |\Psi^{+}\rangle_{AB}$, and the antisymmetric Bell state obtains a minus sign: $|\Psi^{-}\rangle_{BA} = -|\Psi^{-}\rangle_{AB}$; and
3. finally, the antisymmetric state $|\Psi^{-}\rangle_{AB}$ delivers perfect rotationally invariant *exclusive correlations*, i.e. the probability of obtaining the same result $|\nu\rangle$ of arbitrary quantum measurements of each qubit is equal to zero irrespective of the state $|\nu\rangle$: $\mathrm{Tr}_{AB}[(|\nu\rangle_A\langle\nu|_A \otimes |\nu\rangle_B\langle\nu|_B)|\Psi^{-}\rangle_{AB}\langle\Psi^{-}|_{AB}] = 0$. As a consequence, the antisymmetric state is invariant under applying the same unitary transformation U to each qubit, i.e. $|\tilde{i}\rangle = U|i\rangle : |\Psi^{-}\rangle_{AB} = \frac{1}{\sqrt{2}}(|\tilde{0}\rangle_A|\tilde{1}\rangle_B - |\tilde{1}\rangle_A|\tilde{0}\rangle_B) = \frac{1}{\sqrt{2}}(|0\rangle_A|1\rangle_B - |1\rangle_A|0\rangle_B)$.

The Bell states are a rather simple example of entanglement, nevertheless, they are widely used in both theoretical and experimental work. For a number of applications it is useful to consider possible generalizations of the Bell states. A significant amount of work in this direction is concentrated on the investigation of entanglement between several qubits, as this approach is very natural for certain applications such as quantum computation [8]. For other situations (e.g. quantum cryptography), it would be more natural to consider entanglement between two multidimensional systems, or *two-qudit* entanglement [9]–[12].

There are several directions towards the generalization of Bell states and Bell basis to higher dimensions. The most obvious one is to consider a state $|\phi\rangle_{AB} = \frac{1}{\sqrt{D}}\sum_{k=0}^{D-1}|k\rangle_A|k\rangle_B$ as a straightforward generalization of the symmetric Bell state $|\Phi^{+}\rangle_{AB}$. As far as all basis maximally entangled multidimensional bipartite states (MEMBS) can be transformed into each other by local unitary transformations, in certain situations it is enough to consider this symmetric state to demonstrate properties of multidimensional entanglement.

In other situations it is important to have a particular property of (anti)symmetry. For example, the antisymmetric singlet Bell state $|\Psi^{-}\rangle_{AB}$ can be thought as the state of two particles with individual spin $1/2$ and zero total spin. An interesting multidimensional generalization of the singlet Bell state is the state $|\phi\rangle_{AB} = \frac{1}{\sqrt{2j+1}}\sum_{m=-j}^{j}(-1)^{j-m}|m\rangle_A|-m\rangle_B$, which was mentioned as a rotationally invariant state with zero total spin for $j = N/2$, with arbitrary integer N (if states $|m\rangle$ are associated with spin projections m) [13]. Interestingly, it is either symmetric (for even N) or antisymmetric (for odd N). This state was further analyzed in the context of the Bell inequality [14]. The property of rotational invariance of the generalized singlet state was also investigated in the context of EPR correlations and hidden-variable theories [15].

An important generalization of the complete Bell basis was constructed for the qudit teleportation scheme [16]. The basis of MEMBS was chosen to be of the form $|\psi\rangle^{mn}_{AB} = \frac{1}{\sqrt{D}}\sum_{k=0}^{D-1} \mathrm{e}^{\mathrm{i}\frac{2\pi}{D}mk}|k\rangle_A|k-n\rangle_B$. Later this special basis was associated with 'generalized EPR states' or 'generalized Bell states' and widely used in various quantum information processing schemes with two qudits such as teleportation, dense coding, cryptography.

Another interesting choice of the generalized Bell states was suggested for a set of 2^n qubits—the 'Bell gems' [17]. An iterative method for construction of these Bell gems was chosen in such a way that it possesses either subsystem exchange symmetry or antisymmetry.

The property of (anti)symmetry of the Bell states arises in various contexts. For instance, in atomic physics the two natural classes of joint states of two spins $1/2$ are those with the total spin 0 (represented by the antisymmetric singlet) and the total spin 1 (and its projections $1, 0, -1$ represented by the symmetric triplet).

