Characterization of the positivity of the density matrix in terms of the coherence vector representation

Mark S. Byrd and Navin Khaneja

Division of Engineering and Applied Science, Harvard University, 33 Oxford Street, Cambridge, Massachusetts 02138, USA

A parametrization of the density operator, a coherence vector representation, which uses a basis of orthogonal, traceless, Hermitian matrices is discussed. Using this parametrization we find the region of permissible vectors which represent a density operator. The inequalities which specify the region are shown to involve the Casimir invariants of the group. In particular cases, this allows the determination of degeneracies in the spectrum of the operator. The identification of the Casimir invariants also provides a method of constructing quantities which are invariant under *local* unitary operations. Several examples are given which illustrate the constraints provided by the positivity requirements and the utility of the coherence vector parametrization.

I. INTRODUCTION

The density operator must satisfy three important requirements: (1) It must be Hermitian; (2) the trace of the density operator, when appropriately normalized, must be 1; (3) it must be positive semidefinite. The third of these requirements has been found to be vital in quantum information theory, and in quantum mechanics itself [1]. Perhaps the most important place this has arisen is in the identification of positive and completely positive maps which can be used to identify entangled states [2,3] and to classify quantum channels (Refs. [4,5] and references therein). For both of these problems, but in particular the latter, a parametrization of the density operator is often useful. This provides an explicit way in which to identify when the channel is unital, trace preserving, and/or completely positive (see, for example, Ref. [6]). In addition, positivity requirements place restrictions on physically realizable quantum transformations [7].

Here we represent the density operator using a basis of orthogonal, traceless, Hermitian matrices. This representation is the generalization of the Bloch or coherence vector for two-state systems which is commonly used (see Ref. [8]). While the geometry of the space of density operators for two-state systems is relatively simple, the geometry of the space of density operators for higher-dimensional systems is considerably more complicated. The positivity (or more precisely, positive semidefiniteness) conditions are therefore more difficult to express succinctly for higher-dimensional systems. The inequalities given in this paper give necessary and sufficient conditions for a Hermitian operator to be positive semidefinite.

This set of inequalities can be expressed in terms of a distinguished set of unitary invariants, the Casimir invariants. This is a particularly notable relationship since the Casimir invariants are associated with the "good" quantum numbers of a quantum system [9] and thus have direct experimental interpretation. They specify the set of quantities which are invariant under a given set of unitary transformations. This has found many important applications for modeling of physical systems, and more recently, in quantum control of spin systems [10]. In addition, the Casimir invari-

ants and positivity requirements are expressed in terms of the coefficients of the characteristic polynomials. These coefficients, and their ratios, were found to be entanglement monotones [11]. Entanglement monotones could provide some insight into the problem of finding suitable entanglement measures since they satisfy an important requirement of such measures; they do not increase, on average, under local operations and classical communication [12].

This paper can be divided into three main parts (excluding the Introduction and Conclusion). The first part gives the generalized coherence vector representation of the density operator and the Casimir invariants in terms of the coherence vector. The second part gives positivity conditions for the density operator in terms of the trace invariants as well as the coherence vector. The third part provides examples of the utility of the structures presented in the first two parts.

II. COHERENCE VECTOR/CASIMIR INVARIANTS

In this section we present a coherence vector representation for an N-state system with particular normalization relationships which differ, for example, from Ref. [8]. This is the generalization of the Bloch sphere representation for two-state systems. The coherence vector, in our parametrization, has unit magnitude for pure states and has magnitude strictly less than one for mixed states. We will then show how to construct the Casimir invariants of the system in this parametrization. Using a completely analogous construction, we are able to provide a distinguished set of *local* unitary invariants for composite quantum systems.

A. Pure states in *N* dimensions

Any density operator can be expanded in any basis of orthogonal, traceless, Hermitian matrices. Here we adhere to the following conventions. We will use the following normalization condition for the elements of the Lie algebra of SU(N):

$$\mathrm{Tr}(\lambda_i \lambda_j) = 2\,\delta_{ij}. \tag{1}$$

We will also choose the following relations for commutation and anticommutation relations:

$$[\lambda_i, \lambda_j] = 2if_{ijk}\lambda_k \qquad (2)$$

and

$$\{\lambda_i, \lambda_j\} = \frac{4}{N}\delta_{ij}\mathbb{1} + 2d_{ijk}\lambda_k, \qquad (3)$$

where the f_{ijk} are the structure constants and the d_{ijk} are the components of the totally symmetric "d tensor," and by convention we sum over repeated indices. These two equations may be combined more succinctly as

$$\lambda_i\lambda_j = \frac{2}{N}\delta_{ij}\mathbb{1} + if_{ijk}\lambda_k + d_{ijk}\lambda_k. \qquad (4)$$

Using these conventions, we may express a pure state for an $N \times N$ density operator as

$$\rho = \frac{1}{N}\left(\mathbb{1} + \sqrt{\frac{N(N-1)}{2}}\vec{n}\cdot\vec{\lambda}\right). \qquad (5)$$

This representation is called a coherence vector representation with $\vec{n}$ the coherence vector. The constant is a convenient one such that for pure states

$$\vec{n}\cdot\vec{n} = 1 \quad \text{and} \quad \vec{n}*\vec{n} = \vec{n}, \qquad (6)$$

where the "star" product is defined by

$$(\vec{a}*\vec{b})_k = \sqrt{\frac{N(N-1)}{2}}\frac{1}{N-2}d_{ijk}a_ib_j. \qquad (7)$$

This can be proved by direct computation using Eq. (4).

Orthogonal pure states, e.g., $|a_1\rangle$ and $|a_2\rangle$ with corresponding density operators $\rho_1 = (1/N)(\mathbb{1} + \vec{n}_1\cdot\vec{\lambda})$ and $\rho_2 = (1/N)(\mathbb{1} + \vec{n}_2\cdot\vec{\lambda})$ are orthogonal if

$$\theta = \cos^{-1}\left(\frac{-1}{N-1}\right), \qquad (8)$$

where θ is defined by $\vec{n}_1\cdot\vec{n}_2 = \cos\theta$. Note that for $N=2$ this reduces to the well-known fact that for two-state systems the orthogonal states are represented by antipodal points on the Bloch sphere.

The first condition in Eq. (6) implies that the coherence vector must have unit magnitude. This restricts the set of vectors to those that lie on the surface of the unit sphere S^{N-1}. The second condition restricts the set of allowable rotations to a proper subset of the group $SO(N^2-1)$. The equations are nonlinear and give a set of constraints which restrict to the manifold $\mathbb{C}P^{N-1}$ having $2N-2$ dimensions. The second condition is also related to the positivity of density operators, a fact which is discussed further below.

B. Mixed states in N dimensions

The mixed state density operator in N dimensions can be written in the same form as the pure state case:

$$\rho = \frac{1}{N}\left(\mathbb{1} + \sqrt{\frac{N(N-1)}{2}}\vec{n}\cdot\vec{\lambda}\right) \qquad (9)$$

with $\vec{n}\cdot\vec{n} < 1$. However, unlike the case for a two-state system, there are more constraints on the coherence vector for dimensions greater than two for the Hermitian matrix here to represent a positive, semidefinite operator. This will be given in Sec. III.

C. Casimir invariants

The Casimir operators are invariant operators constructed from the Lie algebra elements. In particular, they form a maximal set of algebraically independent elements of the center of the algebra, formed by homogeneous polynomials in the generators. A very general discussion may be found in Ref. [13], and they were first constructed in Ref. [9]. General expressions for these are given in Appendix A. Here we note that the values of these operators can be determined by their relation to the trace invariants. For example, let us consider a density matrix ρ. For all ρ,

$$\text{Tr}(\rho^2) = \frac{1}{N}[1 + (N-1)\vec{n}\cdot\vec{n}]. \qquad (10)$$

The quantity $\vec{n}\cdot\vec{n}$ is the value of the quadratic Casimir operator (see Appendix A), which we refer to as the quadratic Casimir invariant. An example of the quadratic Casimir operator is the total angular momentum operator. The Casimir invariants are unchanged by unitary transformations on the density operator. Similarly,

$$\text{Tr}(\rho^3) = \frac{1}{N^2}[1 + 3(N-1)\vec{n}\cdot\vec{n} + (N-1)(N-2)(\vec{n}*\vec{n})\cdot\vec{n}] \qquad (11)$$

is clearly invariant under unitary operations. The quantity $\vec{n}*\vec{n}\cdot\vec{n}$ is the cubic Casimir invariant. In Appendix B we give the expressions for $\text{Tr}(\rho^n)$, $n \leq 9$. One may then recursively find higher-order Casimir invariants and show that they are indeed unchanged by unitary operators. The trace invariants $\text{Tr}(\rho^n)$ here were discussed in Ref. [14] where some discussion of the local unitary invariants were given for Greenberger-Horne-Zeilinger states.

