Abstract. We analyze some special properties of a system of two qubits, and in particular of the so-called Bell basis for this system, which have played an important role in recent papers on entanglement of qubits. In particular, we show which of these properties may be generalized to higher dimension. We give a general construction for bases of maximally entangled vectors in any dimension, but show that none of the properties related to complex conjugation in Bell basis can be realized for higher dimensional analogs.
I. Introduction

The qubit system is the smallest non-trivial quantum system. Formerly known as a two-level system, it has often served as an example for basic quantum phenomena\(^1\). Many of the basic ideas of quantum information theory were first tested on qubits. Indeed, for the invention of processes like entanglement enhanced teleportation and dense coding it was very helpful to have an explicit example, in which every detail could be explicitly worked out. For these two processes the generalization to higher dimensional systems was not difficult, hence the intuition gained from the qubit case turned out to be valid.

On the other hand, in the theory of entanglement there have been two achievements, which were so far only possible for qubits, and probably have no higher dimensional analogs. These are the “partial transpose”\(^2\) form of the criterion for separable (classically correlated) states, and the remarkable formula of Wootters\(^3,4\) for the entanglement of formation of an arbitrary state of two qubits. Hence in these cases it may be dangerous to rely too much on the intuitions gained from the qubit case. The purpose of this paper is to state as clearly as possible, which of the ingredients of Wootters’ proof and, in particular, which properties of the “Bell basis” of \(\mathbb{C}^2 \otimes \mathbb{C}^2\) have a chance of generalization to higher dimensions.

Unfortunately, some crucial properties turn out to be specific to two dimensions. We will show this by taking properties of the Bell basis, stated in a form not referring to dimension, and proving that the corresponding property can only hold in dimension two. We hope that this will serve as a caveat and will help researchers in the field to develop more accurate intuitions for higher dimensional entanglement. As a first step we consider in Section 3 a property of the Bell basis which does generalize: it is an orthonormal basis consisting of maximally entangled vectors. In fact, up to a choice of phases and a local unitary transformation the Bell basis is uniquely characterized by this property. After collecting definitions and some basic properties of maximally entangled vectors, we show this uniqueness, and give a fairly general construction for bases of maximally entangled vectors, which works in any dimension.

In Section 4 we look at Bell bases. Their most surprising and at the same time most useful properties are two characterizations of objects which have real components in this basis: real unitary operators with determinant 1 factorize, and real unit vectors are maximally entangled. Our main result is that even weak forms of either of these properties cannot be generalized to higher dimensions.
II. How single qubits are special

In this section we will describe some of the properties of single qubits, which are false for systems with more than two dimensional Hilbert space. Some of these are well-known, and we only recall them because they are referred to later on. Others will have to be treated in more detail for application in Section 4. Throughout we will denote by \( d \) the dimension of the Hilbert space of the systems under consideration, so that qubits are characterized by \( d = 2 \).

Of course, everybody working in quantum information theory or indeed quantum physics as a whole is familiar with the Poincaré ball (or Bloch or Stokes sphere) representing the state space (space of density matrices) of a two-level system. It is so well circulated as the paradigm of a quantum state space that one must perhaps warn students about its not so typical features. The most conspicuous of these, which is in fact at the root of several others, is that the ball has a center. That is, there is a density matrix \( \rho = (1/2) \mathbb{I} \) such that for every density matrix \( \rho \) there is an opposite one, \( \rho' \), such that \( \rho = (\rho + \rho')/2 \).

In the language of Jordan algebras, an axiomatic approach in which more exotic state spaces than usual can arise, the \( d \times d \)-matrices are a “spin factor” iff and only if \( d = 2 \). Another geometrical feature which is only valid in \( d = 2 \) is that the extreme points (pure states) form the complete (topological) boundary of the state space: in higher dimension every density matrix with some zero eigenvalue is on the boundary, whereas the extreme points are those with all but one eigenvalue equal to zero.

A consequence of the fact that for \( d = 2 \) every one-dimensional projection has only one one-dimensional projection in its orthogonal complement is the failure of Gleason’s Theorem. This Theorem says that for \( d > 2 \) any real valued function on one-dimensional projections, which sums to 1 on every maximal set of orthogonal one-dimensional projections, is given by the expectations of a density matrix. Again, this has had some repercussions in Axiomatic Quantum Mechanics.

Since in \( d = 2 \) every pure state \( \rho = |\varphi\rangle\langle\varphi| \) has a unique complement it is natural to ask for a “Quantum NOT” operation, i.e., a map \( \varphi \mapsto \varphi^\perp \), which takes every vector \( \varphi \in \mathbb{C}^d \) to an orthogonal one, \( \varphi^\perp \). It is easy to see that there can be no linear operator \( A \) such that \( \varphi^\perp = A\varphi \): By definition, such an operator would satisfy the equation \( \langle \varphi, A\varphi \rangle = 0 \) for all \( \varphi \), from which one gets \( A = 0 \) by polarization, i.e., by inserting complex linear combinations for \( \varphi \). However, the polarization trick uses complex linearity in a crucial way, and it is indeed possible to find conjugate linear (“antilinear”) operators \( \Theta \) such that

\[
\langle \varphi, \Theta\varphi \rangle = 0 \quad ,
\]