An important aspect of (anti)symmetry is that the symmetric and antisymmetric subspaces are orthogonal to each other. By a single projection of an unknown state to these subspaces one can obtain unambiguous information about the state. As an example, this feature is used in the experimental determination of entanglement with a single measurement [18] by the entanglement concurrence measure [19]. Another interesting example which exploits the property of (anti)symmetry of the Bell states is the adaptive state estimation [20].

The purpose of this paper is to demonstrate a special way of constructing a basis of MEMBS, which naturally preserves all above mentioned basic properties of the standard Bell states. We construct a basis of MEMBS in such a way that it consists only of either symmetric or antisymmetric states. We prove that the antisymmetric MEMBS possess rotationally invariant exclusive correlations. This property is a generalization of rotationally invariant anticorrelations of the singlet Bell state. We also note a close connection between the generalized Pauli matrices and the generalized Bell states.

2. Structure of maximally entangled bipartite states

Let us start with a note that a pure state $|\phi\rangle_{AB}$ of a bipartite system $A+B$ is maximally entangled if and only if the Schmidt number is equal to the dimension D, or, equally, the state can be transformed by local operations to the form

$$|\phi\rangle_{AB} = \frac{1}{\sqrt{D}}\sum_{k,l=0}^{D-1} \lambda_{kl}|k\rangle_A|l\rangle_B, \qquad (1)$$

where in each row k and each column l of the matrix λ there is a single nonzero element $\lambda_{kl} = \mathrm{e}^{\mathrm{i}\alpha_{kl}}$ with arbitrary real parameter α_{kl}. Indeed, tracing a bipartite state (1) over one system we obtain an identity density matrix (normalized to the dimension D) of another system: $\hat{\rho}_A = \mathrm{Tr}_B|\phi\rangle_{AB}\langle\phi|_{AB} = \hat{1}_A/D$, $\hat{\rho}_B = \mathrm{Tr}_A|\phi\rangle_{AB}\langle\phi|_{AB} = \hat{1}_B/D$. The above mentioned symmetric state $|\phi\rangle_{AB} = \frac{1}{\sqrt{D}}\sum_{k=0}^{D-1}|k\rangle_A|k\rangle_B$ is a special case of (1), when $\lambda_{kl} = \delta_{kl}$, i.e. λ is a diagonal unit matrix.

Thus we can represent, according to (1), a pure maximally entangled state $|\phi\rangle_{AB}$ by a $D\times D$ matrix λ. This matrix representation turns out to be very convenient for the analysis of the properties of entangled states. The symmetry of the state $|\phi\rangle_{AB}$ with respect to permutation of systems A and B is equal to the symmetry of the corresponding matrix λ with respect to its transposition: a symmetric matrix corresponds to a symmetric state, while an antisymmetric matrix relates to an antisymmetric state. For example, matrix representation $\{\lambda^{\Phi^+}, \lambda^{\Phi^-}, \lambda^{\Psi^+}, \lambda^{\Psi^-}\}$ of the Bell states $\{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle\}$ is the following set of matrices:

$$\left\{\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}, \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}, \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}, \begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}\right\}. \tag{2}$$

In order to form a basis of two-qudit states it is sufficient to form a basis of $D \times D$ matrices, i.e. to define a set $\{\lambda\}$ of D^2 linearly independent matrices. The question of forming a basis has no unique solution, because we can fix phases α_{kl} in (1) quite arbitrarily to satisfy the linear independence of all matrices. Generally speaking, a basis of MEMBS can be associated with a basis of unitary transformations. Here, we mention two particularly useful constructions of unitary bases—nice error bases [21] and 'shift-and-multiply' bases [22]. A complete classification of unitary bases for small dimensions was investigated in [23].