D. Constructing local invariants

We can now construct a set of quantities which are invariant under *local* unitary transformations. These invariants, like the Casimir invariants, are a *distinguished* set. Clearly local unitary operations preserve the Casimir invariants of the marginal density operators. However, in this section we discuss invariants associated with the correlation matrix.

As an example, consider the quadratic Casimir invariant

$$c_2 = \vec{n} \cdot \vec{n}. \tag{12}$$

A two-qubit density operator can be expressed in a tensor product basis as

$$\rho = \tfrac{1}{4}(1 \otimes 1 + \vec{n}_A \cdot \vec{\sigma} \otimes 1 + 1 \otimes \vec{n}_B \cdot \vec{\sigma} + C_{ij}\sigma_i \otimes \sigma_j). \tag{13}$$

Note that local unitary transformations on systems A and B, denoted U_A and U_B, conserve $\vec{n}_A \cdot \vec{n}_A$ and $\vec{n}_B \cdot \vec{n}_B$, respectively. This can be seen as follows,

$$U_A n_A^{(i)} \sigma_i U_A^\dagger = n_A^{(i)} R_i^j \sigma_j, \tag{14}$$

where $R \in SO(3)$. We can therefore rewrite

$$n_A^{(i)} R_i^j = m_A^{(i)} \tag{15}$$

and note that $\vec{n}_A \cdot \vec{n}_A = \vec{m}_A \cdot \vec{m}_A$ since the transformation is orthogonal. We also know that the set of all unitary transformations acting on the composite system will be a subset of the matrices in $SO(15)$. This implies that

$$\vec{n}_A \cdot \vec{n}_A + \vec{n}_B \cdot \vec{n}_B + \sum_{ij} C_{ij}C_{ij} \tag{16}$$

is also a conserved quantity. However, we may want to ask what quantities associated with the correlation matrix C_{ij} are conserved under local unitary transformations. The correlation matrix has rows and columns labeled by the indices i and j, respectively. Now consider the vector formed from the elements in each. Examining Eq. (14), we see that the magnitude of the vector, is conserved by U_A. Similarly, the magnitude of the vectors formed by the columns is conserved. We may express these relations as

$$U_A C_{ij}\sigma_i \otimes \sigma_j U_A^\dagger = C'_{lj}\sigma_l \otimes \sigma_j, \tag{17}$$

where $C'_{lj} \equiv R_l^i C_{ij}$ implies

$$\sum_i C_{ij}C_{ij} = \sum_l C'_{lj}C'_{lj}. \tag{18}$$

Similarly for U_B acting on the vectors formed from the columns of C_{ij}. Therefore under local unitary transformations of the form $U_A \otimes U_B$, the following quantity is conserved:

$$\sum_{ij} C_{ij}C_{ij}. \tag{19}$$

More generally, we may determine conserved quantities formed from the correlation matrix which are analogs of the Casimir invariants. For the cubic Casimir invariant, for example, the following quantity is invariant under local unitary transformations:

$$\sum_{ijk,lmn} d_{ijk}d_{lmn}C_{il}C_{jm}C_{kn}. \tag{20}$$

Similarly, we could construct invariants for arbitrary dimensional systems as well as systems with any number of subsystems.

The number polynomial invariants under unitary transformations grows rather rapidly with the dimension of the system under consideration [15]. One might suppose that only a subset is required for constructing entanglement measures given that, for example, the square of the concurrence [16,17] for two qubits (see Sec. IV C), are constructed from only three quantities which are invariant under local unitary transformations. Here we have given a subset of local invariants which may well be useful for many quantum information processing tasks. The set of invariants given by Makhlin [18] (see also Refs. [15,19]) to determine equivalence under local unitary operations is larger than the number of Casimir invariants, which are included as a subset, and are a complete set for determining the ability of two density operators to be transformed into one another by local unitary transformations. However, since the concurrence and I concurrence [20] do not rely on this large set of invariants, one may expect, generally, that the number of invariants needed for the construction of entanglement measures may be far less than the number required for other purposes, such as local unitary equivalence.

We have now shown that a density operator can be parametrized in terms of a set of traceless, orthogonal, Hermitian matrices and have constructed associated invariant quantities. Our next goal is to give positivity constraints for the density operators that determine the allowable sets of coherence vectors $\vec{n}$.

III. CHARACTERISTIC POLYNOMIAL/POSITIVITY

In this section the characteristic polynomial of the density matrix is expressed in terms of the multinomial expansion, the trace invariants, and the Casimir invariants.

A. The characteristic polynomial

In this subsection we express the characteristic polynomial in several different ways in terms of invariants of the group. Consider an $n \times n$ complex matrix A of arbitrary dimension with eigenvalues p_i. The characteristic equation for the matrix can be written as (for a similar expression, see Ref. [21])

$$\det(A - \lambda 1) = \lambda^n - S_1\lambda^{n-1} + S_2\lambda^{n-2} - + \cdots + (-1)^n S_n = 0, \tag{21}$$

where the S_k are the symmetric functions given by [22]

$$S_k = \sum_{1 \le i_1 \le \cdots i_k \le N} \prod_{j=1}^k p_{i_j}. \tag{22}$$

These can be written in terms of $[\mathrm{Tr}(\rho^n)]^m$ as

$$S_1 = \text{Tr}(A), S_2 = (1/2)[\text{Tr}(A)S_1 - \text{Tr}(A^2)] \quad (23)$$

and

$$S_k = (1/k)[\text{Tr}(A)S_{k-1} - \text{Tr}(A^2)S_{k-2} + \cdots$$
$$+ (-1)^{n-1}\text{Tr}(A^n)S_{k-n} + \cdots + (-1)^{k-2}\text{Tr}(A^{k-1})S_1$$
$$+ (-1)^{k-1}\text{Tr}(A^k)]. \quad (24)$$

This can be proved using the fact that

$$[\text{Tr}(\rho)]^N = \left(\sum_{k=1}^{M} p_k \right)^N$$
$$= \sum_{\{m_k\}} (N; m_1, m_2, \ldots, m_M) p_1^{m_1} p_2^{m_2} \cdots p_M^{m_M},$$
$$(25)$$

where $\{m_k\}$ is a set of integers such that $\Sigma_{k=1}^{M} m_k = N$, and

$$(N; m_1, m_2, \ldots, m_M) = \frac{N!}{m_1! m_2! \ldots m_M!}. \quad (26)$$

B. Positivity

For a given set of real numbers $\{n_1, n_2, \ldots, n_N\} \in \mathbb{R}^N$, we would like to know when the set will represent a valid density operator of the form Eq. (9). It is clear that the right-hand side of Eq. (9) has trace 1 and is Hermitian. However, the positive semidefinite property is less trivial.

Theorem. For a Hermitian matrix $\rho = (1/N)(\mathbb{1} + \sqrt{[N(N-1)/2]}\vec{n} \cdot \vec{\lambda})$ to represent a positive semi-definite operator it is necessary and sufficient for $S_k \geq 0$ for all k.

