Detecting maximally entangled states without making the Schmidt decomposition

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The bipartite entanglement of a pure quantum state is known to be characterized by its Schmidt decomposition. In particular the state is maximally entangled when all the Schmidt coefficients are equal. We point out a convenient method which always yields a single analytical condition for the state to be maximally entangled, in terms of its expansion coefficients in any basis. The method works even when the Schmidt coefficients cannot be calculated analytically, and does not require their calculation. As an example this technique is used to derive the Bell basis for a system of two qubits. In a second example the technique shows a particular state to never be maximally entangled, a general conclusion that cannot be reached using the Schmidt decomposition.

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I. INTRODUCTION

Entanglement or the existence of quantum correlations between physical systems is currently of great interest both theoretically and experimentally, see Ref. [1] and references therein. From the theoretical point of view the study of entanglement is shedding light on the basic nature of quantum mechanics [2], and providing surprising connections to other areas, such as the study of black holes [3]. From a practical point of view it has been realized that entanglement is a resource that can enable information processing tasks that turn out to be impossible or inefficient when tackled by classical machines [4]. These capabilities include teleportation, cryptography, and computation [1].

In this article we will consider the entanglement of pure bipartite states, i.e. states which describe globally pure quantum mechanical systems which have been partitioned into two subsystems. As is known, the Schmidt decomposition of a pure bipartite state provides a qualitative measure of its entanglement [1, 2]. On the other hand the von Neumann entropy of either subsystem provides a unique quantitative measure of the degree of entanglement of the whole quantum state [1, 2].

In particular we will consider maximally entangled states i.e. those states of a quantum system which contain the largest amount of entanglement possible. Since entanglement is a resource for information processing, these states are of particular importance. Indeed protocols for quantum key distribution, dense coding and teleportation rely on maximally entangled states [2]. In view of the inevitable noise and decoherence that accompanies an experiment, maximally entangled states also provide a benchmark for other, less entangled, states, as in the process of distillation [1]. The Bell states are perhaps the best known example of maximally entangled bipartite pure states.

How do we know if a pure bipartite state is maximally entangled? We can decide using either of the measures mentioned above. If the state is entangled maximally all the coefficients in the Schmidt decomposition are equal; also the reduced von Neumann entropy is maximised to its upper bound $\log d$, where $d$ is the dimension of the smaller partition. However if $d > 4$ neither of these measures can provide analytical conditions (on the expansion coefficients of the state in some basis), and have to be computed numerically.

In this article we point out an existing technique from algebra that can provide a single analytical condition (for arbitrary but finite $d$) that the coefficients (in any basis) of a maximally entangled state have to obey. The method therefore is capable of deciding quite generally if a certain state is maximally entangled or not. We demonstrate below how this method shows a certain state can never be maximally entangled, a general conclusion that cannot be reached using the Schmidt decomposition or the von Neumann entropy. In addition the method can also be used to obtain the maximally entangled basis given the dimensions of the two subsystems. As an example below we use the method to derive the Bell basis for a system of two qubits.

The rest of the article is arranged as follows. In Section II we outline the general algorithm. In Section III we use the technique to derive the Bell basis for a system of two qubits providing also a detailed commentary on our method, and its simple implementation in Mathematica. In Section IV we consider a case which cannot be solved analytically using the Schmidt decomposition or the von Neumann entropy. Section V provides a Conclusion.

II. GENERAL FORMALISM

The steps of our technique are as follows:

1. Begin with a quantum state $|\psi\rangle$.
2. Find the density matrix $\rho = |\psi\rangle \langle \psi |$.
3. Trace over the states of one subsystem, say $A$, to find the reduced density matrix $\rho_B = \text{Tr}_A \rho$.
4. Find the characteristic polynomial $P[\rho_B, x]$ of this matrix with respect to a dummy variable $x$. 
5. Find the subdiscriminant sequence $D_q[P]$, of the polynomial $P$, where $q = 1, 2 \ldots d$.

6. If the last but one member of the sequence, i.e. $D_{d-1}[P]$, equals zero then $|\psi\rangle$ is maximally entangled.