Concerning the generalized Bell states, in [16] a basis of MEMBS was chosen of the form

$$|\psi\rangle_{AB}^{mn} = \frac{1}{\sqrt{D}} \sum_{k=0}^{D-1} \mathrm{e}^{\mathrm{i}\frac{2\pi}{D}mk} |k\rangle_A |k \ominus n\rangle_B, \tag{3}$$

where $k \ominus n \equiv (k-n) \bmod D$. In terms of matrix representation (1), states (3) correspond to a set $\{\lambda^{mn}\}$ with matrix elements $\lambda_{kl}^{mn} = \mathrm{e}^{\mathrm{i}(2\pi/D)mk}\delta_{l,k\ominus n}$, where upper indices m, n enumerate states in the basis $\{|\psi\rangle_{AB}^{mn}\}$ and lower indices $k,\ l$ enumerate terms of direct product $|k\rangle_A|l\rangle_B$ in each state $|\psi\rangle_{AB}^{mn} = \frac{1}{\sqrt{D}} \sum_{k,l=0}^{D-1} \lambda_{kl}^{mn} |k\rangle_A |l\rangle_B$. For $D=2$ this basis actually leads to the standard Bell states with matrices (2), but in general the scheme (3) produces neither symmetric nor antisymmetric states, for instance in the case $D=4$ the scheme (3) produces two antisymmetric states, six symmetric ones, whereas the remaining 8 states are of neither symmetric nor antisymmetric form. Thus the states (3) are not the most straightforward generalization of the Bell states.

Fortunately, among an infinite variety of all possible ways to define a basis of MEMBS we can choose a special one, when MEMBS are of only either symmetric or antisymmetric form, just like Bell states for $D=2$. To show the explicit structure of these MEMBS let us choose the dimension of each qudit equal to power of 2 ($D=2^d$) and follow the notation: $\lambda(d)$ is a $2^d \times 2^d$ matrix representing a pure maximally entangled state according to (1) and $\{\lambda(d)\}$ is a basis of these matrices. The choice of the dimension $D=2^d$ allows us to represent each system as a collection of qubits. However, the following idea with proper modifications can be also exploited in the case of other dimensions.

Note the number of basis states in Hilbert space with the dimension $D=2^{d+1}$ is four times greater than with the dimension $D=2^d$. Let $\{\lambda(d)\}$ be a basis consisting of only symmetric and antisymmetric matrices $\lambda(d)$. To construct a four-times-larger basis $\{\lambda(d+1)\}$, we associate each matrix $\lambda(d)$ with four matrices $\lambda(d+1)$ in the following way: $\{\lambda^{\Phi^+} \otimes \lambda(d), \lambda^{\Phi^-} \otimes \lambda(d), \lambda^{\Psi^+} \otimes \lambda(d), \lambda^{\Psi^-} \otimes \lambda(d)\}$, where the symbol $\otimes$ means the tensor product of the matrices. In other words, matrices $\lambda(d+1)$ have the block structure

$$\begin{pmatrix}\lambda(d) & \mathcal{O}\\ \mathcal{O} & \lambda(d)\end{pmatrix}, \begin{pmatrix}\lambda(d) & \mathcal{O}\\ \mathcal{O} & -\lambda(d)\end{pmatrix}, \begin{pmatrix}\mathcal{O} & \lambda(d)\\ \lambda(d) & \mathcal{O}\end{pmatrix}, \begin{pmatrix}\mathcal{O} & \lambda(d)\\ -\lambda(d) & \mathcal{O}\end{pmatrix}, \tag{4}$$

where $\mathcal{O}$ is a $2^d \times 2^d$ matrix (a matrix of the same size as the matrix $\lambda(d)$), consisting of only zero elements.

As far as each of the subsystems can be thought of as a collection of qubits, one can rewrite this recursive scheme in the explicit nonrecursive form:

$$\lambda(d)_{i_1 i_2 \ldots i_d} = \bigotimes_{j=1}^{d} \lambda(1)_{i_j}, \tag{5}$$

where $\{\lambda(1)\}$ are the Bell state matrices numbered by a subscript index $i_j = 1\ldots4$ and $\{\lambda(d)\}$ are the generalized Bell state matrices numbered by a composite subscript index $i_1 i_2 \ldots i_d = 1\ldots4^d$.

If the matrix $\lambda(d)$ is symmetric, then the first three matrices in (4) are also symmetric and the last one is antisymmetric, and vice versa, if $\lambda(d)$ is antisymmetric, then the first three matrices in (4) are antisymmetric and the last is symmetric. Thus all elements in $\{\lambda(d+1)\}$ are of either symmetric or antisymmetric form. From the construction we see that all matrices $\{\lambda(d+1)\}$ are linearly independent and form a complete basis of $2^{d+1}\times 2^{d+1}$ matrices. The basis of entangled states (1) formed by the set $\{\lambda(d+1)\}$ is a complete orthonormal basis in the $2^{d+1}\times 2^{d+1}$ Hilbert space.