for all \( \varphi \). Indeed, if \( \Theta \) acts on the vectors of a basis \( \{e_\alpha\} \) as \( \Theta e_\alpha = \sum_\beta \Theta_{\beta\alpha} e_\beta \) then equation (2.1) is equivalent to \( \Theta_{\beta\alpha} = -\Theta_{\alpha\beta} \). Clearly, for \( d > 2 \), we have many choices for anti-symmetric matrices. A natural additional requirement for a NOT operation would be that double negatives should be the identity. It turns out that \( \Theta^2 = \lambda \mathbb{I} \) can hold for an anti-unitary NOT operation only in even dimension (for odd \( d \) an anti-symmetric matrix is never invertible) and with \( \lambda = -1 \).
For $d = 2$ there is only one antisymmetric matrix, up to a factor, so the anti-unitary Quantum NOT operation is uniquely defined. Because this argument works in any basis, we conclude that the $\Theta$ is the same in every basis, so indeed this operation is universal in a very strong sense. Formally, this universality is expressed by saying that $U \Theta U^* = \omega(U) \Theta$ for all “basis changes”, i.e., all unitaries $U$, where $\omega(U) \in \mathbb{C}$, $|\omega(U)| = 1$, is a suitable phase. By looking at the universality condition in terms of the matrix $\Theta_{\alpha\beta}$, one can see that for $d \geq 3$ a Universal NOT does not exist. However, the following Proposition makes an even stronger claim: for $d \geq 3$ there is no universal anti-unitary at all.

1 Proposition. Let $d > 1$ be natural number, and suppose that there is a non-zero conjugate linear operator $\Theta$ on $\mathbb{C}^d$ such that for any unitary operator $U$ there is a phase $\omega(U)$ satisfying $U \Theta U^* = \omega(U) \Theta$.

Then $d = 2$ and there is a factor $\lambda \in \mathbb{C}$ such that

$$\Theta \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} b \\ -\bar{a} \end{pmatrix}. \quad (2.2)$$

Moreover, $\omega(U) = \det(U)$, and when $|\lambda| = 1$, $\Theta$ is anti-unitary.

Proof : Since $U \Theta U^* = \omega(U) \Theta$, we may take any matrix element of this equation, which is non-zero for $\Theta$, to conclude that $\omega(U)$ is a continuous function of the matrix elements of $U$. Moreover, it is straightforward to verify that $\omega$ is a character, i.e., $\omega(U_1 U_2) = \omega(U_1) \omega(U_2)$. Together with $\omega(I) = 1$, this implies that $\omega(U) = \det(U)^N$ for some integer $N$. Inserting multiples of the identity, $U = \zeta I$ we find $\zeta^2 = \zeta^{Nd}$, i.e. $Nd = 2$. Since we have assumed $d > 1$, this implies $N = 1$ and $d = 2$. That the $\Theta$ in (2.2) satisfies the conditions and is unique up to an factor was already argued above.

A more elementary argument, not relying on the representation theory of the unitary group, is the following. (We omit here the part of the argument dealing with the null space of $\Theta$, so assume $\Theta$ to be non-singular). Suppose that $u_1, \ldots, u_d$ are the eigenvalues of $U$ with eigenvectors $\varphi_\alpha$, then the vectors $\Theta \varphi_\alpha$ are also eigenvectors with eigenvalues $\omega(U) \overline{\varphi_\alpha}$. Note that the conjugate $\overline{\varphi_\alpha}$ appears, due to the conjugate linearity of $\Theta$. It follows that the spectrum of every unitary must be congruent to itself, subject to a reflection followed by a rotation of the complex plane. For $d = 2$ the spectrum consists of two points on the unit circle, and is hence symmetric with respect to a reflection on a line orthogonal to $u_1 - u_2$. Clearly, for $d \geq 3$ a general set of $d$ points on the unit circle has no such symmetry.

Of course, the operator $\Theta$ from equation (2.2) also satisfies the condition (2.1).
III. Maximal entangled states

We define a vector $\Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ in a Hilbert space tensor product to be **maximally entangled**, whenever both of its restrictions are maximally mixed. The restricted density matrices $\rho_1, \rho_2$ are defined by $\text{tr}(\rho_1 A_1) = \langle \Phi, (A_1 \otimes \mathbb{I}) \Phi \rangle$ and $\text{tr}(\rho_2 A_2) = \langle \Phi, (\mathbb{I} \otimes A_2) \Phi \rangle$ for all $A_1, A_2$. Thus $\Phi$ is maximal entangled, if $\rho_1$ and $\rho_2$ are proportional to the identities on $\mathcal{H}_1$ and $\mathcal{H}_2$. By the well-known Schmidt decomposition this is only possible if $\dim \mathcal{H}_1 = \dim \mathcal{H}_2$, so we will set $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^d$ throughout this section. We will denote by $\mathcal{M}$ the set of maximally entangled vectors.

The Schmidt decomposition for an arbitrary maximally entangled vector $\Omega$ now reads

$$\Omega = \frac{1}{\sqrt{d}} \sum_{\alpha=1}^{d} e_\alpha \otimes e'_\alpha ,$$

where $\{e_\alpha\}$ and $\{e'_\alpha\}$ are suitable orthonormal bases in the tensor factors. Generically (i.e., when the reduced density matrices have only non-degenerate eigenvalues) the Schmidt decomposition is unique up to phase factors. Maximally entangled states constitute the opposite case: Since the reduced density matrices are totally degenerate, the bases are only determined up to a common unitary transformation, i.e.,

$$\Omega = (U \otimes \overline{U}) \Omega ,$$

where $\overline{U}$ is defined by the matrix elements $\langle e'_\alpha, \overline{U} e'_\beta \rangle = \overline{\langle e_\alpha, U e_\beta \rangle}$. Note that this operation depends on the bases $\{e_\alpha\}, \{e'_\alpha\}$, and hence on the particular maximally entangled state $\Omega$.

