On the one-particle reduced density matrices of a pure three-qutrit quantum state

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Abstract

We present a necessary and sufficient condition for three qutrit density matrices to be the one-particle reduced density matrices of a pure three-qutrit quantum state. The condition consists of seven classes of inequalities satisfied by the eigenvalues of these matrices. One of them is a generalization of a known inequality for the qubit case. Some of these inequalities are proved algebraically whereas the proof of the others uses the fact that a continuous function of the state must have a minimum. Construction of states satisfying these inequalities relies on a representation of the convex set of the allowed set of eigenvalues in terms of corner points. We also present a result for a more general quantum system concerning the nature of the boundary surface of the set of the allowed set of eigenvalues.

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I. INTRODUCTION

Recently there has been much activity in clarifying the nature of entanglement in quantum systems of finite degrees of freedom in connection with quantum computing, and there have been some results about properties of reduced density matrices of a pure state. In particular, a necessary and sufficient condition has been found for n one-qubit density matrices to be the reduced density matrices of a pure n-qubit quantum state [1, 2] for all n. [The phrase "reduced density matrix" is used to mean "one-particle reduced density matrix". It will be abbreviated as RDM below.] In this paper, as a continuation of this line of investigation we find a necessary and sufficient condition for three one-qutrit density matrices to be the RDMs of a pure three-qutrit quantum state. (Throughout this paper "a state" means "a pure state" unless otherwise stated.)

We consider the space of states spanned by the basis vectors $|ijk\rangle \equiv |i\rangle \otimes |j\rangle \otimes |k\rangle$, where i, j and k are 1, 2 or 3. The one-particle states $|1\rangle$, $|2\rangle$ and $|3\rangle$ are assumed to be orthonormal. A general state can be given by

$$|\Psi\rangle = \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3} c_{ijk}|ijk\rangle \,.$$

We require that $\langle\Psi\,|\,\Psi\rangle = \sum_{ijk}|c_{ijk}|^2 = 1$. Thus, the state $|\Psi\rangle$ is a normalized three-qutrit quantum state. The three RDMs are given by $\rho_{ii'}^{(1)} = \sum_{J,K} c_{iJK}\overline{c_{i'JK}}$, $\rho_{jj'}^{(2)} = \sum_{I,K} c_{IjK}\overline{c_{Ij'K}}$ and $\rho_{kk'}^{(3)} = \sum_{I,J} c_{IJk}\overline{c_{IJk'}}$. We denote the eigenvalues of the ath RDM, $\rho_{ii'}^{(a)}$, by $\lambda_1^{(a)}$, $\lambda_2^{(a)}$ and $\lambda_3^{(a)}$ with the ordering $\lambda_1^{(a)} \le \lambda_2^{(a)} \le \lambda_3^{(a)}$. We now state the main theorem of this paper.

Theorem 1. *A necessary and sufficient condition for nine nonnegative numbers $\lambda_i^{(a)}$, $i = 1, 2, 3$, $a = 1, 2, 3$ satisfying $\lambda_1^{(a)} \le \lambda_2^{(a)} \le \lambda_3^{(a)}$ and $\lambda_1^{(a)} + \lambda_2^{(a)} + \lambda_3^{(a)} = 1$ to be the eigenvalues of the three RDMs of a three-qutrit quantum state is given by the following inequalities:*

$$\lambda_2^{(a)} + \lambda_1^{(a)} \le \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_2^{(c)} + \lambda_1^{(c)}, \tag{1}$$
$$\lambda_3^{(a)} + \lambda_1^{(a)} \le \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_3^{(c)} + \lambda_1^{(c)}, \tag{2}$$
$$\lambda_2^{(a)} + \lambda_3^{(a)} \le \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_2^{(c)} + \lambda_3^{(c)}, \tag{3}$$
$$2\lambda_2^{(a)} + \lambda_1^{(a)} \le 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_2^{(c)} + \lambda_1^{(c)}, \tag{4}$$
$$2\lambda_1^{(a)} + \lambda_2^{(a)} \le 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_1^{(c)} + \lambda_2^{(c)}, \tag{5}$$
$$2\lambda_2^{(a)} + \lambda_3^{(a)} \le 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_2^{(c)} + \lambda_3^{(c)}, \tag{6}$$
$$2\lambda_2^{(a)} + \lambda_3^{(a)} \le 2\lambda_1^{(b)} + \lambda_2^{(b)} + 2\lambda_3^{(c)} + \lambda_2^{(c)}, \tag{7}$$

where (abc) are any permutations of (123).

If $\lambda_1^{(a)} = 0$ for all a, then by writing $\lambda_3^{(a)} = 1 - \lambda_2^{(a)}$, these inequalities can be expressed in terms of $\lambda_2^{(a)}$. We find that the only nontrivial inequalities resulting from Theorem 1 are $\lambda_2^{(a)} \le \lambda_2^{(b)} + \lambda_2^{(c)}$ for all permutations (abc) of (123). This conclusion agrees with Refs. [1, 2]. In Ref. [2] Bravyi solved the corresponding problem for the system $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^4$. His result can be used to find a necessary and sufficient condition for three density matrices to be RDMs of the quantum system $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^3$. This condition can be compared with that

obtained from Theorem 1 by letting $\lambda_1^{(1)} = \lambda_1^{(2)} = 0$. These conditions can be shown to be identical.

The rest of the paper is organized as follows. In Sec. II we represent the set of the allowed set of eigenvalues as a convex set determined uniquely by the corner points. In Sec. III we prove a generalization of inequality (1). Inequality (1) itself follows from this as a corollary. In Sec. IV we provide a proof of inequalities (2) and (3). Our proof of inequalities (1)–(3) is algebraic. The proof of the other inequalities uses the fact that a continuous function of the (ordered) set of coefficients (c_{ijk}) with the constraint $\sum_{i,j,k} |c_{ijk}|^2 = 1$ must have a minimum because the domain can be identified with the 53-dimensional sphere of radius one, which is compact. We explain our method in Sec. V and use it to prove inequalities (4) and (5) in Sec. VI. In Sec. VII we prove inequalities (6) and (7). [Our proof of inequality (6) is rather lengthy.] We then construct states for each set of eigenvalues satisfying (1)–(7) in Secs. VIII and IX. The corner-point representation given in Sec. II is useful in this construction. We conclude this paper in Sec. X by showing that the set of the allowed set of eigenvalues for a more general quantum system is likely to be bounded by hyperplanes.

II. THE CORNER-POINT REPRESENTATION OF THE SET OF THE AL-LOWED SET OF EIGENVALUES

Let us write a set of possible eigenvalues as

$$[\lambda_1^{(1)}\lambda_2^{(1)}\lambda_3^{(1)}, \lambda_1^{(2)}\lambda_2^{(2)}\lambda_3^{(2)}, \lambda_1^{(3)}\lambda_2^{(3)}\lambda_3^{(3)}]. \tag{8}$$

Since the combinations 001 and $0\frac{1}{2}\frac{1}{2}$ and $\frac{1}{3}\frac{1}{3}\frac{1}{3}$ will appear often, we abbreviate them as $O \equiv 001$, $A \equiv 0\frac{1}{2}\frac{1}{2}$ and $B \equiv \frac{1}{3}\frac{1}{3}\frac{1}{3}$. A set of eigenvalues can be regarded as a point in a six-dimensional space with coordinates $\lambda_1^{(a)}$ and $\lambda_2^{(a)}$, $a = 1, 2, 3$. For this reason we call a set given by (8) an eigenvalue point, or an E-point in short. In this representation the set of E-points defined in Theorem 1 is a convex set bounded by hyperplanes. Therefore this set, which will be denoted by S, can also be specified by giving all the corner points, i.e. the points on the boundary of the set where there is no tangent line to the boundary.

If we impose only the conditions $0 \leq \lambda_1^{(a)} \leq \lambda_2^{(a)} \leq \lambda_3^{(a)}$ and $\lambda_1^{(a)} + \lambda_2^{(a)} + \lambda_3^{(a)} = 1$, then the set of all allowed E-points are bounded by the hyperplanes $\lambda_1^{(a)} = 0$, $\lambda_1^{(a)} = \lambda_2^{(a)}$ and $\lambda_2^{(a)} = \lambda_3^{(a)} = 1 - \lambda_1^{(a)} - \lambda_2^{(a)}$, $a = 1, 2, 3$. The set of E-points satisfying these conditions is of the form $L \times L \times L$, where L is given by the triangle shown in Fig. 1.
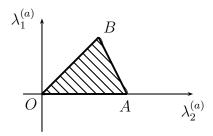

Fig. 1. The set L.

The corner points of the set $L \times L \times L$ are

$$[O,O,O], \ [O,O,A], \ [O,O,B], \ [O,A,A], \ [O,A,B], \ [O,B,B],$$
$$[A,A,A], \ [A,A,B], [A,B,B], \ [B,B,B] \tag{9}$$

and the E-points obtained from these by qutrit permutations. (For example, the E-points $[A,B,A]$ and $[B,A,A]$ are obtained from $[A,A,B]$ by qutrit permutations.)

If $\lambda_3^{(a)} = 1$ and $\lambda_2^{(a)} = \lambda_1^{(a)} = 0$ for some a, the state reduces to a two-qutrit system. It is well known that the two RDMs must have the same eigenvalues for any two-particle state. It can readily be verified that this fact is compatible with Theorem 1. In fact inequalities (1) and (2) imply this fact and the rest are satisfied if $\lambda_3^{(a)} = 1$, $\lambda_i^{(b)} = \lambda_i^{(c)}$, $i = 1, 2, 3$ for some (abc). This implies that the E-points $[O,O,A]$, $[O,O,B]$ and $[O,A,B]$ are not in the set S. All the other E-points in the list (9) satisfy the inequalities of this theorem. Therefore they will remain corner points of S.

Let us give the corner points of S. This will be useful when we construct quantum states satisfying the inequalities of Theorem 1 in Secs. VIII and IX.

Theorem 2. *The convex set S of the E-points characterized by Theorem 1 has the following corner points and those obtained by qutrit permutations from them:*

$$[O,O,O], \ [O,A,A], \ [O,B,B], \ [A,A,A], \ [A,A,B], \ [A,B,B], \ [B,B,B],$$
$$\left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right], \ \left[A, 0\tfrac{1}{4}\tfrac{3}{4}, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}\right], \ \left[A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right], \ \left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right]. \tag{10}$$

Since the E-points in this list that are corner points of $L \times L \times L$, i.e. the first seven E-points, remain corner points of S, we only need to show that the corner points of S that are not corner points of $L \times L \times L$ are given by the last four E-points in (10) and those obtained by qutrit permutations from them. Since each of these new corner points must satisfy one of *equalities* (1)–(7), i.e. equalities obtained by replacing inequality signs by equal signs, the following proposition, which lists all the corner points on the hyperplane given by each of equalities (1)–(7), will imply Theorem 2.

Proposition 1. *The intersection of the set S and the hyperplane bounding each of the inequalities listed in Theorem 1 is a 5-simplex. These 5-simplices are characterized by the corner points given as follows [for $(abc) = (123)$]:*

(1) : $[O,O,O]$, $[B,O,B]$, $[B,B,O]$, $[A,O,A]$, $[A,A,O]$, $\left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right]$;

(2) : $[O,O,O]$, $[B,O,B]$, $[A,O,A]$, $[O,A,A]$, $\left[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A\right]$, $\left[\tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}, 0\tfrac{1}{4}\tfrac{3}{4}, A\right]$;

(3) : $[O,O,O]$ $[B,O,B]$, $[A,O,A]$, $\left[0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}, B\right]$, $\left[A, 0\tfrac{1}{4}\tfrac{3}{4}, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}\right]$, $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, B\right]$;

(4) : $[O,O,O]$, $[B,O,B]$, $[B,B,O]$, $[A,O,A]$, $[A,A,O]$, $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right]$;

(5) : $[O,O,O]$, $[B,O,B]$, $[B,B,O]$, $[A,O,A]$, $\left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right]$, $\left[B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A\right]$;

(6) : $[O,O,O]$, $[B,O,B]$, $[A,O,A]$, $\left[A, 0\tfrac{1}{4}\tfrac{3}{4}, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}\right]$, $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right]$, $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, B\right]$;

(7) : $[A,A,B]$, $[B,O,B]$, $[A,O,A]$, $\left[0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}, B\right]$, $\left[A, 0\tfrac{1}{4}\tfrac{3}{4}, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}\right]$, $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, B\right]$.

Proof. Each set of E-points in this list clearly forms a 5-simplex since there are six E-points each. It is straightforward to check that each simplex is nondegenerate, i.e. five-dimensional. To verify that these simplices form the boundaries, i.e. to show that there are no other E-points contained in the set S on each hyperplane, it is sufficient to show that the six sides of each 5-simplex are on boundary hyperplanes of S. This will be true if any five E-points chosen from the set of corner points of each 5-simplex are on a single boundary hyperplane of S. This fact can readily be verified. We list the hyperplanes bounding each 5-simplex together with the E-point to be removed. For example, for equality (1), "$[O, O, O] : \lambda_2^{(1)} = \lambda_3^{(1)}$" below means that the E-points $[B, O, B]$, $[B, B, O]$, $[A, O, A]$, $[A, A, O]$ and $\left[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}\right]$ are on the hyperplane $\lambda_2^{(1)} = \lambda_3^{(1)}$.

Equality $(1), (abc) = (123)$
$[O, O, O] : \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, O, B] : \lambda_1^{(3)} = 0;$
$[B, B, O] : \lambda_1^{(2)} = 0; \quad [A, O, A] : (5), (abc) = (132);$
$[A, A, O] : (5), (abc) = (123); \quad \left[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}\right] : (4), (abc) = (123);$

Equality $(2), (abc) = (123)$
$[O, O, O] : \lambda_2^{(3)} = \lambda_3^{(3)}; \quad [B, O, B] : \lambda_1^{(3)} = 0;$
$[A, O, A] : \lambda_1^{(1)} = \lambda_2^{(1)}; \quad [O, A, A] : (6), (abc) = (321);$
$\left[\frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}, A\right] : \lambda_1^{(2)} = 0; \quad \left[\frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}, A\right] : (4), (abc) = (321);$

Equality $(3), (abc) = (123)$
$[O, O, O] : (7), (abc) = (123); \quad [B, O, B] : \lambda_1^{(1)} = 0;$
$[A, O, A] : \lambda_1^{(3)} = \lambda_2^{(3)}; \quad \left[0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}, B\right] : (6), (abc) = (123);$
$\left[A, 0\frac{1}{4}\frac{3}{4}, \frac{1}{4}\frac{1}{4}\frac{1}{2}\right] : (5), (abc) = (321); \quad \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, B\right] : \lambda_1^{(2)} = 0;$

Equality $(4), (abc) = (123)$
$[O, O, O] : \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, O, B] : (2), (abc) = (231);$
$[B, B, O] : (2), (abc) = (321); \quad [A, O, A] : \lambda_1^{(3)} = \lambda_2^{(3)};$
$[A, A, O] : \lambda_1^{(2)} = \lambda_2^{(2)}; \quad \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] : (1), (abc) = (123);$

Equality $(5), (abc) = (123)$
$[O, O, O] : \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, O, B] : \lambda_1^{(3)} = 0;$
$[B, B, O] : (3), (abc) = (321); \quad [A, O, A] : \lambda_1^{(1)} = \lambda_2^{(1)};$
$\left[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}\right] : \lambda_1^{(2)} = \lambda_2^{(2)}; \quad \left[B, \frac{1}{6}\frac{1}{6}\frac{2}{3}, A\right] : (1), (abc) = (123);$

Equality $(6), (abc) = (123)$
$[O, O, O] : \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, O, B] : \lambda_1^{(1)} = 0;$
$[A, O, A] : \lambda_1^{(3)} = \lambda_2^{(3)}; \quad \left[A, 0\frac{1}{4}\frac{3}{4}, \frac{1}{4}\frac{1}{4}\frac{1}{2}\right] : \lambda_1^{(2)} = \lambda_2^{(2)};$
$\left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] : (3), (abc) = (123); \quad \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, B\right] : (2), (abc) = (321);$

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Equality $(7), (abc) = (123)$

$[A, A, B] : (3), (abc) = (123); \quad [B, O, B] : \lambda_1^{(1)} = 0;$

$[A, O, A] : \lambda_1^{(3)} = \lambda_2^{(3)}; \quad \left[0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}, B\right] : \lambda_2^{(1)} = \lambda_3^{(1)};$

$\left[A, 0\frac{1}{4}\frac{3}{4}, \frac{1}{4}\frac{1}{4}\frac{1}{2}\right] : \lambda_2^{(3)} = \lambda_3^{(3)}; \quad \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, B\right] : \lambda_1^{(2)} = 0.$

$\square$

III. PROOF OF A GENERALIZATION OF INEQUALITY (1)

Now we start proving the inequalities in Theorem 1, thus establishing that they are necessary conditions for the $\lambda_i^{(a)}$ to be the eigenvalues of the RDMs of a three-qutrit quantum state. Inequality (1) is a corollary of a more general result stated in Ref. [1]. We present a proof of the latter.