Sketch of proof. Since the matrix ρ is Hermitian, all eigenvalues of the operator are real. This implies that the coefficients of the characteristic polynomial are real. They are also non-negative if and only if the signs of the coefficients of the characteristic polynomial alternate. In fact, the number of positive roots of the characteristic polynomial is the number of sign changes in the sequence of coefficients (see pp. 124 and 125 of Ref. [23]). ∎

Constraints on the coherence vector

The set of inequalities $S_k \geq 0$ characterizes the region of permissible vectors which represent valid, i.e., positive semidefinite, density operators. The first few of these conditions, given directly in terms of the coherence vector, are as follows. For a normalized ρ,

$$S_1 = \text{Tr}(\rho) = 1. \quad (27)$$

Here we adhere to the conventions set forth in Secs. II A and II B. Using the symmetric parts of the traces, denoted Tr_{sym} given in Appendix B,

$$S_2 = \frac{1}{2}\{[\text{Tr}(\rho)]^2 - [\text{Tr}(\rho^2)]\} = \frac{N-1}{2N}[1 - \vec{n} \cdot \vec{n}], \quad (28)$$

$$S_3 = \frac{1}{6} \frac{(N-1)(N-2)}{N^2}[1 - 3\vec{n} \cdot \vec{n} + 2\vec{n} * \vec{n} \cdot \vec{n}], \quad (29)$$

$$S_4 = \frac{1}{24} \frac{(N-1)(N-2)(N-3)}{N^3} \left[1 - 6\vec{n} \cdot \vec{n} + 8\vec{n} * \vec{n} \cdot \vec{n} \right.$$
$$\left. + \frac{3(N-1)}{(N-3)}(\vec{n} \cdot \vec{n})^2 - \frac{6(N-2)}{(N-3)}\vec{n} * \vec{n} \cdot \vec{n} * \vec{n} \right]. \quad (30)$$

Higher-order invariants can be calculated using the material from the appendixes in a straightforward albeit somewhat tedious manner. Note that if the two requirements for a density operator to be a pure state are met, $\vec{n} \cdot \vec{n} = 1$ and $\vec{n} * \vec{n} = \vec{n}$, then S_2 through S_4 (as well as all higher S_k) vanish, indicating a characteristic polynomial with the solution, one non-zero eigenvalue. The trace being 1 then demands that this eigenvalue be 1.

It is also noteworthy that two density operators have the same Casimir invariants *if and only if* they have the same eigenvalues. This follows from the fact that two density operators have the same Casimir invariants *if and only if* they satisfy the same characteristic equation. An entanglement measure based upon an entanglement monotone for a bipartite pure state must be a function only of the eigenvalues of the marginal density operators [12]. This relation between Casimir invariants and eigenvalues implies that any entanglement measure based on an entanglement monotone may also be expressed as a function of the S_k or Casimir invariants of the marginal density operator.

C. Symmetric functions and Casimir invariants

The quantities appearing in the S_k are combinations of the Casimir invariants. This relationship is noteworthy for several reasons. Casimir invariants can be used to determine degeneracies in the orbits and emphasize the relation to the physical system and Casimir invariants are conserved quantities used as labels for quantum states. To illustrate the ability of the Casimir invariants to provide information about the degeneracy of the spectrum, we will use the three-state system as an example and then give a brief discussion of four-state systems.

1. Casimir invariants for a system with three states

Since the eigenvalues are invariant under unitary transformations, we can discuss the interpretation of the Casimir invariants in terms of a diagonalized density operator. In three dimensions a common basis for the traceless, diagonal 3×3 Hermitian matrices are the Gell-Mann matrices [24]. In this basis, we denote the two linearly independent, traceless diagonal matrices as

$$\lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad \lambda_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For a mixed state, we may write the diagonalized form as

$$\rho_d \equiv \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix},$$

where $\Sigma_i a_i = 1$. Expanding this using

$$\rho_1 = \frac{1}{3}\left[1 + \frac{\sqrt{3}}{2}(\sqrt{3}\lambda_3 + \lambda_8)\right] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (31)$$

$$\rho_2 = \frac{1}{3}\left[1 + \frac{\sqrt{3}}{2}(-\sqrt{3}\lambda_3 + \lambda_8)\right] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (32)$$

$$\rho_3 = \frac{1}{3}[1 - \sqrt{3}\lambda_8] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (33)$$

yields a density operator of the form

$$\rho_d = \tfrac{1}{3}\{1 + \sqrt{3}[(a_1\sqrt{3}/2 - a_2\sqrt{3}/2)\lambda_3 \\ + (a_1/2 + a_2/2 - a_3)\lambda_8]\}. \quad (34)$$

The coherence vector is given by

$$\vec{n} = (0,0,a_1\sqrt{3}/2 - a_2\sqrt{3}/2,0,0,0,0,a_1/2 + a_2/2 - a_3).$$

Since this is a positive semidefinite, Hermitian matrix, the density operator formed by $\rho_m = U\rho_d U^\dagger = 1/3(1 + \sqrt{3}U\vec{n}\cdot\vec{\lambda}U^\dagger)$ is also a positive semidefinite, Hermitian operator. With the appropriate restrictions on the coefficients, we may parametrize all three-state density matrices (and a direct generalization for higher-dimensional systems) in this way [25,26].

For three-state systems, the following two quantities are two independent Casimir invariants, which, in terms of the coherence vector, are given by

$$\vec{n}\cdot\vec{n} = c_2, \quad \vec{n}*\vec{n}\cdot\vec{n} = c_3. \quad (35)$$

The first is the quadratic Casimir invariant of the group and the second is the cubic Casimir invariant of the group (see also Refs. [8,21]). The generic orbits are given by [21]

$$\vec{n}\cdot\vec{n} = c_2 \quad \text{and} \quad \vec{n}*\vec{n}\cdot\vec{n} = c_3 \neq c_2. \quad (36)$$

The values of c_2 and c_3 are unchanged, i.e., invariant, under unitary transformations of the density operator. One should note that the Hamiltonian and the density operator are both Hermitian and thus can both be expanded in the same basis of traceless, orthogonal, Hermitian matrices. However, the positive semidefiniteness of the density operator puts further restrictions on the space of allowable sets of coefficients $\vec{n}$ of the Hermitian operator. Whereas, in general, $-|\vec{n}|^3 \leq \vec{n}*\vec{n}\cdot\vec{n} \leq |\vec{n}|^3$ [21] for a Hermitian operator, for a density

operator, one must preserve positivity. This restricts the set of coherence vectors such that the limit $-|\vec{n}|^3$ can never be reached for certain values of $|\vec{n}|$. This will be discussed in Sec. IV A.

The square of the coherence vector is

$$\vec{n}\cdot\vec{n} = a_1^2 + a_2^2 + a_3^2 - a_1a_2 - a_1a_3 - a_2a_3 \leq 1.$$

We may also calculate

$$\vec{n}*\vec{n}\cdot\vec{n} = a_1^3 + a_2^3 + a_3^3 + 6a_1a_2a_3 - (3/2)(a_1^2a_2 + a_2^2a_1 + a_1^2a_3 \\ + a_2^2a_3 + a_3^2a_1 + a_3^2a_2).$$

Note that $-|\vec{n}|^3 \leq \vec{n}*\vec{n}\cdot\vec{n} \leq |\vec{n}|^3$ since

$$(\vec{n}*\vec{n}\cdot\vec{n})^2 - |\vec{n}|^6 = \tfrac{27}{4}(a_1 - a_2)^2(a_1 - a_3)^2(a_2 - a_3)^2 \geq 0.$$

Degenerate eigenvalues imply the following relations.
(1) If $a_1 = a_2$,

$$\vec{n}\cdot\vec{n} = (a_1 - a_3)^2 \quad \text{and} \quad \vec{n}*\vec{n}\cdot\vec{n} = -(a_1 - a_3)^3. \quad (37)$$

(2) If $a_2 = a_3$

$$\vec{n}\cdot\vec{n} = (a_1 - a_3)^2 \quad \text{and} \quad \vec{n}*\vec{n}\cdot\vec{n} = (a_1 - a_3)^3. \quad (38)$$

(3) If $a_1 = a_3$

$$\vec{n}\cdot\vec{n} = (a_2 - a_3)^2 \quad \text{and} \quad \vec{n}*\vec{n}\cdot\vec{n} = (a_2 - a_3)^3. \quad (39)$$

Therefore, when the two degenerate eigenvalues are greater than the third, the quantity $\vec{n}*\vec{n}\cdot\vec{n}$ is negative and when they are smaller, $\vec{n}*\vec{n}\cdot\vec{n}$ is positive. Thus by investigating the values of the Casimir invariants, we are able to extract information about degeneracies in the spectrum. These degeneracies correspond to invariant subspaces since an eigenvalue subspace spanned by degeneracies is invariant under unitary transformations on that subspace [25]. We next comment briefly on the four-state and general cases of identifying degeneracies.