It is clear from the definition of maximal entanglement that local unitary transformations, i.e., $U_1 \otimes U_2$ with $U_1, U_2$ unitary, take maximally entangled vectors into maximally entangled ones. In view of equation (3.2) we get the same transformations, by performing a unitary rotation only of one factor. Other vectors, too, can be represented in this form. The salient facts are collected in the following Lemma, the proof of which relies completely on writing out everything in components with respect to the bases $\{e_\alpha\}$ and $\{e'_\alpha\}$ appearing in (3.1), and is left to the reader.

**2 Lemma.** Let $\Omega \in \mathbb{C}^d \otimes \mathbb{C}^d$ be a maximally entangled unit vector. Then every vector $\Phi \in \mathbb{C}^d \otimes \mathbb{C}^d$ can be written as

$$\Phi = (X_\Phi \otimes \mathbb{I}) \Omega ,$$

with a uniquely determined linear operator $X_\Phi$. Moreover,

1. $\langle \Phi, \Psi \rangle = \text{tr}(X_\Phi^T X_\Psi)$.
2. $(X_\Phi \otimes \mathbb{I}) \Omega = (\mathbb{I} \otimes X_\Phi^T) \Omega$
(3) the restrictions of the state $\Phi$ are given by the density matrices $\frac{1}{d}X_\Phi^*X_\Phi$ and $\frac{1}{d}X_\Phi^T X_\Phi^T$.

(4) $\Phi$ is maximally entangled iff $X_\Phi$ is unitary.

$X_\Phi$ and $X_\Phi^T$ are defined by there matrix elements in the basis given by the Schmidt decomposition of $\Omega$ (3.1), in the same way as the above complex conjugation (3.2).

How many maximally entangled states are there? Since the maximally entangled vectors $\Phi$ are in on-to-one correspondence with the unitaries $X_\Phi$, the manifold $\mathcal{M}$ has the same dimension as the unitary group, i.e., $d^2$. But this says very little about how $\mathcal{M}$ is embedded into $\mathbb{C}^d \otimes \mathbb{C}^d$. For example, can we find an orthonormal basis of maximally entangled vectors? In dimension $d = 2$ the well-known Bell basis is an example: it consists of the vectors

$$
\Phi_0 = \frac{\Omega}{\sqrt{2}}(\left| \uparrow \downarrow \right> + \left| \downarrow \uparrow \right>) \quad \Phi_1 = (i\sigma_1 \otimes 1)\Omega = \frac{i}{2}(\left| \downarrow \uparrow \right> + \left| \uparrow \downarrow \right>) \\
\Phi_2 = (i\sigma_2 \otimes 1)\Omega = \frac{i}{2}(\left| \downarrow \uparrow \right> - \left| \uparrow \downarrow \right>) \quad \Phi_3 = (i\sigma_3 \otimes 1)\Omega = \frac{i}{2}(\left| \uparrow \uparrow \right> - \left| \downarrow \downarrow \right>) .
$$

The factors $i$ are, of course, irrelevant at this stage, but will turn out to be crucial for the further properties of this basis studied in the next section.

III.2. Constructing Bases of maximally entangled vectors

By Lemma 1 the task of constructing a basis $\{\Phi_\alpha\} \subset \mathcal{M}$ is equivalent to finding a basis of unitary operators $X_\alpha$ on $\mathbb{C}^d$, satisfying the orthonormality condition

$$
\text{tr}(X_\alpha^* X_\beta) = d \delta_{\alpha\beta} \quad , \quad \alpha, \beta = 1, \ldots, d^2 .
$$

It turns out that such bases exist in any dimension. Indeed, a rough dimension count indicates that there should be many bases of this kind: the manifold of $d^2$-tuples of maximally entangled vectors has dimension $d^2(d^2 - 1)$, where we subtracted 1 for the phase ambiguity in each basis vector. The only remaining conditions are the $d^2(d^2 - 1)/2$ orthogonality conditions between different vectors. If we want to identify bases which can be transformed into each other by local unitaries we should subtract furthermore the dimension of this group, $2d^2 - 1$. So we are left with a dimension count for the manifold of maximally entangled bases growing in leading order like $d^4/2$.

There are several general constructions for bases of unitaries. Since such bases are precisely what is needed for generalization of the entanglement enhanced teleportation scheme to dimensions $d > 2$, one such construction (working for any $d$) has been noted in 9. Here we give the most general construction known to us. A Hadamard matrix $H$ is, by definition, a square matrix, in which all entries have modulus one, and which is unitary up to a factor:

$$
|H_{k\ell}| = 1 \quad , \quad k, \ell = 1, \ldots, d \quad , \quad HH^* = dI .
$$

From this we construct what we call shift-and-multiply bases of $d^2$ unitary operators $\{U^{ij}\}_{i,j=1,\ldots,d}$. The construction depends on a collection of $d$ Hadamard matrices $H^j$ of dimension $d \times d$, and a bi-injective composition $\tau : I_d \times I_d \rightarrow I_d$, where
$I_d = \{1, \ldots, d\}$. This composition need be neither commutative nor associative, but we require “bi-injectivity”, defined as the cancellation laws $(\tau(i, k) = \tau(j, k)) \Rightarrow (i = j)$ and $(\tau(k, i) = \tau(k, j)) \Rightarrow (i = j)$. In other words, every symbol appears exactly once in each row or column of the composition table. With $\{e_k\}_{k=1}^d$ the canonical basis of $\mathbb{C}^d$, we define the operators

$$U^{ij} e_k = H_{ik}^j e_{\tau(k,j)}.$$  \hfill (3.6)

We leave to the reader the verification that in this way any collection of Hadamard matrices $H^j$ and a composition $\tau$ generates an orthonormal basis of unitaries, and hence a basis of maximally entangled vectors.