The basic tool we use is the subdiscriminant sequence of the characteristic polynomial of the reduced density matrix of either subsystem. The subdiscriminant sequence of any polynomial can be found in textbooks on algebraic geometry such as Ref. [5]. A detailed introduction for physicists has been provided in Ref. [6] and will not be repeated here, although we will discuss a few important points. In general the sequence contains $d$ members. The various members denote the number of repeating zeros of the polynomial. For example the first member of the sequence is the discriminant of the polynomial $P$

$$D_1[P] = \prod_{i<j}^d (\lambda_i - \lambda_j)^2, \quad (1)$$

where $\lambda_i$ are the roots of the polynomial $P$. Since density matrices are Hermitian, the $\lambda_i$ are all real. From Eq. (1) we can see that $D_1[P]$ vanishes whenever two or more roots of $P$ are equal.

For the purpose of this article the most important member of the subdiscriminant sequence is its second to last entry

$$D_{d-1}[P] = \sum_{i<j}^d (\lambda_i - \lambda_j)^2, \quad (2)$$

which equals zero only if all the eigenvalues of the reduced density matrix are equal. In turn this implies the equality of the Schmidt coefficients and maximal entanglement of the state. It is an important fact that $D_1[P], D_{d-1}[P]$, and actually the whole subdiscriminant sequence $D_q[P]$ can always be found analytically in terms of the coefficients of the polynomial $P$. Significantly this does not require calculation of the eigenvalues $\lambda_i$, i.e. one need not make the Schmidt decomposition.

Generally $D_{d-1}[P]$, which has to vanish for a maximally entangled state, is itself a polynomial in the coefficients of expansion of the given quantum state written in an arbitrary basis. It follows that from a broader perspective the present technique maps the problem of finding maximally entangled states of a bipartite system to that of finding the roots of a multivariate polynomial. In order to expose the working details of our procedure we present two examples. We first rederive the familiar Bell states using our method; then we consider a more involved example which cannot be solved analytically using Schmidt decomposition or the von Neumann entropy.

### III. A $2 \times 2$ SYSTEM: THE BELL BASIS

We consider a system which is divided into two subsystems $A$ and $B$. Each subsystem contains a qubit which can exist in a superposition of the states $|0\rangle$ and $|1\rangle$. An arbitrary unnormalized pure quantum state of this system can be written as

$$|\psi\rangle = p|00\rangle + q|11\rangle + r|10\rangle + s|01\rangle. \quad (3)$$

Here we have used the product basis, which is often a convenient one to use, although for the method to be demonstrated $|\psi\rangle$ can be expressed in any basis. For the particular task of deriving the Bell states we have chosen the coefficients $(p, q, r, s)$ to be all real.

The density matrix corresponding to the state in Eq. (3) can be written easily and its trace over the first qubit yields the reduced density matrix

$$\rho_B = \begin{pmatrix} p^2 + r^2 & ps + qr \\ ps + qr & q^2 + s^2 \end{pmatrix}, \quad (4)$$

where we have used the representation

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, |0\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (5)$$

etc. The characteristic polynomial of $\rho_B$ [Eq. (4)] is

$$P[\rho_B, x] = x^2 - (p^2 + q^2 + r^2 + s^2) x + (pq - rs)^2, \quad (6)$$

where $x$ is a dummy variable. Clearly $P$ is quadratic in $x$ and has two roots which are non-zero in general. They are the eigenvalues of $\rho_B$ and yield the Schmidt coefficients $\{2\}$; as promised, we will not calculate them.

The Subresultants $[P, P', x]$ function in Mathematica directly yields the subdiscriminant sequence with the polynomial $P$ and its derivative $P'$ with respect to $x$ as inputs. We note that Mathematica requires that the coefficients of the highest power of $x$ in $P$ as well as $P'$ to be 1. This can be arranged easily. Also in the general case the number of terms in the sequence equals the degree of $P$, i.e. $d$. In the present example therefore there are two terms in the sequence. The penultimate term in the subdiscriminant sequence of $P$ in Eq. (6) is the discriminant of $P$, $D_1[P]$, which equals zero whenever the two roots of $\rho_B$ coincide [6]. We find

$$D_1[P] = [(p + q)^2 + (r - s)^2] \left[(p - q)^2 + (r + s)^2\right]. \quad (7)$$