2. Higher dimensions

For N-state systems, there are $N-1$ Casimir invariants. This is the rank of the group of transformations, SU(N) on the space of density operators, and corresponds to the number of elements in a complete set of commuting operators. Each S_k, when expressed in terms of the coherence vector, will contain a term of the form $(\vec{n}*)^{\times(k-2)}\vec{n}\cdot\vec{n}$ which is absent from $S_j, j<k$. In the preceding section it was shown that a degeneracy in the spectrum of the density operator was manifest in the values of the Casimir invariants. When a degeneracy in the spectrum exists, an added symmetry of the density operator under a subgroup of the group of all unitary transformations exists. This will determine a relation between the Casimir invariants, and thus reduce the number of independent polynomial invariants.

Let us discuss the example of four-state systems. If the density operator for a four-state system has the spectrum (a,b,b,b) then each of the four Casimir invariants is proportional to powers of $|\vec{n}|$ ($c_i \propto |\vec{n}|^i$). If the spectrum is (a,a,b,b), then all Casimir invariants are zero except the quadratic. Spectra of the form (a,b,c,c), or nondegenerate spectra are not as easily identified by their Casimir invariants. However, there exists a readily available program, *Macaulay*, which can check the independence of the invariants, thereby determining the degeneracies. Of course, if the spectrum is completely degenerate, then all Casimir invariants vanish since $\vec{n} = 0$ for the completely degenerate case. The advantage of obtaining this information through the use of invariants is that *one may not always solve directly for the eigenvalues of a matrix, but the Casimir invariants may still be obtained.*

For the convenience of the reader, the Casimir operators are given in terms of the Lie algebra elements in Appendix A. In Appendix B we give the trace formulas from which these can be calculated and the coefficients of the characteristic polynomial can be found.

Note that a map from a density operator to a density operator may be expressed as an affine map,

$$\vec{n} \rightarrow \vec{n}' = T\vec{n} + \vec{t}, \tag{40}$$

where T is a matrix and $\vec{t}$ is a translation. The positivity of the mapping is determined by the positivity of the density operator formed by $\vec{n}'$ [6].

IV. EXAMPLES

In this section we give the following results. First, we show how the positivity of the S_k restricts the coherence vector for two particularly interesting examples, $\vec{n} * \vec{n} \cdot \vec{n} = -|\vec{n}|^3$ and inversion. This gives, in terms of the coherence vector, the same bound obtained by Rungta *et al.* [20] on the ability to construct a "universal inverter." Second, we show that the positivity of the density operator of two qubits can be determined by the positivity of S_3 and S_4 for the general case and for the Werner state. Third, we present an alternative derivation of the three-tangle of Coffman, Kundu, and Wootters [27] using the coherence vector description.

A. Inversion of the coherence vector

Here we show that, due to positivity requirements, the limit $\vec{n} * \vec{n} \cdot \vec{n} = -|\vec{n}|^3$ *cannot* be reached for certain $\vec{n}$. This follows from the positivity requirements $S_k \geq 0$ and restricts the set of positive maps for the set of density matrices. An example of this is the universal inverter and universal NOT gate.

1. Universal inversion

The universal inverter and universal NOT gate [20] are related to a mapping of the form

$$\rho \rightarrow 1 - \rho, \tag{41}$$

which is positive but not completely positive. In terms of the coherence vector representation,

$$\rho \rightarrow \frac{1}{N}[1(N-1) - c\vec{n} \cdot \vec{\lambda}] = \frac{(N-1)}{N}\left(1 - \frac{c}{N-1}\vec{n} \cdot \vec{\lambda}\right), \tag{42}$$

where $c = \sqrt{N(N-1)/2}$. Thus, up to an overall constant, the mapping corresponds to a change in sign of the coherence vector and a reduction of the magnitude of the coherence vector.

2. Inverting the coherence vector

We might ask if there exists a physical map which will properly invert the coherence vector. (Inversion of the coherence vector as a possible generalization of the concurrence [16,17] was studied by Rungta *et al.* [20].) This would be of the form

$$\rho = \frac{1}{N}(1 + c\vec{n} \cdot \vec{\lambda}) \rightarrow \rho = \frac{1}{N}(1 - c\vec{n} \cdot \vec{\lambda}). \tag{43}$$

However, this is not positive. To see this, consider the matrix

$$\rho = \frac{1}{N}\left[1 + \begin{pmatrix} a & 0 & \cdots & \\ 0 & a & 0 & \cdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & -(N-1)a \end{pmatrix}\right]. \tag{44}$$

For this matrix $\vec{n} \cdot \vec{n} = a^2$ and $\vec{n} * \vec{n} \cdot \vec{n} = a^3$. This gives the symmetric polynomial

$$S_3 \propto 1 - 3\vec{n} \cdot \vec{n} + 2\vec{n} * \vec{n} \cdot \vec{n} = 1 - 3a^2 + 2a^3. \tag{45}$$

This function of $\vec{n}$ is minimum when $\vec{n} * \vec{n} \cdot \vec{n} = -|\vec{n}|^3 < 0$ so that

$$S_3 \propto 1 - 3\vec{n} \cdot \vec{n} - 2|\vec{n} * \vec{n} \cdot \vec{n}| = 1 - 3a^2 - 2a^3. \tag{46}$$

For this to be positive, $a \geq 1/2$ showing that for certain $\vec{n}$ the limit $\vec{n} * \vec{n} \cdot \vec{n} = -|\vec{n}|^3$ cannot be obtained. This is unlike the case of a Hamiltonian, or general Hermitian matrix, where it is acceptable to have $\vec{n} * \vec{n} \cdot \vec{n} = -|\vec{n}|^3$. For a system with three states, and no zero eigenvalues, S_3 is the non-zero determinant of the matrix.

For higher-dimensional systems the requirement that ρ in Eq. (44) be positive corresponds to

$$\frac{1}{N-1} \geq a \geq -1. \tag{47}$$

Now if we ask for an inversion map which is positive, we seek a mapping of the form

$$\rho \rightarrow \frac{1}{N}(b1 - c\vec{n} \cdot \vec{\lambda}). \tag{48}$$

Choosing an operator of the form Eq. (44), for the map to be positive we require

$$b \geq (1-N)a \geq (N-1). \tag{49}$$

This is the condition found by Rungta *et al.* [20] for positivity and restricts inversion to a map of the form in Eq. (41). This is a condition on the positivity of the determinant which we have shown is S_N for an N-state system.

3. Three-state example

For example, let us consider a three-state density matrix of the form

$$\rho = \begin{pmatrix} 0.152\,78 & 0.036\,084 - i0.062\,50 & -0.072\,169 + i0.125\,00 \\ 0.036\,084 + i0.062\,50 & 0.236\,11 & -0.25 \\ -0.072\,168 - i0.125\,00 & -0.25 & 0.611\,11 \end{pmatrix}. \tag{50}$$

Using $n_i = (\sqrt{3}/2)\mathrm{Tr}(\rho\lambda_i)$, direct calculation gives

$$S_3 \propto 1 - 3(0.666)^2 + 2(0.666)^3.$$

However, when $0.666 \rightarrow -0.666$ then $S_3 < 0$ showing that inversion is not a positive map for this density operator.

B. Two-qubit entanglement

In the Sec. IV B 2 the example of the Werner states for two qubits is investigated. This mixture of a completely mixed and singlet state is separable if and only if the partially transposed density operator is positive semidefinite according to the Peres-Horodecki criterion [2,3]. In this case, S_3 and S_4 determine positivity. This will be shown using the coherence vector representation.