The problem is now shifted to constructing Hadamard matrices. For the case of real entries ($H_{k\ell} = \pm 1$) this is a well-known problem arising in coding theory. Several families are known, but no general construction. The complex case is less well-studied. A simple construction is based on the theory of (finite) abelian groups: If $G$ is an abelian group of order $d$, then there are exactly $d$ different characters, i.e., mappings $\gamma : G \to \mathbb{C}$ such that $|\gamma(g)| = 1$, and $\gamma(g_1g_2) = \gamma(g_1)\gamma(g_2)$. The set of characters is called the dual group $\Gamma$, and the Fourier transform $\mathcal{F}$ takes functions on $G$ into functions on $\Gamma$ via $(\mathcal{F}f)(\gamma) = \sum_g \gamma(g)f(g)$. It is well known that this transformation is unitary up to a normalization factor. Hence the $d \times d$ coefficients $\gamma(g)$ for $\gamma \in \Gamma, g \in G$ form a Hadamard matrix. The simplest choice of this kind (which works in any dimension $d$) is based on the cyclic group of order $d$, which is its own dual. The associated Fourier matrix is then

$$H_{k\ell} = \exp\left(\frac{2\pi i}{d} k\ell\right).$$ \hfill (3.7)

The direct product of groups in this construction leads to the tensor product of Hadamard matrices. More generally, the tensor product for Hadamard matrices is again a Hadamard matrix. Similarly, the tensor product of bases of unitaries (or maximally entangled states) is again a basis of the required type. Thus whenever $d$ is a composite number, bases can be constructed from bases of smaller dimensions (the factors of $d$). The only abelian groups of prime order are the cyclic groups. For $d = 2, 3$ this also leads to the only Hadamard matrix (up to trivial transformations). However, already for order 5 there are Hadamard matrices not arising from the cyclic group, so the shift-and-multiply construction of bases of unitaries is strictly more general than the one based on abelian groups. On the other hand, the dimension count described above suggests, that the shift-and-multiply construction is still not the most general one. In fact, it seems to be an open problem to characterize all bases of unitaries for $d = 3$. Only for $d = 2$ the Bell basis is essentially the only basis of maximally entangled vectors.

3 Lemma. Let $\{\Psi_\alpha\}, \alpha = 0 \ldots 3$ be a maximal entangled basis of $\mathbb{C}^2 \otimes \mathbb{C}^2$ and let $X_\alpha$ denote the unitaries such that $\Psi_\alpha = (X_\alpha \otimes 1)\Omega$.

(1) Then there are unitaries $U_1, U_2$ and phases $\chi_\alpha$ such that $\Psi_\alpha = \chi_\alpha(U_1 \otimes U_2)\Phi_\alpha$, where $\{\Phi_\alpha\}$ denotes the standard Bell basis (3.3).
(2) If all $X_{\alpha}$ have the same determinant then either (a) the phases $\chi_{\alpha}$ may all be chosen equal to 1 or (b) the phases may be chosen as \{1, 1, -1, 1\} or, equivalently, $U_1 \otimes U_2 \Phi_{\alpha}$ may be made into an odd permutation of the given basis.

\textbf{Proof}: From Lemma 2.(2) a local unitary transformation of the vector $\Psi_{\alpha}$ affect the $X_{\alpha}$ matrix like

\[ U_1 \otimes U_2 \Psi_{\alpha} = ((U_1 X_{\alpha} U_2^T) \otimes \mathbb{1}) \Omega, \tag{3.8} \]

i.e., $X_{\alpha} \mapsto (U_1 X_{\alpha} U_2^T)$. By choosing $U_1 = \mathbb{1}$ and $U_2 = X_0^*$, we may assume that $X_0 = \mathbb{1}$. Note that under the assumptions of part (2) this also achieves $\det X_{\alpha} = 1$ for all $\alpha$. The local unitary transformations leaving the condition $X_0 = \mathbb{1}$ invariant are $X_{\alpha} \mapsto U X_{\alpha} U^*$. Moreover, from orthogonality with $X_0$ we get $\text{tr}(X_{\alpha}) = 0$. This means that each of the unitaries $X_{\alpha}$, $\alpha = 1, 2, 3$ has two eigenvalues adding up to 0, and is hence of the form $X_{\alpha} = i \chi_{\alpha} \vec{r}_{\alpha} \cdot \vec{\sigma}$, where the $\vec{r}_{\alpha} \in \mathbb{R}^3$ are real three dimensional unit vectors, and $\vec{\sigma}$ is the vector of Pauli matrices. Orthogonality of the $\Psi_{\alpha}$ implies these three vectors to be orthogonal, too. Moreover, condition (2) is equivalent to $\chi_{\alpha} = \pm 1$, or $\chi_{\alpha} = 1$, since a sign can be absorbed in $\vec{r}_{\alpha}$.