If $|\psi\rangle$ is to be maximally entangled $D_1[P] = 0$. We can extract the Bell basis using this criterion. Specifically, we can see that $(p = q = 0, r = \pm s)$ is a solution set and yields, using Eq. (5), the states

$$|\psi_{1,2}\rangle = \frac{|10\rangle \pm |01\rangle}{\sqrt{2}}, \quad (8)$$

after normalization. Similarly, $(p = \pm q, r = s = 0,)$ is a solution set and yields the states

$$|\psi_{3,4}\rangle = \frac{|00\rangle \pm |11\rangle}{\sqrt{2}}, \quad (9)$$
after normalization. As is well known, the states $|\psi_{1,2,3,4}\rangle$ constitute the Bell basis [1]. Any state, and therefore any maximally entangled state can be expressed in this basis. For example, the solution set $(p = -q, r = s)$ yields the (unnormalized) maximally entangled state

$$|\psi\rangle = p\sqrt{2}|\psi_4\rangle + r\sqrt{2}|\psi_1\rangle.$$  

(10)

We note that $(p, q, r, s)$ can be complex in general; however, the analysis in that case is not very different from that presented here (also see below).

### IV. A 5 × 5 SYSTEM

The superiority of the method proposed in this article over that of Schmidt decomposition or von Neumann entropy calculation becomes clearer for systems of higher dimension, i.e., qudits. Physically qudits are of interest as some of the proposed candidates for quantum computation possess $d > 2$, such as a molecule with ro-vibrational states [8] and an alkali atom with hyperfine-Zeeman levels [8].

Here we consider a system with two parts each containing a 5-level system with states $|0\rangle, |1\rangle, |2\rangle, |3\rangle$, and $|4\rangle$. Specifically, we consider the unnormalized state

$$|\psi\rangle = |02\rangle + 2|10\rangle + |21\rangle + |22\rangle + |23\rangle + |24\rangle + 3|33\rangle + p|44\rangle,$$  

(11)

where $p$ is the only unknown real coefficient of expansion in the product basis. Tracing the density matrix over the five levels of system $A$, we obtain

$$\rho_B = \begin{pmatrix} 5 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 & 1 \\ 1 & 1 & 1 & 10 & 1 \\ 1 & 1 & 1 & 1 & p^2 + 1 \end{pmatrix},$$  

(12)

where we have used a matrix representation analogous to Eq. (5). The characteristic polynomial of $\rho_B$ [Eq. (12)] is

$$P[\rho_B, x] = -x^5 + (p^2 + 19) x^4 - (18p^2 + 105) x^3 + (91p^2 + 183) x^2 - (134p^2 + 72) x + 36p^2.$$  

(13)

$P$ is a quintic, and not generally solvable analytically in terms of radicals [3]. This implies that the Schmidt coefficients have to be found numerically. However the subdiscriminant sequence can be found analytically and its fourth member, apart from an irrelevant numerical prefactor, is

$$D_4[P] = 2p^4 - 14p^2 + 197.$$  

(14)

$|\psi\rangle$ is therefore maximally entangled when $D_4[P] = 0$, which yields the four roots

$$p = \pm \left( \frac{7 + i\sqrt{345}}{2} \right)^{1/2}, \pm \left( \frac{7 - i\sqrt{345}}{2} \right)^{1/2}.$$  

(15)

Since none of these solutions are real, $|\psi\rangle$ can never be maximally entangled.

We note that if we had assumed $p$ to be complex in Eq. (11), then Eqs. (12), (13), and (14) would undergo the transform $p^2 \rightarrow |p|^2$. The conditions presented in Eq. (15) would then hold for $|p|$ and would be impossible to achieve since by definition $|p|$, the modulus of $p$, is real. Therefore even if $p$ is allowed to be complex $|\psi\rangle$ can never be entangled maximally. We also note that the case of Eq. (14) is exceptional in that it is an analytically solvable equation, i.e., a quartic, in the variable of interest, $p$. This is atypical. Although the subdiscriminant sequence can always be obtained analytically, the roots of its members typically have to be found numerically.

The above demonstration, although it uses a somewhat arbitrary quantum state, shows the general usefulness of the method introduced in this article. The inability to maximally entangle the state $|\psi\rangle$ of Eq. (11) for any value of $p$ cannot be established generally by calculating the Schmidt coefficients or the von Neumann entropy.

### V. CONCLUSION

In this article we have pointed out a technique that always yields a single analytical condition that is satisfied by the coefficients of a pure bipartite quantum state if it is maximally entangled. The method is superior to that of Schmidt decomposition and von Neumann entropy for multilevel systems of dimension greater than 4. Further, it can also be used to obtain the maximally entangled basis for systems of arbitrary but finite dimension.

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