1. A basis for two qubits

Let a basis for the Lie algebra of SU(4) be given by

$$\{\lambda_i\}_{i=0}^{15} = \{\sigma_i \otimes \sigma_j\}_{i,j=0}^3, \tag{51}$$

where $\lambda_0 \equiv \mathbb{1}_4$ and $\sigma_0 \equiv \mathbb{1}_2$. The labels correspond in the following way:

$$\lambda_i, i = 0,1,2,3 \leftrightarrow \frac{1}{\sqrt{2}}\sigma_i \otimes \mathbb{1}, \quad i = 0,1,2,3,$$

$$\lambda_i, i = 4,5,6 \leftrightarrow \frac{1}{\sqrt{2}}\mathbb{1} \otimes \sigma_i, \quad i = 1,2,3,$$

$$\lambda_i, i = 7,8,9 \leftrightarrow \frac{1}{\sqrt{2}}\sigma_1 \otimes \sigma_i, \quad i = 1,2,3, \tag{52}$$

$$\lambda_i, i = 10,11,12 \leftrightarrow \frac{1}{\sqrt{2}}\sigma_2 \otimes \sigma_i, \quad i = 1,2,3,$$

$$\lambda_i, i = 13,14,15 \leftrightarrow \frac{1}{\sqrt{2}}\sigma_3 \otimes \sigma_i, \quad i = 1,2,3.$$

This forms an orthogonal basis with respect to the trace and has normalization given by

$$\mathrm{Tr}(\lambda_i \lambda_j) = 2\,\delta_{ij}. \tag{53}$$

The nonzero, totally symmetric d-tensor components in this basis are given by

$$\frac{1}{\sqrt{2}} = d_{1,4,7} = d_{1,5,8} = d_{1,6,9} = d_{2,4,10} = d_{2,5,11} = d_{2,6,12} = d_{3,4,13}$$

$$= d_{3,5,14} = d_{3,6,15} = -d_{7,11,15} = -d_{8,12,13} = d_{7,12,14}$$

$$= -d_{9,10,14} = d_{8,10,15} = d_{9,11,13}. \tag{54}$$

2. Werner states: A case study

Under partial transpose of the first subsystem in the density operator, only elements $n_2, n_{10}, n_{11}, n_{12}$ change sign (in the given basis Sec. IV B 1). Therefore under the partial transpose, one may readily determine which elements of the products $\vec{n} * \vec{n} \cdot \vec{n}$ and $\vec{n} * \vec{n} \cdot \vec{n} * \vec{n}$ change sign.

The inequalities $S_3 \geq 0$ and $S_4 \geq 0$ depend only on the nonlocal invariants of the system since S_2 does not change and the local invariants which have the same form of S_2 also do not change. This shows that the negativity arises in the nonlocal invariants (as it should). As noted before, the partial transpose is positive since it preserves local positivity, but is not completely positive. Although this is a low-dimensional example and the higher order S_k become more complicated as the k increases, such an analysis might lead to ways (e.g., numerical and/or analytic searches) for identifying positive, but not completely positive, maps which may witness entanglement.

To clarify the discussions above, concerning the positivity of the coefficients of the characteristic polynomial, we give an example of the calculation for the Werner state of two qubits. The Werner state for two qubits is given by

$$\rho_W = \frac{1-x}{4}\mathbb{1} + xS, \tag{55}$$

where $0 \leq x \leq 1$ is real and S is the singlet state

$$S = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \qquad (56)$$

Therefore when $x=0$ the state is separable and when $x=1$ the state is maximally entangled. We may rewrite this as

$$\rho_W = \frac{1}{4}\mathbb{1} - \frac{x}{4}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)$$

$$= \begin{pmatrix} \dfrac{1-x}{4} & 0 & 0 & 0 \\ 0 & \dfrac{1+x}{4} & -\dfrac{x}{2} & 0 \\ 0 & -\dfrac{x}{2} & \dfrac{1+x}{4} & 0 \\ 0 & 0 & 0 & \dfrac{1-x}{4} \end{pmatrix}. \qquad (57)$$

The partial transpose condition (Peres-Horodeckis) [2,3] is equivalent (up to a local unitary transformation) to the inversion of the coherence vector, which is also known as spin flip or inversion. In terms of the coherence vector for the combined system, if we write the density operator in terms of the basis given in the preceding section,

$$\rho_W = \rho_{AB} = \frac{1}{4}(\mathbb{1} + \sqrt{6}\vec{n} \cdot \vec{\lambda}), \qquad (58)$$

the partial transpose corresponds to $\vec{n}_2 \rightarrow -\vec{n}_2$, $\vec{n}_{10} \rightarrow -\vec{n}_{10}$, $\vec{n}_{11} \rightarrow -\vec{n}_{11}, \vec{n}_{12} \rightarrow -\vec{n}_{12}$. Calculating the coefficients of the characteristic polynomial, $S_1(\rho_{AB})$ and $S_2(\rho_{AB})$ are unchanged under this transformation. However,

$$S_3(\rho_{AB}) = \left(\frac{1}{4^2}\right)(1 - 3x^2 + 2x^3) \rightarrow \left(\frac{1}{4^2}\right)(1 - 3x^2 - 2x^3) \qquad (59)$$

and

$$S_4(\rho_{AB}) = \left(\frac{1}{4^4}\right)(1 - 6x^2 + 8x^3 - 3x^4)$$

$$\rightarrow \left(\frac{1}{4^4}\right)(1 - 6x^2 - 8x^3 - 3x^4). \qquad (60)$$

This partial transpose condition implies that the density operator is separable *if and only if* the partially transposed density operator (or the spin-flipped density operator) is positive semidefinite. Here we see that the coefficients have following possibilities for sign changes. For $1/3 < x < 1/2$, $S_4 < 0$, $S_3 > 0$, and for $x > 1/2$, $S_4 < 0$ and $S_3 < 0$. However, in each case there is only one change in sign for a S_k and therefore one negative eigenvalue.

C. Distributed entanglement

Coffman, Kundu, and Wootters [27] have studied "distributed entanglement" which concerns the entanglement of various subsystems of a tripartite qubit system. One of their main results is the description of entanglement of a pure state of three qubits which is not expressible in terms of two-qubit relations. Here we wish to streamline their argument using the material presented above and thus derive by alternative means the "tangle" of three qubits. Consider a pure state of three qubits for systems we label A, B, C. We will write the density operator in a tensor product basis,

$$\rho_{ABC} = \tfrac{1}{8}(\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} + \vec{n}_A \cdot \vec{\sigma} \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{n}_B \cdot \vec{\sigma} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes \vec{n}_C \cdot \vec{\sigma}$$

$$+ \vec{n}_{AB} \cdot \vec{\sigma} \otimes \vec{\sigma} \otimes \mathbb{1} + \vec{n}_{AC} \cdot \vec{\sigma} \otimes \mathbb{1} \otimes \vec{\sigma} + \vec{n}_{BC} \cdot \mathbb{1} \otimes \vec{\sigma} \otimes \vec{\sigma}$$

$$+ \vec{n}_{ABC} \cdot \vec{\sigma} \otimes \vec{\sigma} \otimes \vec{\sigma}), \qquad (61)$$

where $\vec{n}_{AB} \cdot \vec{\sigma} \otimes \vec{\sigma} \equiv (n_{AB})_{ij} \sigma_i \otimes \sigma_j$, etc.

Since ρ_{ABC} represents a pure state, the marginal density matrices, e.g., $\rho_{AB} = \text{Tr}_C(\rho_{ABC})$, have only two nonzero eigenvalues, so that the square of the concurrence may be used to write

$$\mathcal{C}_{AB}^2 = (\lambda_1 - \lambda_2)^2 = \lambda_1^2 + \lambda_2^2 - 2\lambda_1\lambda_2 = \text{Tr}(\rho_{AB}\tilde{\rho}_{AB}) - 2\lambda_1\lambda_2$$

$$\leqslant \text{Tr}(\rho_{AB}\tilde{\rho}_{AB}), \qquad (62)$$

where λ_1 and λ_2 are the square roots of the eigenvalues of $\rho_{AB}\tilde{\rho}_{AB}$. The matrix $\tilde{\rho}_{AB}$ is defined by $\tilde{\rho}_{AB} = \sigma_y \otimes \sigma_y \rho_{AB}^* \sigma_y \otimes \sigma_y$.