Since the operation $X \mapsto U X U^*$ is just a three dimensional proper rotation, we can rotate the orthonormal frame ($\vec{r}_1, \vec{r}_2, \vec{r}_3$) to be parallel to the standard basis in $\mathbb{R}^3$. Hence we get $X_{\alpha} = i \chi_{\alpha} \sigma_{\alpha}$, proving part (1), or $X_{\alpha} = \pm i \sigma_{\alpha}$ in case (2). By further rotations we can make all signs but at most one +1. The distinction between cases (a) and (b) is precisely, whether the real orthogonal transformation taking the frame ($\vec{r}_1, \vec{r}_2, \vec{r}_3$) to the standard basis has determinant +1 or -1. In the second case we need an orientation reversing operation (such as reversing one direction or permuting some basis elements) before a proper rotation (implemented by a local unitary) brings the given basis to the standard form.

\[ \blacksquare \]
III.3. Unitaries respecting maximal entanglement

As noted above, all local unitaries map the set $\mathcal{M}$ of maximally entangled vectors into itself. It turns out that the converse is also true, apart from one obvious counterexample, the “flip” unitary defined by $F(\varphi \otimes \psi) = \psi \otimes \varphi$:

4 **Proposition.** Let $U$ be a unitary operator on $\mathbb{C}^d \otimes \mathbb{C}^d$. Then $UM \subset M$ if and only if $U$ is local up to a flip, i.e., there are unitaries $U_1, U_2$ such that either $U = U_1 \otimes U_2$ or $U = (U_1 \otimes U_2)F$.

**Proof:** Every unitary operator $U$ on $\mathbb{C}^d \otimes \mathbb{C}^d$ defines a linear bijective map $f_U$ from the space of all $d \times d$-matrices into itself by $U\Phi = U(X_\Phi \otimes 1)\Omega =: (f_U(X_\Phi) \otimes 1)\Omega$. (3.9)

Then by Lemma 2 the condition $UM \subset M$ is equivalent to $f_U$ taking unitary operators to unitary operators. We have to show that in this case $f_U$ can be written either as $f_U(X) = U_1 X U_2$ or $f_U(X) = U_1 X^T U_2$, which is equivalent to above proposition. From Lemma 2 it is easy to see that in this sense the transposition belongs to the flip operation: $f_F(X) = X^T$. We note that since the implication $UM \supset M$ is trivial, the assumption $UM \subset M$ is actually equivalent to $UM = M$, and hence also to $U^*M \subset M$.

By composing $U$ with a local unitary map we may assume that $f_U(1) = 1$ or, equivalently that the reference vector $\Omega$ from Lemma 2 is invariant under $U$. Consider a unitary $X = e^{iA} = 1 + iA - \frac{1}{2}A^2 + O(A^3)$ close to the identity (with $A = A^*$ small). Then $f_U(X)$ also has to be unitary, and we will evaluate this condition to second order in $A$, using the linearity of $f_U$:

$$1 = f_U(X)^* f_U(X)$$

$$= 1 + f_U(iA)^* + f_U(iA) - \frac{1}{2}(f_U(A^2) + f_U(A^2)^*) + f_U(iA)^* f_U(iA) + O(A^3). \quad (3.10)$$

From the first order, $f_U(A) = f_U(A)^*$ for $A = A^*$. Hence from the second order $f_U(A^2) = \frac{1}{2}(f_U(A^2) + f_U(A^2)^*) = f_U(iA)^* f_U(iA)$ is a positive operator. Since every positive operator can be written as $A^2$ for some $A = A^*$, we find that $f_U$, and by the same token its inverse, map positive operators to positive operators. Hence by Wigner’s Theorem \footnote{11} $f_U$ can be written either as $f_U(X) = SXS^*$ or $f_U(X) = SXTS^*$ with some unitary $S$. (We use a form of Wigner’s Theorem with is formulated with positive and invertible maps. \footnote{12,13})
IV. Bell bases

IV.1. Characterization Theorem

The most surprising properties of the Bell basis are related to the anti-unitary operation of complex conjugation in this basis: a vector is maximally entangled iff its components with respect to the Bell basis are real up to a factor, and a unitary operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$ is local iff, after multiplication with a suitable phase, it becomes real in Bell basis and has determinant $+1$ (In the folklore on this subject, the determinant condition is sometimes forgotten, inviting the flip $\mathbf{F}$ as an obvious counterexample, see Proposition 7). Both these properties are extremely useful and play a crucial role in the Wootters-formula for the two qubit system. It is thus highly desirable to find extensions to higher dimensional systems. One direction in which a generalization might be sought is to break the above “iff” statements, and to require in higher dimensions maybe only one direction of implication. This leaves four possibilities to be tested. However, as the following Theorem shows, none of them can be realized in any dimension $d > 2$.

5 Theorem. Let $d \in \mathbb{N}$, and $\Psi_\alpha, \alpha = 0, \ldots, d^2 - 1$ a basis of maximally entangled vectors in $\mathbb{C}^d \otimes \mathbb{C}^d$. Let $X_\alpha$ denote the unitaries such that $\Psi_\alpha = (X_\alpha \otimes 1)\Omega$, with a maximal entangled vector $\Omega$ (see Lemma 2). Then the following conditions are equivalent:

(1) $d = 2$, and there are unitary operators $U_1, U_2$ and a permutation $\pi$ such that the $\Psi_\alpha$ can be written as $(U_1 \otimes U_2)\Psi_\alpha = \Phi_{\pi(\alpha)}$ with $\alpha = 0, \ldots, 3$.
(2) $U_1, U_2 \in SU_d \Rightarrow \forall \alpha, \beta \langle \Psi_\alpha, U_1 \otimes U_2 \Psi_\beta \rangle \in \mathbb{R}$
(3) $U \in SU_{d^2}$ and $\forall \alpha, \beta \langle \Psi_\alpha, U \Psi_\beta \rangle \in \mathbb{R} \Rightarrow U = U_1 \otimes U_2$ or $U = (U_1 \otimes U_2)\mathbf{F}$
(4) $\varphi \in \mathcal{M} \Rightarrow \exists \omega, |\omega| = 1 \forall \alpha \omega \langle \Psi_\alpha, \varphi \rangle \in \mathbb{R}$
(5) $\forall \alpha < \langle \Psi_\alpha, \varphi \rangle \in \mathbb{R} \Rightarrow \varphi \in \mathcal{M}$
(6) $X_\alpha^* X_\beta + X_\beta^* X_\alpha = 2 \delta_{\alpha\beta} 1$.