Theorem 3. *Consider an n-qudit state given by*

$$|\Psi\rangle = \sum_{1 \leq i_1, \dots, i_n \leq d} c_{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \,,$$

where the set $\{|1\rangle, |2\rangle, \dots, |d\rangle\}$ is an orthonormal basis for a d-dimensional vector space. Let $\lambda_i^{(a)}$, $i = 1, 2, \dots, d$, be the eigenvalues of the ath RDM with $\lambda_i^{(a)} \leq \lambda_j^{(a)}$ if $i < j$. Then

$$\sum_{a=1}^{n-1} \sum_{i=1}^{d-1} \lambda_i^{(a)} \geq \lambda_1^{(n)} + \lambda_2^{(n)} + \cdots + \lambda_{d-1}^{(n)} \,. \tag{11}$$

Proof. The basis states can be chosen in such a way that the RDMs are all diagonal [3, 4, 5]. We work in this basis. Define

$$G \equiv \sum_{a=1}^{n-1} \sum_{i=1}^{d-1} \lambda_i^{(a)} \,.$$

Note that

$$\lambda_i^{(a)} = \sum_{i_1, \dots, i_{a-1}, i_{a+1}, \dots i_n} \left| c_{i_1 \cdots i_{a-1} i\, i_{a+1} \cdots i_n} \right|^2 \,.$$

Let us write

$$c_{i_1 i_2 \cdots i_{n-1} i} = \sqrt{\lambda_i^{(n)}} \, a_{i_1 i_2 \cdots i_{n-1} i} \,.$$

If $\lambda_i^{(n)} > 0$ for all i, we have

$$\sum_{i_1 i_2 \cdots i_{n-1}} \left| a_{i_1 i_2 \cdots i_{n-1} i} \right|^2 = 1 \,, \tag{12}$$

$$\sum_{i_1 i_2 \cdots i_{n-1}} a_{i_1 i_2 \cdots i_{n-1} i} \, \overline{a_{i_1 i_2 \cdots i_{n-1} i'}} = 0 \quad \text{if } i \neq i' \,. \tag{13}$$

The latter follows from the fact that the nth RDM is diagonal. If $\lambda_j^{(n)} = 0$ for some j, then the coefficients $a_{i_1 i_2 \cdots i_{n-1} j}$ are undefined. However, we can choose them so that Eqs. (12) and (13) are satisfied for all i and i' even in this case. For $a \neq n$ we have

$$\lambda_i^{(a)} = \sum_{i_n=1}^{d} \lambda_{i_n}^{(n)} \sum_{i_1,\cdots,i_{a-1},i_{a+1},\cdots,i_{n-1}} |a_{i_1 \cdots i_{a-1} i\, i_{a+1} \cdots i_n}|^2 .$$

Then we find

$$G = \sum_{a=1}^{n-1} \sum_{i=1}^{d-1} \lambda_i^{(a)} = \sum_{i_1,i_2 \cdots i_{n-1}, i_n} g(i_1, i_2, \ldots, i_n) \lambda_{i_n}^{(n)} |a_{i_1 i_2 \cdots i_n}|^2 ,$$

where $g(i_1, i_2, \ldots, i_n) \geq 1$ unless $i_1 = i_2 = \cdots = i_{n-1} = d$, and where $g(d, d, \ldots, d, i_n) = 0$. Thus

$$G \geq \sum_{i_n=1}^{d} \lambda_{i_n}^{(n)} \left\{ \left(\sum_{i_1,\cdots i_{n-1}} |a_{i_1 i_2 \cdots i_n}|^2 \right) - |a_{dd \cdots d\, i_n}|^2 \right\}$$

$$= \sum_{i_n=1}^{d} \lambda_{i_n}^{(n)} (1 - |a_{dd \cdots d\, i_n}|^2)$$

$$= 1 - \sum_{i_n=1}^{d} \lambda_{i_n}^{(n)} |a_{dd \cdots d\, i_n}|^2 , \qquad (14)$$

where we have used (12). Eqs. (12) and (13) allow us to consider $a_{i_1 i_2 \cdots i_{n-1} i}$ as components of orthonormal vectors labelled by i in d^{n-1} dimensions. This implies, in particular, that $(a_{dd \cdots d1}, a_{dd \cdots d2}, \ldots, a_{dd \cdots dd})$ is part of a $d^{n-1} \times d^{n-1}$ unitary matrix. Hence we have

$$\sum_{i_n=1}^{d} |a_{dd \cdots d\, i_n}|^2 \leq 1 . \qquad (15)$$

The quantity $\sum_{i_n=1}^{d} \lambda_{i_n}^{(n)} |a_{dd \cdots d\, i_n}|^2$ takes the maximum value under the constraint (15) if $|a_{dd \cdots dd}| = 1$ and $a_{dd \cdots d\, i_n} = 0$ for $i_n \neq d$ since $\lambda_d^{(n)}$ is the largest among $\lambda_{i_n}^{(n)}$ by definition. Then from (14) we find

$$G \geq 1 - \lambda_d^{(n)} = \lambda_1^{(n)} + \lambda_2^{(n)} + \cdots \lambda_{d-1}^{(n)}$$

as required. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Inequality (1) follows from this theorem by letting $d = 3$ and $n = 3$.

IV.   PROOF OF INEQUALITIES (2) AND (3)

We work in the basis for which the RDMs are all diagonal unless otherwise stated. We let $(abc) = (231)$ in inequality (3) and $(abc) = (132)$ in inequality (2) to find

$$\lambda_2^{(2)} + \lambda_3^{(2)} \leq \lambda_1^{(3)} + \lambda_2^{(3)} + \lambda_2^{(1)} + \lambda_3^{(1)} ,$$
$$\lambda_3^{(1)} + \lambda_1^{(1)} \leq \lambda_1^{(3)} + \lambda_2^{(3)} + \lambda_3^{(2)} + \lambda_1^{(2)} .$$

These are equivalent to the following proposition.

Proposition 2. $\lambda_3^{(3)} - \lambda_1^{(2)} \leq \lambda_2^{(1)} + \lambda_3^{(1)}$ *and* $\lambda_3^{(3)} - \lambda_1^{(2)} \leq \lambda_2^{(1)} + \lambda_3^{(2)}$.

Proof. First we note that

$$\lambda_3^{(3)} - \lambda_1^{(2)} \leq |c_{123}|^2 + |c_{133}|^2 + |c_{223}|^2 + |c_{233}|^2 + |c_{323}|^2 + |c_{333}|^2 \,.$$

Define

$$x \equiv |c_{123}|^2 + |c_{133}|^2 + |c_{223}|^2 + |c_{233}|^2 + |c_{323}|^2 + |c_{333}|^2 \,.$$

Then it is sufficient to show that

$$x \leq \lambda_2^{(1)} + \lambda_3^{(1)} \,, \tag{16}$$
$$x \leq \lambda_2^{(1)} + \lambda_3^{(2)} \,. \tag{17}$$

To prove (16) we define b_{ijk} by $c_{ijk} \equiv \sqrt{\lambda_i^{(1)}}\, b_{ijk}$ if $\lambda_i^{(1)} \neq 0$ for all i. Then we have

$$\sum_{j=1}^{3} \sum_{k=1}^{3} b_{ijk} \overline{b_{i'jk}} = \delta_{ii'} \,.$$

If $\lambda_i^{(1)} = 0$ for some i, then b_{ijk} are arbitrary, but we can still choose them to satisfy these equations. Hence the following matrix is part of a 9×9 unitary matrix:

$$M_1 \equiv \begin{pmatrix} b_{133} & b_{233} & b_{333} \\ b_{123} & b_{223} & b_{323} \end{pmatrix} \,.$$

Thus, we have the following inequalities:

$$|b_{133}|^2 + |b_{233}|^2 + |b_{333}|^2 \leq 1 \,, \tag{18}$$
$$|b_{123}|^2 + |b_{223}|^2 + |b_{323}|^2 \leq 1 \tag{19}$$

and

$$|b_{i33}|^2 + |b_{i23}|^2 \leq 1 \quad \text{for all } i \,. \tag{20}$$

Note that

$$x = \lambda_1^{(1)}(|b_{133}|^2 + |b_{123}|^2) + \lambda_2^{(1)}(|b_{233}|^2 + |b_{223}|^2) + \lambda_3^{(1)}(|b_{333}|^2 + |b_{323}|^2) \,. \tag{21}$$

From (18) and (19) we find

$$|b_{133}|^2 + |b_{123}|^2 \leq 2 - (|b_{233}|^2 + |b_{223}|^2 + |b_{333}|^2 + |b_{323}|^2) \,.$$

By using this in (21) we obtain

$$\begin{aligned} x &\leq 2\lambda_1^{(1)} + (\lambda_2^{(1)} - \lambda_1^{(1)})(|b_{233}|^2 + |b_{223}|^2) + (\lambda_3^{(1)} - \lambda_1^{(1)})(|b_{333}|^2 + |b_{323}|^2) \\ &\leq \lambda_2^{(1)} + \lambda_3^{(1)} \,, \end{aligned} \tag{22}$$

where we have used (20) with $i = 2$ and 3. Thus we have established inequality (16).

To establish (17) we first make a unitary transformation on the first and second rows of M_1 and obtain

$$\tilde{M}_1 = \begin{pmatrix} \overline{\alpha} b_{133} + \overline{\beta} b_{123} & \overline{\alpha} b_{233} + \overline{\beta} b_{223} & \overline{\alpha} b_{333} + \overline{\beta} b_{323} \\ -\beta b_{133} + \alpha b_{123} & -\beta b_{233} + \alpha b_{223} & -\beta b_{333} + \alpha b_{323} \end{pmatrix} \,,$$

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where $|\alpha|^2+|\beta|^2 = 1$. We choose α and β so that $-\beta b_{333}+\alpha b_{323} = 0$. If $b_{333} = c_{333}/\sqrt{\lambda_3^{(1)}} \neq 0$ or $b_{323} = c_{323}/\sqrt{\lambda_3^{(1)}} \neq 0$, then α and β can be chosen as follows:

$$\alpha = \frac{c_{333}}{\sqrt{|c_{333}|^2 + |c_{323}|^2}}, \tag{23}$$

$$\beta = \frac{c_{323}}{\sqrt{|c_{333}|^2 + |c_{323}|^2}}. \tag{24}$$

If $c_{333} = c_{323} = 0$, then (α, β) can be chosen, for example, to be $(1, 0)$. Then we have from the second row of $\tilde{M}_1$

$$| -\beta b_{133} + \alpha b_{123}|^2 + | -\beta b_{233} + \alpha b_{223}|^2 \leq 1 \,.$$

By multiplying this by $\lambda_2^{(1)}$ and remembering that $\lambda_1^{(1)} \leq \lambda_2^{(1)}$ we obtain

$$| -\beta c_{133} + \alpha c_{123}|^2 + | -\beta c_{233} + \alpha c_{223}|^2 \leq \lambda_2^{(1)} \,. \tag{25}$$

Next we define d_{ijk} by $c_{ijk} \equiv \sqrt{\lambda_j^{(2)}} \, d_{ijk}$. Then the following matrix is part of a unitary matrix if $\lambda_2^{(2)} \neq 0$:

$$M_2 \equiv \begin{pmatrix} d_{133} & d_{233} & d_{333} \\ d_{123} & d_{223} & d_{323} \end{pmatrix} \,.$$

If $\lambda_2^{(2)} = 0$, we can still choose d_{ijk} so that M_2 is part of a unitary matrix. Again we perform a unitary transformation on the first and second rows as follows:

$$\tilde{M}_2 = \begin{pmatrix} \overline{\alpha'}d_{133} + \overline{\beta'}d_{123} & \overline{\alpha'}d_{233} + \overline{\beta'}d_{223} & \overline{\alpha'}d_{333} + \overline{\beta'}d_{323} \\ -\beta'd_{133} + \alpha'd_{123} & -\beta'd_{233} + \alpha'd_{223} & -\beta'd_{333} + \alpha'd_{323} \end{pmatrix} \,,$$

where

$$\alpha' = \frac{\sqrt{\lambda_3^{(2)}} \, \alpha}{\sqrt{\lambda_3^{(2)}|\alpha|^2 + \lambda_2^{(3)}|\beta|^2}}, \tag{26}$$

$$\beta' = \frac{\sqrt{\lambda_2^{(2)}} \, \beta}{\sqrt{\lambda_3^{(2)}|\alpha|^2 + \lambda_2^{(3)}|\beta|^2}}. \tag{27}$$

From the first row of $\tilde{M}_2$ we obtain

$$|\overline{\alpha'}d_{133} + \overline{\beta'}d_{123}|^2 + |\overline{\alpha'}d_{233} + \overline{\beta'}d_{223}|^2 + |\overline{\alpha'}d_{333} + \overline{\beta'}d_{323}|^2 \leq 1 \,.$$

By substituting (26) and (27), and by recalling the definition of d_{ijk}, we find

$$|\overline{\alpha}c_{133} + \overline{\beta}c_{123}|^2 + |\overline{\alpha}c_{233} + \overline{\beta}c_{223}|^2 + |\overline{\alpha}c_{333} + \overline{\beta}c_{323}|^2 \leq \lambda_3^{(2)}|\alpha|^2 + \lambda_2^{(2)}|\beta|^2 \,.$$

Adding this and (25) and using (23) and (24) we find

$$|c_{133}|^2 + |c_{123}|^2 + |c_{233}|^2 + |c_{223}|^2 + |c_{333}|^2 + |c_{323}|^2 \leq \lambda_2^{(1)} + \lambda_3^{(2)}|\alpha|^2 + \lambda_2^{(2)}|\beta|^2 \,.$$

Since the left-hand side is equal to x, we obtain $x \leq \lambda_2^{(1)} + \lambda_3^{(2)}$ by using $|\alpha|^2+|\beta|^2 = 1$. This proves inequality (17). $\qquad\square$

The following result will be useful later.

Corollary 1. $\lambda_2^{(b)} + \lambda_3^{(c)} \geq \lambda_2^{(a)}$ *for all permutations* (abc) *of* (123).

Proof. Inequality (3) implies

$$
\begin{aligned}
2(\lambda_2^{(b)} + \lambda_3^{(c)}) &\geq \lambda_2^{(b)} + \lambda_1^{(b)} + \lambda_3^{(c)} + \lambda_2^{(c)} \\
&\geq \lambda_3^{(a)} + \lambda_2^{(a)} \\
&\geq 2\lambda_2^{(a)} .
\end{aligned}
$$

From this the corollary immediately follows. $\qquad\square$

V. THE METHOD FOR PROVING INEQUALITIES (4)–(7)

All our inequalities have the form

$$
F \equiv \sum_{i=1}^{3} \left(p_i \lambda_i^{(1)} + q_i \lambda_i^{(2)} + r_i \lambda_i^{(3)} \right) , \tag{28}
$$

where p_i, q_i and r_i are constants. The function F of the 27 complex variables c_{ijk} with constraint $\sum_{i,j,k} |c_{ijk}|^2 = 1$ is a continuous map from a 53-dimensional unit sphere, which is compact, to $\mathbb{R}$. Therefore there must be a minimum value. For all remaining inequalities we will show that the minimum of the corresponding function F cannot be negative.

Consider a three-qutrit state $|\Psi\rangle$ given as in Sec. I with three diagonal RDMs. Then the coefficients c_{ijk} satisfy the orthogonality relations, $c_{iJK}\overline{c_{i'JK}} = 0$, $c_{IjK}\overline{c_{Ij'K}} = 0$ and $c_{IJk}\overline{c_{IJk'}} = 0$, where the repeated indices are summed over. The state gives the minimum value of F only if the variation of F is nonnegative under any variation δc_{ijk} (not necessarily maintaining the orthogonality relations) of the coefficients c_{ijk}. ("A variation" means "a first-order variation" throughout this paper.)

To examine the variation of the eigenvalues $\lambda_i^{(a)}$ under a variation of c_{ijk} we use first-order perturbation theory in quantum mechanics. An RDM for the ath qutrit, $\rho_{ii'}^{(a)}$, of a given quantum state corresponds to the "unperturbed Hamiltonian", and the variation of an RDM under a variation of c_{ijk} to the "perturbation". The eigenvalues $\lambda_i^{(a)}$ correspond to the "energy eigenvalues". If there are no degenerate eigenvalues, then the variation of $\lambda_i^{(a)}$ can be read off from the diagonal elements of $\delta\rho_{ii'}^{(a)}$. We obtain the following result by this argument.

Proposition 3. *Suppose that* $\lambda_1^{a)} < \lambda_2^{(a)} < \lambda_3^{(a)}$. *Then the variation of the eigenvalues,* $\delta\lambda_i^{(a)}$, *under a variation* δc_{ijk} *of the coefficients* c_{ijk} *satisfying* $\sum_{I,J,K} \mathrm{Re}\,(\delta c_{IJK}\overline{c_{IJK}}) = 0$ *are given by*

$$
\begin{aligned}
\delta\lambda_i^{(1)} &= 2 \sum_{J,K} \mathrm{Re}\,(\delta c_{iJK}\overline{c_{iJK}}) , \\
\delta\lambda_j^{(2)} &= 2 \sum_{I,K} \mathrm{Re}\,(\delta c_{IjK}\overline{c_{IjK}}) , \\
\delta\lambda_k^{(3)} &= 2 \sum_{I,J} \mathrm{Re}\,(\delta c_{IJk}\overline{c_{IJk}}) .
\end{aligned}
$$

Proof. It is enough to note that the right-hand sides give the variation of the diagonal elements of the RDMs. □

For the function F given by (28) we define the level $L(i, j, k)$ of the triple $[ijk]$ by

$$L(i, j, k) \equiv p_i + q_j + r_k \,. \tag{29}$$

Lemma 1. *Suppose that the function F of c_{IJK} defined by (28) has its minimum value at a state with nondegenerate eigenvalues $\lambda_I^{(a)}$ for all a. If c_{ijk} and $c_{i'j'k'}$ are nonzero for this state, then $L(i, j, k) = L(i', j', k')$.*

Proof. Assume first that $i \neq i'$, $j \neq j'$ and $k \neq k'$. Consider the variation of coefficients c_{IJK} given by

$$\delta c_{ijk} = \alpha c_{i'j'k'}, \quad \delta c_{i'j'k'} = -\overline{\alpha} c_{ijk}$$

and $\delta c_{IJK} = 0$ if $[IJK] \neq [ijk], [i'j'k']$. Then by Proposition 3 we have the following variation of $\lambda_I^{(a)}$:

$$\delta \lambda_i^{(1)} = \delta \lambda_j^{(2)} = \delta \lambda_k^{(3)} = \Delta \,,$$
$$\delta \lambda_{i'}^{(1)} = \delta \lambda_{j'}^{(2)} = \delta \lambda_{k'}^{(3)} = -\Delta \,,$$

where $\Delta = 2\mathrm{Re}\,(\alpha c_{i'j'k'} \overline{c_{ijk}})$, with all other $\delta \lambda_I^{(a)}$ vanishing. Hence the variation of F is

$$\delta F = (p_i + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta$$
$$= [L(i, j, k) - L(i', j', k')]\,\Delta \,.$$

It can readily be verified that this formula is valid even if $i = i'$, $j = j'$ or $k = k'$. Since $c_{ijk} \neq 0$ and $c_{i'j'k'} \neq 0$, we can make Δ positive or negative by adjusting the phase of α, thus making δF negative if $L(i, j, k) \neq L(i', j', k')$. Therefore, if the function F takes its minimum value at a state with nondegenerate eigenvalues, and if c_{ijk} and $c_{i'j'k'}$ are both nonzero, then we must have $L(i, j, k) = L(i', j', k')$. □

Let us define

$$P_4 = 2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} + \lambda_1^{(3)} - 2\lambda_2^{(1)} - \lambda_1^{(1)} \,, \tag{30}$$
$$P_5 = 2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} - 2\lambda_1^{(1)} - \lambda_2^{(1)} \,, \tag{31}$$
$$P_6 = 2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} + \lambda_3^{(3)} - 2\lambda_2^{(1)} - \lambda_3^{(1)} \,, \tag{32}$$
$$P_7 = 2\lambda_1^{(2)} + \lambda_2^{(2)} + 2\lambda_3^{(3)} + \lambda_2^{(3)} - 2\lambda_2^{(1)} - \lambda_3^{(1)} \,. \tag{33}$$

Our task is to show that the function P_m cannot have a negative minimum for any m. It is useful to note that if the quantum state reduces to a two-qutrit system, then $P_m \geq 0$ as we have mentioned before. We state this fact as a lemma.