At this point our argument will differ from that of Ref. [27]. Since this is a pure state, the Schmidt decomposition can be used to choose a preferred basis for subsystems AB and C. The reduced density matrices may be rewritten as (using an unnormalized coherence vector)

$$\rho_{AB} = \text{Tr}_C(\rho_{ABC}) = \tfrac{1}{4}(\mathbb{1} + \vec{m}_{AB} \cdot \vec{\lambda}), \qquad (63)$$

where $\vec{m}_{AB} \equiv (\vec{n}_A, \vec{n}_B, \vec{n}_{AB})$ and

$$\rho_C = \text{Tr}_{AB}(\rho_{ABC}) = \tfrac{1}{2}(\mathbb{1} + \vec{n}_C \cdot \vec{\sigma}). \qquad (64)$$

Then, by the Schmidt decomposition these two have the same eigenvalues. Therefore they satisfy the same characteristic equation which will have only one non-trivial S_k [$S_1 = \text{Tr}(\rho) = 1$], that being

$$S_2(\rho_C) = S_2(\rho_{AB}), \qquad (65)$$

which implies

$$\tfrac{1}{4}(1 + \vec{m}_{AB} \cdot \vec{m}_{AB}) = \tfrac{1}{2}(1 + \vec{n}_C \cdot \vec{n}_C). \qquad (66)$$

Therefore

$$\vec{n}_{AB} \cdot \vec{n}_{AB} = 1 + 2\vec{n}_C \cdot \vec{n}_C - \vec{n}_A \cdot \vec{n}_A - \vec{n}_B \cdot \vec{n}_B. \qquad (67)$$

Noting that

$$\text{Tr}(\rho_{AB}\tilde{\rho}_{AB}) = \tfrac{1}{4}(1 - \vec{n}_A \cdot \vec{n}_A - \vec{n}_B \cdot \vec{n}_B + \vec{n}_{AB} \cdot \vec{n}_{AB}), \quad (68)$$

we can use Eq. (67) to write

$$\text{Tr}(\rho_{AB}\tilde{\rho}_{AB}) = \tfrac{1}{2}(1 - \vec{n}_A \cdot \vec{n}_A - \vec{n}_B \cdot \vec{n}_B + \vec{n}_C \cdot \vec{n}_C). \quad (69)$$

This is completely equivalent to the results in Eqs. (7) and (8) of Ref. [27], the latter is repeated here:

$$\text{Tr}(\rho_{AB}\tilde{\rho}_{AB}) = 2(\det \rho_A + \det \rho_B - \det \rho_C). \qquad (70)$$

This is needed to derive the "first main result" of Ref. [27]:

$$\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 \leq 4 \det \rho_A, \qquad (71)$$

where we have used Eq. (62).

At this point, we can calculate

$$4\sqrt{S_2(\rho_{AB}\tilde{\rho}_{AB})} = \tau_{ABC} \equiv \mathcal{C}_{(A)BC}^2 - \mathcal{C}_{AB}^2 - \mathcal{C}_{AC}^2.$$

This quantity describes the three-way entanglement of the three qubits and was shown in Ref. [27] to be invariant under the permutation of the qubits.

V. CONCLUSION

The identification of positive, but not complete positive, maps has recently become an active area of research due to the restrictions it places on physically realizable quantum transformations [7] and the question of entanglement of quantum systems [2,3]. To aid in the study of such transformations this paper has presented a representation of the density operator in terms of traceless, Hermitian, orthogonal matrices. We then showed that the Casimir invariants of generalized coherence vector for density operator could be calculated directly and information about degeneracies in the spectrum of the operator could be obtained for some particular cases. It should be noted that we have given a representation of the density operator in bases, but the expressions of the Casimir invariants and symmetric functions do not depend on the choice of the set of traceless, Hermitian, orthogonal matrices in the basis. The region of positive semidefinite density operators is determined by the *necessary and sufficient* conditions $S_k \geq 0$. The S_k were expressed in terms of the coherence vector and Casimir invariants. The positivity conditions given here not only indicate whether a density operator has all positive eigenvalues, but also indicate the number of positive eigenvalues in terms of the number of sign changes of the sequence of coefficients S_k.

Superoperators which map Hermitian operators to Hermitian operators will preserve the reality of the eigenvalues. Since the eigenvalues are real, the coefficients of the characteristic polynomial must alternate in sign if the eigenvalues are to be positive. Therefore changes in the signs of the S_k can indicate positivity or nonpositivity of maps of the density operator. Given the expressions in this paper, this statement

may be utilized directly given an affine map of the coherence vector.

It is interesting to note that the "measure of purity" of a density operator has arisen in several contexts. Consider a pure state, bipartite density operator. The generalized concurrence in Ref. [20] is simply related to the purity of the marginal density operator. If ρ_A is the marginal density operator, then the concurrence is proportional to $S_2(\rho_A)$ which is a measure of the purity of the density operator. The state ρ_A is pure *if and only if* $S_2(\rho_A)$ is zero. The state is "less pure" if this quantity is larger. This measure of purity is also used in the optimal decompositions discussed in Ref. [28]. One might consider generalizations of the "measure of purity." Certainly if S_1 (equal to 1 when the matrix has unit trace) and S_2 are the only nonzero coefficients of the characteristic polynomial, then S_2 is a "good" measure of purity. However, if S_2 and S_3 are both nonzero, then the purity should be measured by two quantities since pure states necessarily have both quantities equal to zero. States that are closer to being pure are those with smaller values of these two quantities. Similar arguments can be made for the higher-dimensional S_k. One might then consider a generalization of measures of entanglement which rely on this modified set of "measures of purity."

The set of algebraic equations given by $S_k \geq 0$ give a set of geometric constraints on the spaces of allowable coherence vectors. This may motivate further exploration of techniques from algebraic geometry which has already been found useful by Miyake [29] for describing pure-state separability.

Due to the generality of the arguments here and the connections made between Casimir invariants, algebraic geometry, and positivity, we believe that this work provides useful relations and insights into the structure of positive operators. We also hope that it will aid in identifying positive, but not completely positive, maps.

Note added in proof. Recently, a detailed independent proof of the positivity conditions [30] was kindly pointed out by Gen Kimura. This includes an independent derivation of Eqs. (28)–(30) and a more thorough discussion of the regions of positivity for three-state systems.

APPENDIX A: CASIMIR INVARIANTS

Here we give expressions for the Casimir operators of a Lie group. For a discussion see Ref. [13].

The *Killing form* G_{ab} gives the *metric* g_{ab} on the vector space. This will determine the *quadratic Casimir* operator

$$C_2 = \sum_{a,b=1}^{N} g_{ab}\lambda^a\lambda^b, \qquad (A1)$$

where N is the dimension of the vector space [$N=n^2-1$ for SU(n) groups], and $\lambda \in \mathcal{L}(G)$. Note that $g_{ab} \propto \Sigma_{c,d} f_d^{ac} f_c^{bd}$ is an invariant, symmetric tensor. To find other invariant, symmetric tensors, one forms

$$\text{Tr}(ad_{\lambda^{a_1}} \circ ad_{\lambda^{a_2}} \circ \cdots \circ ad_{\lambda^{a_n}})$$

$$= \sum_{b_1,b_2,\ldots,b_n=1}^{N} f_{b_2}^{a_1 b_1} f_{b_3}^{a_2 b_2} \cdots f_{b_n}^{a_{n-1}b_{n-1}} f_{b_1}^{a_n b_n}. \qquad (A2)$$

One can express the *cubic Casimir* operator in terms of the totally symmetric tensor d_{abc},

$$C_3 = \sum_{a,b,c=1}^{N} d_{abc}\lambda^a\lambda^b\lambda^c. \qquad (A3)$$

Generally these higher-order operators can be expressed in terms of the symmetric tensor as

$$C_m = \sum_{\substack{b_1,b_2,\ldots,b_m \\ a_1,a_2,\ldots,a_{m-3}}} d_{a_1 b_1 b_2} d_{a_1 a_2 b_3} d_{a_2 a_3 b_4} \cdots$$

$$\times d_{a_{m-2}a_{m-3}b_{m-2}} d_{a_{m-3}b_{m-1}b_m}$$

$$\times \lambda^{b_1}\lambda^{b_2}\cdots\lambda^{b_m}. \qquad (A4)$$

We list the first few here in order to be explicit and to enable the development of the pattern.