Proof: We will prove the inclusions: (1) $\Rightarrow$ (2) $\Rightarrow$ (4) $\Rightarrow$ (5) $\Rightarrow$ (6) $\Rightarrow$ (1), and (4 and 5) $\Rightarrow$ (3) $\Rightarrow$ (5).

(1) $\Rightarrow$ (2) It suffices to take $\Psi_\alpha = \Phi_\alpha$ as the standard Bell basis (3.3) with $\Phi_0 =: \Omega$ and $\Phi_\alpha = (i\sigma_\alpha \otimes 1)\Omega$, ($\alpha = 1, 2, 3$). Since exponentiation is a power series with real coefficients, it suffices to show that the generators of the local unitary group with determinant one, namely $i\sigma_k \otimes 1$ and $1 \otimes i\sigma_k$ ($k = 1, 2, 3$) are real in the standard Bell basis. Computing the matrix elements $\langle \Phi_\alpha, (i\sigma_k \otimes 1)\Phi_\beta \rangle$ of the generators involves a case distinction as to how many of $\alpha, \beta$ are equal to 0. If $\alpha = \beta = 0$ we get $\langle \Phi_0, (i\sigma_k \otimes 1)\Phi_0 \rangle = d^{-1} \text{tr}(i\sigma_k) = 0$, because $\Phi_0$ is maximally entangled, and its restriction to the first factor is $\frac{1}{d} 1$. If exactly one of $\alpha, \beta$ is zero, the matrix element carries an even power of $i$, and we get matrix elements of the form $\langle \Phi_0, (i\sigma_k \otimes 1)\Phi_0 \rangle = -d^{-1} \text{tr}(\sigma_k)$, which is real anyway.
If both are non-zero, we find
\[ \langle \Phi_{\alpha}, i\sigma_k \otimes I \Phi_{\beta} \rangle = \langle \Omega, i(\sigma_\alpha \sigma_k \sigma_\beta) \otimes I \Omega \rangle = \frac{i}{2} \text{tr}(\sigma_\alpha \sigma_k \sigma_\beta). \] (4.1)

where \( \alpha, \beta, k = 1 \ldots 3 \). When two indices are the same this trace is zero, when they are all different, the relations \( \sigma_1 \sigma_2 = i \sigma_3 \) (and cyclic) imply that the trace is imaginary and the matrix element is real.

(2) \( \Rightarrow \) (4) From (3.1) it is easy to see, that all maximally entangled vectors are equivalent by local unitary transformation. So every maximally entangled vector \( \varphi \) can be written as \( \varphi = \varpi(U_1 \otimes U_2)\Psi_0 \), with \( U_1, U_2 \in SU_d \) and a phase \( \varpi \). \( \omega(\Psi_{\alpha}, \varphi) \) is hence the \((\alpha, 0)\)-row of matrix elements of \( U_1 \otimes U_2 \) in the \( \{\Psi_{\alpha}\} \) basis. Condition (2) guarantees that these matrix elements are real.

(4) \( \Rightarrow \) (5) Condition (4) refers to two different sets of vectors in \( C^d \otimes C^d \): on the one hand, the space of maximally entangled vectors \( M \), which by Lemma 2 can be parameterized by the unitary group \( U_d \), and on the other hand the space of “up to an overall phase factor real in \( \{\Psi_{\alpha}\} \)-basis” normalized vectors, which we call \( Q \) for the sake of this proof. So (4) means \( M \subset Q \) and we now have to show \( Q \subset M \). These two manifolds of vectors have the same dimension, namely \( d^2 \): On the one hand this is the dimension of \( U_d \) (the tangent space at the identity is the space of hermitian operators). On the other hand, a real vector has \( d^2 \) real components. The overall phase for vectors in \( Q \) adds an extra dimension, but we have to subtract one for normalization.

Now consider a small neighborhood \( N \subset M \) of some point \( \Phi \in M \). We can parametrize its points uniquely as \( (U \otimes I)\Phi \), with \( U \) in a neighborhood of the identity in \( U_d \). Thereby we get a \( d^2 \)-dimensional set of vectors, which by assumption (4) lies in the \( d^2 \)-dimensional manifold \( Q \), and hence contains an open neighborhood of \( \Phi \) in \( Q \). This shows that \( M \) is an open subset of \( Q \). On the other hand, \( M \) is the continuous image of the compact space \( U_d \), hence compact, hence closed in \( Q \). But \( Q \) is clearly connected. So \( M \), being both open and closed, must be equal to \( Q \).