Lemma 2. *If $\lambda_3^{(a)} = 1$ and $\lambda_2^{(a)} = \lambda_1^{(a)} = 0$ for some a, then $P_m \geq 0$ for all m.*

Let $L(i, j, k)$ be the level of $[ijk]$ defined by (29) for the function P_m. It can readily be seen that

$$P_m = \sum_{i,j,k} L(i, j, k)|c_{ijk}|^2 \,. \tag{34}$$

If P_m takes its minimum value at a state with nondegenerate eigenvalues, the level $L(i, j, k)$ must be the same for all $[ijk]$ with $c_{ijk} \neq 0$ by Lemma 1. This fact can be used to establish that P_m cannot have a negative minimum at a state with nondegenerate eigenvalues.

Proposition 4. *If P_m defined by (30)–(33) for some m has a negative minimum, then the state where this minimum occurs must have at least one pair of degenerate eigenvalues, i.e. $\lambda_i^{(a)} = \lambda_{i+1}^{(a)}$ for some a and i.*

Proof. All P_m have the following general form:

$$P_m = 2\lambda_{j_3}^{(2)} + \lambda_{j_2}^{(2)} + 2\lambda_{k_3}^{(3)} + \lambda_{k_2}^{(3)} - 2\lambda_{i_1}^{(1)} - \lambda_{i_2}^{(1)} \, . \tag{35}$$

Let i_3 be the number in the set $\{1, 2, 3\}$ which differs from i_1 and i_2, and similarly for j_1 and k_1. There are only four triples $[ijk]$ with negative levels $L(i, j, k)$, which are

$$[i_1 j_1 k_1] \text{ with } L = -2 \, ,$$
$$[i_2 j_1 k_1] \, , \ [i_1 j_2 k_1] \, , \ [i_1 j_1 k_2] \text{ with } L = -1 \, .$$

Suppose that all eigenvalues are nondegenerate. Then for the state where the negative minimum occurs, the level L of the triples $[ijk]$ such that $c_{ijk} \neq 0$ must all be -2 or -1 by Lemma 1. We must have $\lambda_3^{(a)} > \lambda_2^{(a)} > 0$ for all a. This cannot be the case if there is only one nonzero coefficient c_{ijk}. Hence we cannot have $L = -2$. Suppose $L = -1$. Then, the coefficients c_{ijk} other than $c_{i_2 j_1 k_1}$, $c_{i_1 j_2 k_1}$ and $c_{i_1 j_1 k_2}$ would be zero. Since $\lambda_3^{(a)}$ and $\lambda_2^{(a)}$ must be nonzero, we must have $i_3 = j_3 = k_3 = 1$. This is not satisfied by any P_m. Hence if P_m has a negative minimum, then the state where the minimum occurs must have at least one pair of degenerate eigenvalues. $\square$

Next we establish some general results for degenerate cases. Note that if there are degenerate eigenvalues, we need to make sure that the variation of the off-diagonal elements in the degenerate sector vanishes in order to use the perturbation theory argument by taking the variation of only the diagonal elements of the RDMs into account.

Remark. We say that the variation of the RDMs is *effectively diagonal* if it has no off-diagonal elements in the degenerate sector.

Lemma 3. *Suppose that $\lambda_i^{(1)} = \lambda_{i+1}^{(1)} \neq \lambda_{i'}^{(1)}$ with no other degeneracy at a state where the function F defined by (28) has its minimum. Suppose further that $(c_{ijk}, c_{i+1,jk})$ and $c_{i'j'k'}$ are nonzero, i.e. $c_{ijk} \neq 0$ or $c_{i+1,jk} \neq 0$, and $c_{i'j'k'} \neq 0$, for this state. Then*

$$L(i, j, k) \leq L(i', j', k') \leq L(i + 1, j, k) \, .$$

Proof. Since $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$, a unitary transformation in the degenerate sector, i.e. between $|i\rangle$ and $|i+1\rangle$ in the first qutrit, leaves the RDMs diagonal. Hence we can let $c_{i+1,jk} = 0$ and $c_{ijk} \neq 0$ using such a unitary transformation. Then consider the variation given in the proof of Lemma 1. Then

$$\delta\rho_{i,i+1}^{(1)} = \delta c_{ijk} \cdot \overline{c_{i+1,jk}} + c_{ijk}\overline{\delta c_{i+1,jk}} = 0 \, ,$$

i.e. the variation of the RDM is effectively diagonal. Define $\Delta \equiv 2\text{Re}\,(\alpha c_{i'j'k'}\overline{c_{ijk}})$. We have $\delta\lambda_j^{(2)} = \delta\lambda_k^{(3)} = \Delta$ and $\delta\lambda_{i'}^{(1)} = \delta\lambda_{j'}^{(2)} = \delta\lambda_{k'}^{(3)} = -\Delta$ as before. However, since $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$, we must have $\delta\lambda_{i+1}^{(1)} \geq \delta\lambda_i^{(1)}$ by definition. Hence we have $\delta\lambda_{i+1}^{(1)} = \Delta$, $\delta\lambda_i^{(1)} = 0$ if $\Delta > 0$ and $\delta\lambda_{i+1}^{(1)} = 0$, $\delta\lambda_i^{(1)} = \Delta$ if $\Delta < 0$. Hence

$$\delta F \ = \ (p_{i+1} + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \ \text{ if } \ \Delta > 0 \, ,$$
$$\delta F \ = \ (p_i + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \ \text{ if } \ \Delta < 0 \, .$$

By requiring that $\delta F \geq 0$ for both cases we find the desired inequalities. $\square$

Remark. Analogous statements for the cases with $\lambda_j^{(2)} = \lambda_{j+1}^{(2)} \neq \lambda_{j'}^{(2)}$ and with $\lambda_k^{(3)} = \lambda_{k+1}^{(3)} \neq \lambda_{k'}^{(3)}$ can readily be established.

Remark. We often use a unitary transformation in the degenerate sector, *which keeps the RDM unchanged.* A unitary transformation on a qutrit is assumed to be in the degenerate sector unless otherwise stated in this and the next two sections.

Lemma 4. *Suppose that* $\lambda_i^{(1)} = \lambda_{i+1}^{(1)} \neq \lambda_{i'}^{(1)}$ *and* $\lambda_j^{(2)} = \lambda_{j+1}^{(2)} \neq \lambda_{j'}^{(2)}$ *with no other degeneracy at a state where the function* F *has its minimum. Suppose further that* $(c_{ijk}, c_{i+1,jk}, c_{i,j+1,k}, c_{i+1,j+1,k})$ *and* $c_{i'j'k'}$ *are nonzero for this state. Then*

$$L(i, j, k) \leq L(i', j', k') \leq L(i+1, j+1, k).$$

Proof. Since $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$ and $\lambda_j^{(2)} = \lambda_{j+1}^{(2)}$, we can use a unitary transformation to have $c_{i+1,jk} = c_{i,j+1,k} = 0$. Then consider the variation given in the proof of Lemma 1 and define Δ as in that lemma. Then, as in the previous lemma, the variation of the RDMs is effectively diagonal, and we have $\delta\lambda_i^{(1)} = \delta\lambda_j^{(2)} = 0$, $\delta\lambda_{i+1}^{(1)} = \delta\lambda_{j+1}^{(2)} = \Delta$ if $\Delta > 0$ and $\delta\lambda_i^{(1)} = \delta\lambda_j^{(2)} = \Delta$, $\delta\lambda_{i+1}^{(1)} = \delta\lambda_{j+1}^{(2)} = 0$ if $\Delta < 0$. Thus,

$$\delta F = (p_{i+1} + q_{j+1} + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \ \text{ if } \ \Delta > 0,$$
$$\delta F = (p_i + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \ \text{ if } \ \Delta < 0.$$

By requiring that $\delta F \geq 0$ for both cases we find the desired inequalities. $\qquad\square$

Lemma 5. *For the function* F *defined by (28) suppose that* $\lambda_i^{(1)} = \lambda_{i+1}^{(1)} \neq \lambda_{i'}^{(1)}$ *and* $\lambda_{j'}^{(2)} = \lambda_{j'+1}^{(2)} \neq \lambda_j^{(2)}$ *and that there is no other degeneracy. If* $(c_{ijk}, c_{i+1,jk})$ *and* $(c_{i'j'k'}, c_{i',j'+1,k'})$ *are nonzero at a state where the function* F *is minimized, then*

$$L(i, j, k) \leq L(i', j'+1, k') \ \text{ and } \ L(i', j', k') \leq L(i+1, j, k).$$

Proof. We can use unitary transformations to have $c_{i,j+1,k} = c_{i',j'+1,k'} = 0$ and $c_{ijk} \neq 0$, $c_{i'j'k'} \neq 0$ without changing the RDMs. Then by using the variation given in the proof of Lemma 1 we find

$$\delta F = (p_{i+1} + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \ \text{ if } \ \Delta > 0,$$
$$\delta F = (p_i + q_j + r_k - p_{i'} - q_{j'+1} - r_{k'})\Delta \ \text{ if } \ \Delta < 0.$$

By requiring $\delta F \geq 0$ for both cases we find the desired inequalities. $\qquad\square$

Lemma 6. *Suppose that* $\lambda_i^{(1)} = \lambda_{i+1}^{(1)} \neq \lambda_{i'}^{(1)}$, $\lambda_j^{(2)} = \lambda_{j+1}^{(2)} \neq \lambda_{j'}^{(2)}$ *and* $\lambda_k^{(3)} = \lambda_{k+1}^{(3)} \neq \lambda_{k'}^{(3)}$ *at a state where the function* F *defined by (28) has its minimum. Suppose further that at least one of the eight coefficients* c_{IJK} *with* $I = i, i+1$, $J = j, j+1$ *and* $K = k, k+1$ *is nonzero and that* $c_{i'j'k'}$ *is also nonzero for this state. Then*

$$L(i, j, k) \leq L(i', j', k') \leq L(i+1, j+1, k+1).$$

Proof. Since $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$, $\lambda_j^{(2)} = \lambda_{j+1}^{(2)}$ and $\lambda_k^{(3)} = \lambda_{k+1}^{(3)}$, a unitary transformation can be used to maximize $|c_{ijk}|^2$. This makes $c_{i+1,jk}$, $c_{i,j+1,k}$ and $c_{ij,k+1}$ vanish. (This argument was used to construct a generalized Schmidt decomposition in Refs. [6, 7].) Then consider the variation given in the proof of Lemma 1. The variation of the RDMs is effectively diagonal, and we have $\delta\lambda_i^{(1)} = \delta\lambda_j^{(2)} = \delta\lambda_k^{(3)} = 0$, $\delta\lambda_{i+1}^{(1)} = \delta\lambda_{j+1}^{(2)} = \delta\lambda_{k+1}^{(3)} = \Delta$ if $\Delta > 0$ and $\delta\lambda_i^{(1)} = \lambda_j^{(2)} = \delta\lambda_k^{(3)} = \Delta$, $\delta\lambda_{i+1}^{(1)} = \delta\lambda_{j+1}^{(2)} = \delta\lambda_{k+1}^{(3)} = 0$ if $\Delta < 0$. Thus,

$$\delta F = (p_{i+1} + q_{j+1} + r_{k+1} - p_{i'} - q_{j'} - r_{k'})\Delta \quad \text{if} \quad \Delta > 0,$$
$$\delta F = (p_i + q_j + r_k - p_{i'} - q_{j'} - r_{k'})\Delta \quad \text{if} \quad \Delta < 0.$$

By requiring that $\delta F \geq 0$ for both cases we find the desired inequalities. $\qquad\square$

The following proposition will also be useful.

Proposition 5. *Suppose that $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$ with no other degeneracy at a state where the function F defined by (28) has its minimum value. Define the reduced level $R^{(1)}(j, k)$ by*

$$R^{(1)}(j, k) \equiv q_j + r_k. \tag{36}$$

If $R^{(1)}(j, k) \neq R^{(1)}(j', k')$, then

$$c_{ijk}\overline{c_{ij'k'}} + c_{i+1,jk}\overline{c_{i+1,j'k'}} = 0, \tag{37}$$

i.e. the vectors $(c_{ijk}, c_{i+1,jk})$ and $(c_{ij'k'}, c_{i+1,j'k'})$ are orthogonal to each other, for this state.

Proof. We consider the following variation:

$$\delta c_{ijk} = \alpha c_{ij'k'}, \quad \delta c_{i+1,jk} = \alpha c_{i+1,j'k'},$$
$$\delta c_{ij'k'} = -\overline{\alpha} c_{ijk}, \quad \delta c_{i+1,j'k'} = -\overline{\alpha} c_{i+1,jk}$$

with all other δc_{IJK} vanishing. Then we find that the variation of the RDM for the first qutrit vanishes. We also find that if we define

$$\Delta \equiv \text{Re}\left[\alpha(c_{ijk}\overline{c_{ij'k'}} + c_{i+1,jk}\overline{c_{i+1,j'k'}})\right],$$

then $\delta\lambda_j^{(2)} = -\delta\lambda_{j'}^{(2)} = \Delta$ and $\delta\lambda_k^{(3)} = -\delta\lambda_{k'}^{(3)} = \Delta$. Hence

$$\delta F = (q_j + r_k - q_{j'} - r_{k'})\Delta = [R^{(1)}(j, k) - R^{(1)}(j', k')]\Delta.$$

If Eq. (37) does not hold and if $R^{(1)}(j, k) \neq R^{(1)}(j', k')$, then the parameter α can be adjusted so that $\delta F < 0$. Hence, at a state where F has its minimum value we must have either (37) or $R^{(1)}(j, k) = R^{(1)}(j', k')$. $\qquad\square$

Remark. The statements obtained from Lemmas 4 and 5 and Proposition 5 by qutrit permutations are also valid.

It is useful to treat some cases with only one pair of degenerate eigenvalues in general.

Lemma 7. *Suppose that the function P_m given by (35) in the proof of Proposition 4 has a negative minimum at a state with $\lambda_{i_2}^{(1)} = \lambda_{i_3}^{(1)}$ and without any other degeneracy. Then $\lambda_{j_3}^{(2)} = \lambda_{k_3}^{(3)} = 0$.*

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Proof. The only triples with negative levels are $[i_1j_1k_1]$, $[i_2j_1k_1]$, $[i_1j_2k_1]$ and $[i_1j_1k_2]$. If $(c_{i_1j_1k_1}, c_{i_1j_2k_1}, c_{i_1j_1k_2})$ and c_{ij_3k} are nonzero, then the preceding lemmas imply that there must be some i' (which is not necessarily equal to i) such that $L(i', j_3, k)$ is less than $L(i_1, j_1, k_1)$, $L(i_1, j_2, k_1)$ or $L(i_1, j_1, k_2)$. This is impossible because $L(i', j_3, k) \geq 0$ for all i' and k. Hence, if $c_{ij_3k} \neq 0$ for some i and k, then $c_{i_1j_1k_1} = c_{i_1j_2k_1} = c_{i_1j_1k_2} = 0$. Then a unitary transformation can be used to have $c_{i_2j_1k_1} = 0$ without changing the RDMs. Thus, we can make all coefficients c_{ijk} with $L(i, j, k) < 0$ vanish. Hence from (34) we conclude that $P_m \geq 0$ if $\lambda_{j_3}^{(2)} > 0$. Thus, if the function P_m were to have a negative minimum, then we must have $\lambda_{j_3}^{(2)} = 0$. In a similar manner it can be shown that $\lambda_{k_3}^{(3)} = 0$. $\square$

Corollary 2. *Suppose that the function P_m given by (35) in the proof of Proposition 4 has a negative minimum at a state with $\lambda_{j_2}^{(2)} = \lambda_{j_3}^{(2)}$ ($\lambda_{k_2}^{(3)} = \lambda_{k_3}^{(3)}$) and without any other degeneracy. Then $\lambda_{i_3}^{(1)} = \lambda_{k_3}^{(3)} = 0$ ($\lambda_{i_3}^{(1)} = \lambda_{j_3}^{(2)} = 0$).*

Proof. The function P_m can be rewritten as

$$P_m = 1 + \lambda_{i_3}^{(1)} - \lambda_{i_1}^{(1)} + \lambda_{j_3}^{(2)} - \lambda_{j_1}^{(2)} + \lambda_{k_3}^{(3)} - \lambda_{k_1}^{(3)} \, .$$

Then it is clear that the proof of Lemma 7 applies here after performing a qutrit permutations. $\square$

Lemma 8. *If the function P_m given by (35) has a negative minimum at a state with $\lambda_{i_1}^{(1)} = \lambda_{i_2}^{(1)}$ and with no other degeneracy, then $\lambda_{i_3}^{(1)} = 0$ or $\lambda_{j_3}^{(2)} = \lambda_{k_3}^{(3)} = 0$.*

Proof. To have $P_m < 0$ we must have $c_{i_1j_1k_1} \neq 0$, $c_{i_2j_1k_1} \neq 0$, $c_{i_1j_2k_1} \neq 0$ or $c_{i_1j_1k_2} \neq 0$. Then from the preceding lemmas we find that if $c_{i_3jk} \neq 0$, then $L(i_3, j, k) \leq 0$. This is true only for $j = j_1$, $k = k_1$. Thus, if we assume that $\lambda_{i_3}^{(1)} \neq 0$, then $c_{i_3j_1k_1} \neq 0$, and orthogonality relations give $c_{i_2j_1k_1} = c_{i_1j_1k_1} = 0$. If the vectors $(c_{i_1j_2k_1}, c_{i_2j_2k_1})$ and $(c_{i_1j_1k_2}, c_{i_2j_1k_2})$ are linearly independent, then there cannot be any other nonzero coefficients of the form c_{i_1jk} or c_{i_2jk} by Proposition 5 because $R^{(1)}(j, k) < 0$ for $[jk] = [j_1k_1]$, $[j_1k_2]$ and $[j_2k_1]$, and $R^{(1)}(j, k) \geq 0$ for all other $[jk]$. This implies that $\lambda_{j_3}^{(2)} = \lambda_{k_3}^{(3)} = 0$. If these vectors are linearly dependent, a unitary transformation can be used to have $c_{i_1j_1k_2} = c_{i_1j_2k_1} = 0$. Then all coefficients c_{ijk} with $L(i, j, k) < 0$ vanish. Hence $P_m \geq 0$. $\square$

Corollary 3. *If the function P_m given by (35) has a negative minimum at a state with $\lambda_{j_1}^{(2)} = \lambda_{j_2}^{(2)}$ ($\lambda_{k_1}^{(3)} = \lambda_{k_2}^{(3)}$) and with no other degeneracy, then $\lambda_{j_3}^{(2)} = 0$ ($\lambda_{k_3}^{(3)} = 0$) or $\lambda_{i_3}^{(1)} = \lambda_{k_3}^{(3)} = 0$ ($\lambda_{i_3}^{(1)} = \lambda_{j_3}^{(2)} = 0$).*

VI. PROOF OF INEQUALITIES (4) AND (5)

Now we are in a position to prove inequalities (4) and (5). The following Proposition, which was used in Ref. [1], will be useful.