The total numbers of symmetric (N_{s}) and antisymmetric (N_{a}) states, formed by the scheme (4), are given by the following recurrence relations:

$$N_{\mathrm{s}}(d+1) = 3N_{\mathrm{s}}(d) + N_{\mathrm{a}}(d), \qquad N_{\mathrm{a}}(d+1) = 3N_{\mathrm{a}}(d) + N_{\mathrm{s}}(d). \tag{6}$$

We can start the scheme (4) from the smallest case $d = 0$ $(D = 2^0 = 1)$. Here, we have a trivial 1×1 matrix, consisting of a single element 1. It is symmetric, thus the initial conditions for (6) are $N_{\mathrm{s}}(0) = 1$, $N_{\mathrm{a}}(0) = 0$. Taking it into account, the non-recurrence solution of (6) is

$$N_{\mathrm{s}} = D(D+1)/2, \quad N_{\mathrm{a}} = D(D-1)/2, \tag{7}$$

which are the dimensions of symmetric and antisymmetric subspaces of a bipartite Hilbert space.

One can calculate the numbers N_{s} and N_{a} in another way. A state is antisymmetric if, in its tensor product representation (5), the number of antisymmetric Bell state matrices is odd, otherwise it is symmetric. Therefore the total number of symmetric states is given by $N_s = \sum_k C(d,k)3^{d-k}$, where we sum over even numbers $0 \leqslant k \leqslant d$, and $C(d,k) = d!/(k!(d-k)!)$ is the binomial coefficient. Respectively, the number of antisymmetric states is $N_{\mathrm{a}} = \sum_k C(d,k)3^{d-k}$, where we sum over odd numbers $1 \leqslant k \leqslant d$. By direct computation one obtains the same values as (7).

In the case $d = 1$ $(D = 2^1 = 2)$ we have the four Bell states (2) obeying (4) with the number of symmetric and antisymmetric states $N_{\mathrm{s}} = 3$, $N_{\mathrm{a}} = 1$. The next case $d = 2$ $(D = 2^2 = 4)$ gives us ten symmetric pairs of quarts ($N_{\mathrm{s}} = 10$) and six antisymmetric ($N_{\mathrm{a}} = 6$). In the limit of infinite-dimensional states the number of symmetric states tends to the number of antisymmetric states, or more accurately $\lim_{D\to\infty} N_{\mathrm{a}}/N_{\mathrm{s}} = \lim_{D\to\infty}(D-1)/(D+1) = 1$.

3. Rotational invariance of antisymmetric MEMBS

Properties of the antisymmetric MEMBS, particularly those formed by the scheme (4), are similar to the properties of the antisymmetric Bell state, namely, they deliver *perfect rotationally invariant exclusive correlations*. By exclusive correlations we mean that any two identical measurements on both subsystems never give the same result, i.e. the case of two identical results is excluded. For the two-dimensional subsystems exclusive correlations simply mean correlations of the orthogonal states, or anticorrelations.

To prove exclusive correlations property of antisymmetric MEMBS, let us calculate the probability $P_{AB}(\alpha,\beta)$ of measuring a state α of system A and a state β of system B. It is equal to the mean value of a joint projector $\hat{E}_A(\alpha)\otimes\hat{E}_B(\beta)$, where $\hat{E}(\alpha)=|\alpha\rangle\langle\alpha|,\ |\alpha\rangle=\sum_{k=0}^{D-1}\alpha_k|k\rangle$ and $\hat{E}(\beta)=|\beta\rangle\langle\beta|,\ |\beta\rangle=\sum_{l=0}^{D-1}\beta_l|l\rangle$:

$$P_{AB}(\alpha,\beta)=\mathrm{Tr}_{AB}\left[\left(\hat{E}_A(\alpha)\otimes\hat{E}_B(\beta)\right)|\phi\rangle_{AB}\langle\phi|_{AB}\right]=\frac{1}{D}\left|\sum_{k,l=0}^{D-1}\lambda_{kl}^*\alpha_k\beta_l\right|^2. \quad (8)$$