(5) \( \Rightarrow \) (6) Condition (5) means that every vector of the form
\[ \varphi = \sum_\alpha a_\alpha \Psi_\alpha = ((\sum_\alpha a_\alpha X_\alpha) \otimes I)\Omega \] (4.2)
with real \( a_\alpha, \sum_\alpha a_\alpha^2 = 1 \) is maximally entangled. Therefore \( \sum_\alpha a_\alpha X_\alpha \) has to be unitary for every normalized real vector \( \vec{a} \). Expanding the unitarity condition, and using the normalization condition to cancel the diagonal, we are left with the condition
\[ \sum_{\alpha > \beta} a_\alpha a_\beta (X_\alpha X_\beta^* + X_\beta X_\alpha^*) = 0 \] (4.3)
Since this holds for all vectors \( \vec{a} \) each term of this sum has to be zero. The relation for \( \alpha = \beta \) is clear from the unitarity of each \( X_\alpha \).

(6) \( \Rightarrow \) (1) Note that unitaries satisfying these relations retain this property under the transformation \( X_\alpha \mapsto UX_\alpha \), with \( U \) unitary. Choosing \( U = X_0^* \), we find that we may assume \( X_0 = I \) without loss of generality. Then the relations for \( \beta = 0 \) say that \( X_\alpha + X_\alpha^* = 0 \). Setting \( X_\alpha = iR_\alpha \quad \alpha > 0 \), the problem is reformulated to finding \( d^2 - 1 \) hermitian, unitary, operators acting on a \( d \)-dimensional Hilbert space satisfying the relations (4.4)
below. Hence by Lemma 6, \( d \) is even, \( N = d^2 - 1 \) is odd, and hence \( d = 2^{d/2-1} \). This is possible only for \( d = 2 \). We can thus invoke Lemma 3 showing that the \( R_\alpha \) must be the Pauli matrices, up to at most a permutation of the indices.

\((4 \text{ and } 5) \Rightarrow (3)\) From (4) and (5) it follows, that a unitary matrix, which is real in the \{\Psi_\alpha\} basis maps \( M \) into itself. Hence (3) follows from Proposition 4.

\((3) \Rightarrow (5)\) Any unit vector \( \varphi \) which is real in some basis \{\Psi_\alpha\} can be obtained by rotating the first basis vector \( \Psi_0 \) in his direction via a in this basis real orthogonal transformation. This is to say that there is a unitary operator \( U \) satisfying the hypothesis of (3) and \( \varphi = U \Psi_0 \). Hence, whether \( \varphi = (U_1 \otimes U_2) \Psi_0 \) or \( \varphi = \mathsf{F}(U_1 \otimes U_2) \Psi_0 \), this vector is maximally entangled.

To complete the proof, especially the crucial step (6) \( \Rightarrow (1) \), in which dimension \( d = 2 \) is forced, we invoked the following Lemma, which belongs to the representation theory of Clifford algebras. It can be found, e.g., in 14. But since it is a crucial step, we will give an independent proof in the following Lemma.

\[\text{6 Lemma. Assume that } R_1, \ldots, R_N \text{ is a set of } N > 1 \text{ hermitian operators(generators) acting irreducibly on a } d\text{-dimensional space, and satisfying the relations } \]
\[ R_\alpha R_\beta + R_\beta R_\alpha = 2 \delta_{\alpha \beta} \mathbb{I}. \quad (4.4) \]

\[\text{Then } d \text{ is even, and if } N \text{ is odd, we have } d = 2^{(N-1)/2}. \]

\[\text{Proof :} \] Cause this Lemma belongs to the representations theories of algebraic groups, we will now denote \( R_\alpha \) as the generators of a group. Consider the generator \( R_1 \): Setting \( \alpha = \beta = 1 \) in (4.4) it can be seen, that \( R_1 \) has two eigenspaces for the eigenvalues \( \pm 1 \), and from the relation \( R_\alpha R_1 = -R_1 R_\alpha \) it is clear that each of the other generators exchanges these two eigenspaces. Since \( R_\alpha \) is unitary, this also shows that the eigenspaces are of equal dimension, so \( d \) is even. Let us take the second generator, \( R_2 \) to furnish a standard mapping between these spaces. Then we can characterize the action of generators \( R_\alpha \) with \( \alpha \geq 3 \) completely by the action of \( R_2 R_\alpha \) inside the “+1”-eigenspace of \( R_1 \). In other words, we consider, for \( \alpha \geq 3 \) the operators \( R'_\alpha = i R_2 R_\alpha \)

It is straightforward to verify that these operators again satisfy the Clifford relations (4.4), and are Hermitian. Moreover, they commute with \( R_1 \). Restricting to the “+1”-eigenspace of \( R_1 \) we are thus left with the same representation problem as before, albeit with \( N' = N - 2 \) generators, and in a representation space of dimension \( d' = d/2 \). Moreover, the \{\( R'_\alpha \)\} are again an irreducible set, because any operator \( C' \) commuting with them all determines an operator \( C \) commuting with the \( R_\alpha \), by extending \( C' \) as \( R_2 C'R_2 \) to the “−1”-eigenspace of \( R_1 \).

This argument can be iterated until exactly one generator is left (since \( N \) is odd). Irreducible representations of the only remaining relations \( R_N^2 = \mathbb{I}, R_N = R_N^* \) are one-dimensional, with \( R = \pm 1 \). (The sign coming out at this stage can also be determined
from the sign of the product $R_1R_2\cdots R_N$, which commutes with all $R_\alpha$ by virtue of (4.4), and is hence a multiple of the identity). Collecting the factors 2 for the dimension then gives $d = 2^{(N-1)/2}$.