Proposition 6. *If $i_1 < i_2$, then $|c_{i_1jk}|^2 + |c_{i_2jk}|^2 \leq \lambda_{i_2}^{(1)}$.*

Proof. If $\lambda_{i_1}^{(1)} = 0$, then $c_{i_1jk} = 0$ for all $[jk]$. Since we have $|c_{i_2jk}|^2 \leq \lambda_{i_2}^{(1)}$, the desired inequality is satisfied. So we assume $\lambda_{i_1}^{(1)} \neq 0$. By applying the Cauchy-Schwarz inequality to the orthogonality relation $c_{i_1JK}\overline{c_{i_2JK}} = 0$, we obtain

$$|c_{i_1jk}|^2|c_{i_2jk}|^2 \leq (\lambda_{i_1}^{(1)} - |c_{i_1jk}|^2)(\lambda_{i_2}^{(1)} - |c_{i_2jk}|^2).$$

Thus,

$$\lambda_{i_2}^{(1)}|c_{i_1jk}|^2 + \lambda_{i_1}^{(1)}|c_{i_2jk}|^2 \leq \lambda_{i_2}^{(1)}\lambda_{i_1}^{(1)}.$$

Hence

$$|c_{i_1jk}|^2 + |c_{i_2jk}|^2 \leq \frac{\lambda_{i_2}^{(1)}}{\lambda_{i_1}^{(1)}}|c_{i_1jk}|^2 + |c_{i_2jk}|^2 \leq \lambda_{i_2}^{(1)}.$$

$\square$

Remark. We can prove similarly that $|c_{ij_1k}|^2 + |c_{ij_2k}|^2 \leq \lambda_{j_2}^{(2)}$ if $j_1 < j_2$ and that $|c_{ijk_1}|^2 + |c_{ijk_2}|^2 \leq \lambda_{k_2}^{(3)}$ if $k_1 < k_2$.

We need the following lemma to prove $P_4 \geq 0$, i.e. inequality (4).

Lemma 9. *The function P_4 has its minimum value at a state with $c_{233} = 0$.*

Proof. If $\lambda_2^{(1)}$, $\lambda_3^{(2)}$ or $\lambda_3^{(3)}$ is degenerate with another eigenvalue, then we can use a unitary transformation to have $c_{233} = 0$. Hence, if $c_{233} \neq 0$ at all states where the minimum of P_4 occurs, then the only possible degeneracies are $\lambda_1^{(2)} = \lambda_2^{(2)}$ and $\lambda_1^{(3)} = \lambda_2^{(3)}$. Suppose that c_{233} and another coefficient c_{ijk} are nonzero. Then we must have $L(i, j', k') \leq L(2, 3, 3)$ for some $[ij'k']$ with $\lambda_{j'}^{(2)} = \lambda_j^{(2)}$ and $\lambda_{k'}^{(3)} = \lambda_k^{(3)}$. This is impossible because [233] is the only triple with $L(2, 3, 3) \leq -2$. Hence there must be a state with $c_{233} = 0$ where P_4 has its minimum value. $\square$

Proposition 7. *The function P_4 is nonnegative.*

Proof. We write P_4 in the following form

$$P_4 = \lambda_1^{(1)} + 2\lambda_3^{(1)} + \lambda_2^{(2)} - \lambda_3^{(2)} + \lambda_2^{(3)} - \lambda_3^{(3)}. \tag{38}$$

By Proposition 6 and the remark following it we obtain

$$\begin{aligned}
|c_{133}|^2 + |c_{333}|^2 &\leq \lambda_3^{(1)}, \\
|c_{213}|^2 + |c_{223}|^2 &\leq \lambda_2^{(2)}, \\
|c_{231}|^2 + |c_{232}|^2 &\leq \lambda_2^{(3)}.
\end{aligned}$$

By using these inequalities in (38) we find

$$\begin{aligned}
P_4 \geq\ &|c_{133}|^2 + |c_{333}|^2 + |c_{213}|^2 + |c_{223}|^2 + |c_{231}|^2 + |c_{232}|^2 \\
&+\lambda_1^{(1)} + \lambda_3^{(1)} - \lambda_3^{(2)} - \lambda_3^{(3)}.
\end{aligned}$$

By letting $\lambda_1^{(1)} = \sum_{j,k} |c_{1jk}|^2$, and similarly for $\lambda_3^{(1)}$, $\lambda_3^{(2)}$ and $\lambda_3^{(3)}$, we find

$$\begin{aligned}
P_4 \geq\ &|c_{111}|^2 + |c_{112}|^2 + |c_{121}|^2 + |c_{122}|^2 - 2|c_{233}|^2 \\
&+|c_{311}|^2 + |c_{312}|^2 + |c_{321}|^2 + |c_{322}|^2. \tag{39}
\end{aligned}$$

By Lemma 9 we can choose a state with $c_{233} = 0$ to achieve the minimum of P_4. Then, Eq. (39) shows that this minimum is nonnegative. $\square$

Our next task is to prove $P_5 \geq 0$.

Lemma 10. *If $c_{133} = c_{132} = 0$, then $P_5 \geq 0$.*

Proof. The function P_5 can be written as

$$P_5 = \lambda_2^{(1)} + 2\lambda_3^{(1)} + \lambda_2^{(2)} - \lambda_3^{(2)} + \lambda_1^{(3)} - \lambda_3^{(3)}. \tag{40}$$

By Proposition 6 and the remark following it we have

$$|c_{233}|^2 + |c_{333}|^2 \leq \lambda_3^{(1)},$$
$$|c_{113}|^2 + |c_{123}|^2 \leq \lambda_2^{(2)}.$$

By using these inequalities in (40) we find

$$\begin{aligned}
P_5 \geq &\ |c_{233}|^2 + |c_{333}|^2 + |c_{113}|^2 + |c_{123}|^2 \\
&+ \lambda_2^{(1)} + \lambda_3^{(1)} - \lambda_3^{(2)} + \lambda_1^{(3)} - \lambda_3^{(3)}.
\end{aligned}$$

By using the expressions of $\lambda_2^{(1)}$, $\lambda_3^{(1)}$, $\lambda_3^{(2)}$ and $\lambda_3^{(3)}$ as sums of $|c_{ijk}|^2$ we find

$$\begin{aligned}
P_5 \geq &\ \lambda_1^{(3)} - |c_{131}|^2 - |c_{132}|^2 - 2|c_{133}|^2 \\
&+ |c_{211}|^2 + |c_{212}|^2 + |c_{221}|^2 + |c_{222}|^2 \\
&+ |c_{311}|^2 + |c_{312}|^2 + |c_{321}|^2 + |c_{322}|^2.
\end{aligned}$$

Since $\lambda_1^{(3)} \geq |c_{131}|^2$, we have $P_5 \geq 0$ if $c_{133} = c_{132} = 0$. $\qquad\square$

Lemma 11. *The function P_5 is nonnegative if $\lambda_2^{(2)} = \lambda_3^{(2)}$, $\lambda_1^{(3)} = \lambda_2^{(3)}$ or $\lambda_2^{(3)} = \lambda_3^{(3)}$.*

Proof. If $\lambda_2^{(2)} = \lambda_3^{(2)}$, then the inequality $P_5 \geq 0$ is equivalent to

$$2\lambda_3^{(2)} + \lambda_1^{(2)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} - 2\lambda_1^{(1)} - \lambda_2^{(1)} \geq 0. \tag{41}$$

Since $\lambda_3^{(2)} \geq 1/3 \geq \lambda_1^{(1)}$, we have $\lambda_3^{(2)} + \lambda_1^{(3)} \geq \lambda_1^{(1)}$. Hence inequality (41) will follow from

$$\lambda_3^{(2)} + \lambda_1^{(2)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_1^{(1)} - \lambda_2^{(1)} \geq 0.$$

This follows from inequality (1) by letting $(abc) = (123)$ and noting that $\lambda_3^{(2)} \geq \lambda_2^{(2)}$. If $\lambda_1^{(3)} = \lambda_2^{(3)}$, then

$$\begin{aligned}
P_5 &= 2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} + \lambda_1^{(3)} - 2\lambda_1^{(1)} - \lambda_2^{(1)} \\
&= P_4 + \lambda_2^{(1)} - \lambda_1^{(1)}.
\end{aligned}$$

This is nonnegative because $P_4 \geq 0$. Finally, let $\lambda_2^{(3)} = \lambda_3^{(3)}$. From Corollary 1 we have

$$\lambda_2^{(2)} + \lambda_3^{(1)} \geq \lambda_2^{(3)}.$$

By adding this to inequality (3) with $(abc) = (321)$ we obtain

$$2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_3^{(1)} + \lambda_2^{(1)} \geq 2\lambda_2^{(3)} + \lambda_3^{(3)} = 2\lambda_3^{(3)} + \lambda_2^{(3)}.$$

This is equivalent to the inequality $P_5 \geq 0$. $\qquad\square$

Thus we only need to deal with the cases with $\lambda_1^{(1)} = \lambda_2^{(1)}$, $\lambda_2^{(1)} = \lambda_3^{(1)}$ or $\lambda_1^{(2)} = \lambda_2^{(2)}$.

Lemma 12. *Suppose that the minimum of P_5 is negative. Then it does not occur in any of the following three cases:*

1. *$\lambda_1^{(1)} = \lambda_2^{(1)}$ with no other degeneracy;*

2. *$\lambda_2^{(1)} = \lambda_3^{(1)}$ with no other degeneracy;*

3. *$\lambda_1^{(2)} = \lambda_2^{(2)}$ with no other degeneracy.*

Proof. Case 1. By Lemma 8 we have either $\lambda_3^{(1)} = 0$ or $\lambda_2^{(2)} = \lambda_1^{(3)} = 0$. The first case is impossible. The second case leads to $\lambda_3^{(2)} = 1$. Then, by Lemma 2 we have $P_5 \geq 0$.

Case 2. By Lemma 7 we must have $\lambda_2^{(2)} = \lambda_1^{(3)} = 0$. This implies that $\lambda_3^{(2)} = 1$. By Lemma 2 we have $P_5 \geq 0$.

Case 3. By Corollary 2 we must have $\lambda_3^{(1)} = \lambda_1^{(3)} = 0$. This is impossible. $\square$

The following lemma completes the proof of inequality (5).

Lemma 13. *Suppose that the minimum of P_5 is negative. Then it does not occur in any of the following three cases:*

1. *$\lambda_1^{(1)} = \lambda_2^{(1)} = \lambda_3^{(1)}$;*

2. *$\lambda_1^{(1)} = \lambda_2^{(1)}$ and $\lambda_1^{(2)} = \lambda_2^{(2)}$ with no other degeneracy;*

3. *$\lambda_2^{(1)} = \lambda_3^{(1)}$ and $\lambda_1^{(2)} = \lambda_2^{(2)}$ with no other degeneracy.*

Proof. We will show that there is a state with $c_{133} = c_{132} = 0$ where the function P_5 has its minimum if it occurs in any of the three cases. Then by Lemma 10 we conclude that the minimum must be nonnegative.

Case 1. Any unitary transformation on the first qutrit leaves the RDMs diagonal. Consider the vectors $(c_{133}, c_{233}, c_{333})$ and $(c_{132}, c_{232}, c_{332})$. By a unitary transformation on the first qutrit we can set $c_{133} = c_{233} = c_{132} = 0$.

Case 2. Suppose that $(c_{132}, c_{232}) = (0, 0)$ or $(c_{133}, c_{233}) = (0, 0)$. Then both c_{132} and c_{133} can be made zero by a unitary transformation on the first qutrit. Hence, all we need to show is that if $(c_{132}, c_{232}) \neq (0, 0)$, then $(c_{133}, c_{233}) = 0$ at a state where the function P_5 is minimized. Suppose $(c_{132}, c_{232}) \neq (0, 0)$ and $c_{33k} \neq 0$ for some k. Then by Lemma 3 we have $L(3, 3, k) \leq L(2, 3, 2) = 0$, which implies that $r_k = 0$, i.e. $k = 3$. Next, suppose that $(c_{31k}, c_{32k}) \neq (0, 0)$. Then, by Lemma 5 we have $L(3, 1, k) \leq L(2, 3, 2)$, i.e. $r_k \leq -1$. This is impossible. Hence $(c_{31k}, c_{32k}) = (0, 0)$ for all k. Thus, c_{333} is the only nonzero coefficient of the form c_{3jk}. Then by orthogonality relations we have $(c_{133}, c_{233}) = (0, 0)$.

Case 3. Note that the triple [133] is not linked to the degenerate sector of the RDMs in the sense that $\lambda_1^{(1)} \neq \lambda_2^{(1)}$, $\lambda_3^{(2)} \neq \lambda_2^{(2)}$ and $\lambda_3^{(3)} \neq \lambda_2^{(3)}$. Since $L(1, 3, 3) = -2$ and $L(i, j, k) > -2$ for all other triples [ijk], if $c_{133} \neq 0$, then $c_{ijk} = 0$ for any other [ijk]. This implies that $\lambda_3^{(1)} = 0$, which is a contradiction. Thus, we can assume that $c_{133} = 0$. Suppose that $c_{132} \neq 0$. If $(c_{33k}, c_{23k}) \neq (0, 0)$ as well, then by Lemma 3 we have $L(2, 3, k) \leq L(1, 3, 2) = -1$, hence $r_k = 0$, i.e. $k = 3$. Next, if $(c_{32k}, c_{31k}, c_{22k}, c_{21k}) \neq (0, 0, 0, 0)$, then by Lemma 4 we have $L(2, 1, k) \leq L(1, 3, 2)$. This is impossible for any k. Hence $c_{32k} = c_{31k} = c_{22k} = c_{21k} = 0$.

Thus, the only nonzero coefficient of the form c_{3jk} (c_{2jk}) is c_{333} (c_{233}). Then, by orthogonality we must have $c_{233} = 0$ since $\lambda_3^{(1)} \neq 0$. Then $\lambda_2^{(1)} = 0$ and hence $\lambda_3^{(1)} \neq \lambda_2^{(1)}$, contradicting the assumption. $\square$

VII.   PROOF OF INEQUALITIES (6) AND (7)

For the case where there are two pairs of degenerate eigenvalues, it is useful to consider the variation of the eigenvalues for some variation of the coefficients c_{IJK} in a general setting.

Proposition 8. *Suppose that $\lambda_i^{(1)} = \lambda_{i+1}^{(1)}$ and $\lambda_j^{(2)} = \lambda_{j+1}^{(2)}$, and that there is no other degeneracy. Suppose further that*

$$\begin{pmatrix} c_{ijk} & c_{i,j+1,k} \\ c_{i+1,jk} & c_{i+1,j+1,k} \end{pmatrix} \text{ and } (c_{ij'k'}, c_{i+1,j'k'}) \text{ are nonzero.}$$

Let $c_{i,j+1,k} = c_{i+1,j,k} = 0$ by using unitary transformations, and let

$$\delta c_{ijk} = \alpha_1 c_{ij'k'} + \alpha_2 c_{i+1,j'k'}, \quad \delta c_{i+1,j+1,k} = \beta_1 c_{ij'k'} + \beta_2 c_{i+1,j'k'},$$
$$\delta c_{ij'k'} = -\overline{\alpha_1} c_{ijk} - \overline{\beta_1} c_{i+1,j+1,k}, \quad \delta c_{i+1,j'k'} = -\overline{\alpha_2} c_{ijk} - \overline{\beta_2} c_{i+1,j+1,k},$$

where $j' \neq j$ and $j' \neq j+1$, but k' may or may not be equal to k. Define $a_{I+1} \equiv 2\mathrm{Re}\,(\alpha_{I+1}\overline{c_{i+I,j'k'}} c_{ijk})$ and $b_{I+1} \equiv 2\mathrm{Re}\,(\beta_{i+I}\overline{c_{i+I,j'k'}} c_{i+1,j+1,k})$, $I = 0, 1$. Then it is possible to arrange the variation of the coefficients $c_{i,j+1,k}$ and $c_{i+1,jk}$ so that the variation of the RDMs is effectively diagonal without making a_1, a_2, b_1 and b_2 all vanish. If $k \neq k'$, the variation of the eigenvalues of the RDMs is given as follows:

$$\delta\lambda_i^{(1)} = -|a_2 - b_1|, \quad \delta\lambda_{i+1}^{(1)} = |a_2 - b_1|,$$
$$\delta\lambda_j^{(2)} = \min\,(a_1 + a_2, b_1 + b_2), \quad \delta\lambda_{j+1}^{(2)} = \max\,(a_1 + a_2, b_1 + b_2),$$
$$\delta\lambda_{j'}^{(2)} = -a_1 - a_2 - b_1 - b_2, \quad \delta\lambda_k^{(3)} = a_1 + a_2 + b_1 + b_2,$$
$$\delta\lambda_{k'}^{(3)} = -a_1 - a_2 - b_1 - b_2.$$

If $k = k'$, then $\delta\lambda_k^{(3)} = \delta\lambda_{k'}^{(3)} = 0$, and the variation of the other eigenvalues remains the same.