$$C_4 = \sum_{a_1,b_1,b_2,b_3,b_4} d_{a_1 b_1 b_2} d_{a_1 b_3 b_4} \lambda^{b_1}\lambda^{b_2}\lambda^{b_3}\lambda^{b_4}, \qquad (A5)$$

$$C_5 = \sum_{\substack{b_1,b_2,b_3,b_4,b_5 \\ a_1,a_2}} d_{a_1 b_1 b_2} d_{a_1 a_2 b_3} d_{a_2 a_4 b_5} \lambda^{b_1}\lambda^{b_2}\cdots\lambda^{b_5}, \qquad (A6)$$

$$C_6 = \sum_{\substack{b_1,b_2,\ldots,b_6 \\ a_1,a_2,a_3}} d_{a_1 b_1 b_2} d_{a_1 a_2 b_3} d_{a_2 a_3 b_4} d_{a_3 b_5 b_6} \lambda^{b_1}\lambda^{b_2}\cdots\lambda^{b_6}. \qquad (A7)$$

Of course the ones that are immediately interesting are C_2, C_3, C_4, C_6, C_9 for the purposes of embedding two qubits into a four-state system, a two-state and a three-state system into a six-state system and the embedding of two three-state systems into a nine-state system. These are useful for examining quantum control for two qubits and entanglement issues for a two qubits, a qubit and a qutrit, and two qutrits.

The above relations can be expressed in terms of adjoint vectors and particular products. We introduce this notation here since it has its own manipulation rules that make it easier to calculate quantities of interest. Note also that since the f_{abc} and d_{abc} tensors are obtained by taking traces of products of elements with anticommutators and commutators respectively, they are easily calculated by analytic methods on a symbolic manipulation program such as MATHEMATICA. These relations are

$$f_{abc} = \left(\frac{-i}{4}\right)\text{Tr}([\lambda_a,\lambda_b]\lambda_c)$$

and

$$d_{abc} = \left(\frac{1}{4}\right)\text{Tr}(\{\lambda_a,\lambda_b\}\lambda_c).$$

The difference between upper and lower indices is not important if we are considering SU(n).

APPENDIX B: TRACE FORMULAS

1. Symmetric traces of basis elements

Here the first few examples of the trace formulas have been given.

$$\text{Tr}(\lambda_i\lambda_j) = 2\delta_{ij}, \qquad (B1)$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k) = 2d_{ijk}, \qquad (B2)$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l) = \frac{4}{N}\delta_{ij}\delta_{kl} + 2d_{ijm}d_{mkl}, \qquad (B3)$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_q) = \frac{4}{N}(\delta_{ij}d_{klq} + \delta_{kl}d_{ijq}) + 2d_{ijm}d_{kln}d_{mnq}, \qquad (B4)$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_q\lambda_s) = \frac{2^3}{N^2}\delta_{ij}\delta_{kl}\delta_{qs} + \frac{4}{N}(d_{ijm}d_{klm}\delta_{qs} + d_{ijm}d_{qsm}\delta_{kl} + d_{klm}d_{qsm}\delta_{ij}) + 2d_{ijm}d_{kln}d_{qst}d_{mnt}, \qquad (B5)$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_q\lambda_s\lambda_u) = \frac{2^3}{N^2}(\delta_{ij}\delta_{kl}d_{qsu} + \delta_{ij}\delta_{qs}d_{klu} + \delta_{qs}\delta_{kl}d_{iju}) + \frac{2^2}{N}(\delta_{qs}d_{ijm}d_{kln}d_{mnu} + \delta_{ij}d_{klm}d_{qsn}d_{mnu}$$

$$+ \delta_{kl}d_{ijm}d_{qsn}d_{mnu}) + \frac{2^2}{N}d_{qsu}d_{ijm}d_{klm} + 2d_{ijm}d_{kln}d_{qst}d_{mnv}d_{vtu}, \tag{B6}$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_q\lambda_s\lambda_u\lambda_w) = \frac{2^4}{N^3}\delta_{ij}\delta_{kl}\delta_{qs}\delta_{uw} + \frac{2^3}{N^2}(\delta_{ij}\delta_{kl}d_{qst}d_{uwt} + \delta_{ij}\delta_{qs}d_{kln}d_{uwn} + \delta_{ij}\delta_{uw}d_{qsn}d_{kln} + \delta_{kl}\delta_{qs}d_{ijn}d_{uwn}$$

$$+ \delta_{kl}\delta_{uw}d_{ijn}d_{qsn} + \delta_{uw}\delta_{qs}d_{kln}d_{ijn}) + \frac{2^2}{N}(\delta_{ij}d_{klm}d_{qst}d_{uwv}d_{tvm} + \delta_{kl}d_{ijm}d_{qst}d_{uwv}d_{tvm}$$

$$+ \delta_{qs}d_{ijm}d_{kln}d_{mnv}d_{uwv} + \delta_{uw}d_{ijm}d_{kln}d_{mnv}d_{qsv}) + 2d_{ijm}d_{kln}d_{mnp}d_{qst}d_{uwv}d_{tvp}, \tag{B7}$$

$$\text{Tr}_{sym}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_q\lambda_s\lambda_u\lambda_w\lambda_y) = \frac{2^4}{N^3}(\delta_{ij}\delta_{kl}\delta_{qs}d_{uyw} + \delta_{ij}\delta_{kl}\delta_{uw}d_{qsy} + \delta_{ij}\delta_{qs}\delta_{uw}d_{kly} + \delta_{kl}\delta_{qs}\delta_{uw}d_{ijy}) + \frac{2^3}{N^2}(\delta_{ij}\delta_{kl}d_{qst}d_{uvw}d_{tvy}$$

$$+ \delta_{qs}\delta_{uw}d_{ijm}d_{kln}d_{mny} + \delta_{ij}\delta_{qs}d_{kln}d_{uvw}d_{nvy} + \delta_{ij}\delta_{uw}d_{kln}d_{qst}d_{nty}) + \frac{2^3}{N^2}(\delta_{ij}d_{kly}d_{qst}d_{uwt}$$

$$+ \delta_{kl}d_{ijy}d_{qst}d_{uwt} + \delta_{qs}d_{ijm}d_{klm}d_{uwy} + \delta_{uw}d_{ijm}d_{klm}d_{qsy}) + \frac{2^2}{N}(\delta_{ij}d_{kln}d_{qst}d_{uvw}d_{tvx}d_{nxy}$$

$$+ \delta_{kl}d_{ijm}d_{qst}d_{uvw}d_{tvx}d_{mxy} + \delta_{qs}d_{ijm}d_{kln}d_{mnp}d_{uwv}d_{pvy} + \delta_{uw}d_{ijm}d_{kln}d_{mnp}d_{qst}d_{pty})$$

$$+ 2d_{ijm}d_{kln}d_{mnp}d_{qst}d_{uwv}d_{tvx}d_{pxy}. \tag{B8}$$

2. Symmetric traces for the density operator

For the density operator these translate to (again only the first few are given)

$$\text{Tr}(\rho^2) = \frac{1}{N}[1 + (N-1)\vec{n}\cdot\vec{n}], \tag{B9}$$

$$\text{Tr}(\rho^3) = \frac{1}{N^2}[1 + 3(N-1)\vec{n}\cdot\vec{n} + (N-1)(N-2)(\vec{n}*\vec{n})\cdot\vec{n}], \tag{B10}$$

$$\text{Tr}(\rho^4) = \frac{1}{N^3}[1 + 6(N-1)\vec{n}\cdot\vec{n} + 4(N-1)(N-2)(\vec{n}*\vec{n})\cdot\vec{n} + (N-1)^2(\vec{n}\cdot\vec{n})^2 + (N-1)(N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n})], \tag{B11}$$