We now want to look back at condition (3) of Theorem 5. It would be nice here to have a simple condition on $U$ distinguishing the two cases. It turns out that this criterion is simply the determinant of $U$.

7 Proposition. Let $U$ be a unitary operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$ which is real in the standard Bell basis. Then $U = (U_1 \otimes U_2)$ iff $\det(U) = 1$ and $U = (U_1 \otimes U_2)\mathbb{F}$ iff $\det(U) = -1$.

Proof: From Theorem 5 we know that $U$ has to factorize in one of the given forms. $U$ lies in the connected component of the identity of $SO_4$ iff its determinant is one, and iff it can be written as the square of another element, say $U = V^2$. Either factorization for $V$ now implies that $U$ is local. Since $SU_2$ is connected, every local unitary $U$ can be written as a square, so $\det U = 1$. This proves the first assertion, and hence the remaining cases, $\det U = -1$ and $U\mathbb{F}$ local must also match. Indeed, $\det \mathbb{F} = -1$, because the dimension of its “$-1$”-eigenspace is one, hence odd.
IV.2. Conjugation in Bell basis

The remarkable properties of the Bell basis described in Theorem 5 are in some sense not so much a property of this basis, but of the anti-unitary operation of complex conjugation in Bell basis. Indeed, if we change the Bell basis by a local unitary transformation, the new basis vectors will also be maximally entangled, hence real in Bell basis (up to a common factor), and the complex conjugation with respect to the new basis will be exactly the same as before (again, up to a common factor). Hence this conjugation operation is “universal” in a way very similar to the Universal NOT of Proposition 1. We would like to formulate the following Proposition in a more general way, so that it also could be applied to multi-particle-systems:

8 Proposition. Let $d_1, d_2 \ldots d_n > 1, n \geq 2$ be natural numbers, and suppose that there is a non-zero conjugate linear operator $\Theta_n$ on $\mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \ldots \otimes \mathbb{C}^{d_n}$ such that for any local unitary operator $U = U_1 \otimes U_2 \ldots \otimes U_n$ there is a phase $\omega(U)$ satisfying $U \Theta_n U^* = \omega(U) \Theta_n$. Then $d_1 = d_2 \ldots = d_n = 2$ and there is a factor $\lambda \in \mathbb{C}$ such that

$$\Theta_n = \lambda \Theta \otimes \Theta \ldots \otimes \Theta =: \Theta^\otimes n$$

and $\omega(U) = \det(U)$, where $\Theta$ denotes the operator described in Proposition 1. For two qubits we get $\Theta_2 = \lambda \Theta \otimes \Theta = \lambda \Theta_{\text{Bell}}$, where $\Theta_{\text{Bell}}$ denotes the complex conjugation in Bell basis.

Note that the antilinear operator-tensor-product is uniquely defined on product vectors and from there it can be extended by antilinearity to arbitrary vectors.

Proof: Similarly to the proof of Proposition 1 we get that $\omega(U)$ is a character, i.e., $\omega(U_1 U_2) = \omega(U_1) \omega(U_2)$. Therefore, it is clear that $\omega(U)$ has to factorize in the following form: $\omega(U_1 \otimes U_2 \ldots \otimes U_n) = \omega_1(U_1) \omega_2(U_2) \ldots \omega_n(U_n)$. $d_1 = 2$ follows by applying exactly the same arguments as in the proof of Proposition 1 to the equation $(U_1 \otimes 1 \ldots \otimes 1) \Theta_n (U_1 \otimes 1 \ldots \otimes 1)^* = \omega_1(U_1) \Theta_n$. Similarly, we get $d_2, \ldots, d_n = 2$ and $\omega(U) = \det(U)$. It is clear that $\Theta_n = \Theta \otimes \Theta \ldots \otimes \Theta$ has the required properties. On the other hand, if $\Theta_n$ and $\Theta'_n$ both satisfy these conditions, the linear operator $C = \Theta_n \Theta'_n$ satisfies the equation $UCU^* = \omega(U) \omega'(U) C = |\det(U)|^2 C = C$. Therefore $C$ commutes with all local unitaries and has to be a multiple of the identity, and therewith $\Theta^2$ and $\Theta'^2$ are multiple of the identity and finally $\Theta'_n$ is a multiple of $\Theta_n$.

For the two qubit-system ($n = 2$) this shows that $\Theta_{\text{Bell}} = \lambda \Theta \otimes \Theta$. However, the Proposition makes the stronger claim that $\lambda = 1$. This is readily verified by checking that the Bell basis is invariant under $\Theta \otimes \Theta$.

Squaring the equation in the proposition, and using anti-unitarity, we find

$$\Theta_n^2 = |\lambda|^2 (\Theta^2)^\otimes n = |\lambda|^2 (-1)^n \mathbf{1},$$
where $|\lambda| = 1$ characterizes the unitary case. From this we see that the $\Theta_n$-operation applied to density matrices ($\rho \mapsto \Theta_n \rho \Theta_n^*$), as it is used in the Wootters formula for two qubits, can have pure fixed points only if $n$ is even. Exactly in these cases $\Theta_n$ can be identified with the complex conjugation in some basis, namely the tensor product of the Bell bases. On the other hand, if $n$ is odd, $\Theta_n$ is a NOT-operation in the sense of Section 2, although, of course, not a universal one with respect to unitaries other than local ones. That is $\langle \Psi, \Theta_n \Psi \rangle = 0$ for all vectors, not just for product vectors. In either case, no application of $\Theta_n$ to multi-particle entanglement is known to us.

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