The probability of obtaining the same result $\alpha=\beta$ in both systems A and B is given by (8) rewritten in a form

$$P_{AB}(\alpha,\alpha)=\mathrm{Tr}\left[\left(\hat{E}_A(\alpha)\otimes\hat{E}_B(\alpha)\right)|\phi\rangle_{AB}\langle\phi|_{AB}\right]=\frac{1}{D}\left|\sum_{k=0}^{D-1}\lambda_{kk}^*\alpha_k^2+\sum_{k>l=0}^{D-1}\alpha_k\alpha_l(\lambda_{kl}^*+\lambda_{lk}^*)\right|^2, \quad (9)$$

which is constant with respect to α (namely, it is equal to zero) if and only if $\lambda_{kl}=-\lambda_{lk}$, i.e. if λ is an antisymmetric matrix. This means that the results of the same measurement of systems A and B never coincide, or, more accurately, the probability (9) of measuring the same result is equal to zero regardless of the measurement. Thus, we have proved *perfect rotationally invariant exclusive correlations* of antisymmetric states.

Here, we note that any antisymmetric state demonstrates rotationally invariant exclusive correlations, not only those formed by the scheme (4). The state must be not necessarily maximally entangled. But the dimension D of the Hilbert space of each system A and B must be even, because there are no antisymmetric matrices with odd rank D. Indeed, all nonzero elements must be pairwise ($\lambda_{lk}=-\lambda_{kl}$), so the total number of nonzero elements is even, thus the dimension D must also be even.

The property of rotationally invariant exclusive correlations (i.e. non-coincident results) can be used in various quantum information processing schemes. For qubits, exclusive correlation means that identical measurements on both subsystems always yield orthogonal results. This is a direct consequence of the two-dimensional Hilbert space. However, in higher dimensions this is not as simple as for qubits.

4. Relation to the Pauli matrices

We note that the matrix representation of the Bell states (2) is very similar to the Pauli matrices (we follow the notation where $\sigma_0=\hat{1}$)

$$\left\{\hat{1},\vec{\sigma}\right\}=\left\{\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}0&1\\1&0\end{pmatrix},\begin{pmatrix}0&\mathrm{i}\\-\mathrm{i}&0\end{pmatrix},\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right\}. \quad (10)$$

The only antisymmetric Pauli matrix σ_2 is multiplied by i with respect to the antisymmetric Bell matrix λ^{Ψ^-} (2). If in the scheme (4) we replace the matrix λ^{Ψ^-} with the Pauli matrix σ_2 and start from $d=0$ with $\lambda(0)=1$, we obtain exactly the set of Pauli matrices (10) for $d=1$. In terms of block elements, all matrices $\lambda(d+1)$ have a block structure very similar to (4):

$$\begin{pmatrix}\lambda(d)&\mathcal{O}\\\mathcal{O}&\lambda(d)\end{pmatrix},\begin{pmatrix}\mathcal{O}&\lambda(d)\\\lambda(d)&\mathcal{O}\end{pmatrix},\begin{pmatrix}\mathcal{O}&\mathrm{i}\lambda(d)\\-\mathrm{i}\lambda(d)&\mathcal{O}\end{pmatrix},\begin{pmatrix}\lambda(d)&\mathcal{O}\\\mathcal{O}&-\lambda(d)\end{pmatrix}. \quad (11)$$

All properties of the scheme (11) are the same as those mentioned for the scheme (4), e.g. the number of symmetric and antisymmetric states, the rotational invariance of antisymmetric states, etc.

Matrices formed by the recursive scheme (11) can be rewritten in a non-recursive way similarly to (5):

$$\lambda(d)_{i_1 i_2 \ldots i_d} = \bigotimes_{j=1}^{d} \sigma_{i_j}, \tag{12}$$

where $\{\sigma_{i_j}\}$ are the standard Pauli matrices numbered by a subscript index $i_j = 0 \ldots 3$ and $\{\lambda(d)\}$ are the generalized Bell state matrices numbered by a composite subscript index $i_1 i_2 \ldots i_d = 1 \ldots 4^d$.

Here, we can see that these matrices corresponding to the generalized Bell states are similar to the matrices of the generalized Pauli group [5], which appear particularly in quantum error correction [24]. The explanation of this fact is our choice of the matrix dimension. We consider a case when the dimension of each qudit is equal to a power of 2. In other words, the qudit can be represented by a collection of qubits.