$$\text{Tr}(\rho^5) = \frac{1}{N^4}[1 + 10(N-1)\vec{n}\cdot\vec{n} + 10(N-1)(N-2)\vec{n}*\vec{n}\cdot\vec{n} + 5(N-1)^2(\vec{n}\cdot\vec{n})^2 + 5(N-1)(N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n})$$

$$+ 2(N-1)^2(N-2)(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}) + (N-1)(N-2)^3\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}], \tag{B12}$$

$$\text{Tr}(\rho^6) = \frac{1}{N^5}[1 + 15(N-1)\vec{n}\cdot\vec{n} + 20(N-1)(N-2)\vec{n}*\vec{n}\cdot\vec{n} + 15(N-1)^2(\vec{n}\cdot\vec{n})^2 + 15(N-1)(N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n})$$

$$+ 12(N-1)^2(N-2)(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}) + 6(N-1)(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ (N-1)^3(\vec{n}\cdot\vec{n})^3 + 3(N-1)^2(N-2)^2(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + (N-1)(N-2)^4(\vec{n}*\vec{n}*\vec{n})^2], \tag{B13}$$

$$\text{Tr}(\rho^7) = \frac{1}{N^6}[1 + 21(N-1)\vec{n}\cdot\vec{n} + 35(N-1)(N-2)\vec{n}*\vec{n}\cdot\vec{n} + 35(N-1)^2(\vec{n}\cdot\vec{n})^2 + 35(N-1)(N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n})$$

$$+ 42(N-1)^2(N-2)(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}) + 21(N-1)(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ 7(N-1)^3(\vec{n}\cdot\vec{n})^3 + 21(N-1)^2(N-2)^2(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 7(N-1)(N-2)^4(\vec{n}*\vec{n}*\vec{n})^2$$

$$+ 3(N-1)^3(N-2)(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}\cdot\vec{n}) + 3(N-1)^2(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}\cdot\vec{n}) + (N-1)$$

$$\times (N-2)^3(\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + (N-1)(N-2)^5(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})], \tag{B14}$$

$$\text{Tr}(\rho^8) = \frac{1}{N^7}[1 + 28(N-1)\vec{n}\cdot\vec{n} + 56(N-1)(N-2)\vec{n}*\vec{n}\cdot\vec{n} + 70(N-1)^2(\vec{n}\cdot\vec{n})^2 + 70(N-1)$$

$$\times (N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n}) + 112(N-1)^2(N-2)(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}) + 56(N-1)(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ 28(N-1)^3(\vec{n}\cdot\vec{n})^3 + 84(N-1)^2(N-2)^2(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n})N^2 + 28(N-1)(N-2)^4(\vec{n}*\vec{n}*\vec{n})^2$$

$$+ 24(N-1)^3(N-2)(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}\cdot\vec{n}) + 24(N-1)^2(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}\cdot\vec{n})$$

$$+ 8(N-1)(N-2)^3(\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 8(N-1)(N-2)^5(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ (N-1)^4(\vec{n}\cdot\vec{n})^4 + 6(N-1)^3(N-2)^2(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 4(N-1)^2(N-2)^4$$

$$\times (\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}) + (N-2)^6(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})], \tag{B15}$$

$$\text{Tr}(\rho^9) = \frac{1}{N^8}[1 + 36(N-1)\vec{n}\cdot\vec{n} + 84(N-1)(N-2)\vec{n}*\vec{n}\cdot\vec{n} + 126(N-1)^2(\vec{n}\cdot\vec{n})^2 + 126(N-1)$$

$$\times (N-2)^2(\vec{n}*\vec{n})\cdot(\vec{n}*\vec{n}) + 252(N-1)^2(N-2)(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}) + 126(N-1)(N-2)^3$$

$$\times (\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}) + 84(N-1)^3(\vec{n}\cdot\vec{n})^3 + 252(N-1)^2(N-2)^2(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 84(N-1)(N-2)^4(\vec{n}*\vec{n}*\vec{n})^2$$

$$+ 108(N-1)^3(N-2)(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}\cdot\vec{n}) + 108(N-1)^2(N-2)^3(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}\cdot\vec{n})$$

$$+ 36(N-1)(N-2)^3(\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 36(N-1)(N-2)^5(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}) + 9(N-1)^4(\vec{n}\cdot\vec{n})^4$$

$$+ 54(N-1)^3(N-2)^2(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 36(N-1)^2(N-2)^4(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}) + 9(N-2)^6$$

$$\times (\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}) + 4(N-1)^4(N-2)(\vec{n}\cdot\vec{n})^3(\vec{n}*\vec{n}\cdot\vec{n}) + 6(N-1)^3(N-2)^3(\vec{n}\cdot\vec{n})^2(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ 4(N-1)^3(N-2)^3(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}) + 2(N-1)^2(N-2)^5(\vec{n}*\vec{n}\cdot\vec{n}*\vec{n})(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})$$

$$+ 4(N-1)^2(N-2)^5(\vec{n}\cdot\vec{n})(\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n}*\vec{n}*\vec{n}) + (N-1)(N-2)^7(\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}*\vec{n}\cdot\vec{n})]. \tag{B16}$$

[1] K. Kraus, *States, Effects and Operations*, Fundamental Notions of Quantum Theory (Academic, Berlin, 1983).

[2] Asher Peres, Phys. Rev. Lett. **77**, 1413 (1996).

[3] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223**, 1 (1996).

[4] Mary Beth Ruskai, e-print quant-ph/0302032.

[5] Michael Horodecki, Peter W. Shor, and Mary Beth Ruskai, e-print quant-ph/0302031.

[6] Christopher King and Mary Beth Ruskai, e-print quant-ph/9901079.

[7] F. De Martini, V. Buzek, F. Sciarrino, and C. Sias, Nature (London) **419**, 815 (2002).

[8] G. Mahler and V.A. Weberruss, *Quantum Networks: Dynamics of Open Nanostructures*, 2nd ed. (Springer-Verlag, Berlin, 1998).

[9] L.C. Biedenharn, J. Math. Phys. **4**, 436 (1963).

[10] N. Khaneja, B. Luy, and S.J. Glaser, e-print quant-ph/0302060.

[11] H. Barnum and N. Linden, e-print quant-ph/0103155.

[12] Guifré Vidal, J. Mod. Opt. **47**, 355 (2000).

[13] Jürgen Fuchs and Christoph Schweigert, *Symmetries, Lie Alge-*

bras and Representations (Cambridge University Press, Cambridge, England, 1997).

[14] J. Schlienz and G. Mahler, Phys. Lett. A **224**, 39 (1996).

[15] Markus Grassl, Martin Rötteler, and Thomas Beth, Phys. Rev. A **58**, 1833 (1998).

[16] Scott Hill and William K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997).

[17] W.K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

[18] Yuriy Makhlin, e-print quant-ph/0002045.

[19] Eric M. Rains, e-print quant-ph/9704042.

[20] Pranaw Rungta, V. Buzek, Carlton M. Caves, M. Hillery, and G.J. Milburn, Phys. Rev. A **64**, 042315 (2001).

[21] E. Ercolessi, G. Marmo, G. Morandi, and N. Mukunda, e-print quant-ph/0105007.

[22] Roger A. Horn and Charles R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, England, 1990).

[23] I.N. Bronshtein and K.A. Semendyayev, *Handbook of Mathematics* (Springer-Verlag, Berlin, 1998).

[24] M. Gell-Mann and Y. Ne'eman, *The Eightfold Way* (Benjamin, New York, 1964).

[25] Mark S. Byrd, Luis J. Boya, Mark Mims, and E.C.G. Sudarshan, e-print quant-ph/9810084.

[26] Mark S. Byrd and Paul B. Slater, Phys. Lett. A **283**, 152 (2001).

[27] Valerie Coffman, Joydip Kundu, and William K. Wootters, Phys. Rev. A **61**, 052306 (2000).

[28] K. Audenaert, F. Verstraete, and B. De Moor, Phys. Rev. A **64**, 052304 (2001).

[29] Akimasa Miyake, Phys. Rev. A **67**, 012108 (2003).

[30] Gen Kimura, e-print quant-ph/0301152 (2003).