Proof. By requiring the variation of the RDMs to be effectively diagonal, we find

$$c_{ijk}\overline{\delta c_{i+1,jk}} + \delta c_{i,j+1,k}\overline{c_{i+1,j+1,k}} = -\delta\,[c_{ij'k'}\overline{c_{i+1,j'k'}}],$$
$$\overline{c_{ijk}}\delta c_{i,j+1,k} + \overline{\delta c_{i+1,jk}}c_{i+1,j+1,k} = 0.$$

Thus, if $|c_{ijk}|^2 \neq |c_{i+1,j+1,k}|^2$, then we can solve for $\delta c_{i+1,jk}$ and $\delta c_{i,j+1,k}$ to make the variation of the RDMs effectively diagonal. If $|c_{ijk}|^2 = |c_{i+1,j+1,k}|^2$, we first use phase transformations to have $c_{ijk} = c_{i+1,j+1,k}$. Then any unitary transformation on the first qutrit can be compensated by a unitary transformation on the second qutrit while maintaining the condition $c_{i+1,jk} = c_{i,j+1,k} = 0$. Thus we can make $c_{i+1,j'k'}$ vanish as well. Then by letting $\delta c_{i+1,j'k'} = \delta c_{i+1,jk} = \delta c_{i,j+1,k} = 0$, the variation of the RDMs can be kept effectively diagonal. We have $\alpha_2 = \beta_2 = 0$ and $a_2 = b_2 = 0$ as a consequence but can have $a_1 \neq 0$ or $b_1 \neq 0$ by the assumption on the coefficients. (Since we have made $c_{i+1,j'k'}$ vanish, the equation $\alpha_2 = \beta_2 = 0$ does not give rise to any further constraint on the variation of the eigenvalues.) The calculation of the variation of the eigenvalues is straightforward. $\square$

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Remark. This proposition remains valid after a qutrit permutation.

Now we prove $P_6 \geq 0$, i.e. inequality (6). Our proof is rather lengthy.

Lemma 14. *If* $\lambda_1^{(1)} = \lambda_2^{(1)}$, $\lambda_2^{(2)} = \lambda_3^{(2)}$ *or* $\lambda_2^{(3)} = \lambda_3^{(3)}$, *then* $P_6 \geq 0$.

Proof. Inequality (3) with $(abc) = (123)$ reads

$$\lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} + \lambda_3^{(3)} \geq \lambda_2^{(1)} + \lambda_3^{(1)}. \tag{42}$$

From inequality (1) we have

$$
\begin{aligned}
\lambda_2^{(2)} + \lambda_2^{(3)} &\geq \frac{1}{2}\left(\lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} + \lambda_1^{(3)}\right) \\
&\geq \frac{1}{2}\left(\lambda_2^{(1)} + \lambda_1^{(1)}\right) \\
&\geq \lambda_1^{(1)}.
\end{aligned}
$$

By adding these two inequalities we obtain

$$2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} + \lambda_3^{(3)} \geq \lambda_1^{(1)} + \lambda_2^{(1)} + \lambda_3^{(1)}.$$

This is equivalent to inequality (6) if $\lambda_1^{(1)} = \lambda_2^{(1)}$. Next we recall that $\lambda_3^{(2)} + \lambda_2^{(3)} \geq \lambda_2^{(1)}$ (Corollary 1). By adding this to (42) we have

$$\lambda_3^{(2)} + \lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} + \lambda_3^{(3)} \geq 2\lambda_2^{(1)} + \lambda_3^{(1)}.$$

This is equivalent to inequality (6) if $\lambda_2^{(2)} = \lambda_3^{(2)}$. Next, if we add the inequality $\lambda_2^{(2)} + \lambda_3^{(3)} \geq \lambda_2^{(1)}$ to inequality (42), we have

$$2\lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} + 2\lambda_3^{(3)} \geq 2\lambda_2^{(1)} + \lambda_3^{(1)}.$$

This is equivalent to inequality (6) if $\lambda_2^{(3)} = \lambda_3^{(3)}$. $\qquad\square$

The following lemmas will be useful in proving $P_6 \geq 0$.

Lemma 15. *The function* P_6 *is nonnegative if* $c_{231} = c_{233} = c_{331} = 0$.

Proof. By Proposition 6 we have $|c_{211}|^2 + |c_{221}|^2 \leq \lambda_2^{(2)}$. Hence

$$
\begin{aligned}
P_6 &= \lambda_1^{(1)} - \lambda_2^{(1)} + 2\lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} - \lambda_1^{(3)} \\
&\geq \lambda_1^{(1)} - \lambda_2^{(1)} + \lambda_1^{(2)} + \lambda_2^{(2)} + \lambda_2^{(3)} - \lambda_1^{(3)} + |c_{221}|^2 + |c_{211}|^2.
\end{aligned}
$$

Then, if we substitute $\lambda_i^{(1)} = \sum_{JK} |c_{iJK}|^2$ and the similar formulae for $\lambda_j^{(2)}$ and $\lambda_k^{(3)}$, the only coefficients that contribute negatively to P_6 are $c_{231}, c_{233}, c_{331}$. Hence, if these coefficients vanish, then $P_6 \geq 0$. $\qquad\square$

Lemma 16. *The function* P_6 *is nonnegative if* $c_{232} = c_{233} = c_{332} = 0$.

Proof. Note first that

$$P_6 \geq \tilde{P}_6 \equiv 2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_1^{(3)} + \lambda_3^{(3)} - 2\lambda_2^{(1)} - \lambda_3^{(1)} .$$

It can be shown that $\tilde{P}_6 \geq 0$ under the assumption of this lemma by the argument in the proof of the previous lemma with $\lambda_1^{(3)} \leftrightarrow \lambda_2^{(3)}$. $\qquad\square$

Lemma 17. *If $c_{233} = c_{333} = 0$, then $P_6 \geq 0$.*

Proof. Since $\lambda_2^{(2)} + \lambda_3^{(3)} \geq \lambda_2^{(1)}$ by Corollary 1, we have

$$\begin{aligned} P_6 &\geq \lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_2^{(3)} - \lambda_2^{(1)} - \lambda_3^{(1)} \\ &\geq \lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} + \lambda_1^{(3)} - \lambda_2^{(1)} - \lambda_3^{(1)} . \end{aligned}$$

Using the formulae for the eigenvalues in terms of $|c_{ijk}|^2$ in the last expression, we find that only $|c_{233}|^2$ and $|c_{333}|^2$ have negative coefficients. Hence $P_6 \geq 0$ if $c_{233} = c_{333} = 0$. $\qquad\square$

First we treat the cases with only one pair of degenerate eigenvalues.

Lemma 18. *If the function P_6 has a negative minimum, then it does not occur at a state with any of the following properties:*

1. $\lambda_2^{(1)} = \lambda_3^{(1)}$ *with no other degeneracy;*

2. $\lambda_1^{(2)} = \lambda_2^{(2)}$ *with no other degeneracy;*

3. $\lambda_1^{(3)} = \lambda_2^{(3)}$ *with no other degeneracy.*

Proof. Case 1. By Lemma 8 we have $\lambda_1^{(1)} = 0$ or $\lambda_2^{(2)} = \lambda_2^{(3)} = 0$. The latter case leads to $\lambda_3^{(1)} = \lambda_3^{(2)} = \lambda_3^{(3)} = 1$, and the inequality is obviously satisfied. Hence we can assume that $\lambda_1^{(1)} = 0$, i.e. $c_{1jk} = 0$ for all $[jk]$. Then $\lambda_2^{(1)} = \lambda_3^{(1)} = 1/2$. If $(c_{231}, c_{331}) = (0, 0)$, then by letting $c_{233} = 0$ by a unitary transformation on the first qutrit and using Lemma 15 we have $P_6 \geq 0$. If $(c_{231}, c_{331}) \neq (0, 0)$, then all other vectors of the form (c_{2jk}, c_{3jk}) must be orthogonal to (c_{231}, c_{331}) by Proposition 5. Thus, if we let $c_{331} = 0$ by using a unitary transformation on the first qutrit, then $c_{2jk} = 0$ for all $[jk]$ except $[31]$. Hence $|c_{231}|^2 = \lambda_2^{(1)} = 1/2$, and $\lambda_1^{(3)} \geq |c_{231}|^2 = 1/2$, which is a contradiction.

Case 2. Corollary 2 implies that $\lambda_1^{(1)} = \lambda_2^{(3)} = 0$, and by Lemma 2 we have $P_6 \geq 0$.

Case 3. Assume that $c_{233} \neq 0$. Then, since there is no $[ij]$ satisfying $L(i, j, 3) = -1$ except $[ij] = [23]$ and since the triple $[233]$ is not connected to the degenerate sector, the c_{233} is the only nonzero coefficient of the form c_{ij3}. Then, by orthogonality relations we have $c_{231} = c_{232} = 0$. If $(c_{ij1}, c_{ij2}) \neq (0, 0)$, by Lemma 4 we must have $L(i, j, 1) \leq L(2, 3, 3)$, i.e. $p_i + q_j \geq -1$. Hence $[ij] = [23]$, which has been rejected, $[21]$ or $[33]$. Then $\lambda_2^{(3)} = 0$, and we have $P_6 \geq 0$ by Lemma 2. Thus, we can assume that $c_{233} = 0$. If $(c_{231}, c_{232}) = (0, 0)$ $[(c_{331}, c_{332}) = (0, 0)]$, then we can have $c_{331} = 0$ $[c_{231} = 0]$ in addition by a unitary transformation on the third qutrit. Then $P_6 \geq 0$ by Lemma 15. Assume that (c_{231}, c_{232}) and (c_{331}, c_{332}) are both nonzero. These vectors are orthogonal to each other by Proposition 5 applied to the case with degeneracy in the third qutrit. Then the only other possible nonzero vector of the form (c_{ij1}, c_{ij2}) is (c_{211}, c_{212}) by the same proposition. For c_{ij3} to be nonzero we must have $L(i, j, 3) \leq \min[L(2, 3, 2), L(2, 1, 2), L(3, 3, 2)] = 1$. All nonzero coefficients of

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the form c_{ij3} must have the same value of $L(i, j, 3)$. In order not to have $\lambda_2^{(2)} = 0$ (and hence $P_6 \geq 0$ by Lemma 2) we must have $L(i, j, 3) = 1$ and the possibly nonzero coefficients of the form c_{ij3} are c_{223}, c_{313} and c_{133}. (We mean, strictly speaking, that c_{ij3} is nonzero only if $[ij3]$ is in the set $\{[223], [313], [133]\}$.) Then $c_{233} = c_{333} = 0$, and by Lemma 17 we have $P_6 \geq 0$. $\qquad\square$

Remark. We abbreviate the phrase "possibly nonzero coefficient" as PNC below.

The following lemma is used in the most degenerate case.

Lemma 19. *If* $c_{231} = c_{211} = c_{233} = c_{213} = 0$, *then* $P_6 \geq 0$.

Proof. First we note inequality (3) with $(abc) = (123)$:

$$\lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} + \lambda_3^{(3)} - \lambda_2^{(1)} - \lambda_3^{(1)} \geq 0.$$

The inequality $P_6 \geq 0$ follows from this if

$$\lambda_2^{(2)} + \lambda_2^{(3)} - \lambda_2^{(1)} \geq 0.$$

By using the expression for $\lambda_2^{(a)}$ in terms of $|c_{ijk}|^2$ we find that this inequality is satisfied if $c_{211} = c_{213} = c_{231} = c_{233} = 0$, as required. $\qquad\square$

Now we treat the most degenerate case.

Proposition 9. *If the minimum value of* P_6 *is negative, then it does not occur at a state with* $\lambda_2^{(1)} = \lambda_3^{(1)}$, $\lambda_1^{(2)} = \lambda_2^{(2)}$, $\lambda_1^{(3)} = \lambda_2^{(3)}$ *and with no other degeneracy.*

Proof. Note that we can make c_{233}, c_{231} and c_{211} vanish by successively using unitary transformations on the first, third and second qutrits. Then the only PNC with a negative level is c_{331}. We will show that if $c_{331} \neq 0$, then $c_{213} = 0$. Then by Lemma 19 we have $P_6 \geq 0$. Thus, we assume that

$$\begin{pmatrix} c_{331} & c_{332} \\ c_{231} & c_{232} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} c_{323} & c_{313} \\ c_{223} & c_{213} \end{pmatrix}$$

are nonzero and derive a contradiction.

Suppose that the first matrix has rank less than two. Then after making c_{233} vanish by using a unitary transformation on the first qutrit, we can make c_{231} and c_{331} vanish simultaneously by a unitary transformation on the third qutrit. Then, by Lemma 15 we have $P_6 \geq 0$. Thus, we can assume that the first matrix has rank two. We set $c_{231} = c_{332} = 0$ by unitary transformations on the first and third qutrits and let $c_{313} = 0$ by using a unitary transformation on the second qutrit. Then, the above matrices become

$$\begin{pmatrix} c_{331} & 0 \\ 0 & c_{232} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} c_{323} & 0 \\ c_{223} & c_{213} \end{pmatrix}$$

with $c_{331} \neq 0$ and $c_{232} \neq 0$. Let us consider the following variation:

$$\begin{aligned}
\delta c_{323} &= -\alpha_1 c_{331} - \alpha_2 c_{232}, \\
\delta c_{213} &= -\beta_1 c_{331} - \beta_2 c_{232}, \\
\delta c_{223} &= -\gamma_1 c_{331} - \gamma_2 c_{232}, \\
\delta c_{331} &= \overline{\alpha_1} c_{323} + \overline{\beta_1} c_{213} + \overline{\gamma_1} c_{223}, \\
\delta c_{232} &= \overline{\alpha_2} c_{323} + \overline{\beta_2} c_{213} + \overline{\gamma_2} c_{223}.
\end{aligned}$$

By requiring that the variation of the RDMs be effectively diagonal we have

$$c_{331}\overline{\delta c_{231}} + \delta c_{332}\overline{c_{232}} + \delta c_{313}\overline{c_{213}} = -\delta\left[c_{323}\overline{c_{223}}\right],$$

$$\delta c_{313}\overline{c_{323}} = -\delta\left[c_{213}\overline{c_{223}}\right],$$

$$c_{232}\overline{\delta c_{231}} + \delta c_{332}\overline{c_{331}} = 0.$$

These equations can be consistently solved for δc_{231}, δc_{332} and δc_{313} provided that $c_{323} \neq 0$ and $|c_{331}|^2 \neq |c_{232}|^2$. (Notice that the variations δc_{231}, δc_{332} and δc_{313} do not contribute to the variation of the diagonal elements.) If $c_{323} = 0$, then we can use a unitary transformation on the second qutrit to eliminate c_{223} as well. Then $\delta[c_{323}\overline{c_{223}}] = \delta[c_{213}\overline{c_{223}}] = 0$ if we set $\gamma_1 = \gamma_2 = 0$. Then we can simply let $\delta c_{332} = \delta c_{313} = \delta c_{231} = 0$. If $|c_{331}|^2 = |c_{232}|^2$, then we can use a phase transformation to have $c_{331} = c_{232}$. Then any unitary transformation in the first qutrit can be compensated by a unitary transformation in the third qutrit to keep c_{331} and c_{232} unchanged and keep the condition $c_{231} = c_{332} = 0$. This means that we can diagonalize the second matrix as well, making c_{223} vanish in addition. Then we again have $\delta[c_{323}\overline{c_{223}}] = \delta[c_{213}\overline{c_{223}}] = 0$ if we let $\gamma_1 = \gamma_2 = 0$. Then we can let $\delta c_{332} = \delta c_{313} = \delta c_{231} = 0$.

Let us introduce the following definitions: $a_i \equiv 2\mathrm{Re}\left(\alpha_i C^{(i)}\overline{c_{323}}\right)$, $b_i \equiv 2\mathrm{Re}\left(\beta_i C^{(i)}\overline{c_{213}}\right)$ and $c_i \equiv 2\mathrm{Re}\left(\gamma_i C^{(i)}\overline{c_{223}}\right)$, where $C^{(1)} \equiv c_{331}$ and $C^{(2)} \equiv c_{232}$. The variation of the function P_6 can be given as follows:

$$\delta P_6 = \delta\lambda_1^{(1)} - \delta\lambda_2^{(1)} + \delta\lambda_2^{(2)} - \delta\lambda_3^{(2)} + \delta\lambda_2^{(3)} - \delta\lambda_1^{(3)}.$$

Assume first that $c_{323} \neq 0$ and $|c_{331}|^2 \neq |c_{232}|^2$ and that the variation of the RDMs is made effectively diagonal. Then, we have

$$\begin{aligned}\delta P_6 = {} & |a_2 - b_1 - c_1| - \min\left(a_1 + a_2 + c_1 + c_2, b_1 + b_2\right)\\ & -(a_1 + b_1 + c_1 + a_2 + b_2 + c_2)\\ & +|a_2 + b_2 + c_2 - a_1 - b_1 - c_1|.\end{aligned}$$

If a_1 can be made nonzero, then so can a_2, and vice versa, and similarly for b_1, b_2, c_1 and c_2 because c_{331} and c_{232} are both nonzero. Hence we can always have $a_2 + b_2 + c_2 = a_1 + b_1 + c_1$ by adjusting α_i, β_i and γ_i, $i = 1, 2$. We can also choose all coefficients to be nonnegative. Then,

$$\delta P_6 \leq |a_2 - b_1 - c_1| - (a_1 + b_1 + c_1 + a_2 + b_2 + c_2).$$

If a_1 and a_2 can be made nonzero, then by choosing the others to be zero (by letting $\beta_i = \gamma_i = 0$, $i = 1, 2$) we find $\delta P_6 \leq -a_1 < 0$. If $a_1 = a_2 = 0$, then $\delta P_6 \leq -b_2 - c_2$. Since b_2 or c_2 can be made positive — otherwise $c_{323} = c_{223} = c_{213} = 0$ — we have $\delta P_6 < 0$. If $c_{323} = 0$, then we have $a_1 = a_2 = 0$ and $c_1 = c_2 = 0$ to make the variation of the RDMs effectively diagonal, but we can still make b_1 and b_2 positive. Then we can have $\delta P_6 < 0$. Similarly, if $|c_{331}|^2 = |c_{232}|^2$, we must have $c_1 = c_2 = 0$, but we can still have either $a_1 \neq 0$, $a_2 \neq 0$ or $b_1 \neq 0$, $b_2 \neq 0$ (or both). Then we can have $\delta P_6 < 0$.

Thus, if $c_{331} \neq 0$ and $c_{213} \neq 0$ at the same time, we can always lower the value of P_6 if it is negative. Hence, if c_{331} and c_{213} are both nonzero, the function P_6 does not have a negative minimum. $\qquad\qquad\Box$

Finally we deal with the cases with two pairs of degenerate eigenvalues to complete the proof of inequality (6).