The matrices formed by the scheme (12) preserve the following properties of the 2×2 Pauli matrices:

1. unitarity ($\lambda^* = \lambda^{-1}$);
2. hermiticity ($\lambda^* = \lambda^T$);
3. trace zero, except the first unit matrix;
4. all matrices are linearly independent and form a complete basis in space of $D \times D$ matrices;
5. the determinant of all matrices is equal to 1, except three 2×2 Pauli matrices $\sigma_{1,2,3}$, whose determinant is equal to -1; and
6. multiplication of any two matrices from the set $\{\lambda(d)\}$ is a matrix which belongs to the same set apart from a certain coefficient ($\pm$i, ± 1).

The last property can be more precisely described by the structure of commutators $[\lambda_k, \lambda_l] \equiv \lambda_k \lambda_l - \lambda_l \lambda_k$ and anticommutators $\{\lambda_k, \lambda_l\} \equiv \lambda_k \lambda_l + \lambda_l \lambda_k$. For convenience we will use slightly modified expressions instead of the standard definitions, namely, we denote

$$\mathcal{C}_{kl} = [\lambda_k, \lambda_l]/(2\mathrm{i}), \qquad \mathcal{A}_{kl} = \{\lambda_k, \lambda_l\}/2. \tag{13}$$

Each element $\mathcal{C}_{kl}$ and $\mathcal{A}_{kl}$ is equal to either 0 or a matrix λ_j from the set $\{\lambda\}$ within a coefficient ± 1, thus we can simply use 0 or a number $\pm j$ of matrix λ_j to express elements of matrices $\mathcal{C}$ and $\mathcal{A}$. It is important to follow the rule for state numbering in $\{\lambda(d+1)\}$: take elements one after another from $\{\lambda(d)\}$ and add, according to (11), four elements to $\{\lambda(d+1)\}$.

For example, in the case $d = 1$ (i.e. the standard 2×2 Pauli matrices) we have the following matrices $\mathcal{C}$ and $\mathcal{A}$:

$$\mathcal{C} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 3 \\ 0 & 4 & 0 & -2 \\ 0 & -3 & 2 & 0 \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 \\ 4 & 0 & 0 & 1 \end{pmatrix}. \tag{14}$$

For any $D = 2^d$ we have:

$$\mathcal{C} = \begin{pmatrix} C_1 & C_2 & C_3 & C_4 \\ C_2 & C_1 & -A_4 & A_3 \\ C_3 & A_4 & C_1 & -A_2 \\ C_4 & -A_3 & A_2 & C_1 \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} A_1 & A_2 & A_3 & A_4 \\ A_2 & A_1 & -C_4 & C_3 \\ A_3 & C_4 & A_1 & -C_2 \\ A_4 & -C_3 & C_2 & A_1 \end{pmatrix}, \tag{15}$$

where C_i and A_i denote the commutator and anticommutator matrices (13) for the one step lower dimension, i.e. $\mathcal{C}$ and $\mathcal{A}$ refer to the dimension $D = 2^d$, whereas C and A refer to the dimension $D = 2^{d-1}$.

We can see that the standard 2×2 Pauli matrices actually have the same structure of commutators and anticommutators (14) as the generalized ones (15), but the one step lower dimension $2^0 = 1$ for them is just a trivial 1×1 matrix consisting of only one element 1, whose commutator and anticommutator (13) are equal to 0 and 1, respectively. Thus in the case of the Pauli matrices, all commutators C_i are equal to zero and all anticommutators A_i are equal to the element number i.

5. Conclusions

We have shown how to generalize Bell states by constructing a special set of MEMBS while preserving the basic properties of the standard Bell states. This can potentially lead to the extension of the previously known schemes of quantum information processing exploiting such properties as (anti)symmetry of the Bell states. Particularly, the antisymmetric MEMBS generalize the rotational invariance of the singlet Bell state and possess perfect rotationally invariant exclusive correlations. We also noticed a close connection between the generalized Bell states and the generalized Pauli matrices.

A possible extension of the obtained results is to consider an arbitrary dimension of the Hilbert space. In our case the dimension is equal to a power of 2, because we are interested in the property of (anti)symmetry of MEMBS, which is uniquely attributed to (anti)symmetry of even-dimensional MEMBS.

In principle, a basis of MEMBS can be constructed in a regular way (similarly to (4) or (5)) for dimensions which are powers of arbitrary numbers. But in this general case the structure of a basis of MEMBS will be irregular and the properties of MEMBS will be incomplete with respect to the standard Bell states. In this sense we carried out the most accurate generalization of the Bell states from qubits to qudits, although with special dimensions.

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