Lemma 20. *Suppose that the minimum of the function P_6 is negative. Then it does not occur at a state with $\lambda_2^{(1)} = \lambda_3^{(1)}$ and $\lambda_1^{(2)} = \lambda_2^{(2)}$ and without any other degeneracy.*

Proof. If $(c_{231}, c_{331}) = (0, 0)$, then we can use a unitary transformation on the first qutrit to make c_{233} vanish. Then $P_6 \geq 0$ by Lemma 15. Thus, we can assume that $(c_{231}, c_{331}) \neq (0, 0)$. If $(c_{233}, c_{333}) = 0$, then we have $P_6 \geq 0$ by Lemma 17. Thus, we can also assume $(c_{233}, c_{333}) \neq 0$. By Proposition 5 we conclude that the vectors (c_{231}, c_{331}) and (c_{233}, c_{333}) are orthogonal to each other. By the same proposition (c_{232}, c_{332}) must be orthogonal to both of these vectors. This implies that $(c_{232}, c_{332}) = (0, 0)$. Then by a unitary transformation on the first qutrit we can have $c_{233} = 0$, and we conclude that $P_6 \geq 0$ by Lemma 16. $\square$

Lemma 21. *Suppose that the minimum of the function P_6 is negative. Then it does not occur at a state with $\lambda_2^{(1)} = \lambda_3^{(1)}$ and $\lambda_1^{(3)} = \lambda_2^{(3)}$ and without any other degeneracy.*

Proof. Suppose that $(c_{231}, c_{331}) = (0, 0)$. Then we can have $c_{233} = 0$ while maintaining $c_{231} = c_{331} = 0$ by a unitary transformation on the first qutrit. Then $P_6 \geq 0$ by Lemma 15. Next, suppose $c_{213} = c_{313} = c_{223} = c_{323} = 0$. First we use a unitary transformation on the first qutrit to let $c_{233} = 0$. Then a unitary transformation on the third qutrit can be used to have $c_{231} = 0$. Since $c_{213} = c_{223} = 0$, by Proposition 6 we have

$$|c_{331}|^2 + |c_{333}|^2 \leq \lambda_3^{(3)} = \lambda_3^{(3)} - |c_{213}|^2 - |c_{223}|^2 \, .$$

We use this together with $|c_{211}|^2 + |c_{221}|^2 \leq \lambda_2^{(2)}$ to have

$$
\begin{aligned}
P_6 &= \lambda_1^{(1)} - \lambda_2^{(1)} + \lambda_2^{(2)} - \lambda_3^{(2)} + 2\lambda_2^{(3)} + \lambda_3^{(3)} \\
&\geq \lambda_1^{(1)} - \lambda_2^{(1)} - \lambda_3^{(2)} + 2\lambda_2^{(3)} \\
&\quad + |c_{211}|^2 + |c_{221}|^2 + |c_{331}|^2 + |c_{333}|^2 + |c_{213}|^2 + |c_{223}|^2 \, .
\end{aligned}
$$

By substituting the expression of $\lambda_I^{(a)}$ in terms of $|c_{ijk}|^2$ we find

$$P_6 \geq -2(|c_{231}|^2 + |c_{233}|^2) = 0 \, .$$

Thus, it is enough to show that if $(c_{231}, c_{331}, c_{232}, c_{332}) \neq (0, 0, 0, 0)$, then $(c_{223}, c_{323}) = (c_{213}, c_{313}) = (0, 0)$.

If the matrix

$$
\begin{pmatrix}
c_{231} & c_{331} \\
c_{232} & c_{332}
\end{pmatrix}
\tag{43}
$$

has rank less than two, then we can set $c_{231} = c_{331} = 0$ by a unitary transformation on the third qutrit. Then a unitary transformation on the first qutrit can be used to let $c_{233} = 0$. Then $P_6 \geq 0$. Therefore we can assume that the matrix (43) is regular.

First we use Proposition 8 after a qutrit permutation $(123) \rightarrow (132)$ with $[ijk] = [213]$ and $[i'j'k'] = [132]$ to show that $(c_{223}, c_{323}) = (0, 0)$. By considering the variation as given in Proposition 8 we find

$$
\begin{aligned}
\delta P_6 &= \delta\lambda_1^{(1)} - \delta\lambda_2^{(1)} + \delta\lambda_2^{(2)} - \delta\lambda_3^{(2)} + \delta\lambda_2^{(3)} - \delta\lambda_1^{(3)} \\
&= |a_2 - b_1| - \max(a_1 + a_2, b_1 + b_2) - 3\min(a_1 + a_2, b_1 + b_2) \, .
\end{aligned}
$$

This can be made negative unless $a_1 + a_2 = 0$ or $b_1 + b_2 = 0$. Since the matrix in (43) is regular, we can have $a_i \neq 0$ if $b_i \neq 0$ and vice versa for both $i = 1$ and 2. Thus, unless

$a_1 = a_2 = b_1 = b_2 = 0$, we can have both $a_1 + a_2$ and $b_1 + b_2$ nonzero. Hence δP_6 can be made negative. Thus, unless $(c_{223}, c_{323}) = (0, 0)$, P_6 cannot have a minimum. Next we change k' from 2 to 1 to show that $(c_{213}, c_{313}) = (0, 0)$. The only difference here is that we have $\delta\lambda_2^{(3)} = 0$ instead of $\lambda_2^{(3)} = -a_1 - a_2 - b_1 - b_2$. Thus we find

$$\delta P_6 = |a_2 - b_1| - 2\min(a_1 + a_2, b_1 + b_2).$$

Again, this can be made negative unless $a_1 + a_2 = 0$ or $b_1 + b_2 = 0$. Hence by the same argument as above we conclude that the function P_6 cannot have a minimum unless $(c_{213}, c_{313}) = (0, 0)$. $\qquad\square$

Lemma 22. *Suppose that the minimum of the function P_6 is negative. Then it does not occur at a state with $\lambda_1^{(2)} = \lambda_2^{(2)}$ and $\lambda_1^{(3)} = \lambda_2^{(3)}$ and without any other degeneracy.*

Proof. Assume that $c_{233} \neq 0$. Then by lemmas in Sec. V we find that the PNCs other than c_{233} are (c_{231}, c_{232}), $(c_{211}, c_{212}, c_{221}, c_{222})$ and (c_{331}, c_{332}). By a unitary transformation we can let $c_{212} = c_{221} = 0$. By orthogonality relations $c_{233}\overline{c_{23i}} = 0$, $i = 1, 2$, we have $c_{231} = c_{232} = 0$. Hence the PNCs are $c_{233}, c_{211}, c_{222}, c_{331}$ and c_{332}. If $c_{332} = 0$, then $|c_{331}|^2 \geq |c_{222}|^2 + |c_{233}|^2 + |c_{211}|^2$ but $|c_{233}|^2 \geq |c_{331}|^2$ and $|c_{222}|^2 \geq |c_{331}|^2$. These imply that $c_{331} = c_{233} = c_{211} = c_{222} = 0$, which is a contradiction. Hence $c_{332} \neq 0$ and by an orthogonality relation we have $c_{331} = 0$. Then

$$P_6 = -|c_{233}|^2 - |c_{211}|^2 + 2|c_{222}|^2 + |c_{332}|^2 \geq 0$$

because $|c_{332}|^2 \geq |c_{233}|^2 + |c_{211}|^2 + |c_{222}|^2$.

Next suppose that $c_{233} = 0$. Suppose further that $(c_{231}, c_{232}) = (0, 0)$. Then, we can use a unitary transformation on the third qutrit to have $c_{331} = 0$. Then $P_6 \geq 0$ by Lemma 15. Hence we assume that $(c_{231}, c_{232}) \neq (0, 0)$. Let us use a unitary transformation to let $c_{232} = 0$ for convenience. Note that $L(2, 3, 1) = -2$ and $L(2, 3, 2) = 0$. Since $L(1, 3, 3) = 1$, we must have $c_{133} = 0$ by Lemma 3. For (c_{113}, c_{123}) to be nonzero, we must have $L(1, 1, 3) < L(2, 3, 2)$, which is false, by Lemma 5. Hence $(c_{113}, c_{123}) = (0, 0)$. Similarly, for $(c_{313}, c_{323}) \neq (0, 0)$ we must have $L(3, 1, 3) < L(2, 3, 2)$, which is false. Hence $(c_{313}, c_{323}) = (0, 0)$. Thus, the PNCs of the form c_{ij3} are c_{213}, c_{223} and c_{333}. (We have already shown that $c_{233} = 0$.)

By applying Proposition 5 to the case with degeneracy in the third qutrit, we find that (c_{131}, c_{132}) and (c_{331}, c_{332}) are mutually orthogonal and are both orthogonal to (c_{231}, c_{232}). Since we have let $c_{232} = 0$, we obtain $c_{131} = c_{331} = 0$ and either c_{332} or c_{132} must vanish. However, if $c_{332} = 0$, then we have $P_6 \geq 0$ by Lemma 16. Hence we can assume that $c_{332} \neq 0$ and $c_{132} = 0$. Next, we use Proposition 8 after a qutrit permutation $(123) \to (321)$ with $[ijk] = [111]$ and $k' = 2$. Then we find

$$\delta P_6 = 3(a_1 + a_2 + b_1 + b_2) + 2|a_2 - b_1| + \max(a_1 + a_2, b_1 + b_2).$$

By making all a_i and b_i nonpositive, we obtain

$$\delta P_6 \leq 3a_1 + a_2 + b_1 + 3b_2.$$

The right-hand side can be made negative unless $a_1 = a_2 = b_1 = b_2 = 0$. Hence $c_{111} = c_{112} = c_{121} = c_{122} = 0$.

Next we apply Proposition 8 with $[ijk] = [113]$. The only difference is that we have $\delta\lambda_1^{(1)} = 0$ instead of $\delta\lambda_1^{(1)} = a_1 + a_2 + b_1 + b_2$. Hence

$$\delta P_6 = 2(a_1 + a_2 + b_1 + b_2) + 2|a_2 - b_1| + \max(a_1 + a_2, b_1 + b_2).$$

If a_1 or b_2 is nonzero, then δP_6 can be made negative by making the nonzero one large and negative. If a_2 and b_1 are both nonzero, then we can let $a_2 = b_1 < 0$ $a_1 = b_2 = 0$ to make $\delta P_6 < 0$. If $\delta P_6 \geq 0$ and if $c_{231} \neq 0$ and $c_{232} = 0$, then the PNCs among c_{3jk}, $j, k = 1, 2$, is c_{322} *after using a unitary transformation in the second qutrit.* If we undo this transformation, we have $c_{312} \neq 0$ as well.

Next let $[ijk] = [112]$ in Proposition 8. Then $\delta\lambda_1^{(1)} = \delta\lambda_2^{(1)} = 0$ and all other variations of the eigenvalues are the same. Hence

$$\delta P_6 = a_1 + a_2 + b_1 + b_2 + 2|a_2 - b_1| + \max(a_1 + a_2, b_1 + b_2).$$

If a_1 or b_2 is nonzero, then by letting the nonzero one be negative and letting $a_2 = b_1 = 0$ we have

$$\delta P_6 \leq a_1 + b_2 < 0.$$

If $a_1 = b_2 = 0$, then

$$\delta P_6 = a_2 + b_1 + 2|a_2 - b_1| + \max(a_2, b_1).$$

If both a_2 and b_1 are nonzero, then by letting $a_2 = b_1$ and letting them be negative, we find

$$\delta P_6 < a_2 + b_1 < 0.$$

By the same argument as in the $k = 3$ case, we have only c_{212} and c_{222} among c_{2jk}, $j, k = 1, 2$, possibly nonzero if $\delta P_6 \geq 0$. Here we can use a unitary transformation on the second qutrit to let $c_{212} = 0$.

Thus, the following coefficients are the PNCs:

$$c_{332}, c_{322}, c_{312}, c_{222}, c_{213}, c_{223}, c_{333}, c_{231}.$$

Recall that $c_{332} \neq 0$. Hence, by orthogonality relations we have $c_{322} = c_{312} = 0$. We may assume that $c_{213} \neq 0$ because otherwise $\lambda_1^{(2)} = \lambda_2^{(2)} = 0$ and $P_6 \geq 0$ by Lemma 2. Then by the orthogonality relation $c_{213}\overline{c_{223}} = 0$, we have $c_{223} = 0$. From $c_{332}\overline{c_{333}} = 0$ we have $c_{333} = 0$. Then $c_{233} = c_{333} = 0$, and by Lemma 17 we have $P_6 \geq 0$. $\square$

Now we turn our attention to inequality (7), i.e. $P_7 \geq 0$.

Lemma 23. *The function P_7 is nonnegative if $\lambda_1^{(1)} = \lambda_2^{(1)}$, $\lambda_1^{(2)} = \lambda_2^{(2)}$ or $\lambda_2^{(2)} = \lambda_3^{(2)}$.*

Proof. If $\lambda_1^{(1)} = \lambda_2^{(1)}$, then $P_7 \geq 0$ is equivalent to

$$2\lambda_1^{(2)} + \lambda_2^{(2)} + 2\lambda_3^{(3)} + \lambda_2^{(3)} \geq 2\lambda_1^{(1)} + \lambda_3^{(1)}.$$

Since $\lambda_3^{(3)} \geq 1/3 \geq \lambda_1^{(1)}$ and $\lambda_1^{(2)} \geq 0$, it is enough to show that

$$\lambda_1^{(2)} + \lambda_2^{(2)} + \lambda_3^{(3)} + \lambda_2^{(3)} \geq \lambda_1^{(1)} + \lambda_3^{(1)}.$$

This follows from inequality (3) since $\lambda_2^{(1)} \geq \lambda_1^{(1)}$. If $\lambda_1^{(2)} = \lambda_2^{(2)}$, then $P_7 \geq 0$ is equivalent to

$$2\lambda_2^{(2)} + \lambda_1^{(2)} + 2\lambda_3^{(3)} + \lambda_2^{(3)} \geq 2\lambda_2^{(1)} + \lambda_3^{(1)},$$

which follows from inequality (6). Finally, if $\lambda_2^{(2)} = \lambda_3^{(2)}$, then $\lambda_1^{(2)} = 1 - 2\lambda_2^{(2)}$. Hence

$$\begin{aligned}
P_7 &= 2 - 3\lambda_2^{(2)} + 2\lambda_3^{(3)} + \lambda_2^{(3)} - 2\lambda_2^{(1)} - \lambda_3^{(1)} \\
&= 2 - 3\lambda_2^{(2)} + \lambda_3^{(3)} - \lambda_1^{(3)} - \lambda_2^{(1)} + \lambda_1^{(1)}.
\end{aligned}$$

Since $\lambda_2^{(2)}$ and $\lambda_2^{(1)}$ are both less than or equal to $1/2$, we have $P_7 \geq 0$. $\qquad \square$

Thus, the only degeneracies we need to consider are $\lambda_2^{(1)} = \lambda_3^{(1)}$, $\lambda_1^{(3)} = \lambda_2^{(3)}$ and $\lambda_2^{(3)} = \lambda_3^{(3)}$.

Lemma 24. *If $c_{231} = c_{221} = c_{331} = 0$, then $P_7 \geq 0$.*

Proof. Writing P_7 as

$$P_7 = \lambda_1^{(1)} - \lambda_2^{(1)} + \lambda_1^{(2)} - \lambda_3^{(2)} + 2\lambda_3^{(3)} + \lambda_2^{(3)}$$

and noting that $|c_{232}|^2 + |c_{233}|^2 \leq \lambda_3^{(3)}$, which follows from Proposition 6 and the remark following it, we have

$$P_7 = \lambda_2^{(3)} + \lambda_3^{(3)} + \lambda_1^{(1)} - \lambda_2^{(1)} + \lambda_1^{(2)} - \lambda_3^{(2)} + |c_{232}|^2 + |c_{233}|^2.$$

Then, by expressing the eigenvalues in terms of $|c_{ijk}|^2$ we find that the negative terms are $-2|c_{231}|^2 - |c_{221}|^2 - |c_{331}|^2$. Hence, if $c_{231} = c_{221} = c_{331} = 0$, then $P_7 \geq 0$. $\qquad \square$

Lemma 25. *If $\lambda_2^{(1)} = \lambda_3^{(1)}$ and $\lambda_1^{(3)} = \lambda_2^{(3)} = \lambda_3^{(3)}$, then $P_7 \geq 0$.*

Proof. Consider the vectors $(c_{231}, c_{232}, c_{233})$ and $(c_{331}, c_{332}, c_{333})$. We can use a unitary transformation on the third qutrit to make c_{231} and c_{331} both vanish. Then we use a unitary transformation on the first qutrit to let $c_{221} = 0$. Note that the condition $(c_{231}, c_{331}) = (0, 0)$ is preserved. Hence, $c_{231} = c_{331} = c_{221} = 0$ and $P_7 \geq 0$ by the previous lemma. $\qquad \square$

Lemma 26. *Suppose that the minimum of the function P_7 is negative. Then it does not occur at a state satisfying any of the following conditions:*

1. *$\lambda_2^{(1)} = \lambda_3^{(1)}$ with no other degeneracy;*

2. *$\lambda_1^{(3)} = \lambda_2^{(3)}$ with no other degeneracy;*

3. *$\lambda_2^{(3)} = \lambda_3^{(3)}$ with no other degeneracy.*

Proof. Case 1. If $(c_{231}, c_{331}) = (0, 0)$, then a unitary transformation on the first qutrit can be used to have $c_{221} = 0$. Then we have $P_7 \geq 0$ by Lemma 24. Next let $(c_{231}, c_{331}) \neq (0, 0)$. By Lemma 8 we have $\lambda_1^{(1)} = 0$ or $\lambda_1^{(2)} = \lambda_3^{(3)} = 0$. The latter is impossible. Hence $\lambda_1^{(1)} = 0$. Then $\lambda_2^{(1)} = \lambda_3^{(1)} = 1/2$. Use a unitary transformation to let $c_{331} = 0$. Then, since all (c_{2jk}, c_{3jk}) must be orthogonal to (c_{231}, c_{331}) for $[jk] \neq [31]$ by Proposition 5, we have $c_{2jk} = 0$ except for c_{231}. This implies that $|c_{231}|^2 = \lambda_2^{(1)} = 1/2$. Hence $\lambda_1^{(3)} \geq 1/2$. This is impossible.

Case 2. Assume that $(c_{231}, c_{232}) \neq (0,0)$. If $c_{ij3} \neq 0$ for some $[ij]$, then we must have $L(i,j,3) \leq L(2,3,2) = -1$. This is impossible because $r_3 = 2$. If $c_{ij3} = 0$ for all $[ij]$, then $\lambda_3^{(3)} = 0$, which is impossible. Hence $c_{231} = c_{232} = 0$. If $c_{ij3} \neq 0$ and if (c_{221}, c_{222}) or (c_{331}, c_{332}) is not $(0,0)$, then we must have $L(i,j,3) \leq L(2,2,2) = L(3,3,2) = 0$. Since $r_3 = 2$, we must have $p_i = -2$, $q_j = 0$, i.e. $[ij] = [23]$. Thus, if (c_{221}, c_{222}) or (c_{331}, c_{332}) is not $(0,0)$, then the only nonzero coefficient of the form c_{ij3} is c_{233}. If the vectors (c_{221}, c_{222}) and (c_{331}, c_{332}) are linearly dependent, then a unitary transformation can be used to have $c_{221} = c_{331} = 0$. Then by Lemma 24 we have $P_7 \geq 0$. If they are linearly independent, by Proposition 5 applied to the case with degeneracy in the third qutrit we conclude that all the other vectors (c_{ij1}, c_{ij2}) must vanish since $[ij] = [22]$ and $[33]$ are the only pairs with $R^{(3)}(i,j) \equiv p_i + q_j = -1$. Then the PNCs are

$$c_{221}, c_{222}, c_{331}, c_{332}, c_{233}.$$

We can let $c_{221} = 0$ by a unitary transformation on the third qutrit. Then by an orthogonality relation we find $c_{332} = 0$. [Note that the vectors (c_{221}, c_{222}) and (c_{331}, c_{332}) are linearly independent.] Hence, c_{222}, c_{233} and c_{331} are the PNCs. Then $|c_{331}|^2 = \lambda_1^{(3)} = \lambda_3^{(1)} = 1/3$ and $\lambda_2^{(1)} = |c_{222}|^2 + |c_{233}|^2 = 2/3$. This is impossible. Hence, we must have $c_{231} = c_{221} = c_{331} = 0$ and $P_7 \geq 0$ by Lemma 24.

Case 3. Assume that $c_{231} \neq 0$. If $(c_{ij2}, c_{ij3}) \neq (0,0)$, then $L(i,j,2) \leq L(2,3,1) = -2$. This is impossible. Since $c_{ij3} = 0$ for all $[ij]$ would imply that $\lambda_3^{(3)} = 0$, we conclude that $c_{231} = 0$. If c_{221} or c_{331} is nonzero and if $(c_{ij2}, c_{ij3}) \neq (0,0)$, then we must have $L(i,j,2) \leq L(2,2,1) = L(3,3,1) = -1$. This is satisfied only by (c_{232}, c_{233}). Then, by an orthogonality relation we have $c_{232} = 0$ or $c_{233} = 0$. Hence, either $\lambda_2^{(3)} = 0$, which yields $P_7 \geq 0$ by Lemma 2, or $\lambda_3^{(3)} = 0$, which is impossible. Thus, $c_{231} = c_{221} = c_{331} = 0$ and $P_7 \geq 0$ by Lemma 24. $\square$

Lemma 27. *Suppose that the minimum of the function P_7 is negative. Then it does not occur at a state with $\lambda_1^{(3)} = \lambda_2^{(3)} = \lambda_3^{(3)}$ and without any other degeneracy.*

Proof. First we establish the following result, which is similar to Proposition 5: if $(c_{ij1}, c_{ij2}, c_{ij3})$ and $(c_{i'j'1}, c_{i'j'2}, c_{i'j'3})$ are nonzero, then either $R^{(3)}(i,j) = R^{(3)}(i'j')$ or these vectors are orthogonal to each other. This can be shown as follows. Consider the variation

$$\delta c_{ijK} = \alpha c_{i'j'K}, \quad \delta c_{i'j'K} = -\overline{\alpha} c_{ijK} \quad \text{for all } K$$

and $\delta c_{IJK} = 0$ for all other coefficients. We note first that the variation of the third RDM vanishes, The variation of P_7 is found to be

$$\delta P_7 = 2[R^{(3)}(i,j) - R^{(3)}(i',j')] \sum_{k=1}^{3} \mathrm{Re}\left(\alpha c_{i'j'k}\overline{c_{ijk}}\right).$$

Hence, if $\delta P_7 \geq 0$ for all α, we must have either $R^{(3)}(i,j) = R^{(3)}(i',j')$ or $\sum_{k=1}^{3} c_{i'j'k}\overline{c_{ijk}} = 0$. We note that $R^{(3)}(2,3) = -2$, $R^{(3)}(2,2) = R^{(3)}(3,3) = -1$, and $R^{(3)}(i,j) \geq 0$ for all other $[ij]$.

If $c_{23k} = 0$ for all k, then we can have $c_{221} = c_{331} = 0$ by a unitary transformation on the third qutrit and have $P_7 \geq 0$ by Lemma 24. Assume that $(c_{233}, c_{232}, c_{231})$ is nonzero. Let $c_{232} = c_{231} = 0$ by a unitary transformation on the third qutrit. Then, if $c_{33k} = 0$ for

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all k, we can use a third-qutrit unitary transformation between $|1\rangle$ and $|2\rangle$ to have $c_{221} = 0$ while keeping $c_{232} = c_{231} = c_{331} = 0$. Then we have $P_7 \geq 0$ by Lemma 24. So we assume that $c_{33k} \neq 0$ for some k. By orthogonality of $(c_{231}, c_{232}, c_{233})$ and $(c_{331}, c_{332}, c_{333})$ and by the condition $c_{231} = c_{232} = 0$ we have $c_{333} = 0$. We choose $c_{332} \neq 0$ and $c_{331} = 0$. If $c_{221} = 0$ for the vector $(c_{221}, c_{222}, c_{223})$, then $P_7 \geq 0$ by Lemma 24. So let $c_{221} \neq 0$. Then, all the other vectors $(c_{ij1}, c_{ij2}, c_{ij3})$ are orthogonal to three linearly independent vectors. Hence they must all vanish. Then, the PNCs are c_{233}, c_{332} and c_{221} since $c_{222} = 0$ due to the relation $c_{222}\overline{c_{221}} = 0$. Then, $|c_{332}|^2 \geq |c_{233}|^2 + |c_{221}|^2$ and $|c_{233}|^2 \geq |c_{332}|^2$ imply that $|c_{332}|^2 = |c_{233}|^2$, $c_{221} = 0$. Hence $\lambda_1^{(3)} = 0$, which contradicts the degeneracy assumption. $\qquad\square$

The following lemma completes the proof of inequality (7).

Lemma 28. *Suppose that the minimum of P_7 is negative. Then it does not occur in either of the following two cases:*

1. $\lambda_2^{(1)} = \lambda_3^{(1)}$ *and* $\lambda_2^{(3)} = \lambda_3^{(3)}$ *with no other degeneracy;*

2. $\lambda_2^{(1)} = \lambda_3^{(1)}$ *and* $\lambda_1^{(3)} = \lambda_2^{(3)}$ *with no other degeneracy.*

Proof. Case 1. If $(c_{231}, c_{331}) = (0, 0)$, then we can use a unitary transformation on the first qutrit to have $c_{221} = 0$, and use Lemma 24 to conclude that $P_7 \geq 0$. Suppose $(c_{231}, c_{331}) \neq (0, 0)$. If $(c_{1j2}, c_{1j3}) \neq (0, 0)$, then we must have $L(1, j, 2) \leq L(3, 3, 1) = -1$, which is impossible. Hence $(c_{1j2}, c_{1j3}) = (0, 0)$ for all j. Next let $(c_{2j2}, c_{3j2}, c_{2j3}, c_{3j3}) \neq (0, 0, 0, 0)$. Then by considering the variation given in Proposition 8 after a qutrit permutation $(123) \rightarrow (132)$ with $[ijk] \rightarrow [22j]$ and $j' = 1$, we find

$$\begin{aligned}
\delta P_7 &= \delta\lambda_1^{(1)} - \delta\lambda_2^{(1)} + \delta\lambda_1^{(2)} - \delta\lambda_3^{(2)} + \delta\lambda_3^{(3)} - \delta\lambda_1^{(3)} \\
&= |a_2 - b_1| + \max(a_1 + a_2, b_1 + b_2) + (4 - j)(a_1 + a_2 + b_1 + b_2).
\end{aligned} \tag{44}$$

If $j = 1$ or 2, then by choosing a_i and b_i to be nonpositive, we have

$$\delta P_7 \leq |a_2 - b_1| + 2(a_1 + a_2 + b_1 + b_2) < 0$$

if some of a_i and b_i is nonzero. For $j = 3$, if a_i and b_i are nonpositive, then

$$\delta P_7 = |a_2 - b_1| + 2\max(a_1 + a_2, b_1 + b_2) + \min(a_1 + a_2, b_1 + b_2).$$

If $a_1 \neq 0$ or $b_2 \neq 0$ or if both a_2 and b_1 are nonzero, then we can have $\delta P_7 < 0$. If a_2 is the only nonzero coefficient, then we find $\delta P_7 = |a_2| + a_2 = 0$, and similarly for b_1. The cases $a_2 \neq 0$ and $b_1 \neq 0$ are related by unitary transformations. By choosing the latter, we find that $c_{233} = c_{332} = c_{333} = 0$. Since we have already concluded that there are no coefficients of the form c_{ij3} other than c_{233} and c_{333}, we have $\lambda_3^{(3)} = 0$, which is a contradiction.

Case 2. It is enough to show that $(c_{231}, c_{331}) = (0, 0)$ for the same reason as in case 1. Assume that

$$\begin{pmatrix} c_{231} & c_{331} \\ c_{232} & c_{332} \end{pmatrix} \neq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \tag{45}$$

If this matrix has rank one, then we can use a unitary transformation on the third qutrit to have $c_{231} = c_{331} = 0$. Then, we can have $c_{221} = 0$ using a unitary transformation on the first qutrit and conclude that $P_7 \geq 0$ by Lemma 24. Therefore we may assume

that the matrix (45) has rank two. Suppose further that $c_{1j3} \neq 0$. Then we must have $L(1, j, 3) \leq L(3, 3, 2) = 0$, which is impossible. Hence $c_{1j3} = 0$ for all j. Next, suppose that $(c_{2j3}, c_{3j3}) \neq (0, 0)$. Then by letting $(abc) = (132)$ and $[ijk] \rightarrow [213]$ and $j' = 3$, $k' \rightarrow j$ in Proposition 8, we find

$$\delta P_7 = |a_2 - b_1| - \min(a_1 + a_2, b_1 + b_2) - (4 - j)(a_1 + a_2 + b_1 + b_2).$$

This formula will be identical with (44) if we let $a_i \rightarrow -a_i$ and $b_i \rightarrow -b_i$. Hence δP_7 can be made negative if (c_{213}, c_{313}) or (c_{223}, c_{323}) is nonzero. For $j = 3$, then we can have $\delta P_7 < 0$ unless a_2 or b_1 is the only possibly nonzero one among a_i and b_i. Since the matrix (45) has rank two, we must have both c_{231} and c_{332} nonzero after diagonalizing it. Hence, if a_i can be made nonzero, then so can b_i, and vice versa. Hence we can conclude that unless a_i and b_i, $i = 1, 2$, are all zero, we can have $\delta P_7 < 0$. Hence we must have $c_{ij3} = 0$ for all $[ij]$, i.e. $\lambda_3^{(3)} = 0$, which is a contradiction. $\qquad\square$

VIII.   CONSTRUCTION OF SOME STATES

We have shown that the inequalities listed in Theorem 1 are necessary for a state to exist with a given E-point. Our next task is to show that these inequalities guarantee that there is a quantum state having these eigenvalues. The following elementary fact will be useful.

Lemma 29. *Suppose that the angles θ and φ are constrained by*

$$u \sin 2\theta - v \sin 2\varphi = 0,$$

where u and v are real constants, and that there are no other constraints on them. Then, $\theta + \varphi$ can take any value and the range of the function

$$f \equiv u \cos 2\theta + v \cos 2\varphi$$

is given by $||u| - |v|| \leq |f| \leq |u| + |v|$.

Proof. The constraint equation can be written as

$$(u - v) \sin(\theta + \varphi) \cos(\theta - \varphi) + (u + v) \cos(\theta + \varphi) \sin(\theta - \varphi) = 0.$$

For any value of $\theta + \varphi$, we can find a value of $\theta - \varphi$ so that this equation is satisfied. Hence, the combination $\theta + \varphi$ is unconstrained. Note that

$$\begin{aligned} f^2 &= (u \cos 2\theta + v \cos 2\varphi)^2 + (u \sin 2\theta - v \sin 2\varphi)^2 \\ &= u^2 + v^2 + 2uv \cos 2(\theta + \varphi). \end{aligned}$$

This shows that $|f|$ ranges between $(u + v)^2$ and $(u - v)^2$. Hence, the range of f is given by $||u| - |v|| \leq |f| \leq |u| + |v|$. (Since $f \rightarrow -f$ for $\theta \rightarrow \theta + \pi/2$ and $\varphi + \pi/2$, the range is invariant under $f \rightarrow -f$.) $\qquad\square$

First we construct a convex subset of S.

Proposition 10. *There is a state with any E-point in the convex set S_0 bounded by hyperplanes with the following corner points:*

$$[B, B, B], \ [B, A, A], \ [A, B, B], \ [O, B, B], \ [A, A, A],$$
$$[O, A, A], \ [O, O, O], \ [A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}], \ [A, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}, 0\tfrac{1}{4}\tfrac{3}{4}]$$

and those obtained by qutrit permutations from them.

Proof. First consider the following PNCs: $c_{333}, c_{322}, c_{232}, c_{223}, c_{311}, c_{131}, c_{113}$. Suppose that we add c_{122}, c_{212} and c_{221} to this list. Then the only off-diagonal elements in the RDMs that become nonzero are the ones connecting $|1\rangle$ and $|3\rangle$ in each qutrit. Thus, each RDM can be diagonalized by a simple unitary transformation. Motivated by this observation, we consider the state with the PNCs given as follows. First let

$$\begin{pmatrix} b_{333} \\ b_{133} \end{pmatrix} = \begin{pmatrix} a\cos\theta_1 \\ a\sin\theta_1 \end{pmatrix}, \quad \begin{pmatrix} b_{331} \\ b_{131} \end{pmatrix} = \begin{pmatrix} -g\sin\theta_1 \\ g\cos\theta_1 \end{pmatrix},$$
$$\begin{pmatrix} b_{313} \\ b_{113} \end{pmatrix} = \begin{pmatrix} -h\sin\theta_1 \\ h\cos\theta_1 \end{pmatrix}, \quad \begin{pmatrix} b_{311} \\ b_{111} \end{pmatrix} = \begin{pmatrix} f\cos\theta_1 \\ f\sin\theta_1 \end{pmatrix},$$

where a, h, g and f are real constants. Next we define

$$\begin{pmatrix} d_{i3k} \\ d_{i1k} \end{pmatrix} = \begin{pmatrix} \cos\varphi_1 & -\sin\varphi_1 \\ \sin\varphi_1 & \cos\varphi_1 \end{pmatrix} \begin{pmatrix} b_{i3k} \\ b_{i1k} \end{pmatrix},$$

where $[ik] = [11]$, $[13]$, $[31]$ or $[33]$. Finally we let

$$\begin{pmatrix} c_{ij3} \\ c_{ij1} \end{pmatrix} = \begin{pmatrix} \cos\chi_1 & -\sin\chi_1 \\ \sin\chi_1 & \cos\chi_1 \end{pmatrix} \begin{pmatrix} d_{ij3} \\ d_{ij1} \end{pmatrix}$$

with $[ij] = [11]$, $[13]$, $[31]$ or $[33]$. We also let

$$c_{322} = b\cos\theta_2, \quad c_{122} = b\sin\theta_2, \quad c_{232} = c\cos\varphi_2, \quad c_{212} = c\sin\varphi_2,$$
$$c_{223} = d\cos\chi_2, \quad c_{221} = d\sin\chi_2,$$

where b, c and d are real constants. Then we find $a^2 + b^2 + c^2 + d^2 + f^2 + g^2 + h^2 = 1$ and

$$\lambda_2^{(1)} = c^2 + d^2,$$
$$\lambda_2^{(2)} = b^2 + d^2,$$
$$\lambda_2^{(3)} = b^2 + c^2,$$

and

$$\lambda_3^{(1)} - \lambda_1^{(1)} = b^2\cos 2\theta_2 + (a^2 + f^2 - g^2 - h^2)\cos 2\theta_1,$$
$$\lambda_3^{(2)} - \lambda_1^{(2)} = c^2\cos 2\varphi_2 + (a^2 + g^2 - f^2 - h^2)\cos 2\varphi_1,$$
$$\lambda_3^{(3)} - \lambda_1^{(3)} = d^2\cos 2\chi_2 + (a^2 + h^2 - f^2 - g^2)\cos 2\chi_1.$$

The orthogonality relations are

$$b^2\sin 2\theta_2 + (a^2 + f^2 - g^2 - h^2)\sin 2\theta_1 = 0,$$
$$c^2\sin 2\varphi_2 + (a^2 + g^2 - f^2 - h^2)\sin 2\varphi_1 = 0,$$
$$d^2\sin 2\chi_2 + (a^2 + h^2 - f^2 - g^2)\sin 2\chi_1 = 0.$$

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We require that

$$a^2 + f^2 - g^2 - h^2 \geq 0,$$
$$a^2 + g^2 - f^2 - h^2 \geq 0,$$
$$a^2 + h^2 - f^2 - g^2 \geq 0.$$

Then, by Lemma 29 we conclude that $\lambda_3^{(a)} - \lambda_1^{(a)}$ have the ranges given by the following inequalities:

$$|a^2 + f^2 - g^2 - h^2 - b^2| \leq \lambda_3^{(1)} - \lambda_1^{(1)} \leq a^2 + f^2 - g^2 - h^2 + b^2, \tag{46}$$

$$|a^2 + g^2 - f^2 - h^2 - c^2| \leq \lambda_3^{(2)} - \lambda_1^{(2)} \leq a^2 + g^2 - f^2 - h^2 + c^2, \tag{47}$$

$$|a^2 + h^2 - f^2 - g^2 - d^2| \leq \lambda_3^{(3)} - \lambda_1^{(3)} \leq a^2 + h^2 - f^2 - g^2 + d^2. \tag{48}$$

The equations for $\lambda_2^{(a)}$ and the inequalities for $\lambda_3^{(a)} - \lambda_1^{(a)}$ can be satisfied for all corner points listed here. We give a^2, b^2 etc. that are nonzero for each corner point:

$$[B, B, B] : a^2 = 1/4, \ b^2 = c^2 = d^2 = 1/6, \ f^2 = g^2 = h^2 = 1/12,$$
$$[B, A, A] : a^2 = b^2 = 1/3, \ c^2 = d^2 = 1/6,$$
$$[A, B, B] : a^2 = 1/3, \ b^2 = 1/12, \ c^2 = d^2 = 1/4, \ f^2 = 1/12,$$
$$[O, B, B] : a^2 = b^2 = f^2 = 1/3,$$
$$[A, A, A] : a^2 = b^2 = c^2 = d^2 = 1/4,$$
$$[O, A, A] : a^2 = b^2 = 1/2,$$
$$[O, O, O] : a^2 = 1,$$
$$\left[A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] : a^2 = d^2 = 1/3, \ c^2 = f^2 = 1/6,$$
$$\left[A, 0\tfrac{1}{4}\tfrac{3}{4}, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}\right] : a^2 = 1/2, \ c^2 = d^2 = 1/4.$$

The E-points obtained by qutrit permutations can be realized because this construction is invariant under qutrit permutations. If two sets of eigenvalues $\lambda_i^{(a)I}$ and $\lambda_i^{(a)II}$ are given by $a^2 = a_I^2$, $b^2 = b_I^2$, etc. and $a^2 = a_{II}^2$, $b^2 = b_{II}^2$, etc., respectively, then any set of eigenvalues of the form $\lambda_i^{(a)} = \alpha\lambda_i^{(a)I} + (1 - \alpha)\lambda_i^{(a)II}$ with $0 \leq \alpha \leq 1$ is given by $a^2 = \alpha a_I^2 + (1 - \alpha)a_{II}^2$, $b^2 = \alpha b_I^2 + (1 - \alpha)b_{II}^2$, etc. with inequalities (46)–(48) being satisfied. Hence the set of states constructed here forms a convex set in the space of E-points. $\square$

It will be useful later to construct states whose E-points are on the boundary of inequality (1). This inequality with $(abc) = (123)$ reads

$$P_1 \equiv \lambda_1^{(2)} + \lambda_2^{(2)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_1^{(1)} - \lambda_2^{(1)} \geq 0.$$

From the proof of Theorem 3 we find that to have $P_1 = 0$ we need $c_{ijk} = 0$ for all $[ijk]$ except those with $i = 3$ or $j = 3$. We also find that unless $\lambda_2^{(1)} = \lambda_3^{(1)}$, we must have $c_{332} = c_{331} = 0$. Thus, a generic state satisfying the equality $P_1 = 0$ has only the following PNCs:

$$c_{131}, c_{231}, c_{132}, c_{232}, c_{113}, c_{213}, c_{123}, c_{223}, c_{333}. \tag{49}$$

Notice that for all these coefficients c_{ijk} we have $L(i, j, k) = 0$. The orthogonality relations are as follows:

$$c_{131}\overline{c_{231}} + c_{132}\overline{c_{232}} + c_{113}\overline{c_{213}} + c_{123}\overline{c_{223}} = 0, \tag{50}$$

$$c_{113}\overline{c_{123}} + c_{213}\overline{c_{223}} = 0, \tag{51}$$

$$c_{131}\overline{c_{132}} + c_{231}\overline{c_{232}} = 0. \tag{52}$$

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The last two constraints are satisfied by letting

$$c_{113} = a\cos\theta, \quad c_{213} = a\sin\theta, \quad c_{123} = -b\sin\theta, \quad c_{223} = b\cos\theta,$$
$$c_{131} = d\cos\varphi, \quad c_{231} = -d\sin\varphi, \quad c_{132} = f\sin\varphi, \quad c_{232} = f\cos\varphi,$$

where a, b, d, f, *theta* and φ are real numbers. Let us write the eigenvalues $\lambda_i^{(a)}$ as $\Lambda_i^{(a)}$ for later purposes. Then

$$\Lambda_1^{(2)} = a^2, \quad \Lambda_2^{(2)} = b^2, \quad \Lambda_1^{(3)} = d^2, \quad \Lambda_2^{(3)} = f^2$$

and

$$\Lambda_2^{(1)} + \Lambda_1^{(1)} = \Lambda_2^{(2)} + \Lambda_1^{(2)} + \Lambda_2^{(3)} + \Lambda_1^{(3)}, \tag{53}$$
$$\Lambda_2^{(1)} - \Lambda_1^{(1)} = (\Lambda_2^{(2)} - \Lambda_1^{(2)})\cos 2\theta + (\Lambda_2^{(3)} - \Lambda_1^{(3)})\cos 2\varphi. \tag{54}$$

The constraint (50) reads

$$(\Lambda_2^{(2)} - \Lambda_1^{(2)})\sin 2\theta = (\Lambda_2^{(3)} - \Lambda_1^{(3)})\sin 2\varphi.$$

Hence, by Lemma 29 the range of $\Lambda_2^{(1)} - \Lambda_1^{(1)}$ is given by

$$|(\Lambda_2^{(2)} - \Lambda_1^{(2)}) - (\Lambda_2^{(3)} - \Lambda_1^{(3)})| \leq \Lambda_2^{(1)} - \Lambda_1^{(1)} \leq \Lambda_2^{(2)} - \Lambda_1^{(2)} + \Lambda_2^{(3)} - \Lambda_1^{(3)}. \tag{55}$$

In summary, there is a state with any E-point satisfying (53) and (55), and $\Lambda_2^{(a)} \geq \Lambda_1^{(a)}$ for all a. Notice that it is not necessary for the eigenvalues to satisfy $\Lambda_3^{(a)} \geq \Lambda_2^{(a)}$, or even $\Lambda_3^{(a)} \geq \Lambda_1^{(a)}$. It is clear that the states constructed here form a convex set in the space of E-points. It can readily be seen that the corner points of this boundary hyperplane listed in the proof of Proposition 1 all satisfy (55) and, of course, (53). Hence all E-points on the boundary hyperplane (53) have corresponding states. This construction of states can be slightly generalized to prove the following lemma, which will be useful later.

Lemma 30. *There is a state with any E-point in the simplex with the following corner points:*

$$[O,O,O] \ \ [B,O,B] \ \ [B,B,O] \ \ [A,O,A] \ \ [A,A,O] \ \ \left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right], \ [B,A,A].$$

Proof. Let us add c_{322} to the list of PNCs (49). Then we find that no new orthogonality relation will be introduced. Let us define $\Lambda_i^{(1)}$ to be the sum over J and K of $|c_{iJK}|^2$, where c_{iJK} appear in the list (49), and similarly for $\Lambda_j^{(2)}$ and $\Lambda_k^{(3)}$. Then the eigenvalues $\lambda_i^{(a)}$ can be expressed as follows:

$$\lambda_1^{(1)} = \Lambda_1^{(1)}, \quad \lambda_2^{(1)} = \Lambda_2^{(1)}, \quad \lambda_3^{(1)} = \Lambda_3^{(1)} + |c_{322}|^2,$$
$$\lambda_1^{(2)} = \Lambda_1^{(2)}, \quad \lambda_2^{(2)} = \Lambda_2^{(2)} + |c_{322}|^2,$$
$$\lambda_1^{(3)} = \Lambda_1^{(3)}, \quad \lambda_2^{(3)} = \Lambda_2^{(3)} + |c_{322}|^2. \tag{56}$$

The preceding construction shows that if $\lambda_i^{(a)}$ are given in this manner and if $\Lambda_i^{(a)}$ satisfy (53) and (55), then there is a state with the eigenvalues $\lambda_i^{(a)}$. Furthermore, if we require that $\Lambda_2^{(a)} \geq \Lambda_1^{(a)}$ for all a, then the set of E-points satisfying all these conditions is convex.

All points except $[B, A, A]$ satisfy the conditions given here with $c_{322} = 0$ since they are on the boundary (53) with $\lambda_i^{(a)} = \Lambda_i^{(a)}$ for all i and a. Thus, all we need to do is find $\Lambda_i^{(a)}$ [which satisfy (53) and (55)] and c_{322} such that the eigenvalues $[B, A, A]$ are expressed as in (56). We can do so with $|c_{322}|^2 = 1/6$, $\Lambda_1^{(1)} = \Lambda_2^{(1)} = 1/3$, $\Lambda_3^{(1)} = 1/6$, $\Lambda_1^{(2)} = \Lambda_1^{(3)} = 0$, $\Lambda_2^{(2)} = \Lambda_2^{(3)} = 1/3$ (and with $\Lambda_3^{(2)} = \Lambda_3^{(3)} = 1/2$ as a result). $\qquad\square$

We will need the states given by the following PNCs:

$$c_{132} = a\cos\theta, \quad c_{232} = -a\sin\theta,$$
$$c_{112} = r\sin\alpha\sin\theta, \quad c_{212} = r\sin\alpha\cos\theta,$$
$$c_{122} = r\cos\alpha\sin\theta, \quad c_{222} = r\cos\alpha\cos\theta,$$
$$c_{131} = f\sin\theta, \quad c_{231} = f\cos\theta,$$
$$c_{113} = p\sin\alpha\cos\theta - q\cos\alpha\cos\varphi,$$
$$c_{213} = -p\sin\alpha\sin\theta - q\cos\alpha\sin\varphi,$$
$$c_{123} = p\cos\alpha\cos\theta + q\sin\alpha\cos\varphi,$$
$$c_{223} = -p\cos\alpha\sin\theta + q\sin\alpha\sin\varphi, \quad c_{333} = g,$$

where a, f, g, p, q, r, θ, φ and α are real numbers. (Note that the PNCs will be those for the boundary $P_1 = 0$ if $r = 0$ although the parametrization is slightly different.) The only nontrivial orthogonality relations are

$$(r^2 + f^2 - a^2 - p^2)\sin 2\theta = -q^2\sin 2\varphi, \tag{57}$$
$$(r^2 + p^2 - q^2)\sin 2\alpha = 2pq\cos(\theta + \varphi)\cos 2\alpha. \tag{58}$$

The eigenvalues are given by

$$\lambda_1^{(1)} = (a^2 + p^2)\cos^2\theta + (r^2 + f^2)\sin^2\theta + q^2\cos^2\varphi,$$
$$\lambda_2^{(1)} = (a^2 + p^2)\sin^2\theta + (r^2 + f^2)\cos^2\theta + q^2\sin^2\varphi,$$
$$\lambda_1^{(2)} = (r^2 + p^2)\sin^2\alpha + q^2\cos^2\alpha - pq\sin 2\alpha\,\cos(\theta + \varphi),$$
$$\lambda_2^{(2)} = (r^2 + p^2)\cos^2\alpha + q^2\sin^2\alpha + pq\sin 2\alpha\,\cos(\theta + \varphi),$$
$$\lambda_1^{(3)} = f^2,$$
$$\lambda_2^{(3)} = a^2 + r^2.$$

Let us introduce the variable $s^2 \equiv p^2 + q^2$. Then we have

$$\lambda_1^{(1)} + \lambda_2^{(1)} = a^2 + r^2 + f^2 + s^2, \tag{59}$$
$$\lambda_1^{(2)} + \lambda_2^{(2)} = r^2 + s^2, \tag{60}$$
$$\lambda_2^{(3)} = a^2 + r^2, \tag{61}$$
$$\lambda_1^{(3)} = f^2. \tag{62}$$

Notice that these equations can be solved for a^2, r^2, f^2 and s^2. Then note that Eq. (58) can be satisfied by letting

$$\sin 2\alpha = \frac{2pq\cos(\theta + \varphi)}{\sqrt{(r^2 + p^2 - q^2)^2 + 4p^2q^2\cos^2(\theta + \varphi)}},$$
$$\cos 2\alpha = \frac{r^2 + p^2 - q^2}{\sqrt{(r^2 + p^2 - q^2)^2 + 4p^2q^2\cos^2(\theta + \varphi)}}$$

unless $r^2 + p^2 - q^2 = pq\cos(\theta + \varphi) = 0$. The eigenvalues $\lambda_1^{(2)}$ and $\lambda_2^{(2)}$ can be given as

$$\lambda_1^{(2)} = \frac{1}{2}\left[r^2 + p^2 + q^2 - \sqrt{(r^2 + p^2 - q^2)^2 + 4p^2q^2\cos^2(\theta + \varphi)}\right],$$

$$\lambda_2^{(2)} = \frac{1}{2}\left[r^2 + p^2 + q^2 + \sqrt{(r^2 + p^2 - q^2)^2 + 4p^2q^2\cos^2(\theta + \varphi)}\right].$$

These equations are valid even if $r^2 + p^2 - q^2 = pq\cos(\theta + \varphi) = 0$.

Suppose that a^2, r^2, f^2 and s^2 are fixed at some values satisfying

$$s^2 - r^2 \geq 0,$$
$$a^2 - f^2 - 2r^2 \geq 0.$$

We first show that $\lambda_1^{(2)}$ can take any value between 0 and $(r^2 + s^2)/2$. By the first part of Lemma 29 we find that the combination $\theta + \varphi$ can vary freely. Hence $\lambda_1^{(2)}$ can take any value as long as

$$\frac{1}{2}\left[r^2 + s^2 - \sqrt{(r^2 + p^2 - q^2)^2 + 4p^2q^2}\right] \leq \lambda_1^{(2)} \leq \frac{1}{2}\left[r^2 + s^2 - |r^2 + p^2 - q^2|\right].$$

By varying q^2 from 0 to $(r^2 + s^2)/2$, which is possible by the assumption that $r^2 \leq s^2$, we can see that $\lambda_1^{(2)}$ varies from 0 to $(r^2 + s^2)/2$.

However, let us impose the condition $r^2 \leq \lambda_1^{(2)}$ or, equivalently, $\lambda_2^{(2)} \leq s^2$. We will show, under this condition, that $\lambda_2^{(1)} - \lambda_1^{(1)}$ can take any value between $|a^2 - f^2 - 2r^2 - \lambda_2^{(2)} + \lambda_1^{(2)}|$ and $|a^2 - f^2 - 2r^2 + \lambda_2^{(2)} - \lambda_1^{(2)}|$. Note first that

$$\lambda_1^{(2)}\lambda_2^{(2)} = q^2[r^2 + p^2\sin^2(\theta + \varphi)]. \tag{63}$$

This equation to have a solution for $\theta + \varphi$ if and only if

$$q^2r^2 \leq \lambda_1^{(2)}\lambda_2^{(2)} \leq q^2(r^2 + p^2) = q^2(\lambda_1^{(2)} + \lambda_2^{(2)} - q^2).$$

These inequalties are satisfied if $\lambda_1^{(2)} \leq q^2 \leq \lambda_2^{(2)}$. Assuming that $\lambda_1^{(2)} > r^2$, we have $q^2 > r^2 \geq 0$ and $p^2 = s^2 - q^2 \geq s^2 - \lambda_2^{(2)} = \lambda_1^{(2)} - r^2 > 0$. Then from (63) we find $\sin^2(\theta + \varphi)$ as a function of q^2 with $\lambda_1^{(2)}$ fixed as

$$\sin^2(\theta + \varphi) = \frac{\lambda_1^{(2)}\lambda_2^{(2)} - q^2r^2}{p^2q^2}.$$

By substituting this in

$$|\lambda_2^{(1)} - \lambda_1^{(1)}|^2 = \left[(r^2 + f^2 - a^2 - p^2)\cos 2\theta - q^2\cos 2\varphi\right]^2$$
$$+ \left[(r^2 + f^2 - a^2 - p^2)\sin 2\theta + q^2\sin 2\varphi\right]^2$$
$$= (r^2 + f^2 - a^2 - p^2 - q^2)^2$$
$$+ 4(r^2 + f^2 - a^2 - p^2)q^2\sin^2(\theta + \varphi),$$

we obtain

$$|\lambda_2^{(1)} - \lambda_1^{(1)}|^2 = (r^2 + f^2 - a^2 - p^2 - q^2)^2$$
$$+ 4(r^2 + f^2 - a^2 - p^2)\frac{\lambda_1^{(2)}\lambda_2^{(2)} - q^2r^2}{p^2}.$$

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If we substitute $q^2 = \lambda_1^{(2)}$ and $q^2 = \lambda_2^{(2)}$, then the right-hand side becomes $|a^2 - f^2 - 2r^2 + \lambda_2^{(2)} - \lambda_1^{(2)}|^2$ and $|a^2 - f^2 - 2r^2 - \lambda_2^{(2)} + \lambda_1^{(2)}|^2$, respectively. Hence, by continuity, $|\lambda_2^{(1)} - \lambda_1^{(1)}|^2$ takes any value between these values as q^2 ranges from $\lambda_1^{(2)}$ to $\lambda_2^{(2)}$. If $\lambda_1^{(2)} = r^2$, then Eq. (63) can be solved by letting $q^2 = s^2 = \lambda_2^{(2)}$. Then we have $p^2 = 0$, and $\sin^2(\theta + \varphi)$ can take any value in $[0, 1]$. Hence, $\lambda_2^{(2)} - \lambda_1^{(2)}$ can take any value between $|a^2 - f^2 - 2r^2 - \lambda_2^{(2)} + \lambda_1^{(2)}|$ and $|a^2 - f^2 - 2r^2 + \lambda_2^{(2)} + \lambda_1^{(2)}|$. This range contains the desired range. The result obtained here can be summarized as follows.

Lemma 31. *Suppose that*

$$
\begin{aligned}
r^2 &\equiv \lambda_1^{(2)} + \lambda_2^{(2)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_1^{(1)} - \lambda_2^{(1)} \geq 0 \,, \\
a^2 &\equiv \lambda_1^{(1)} + \lambda_2^{(1)} - \lambda_1^{(2)} - \lambda_2^{(2)} - \lambda_1^{(3)} \geq 0 \,, \\
s^2 &\equiv \lambda_1^{(1)} + \lambda_2^{(1)} - \lambda_1^{(3)} - \lambda_2^{(3)} \geq 0 \,.
\end{aligned}
$$

Let $f^2 \equiv \lambda_1^{(3)}$. If $r^2 \leq \lambda_1^{(2)} \leq \lambda_2^{(2)} \leq s^2$, $a^2 - f^2 - 2r^2 \geq 0$ and

$$
|a^2 - f^2 - 2r^2 - \lambda_2^{(2)} + \lambda_1^{(2)}| \leq \lambda_2^{(1)} - \lambda_1^{(1)} \leq a^2 - f^2 - 2r^2 + \lambda_2^{(2)} - \lambda_1^{(2)} \,,
$$

then there is a state with these eigenvalues. The set of E-points satisfying these conditions is convex.

Proof. The first three conditions guarantee that Eqs. (59), (60) and (61) can be solved for a^2, r^2 and s^2. Convexity is obvious from the form of the conditions imposed. $\square$

The following fact, emphasized by Bravyi [2], is useful in constructing states.

Lemma 32. *Consider the set of states such that $c_{ijk} \neq 0$ only if the triple $[ijk]$ is in a set E. Suppose that if $[ijk]$ and $[i'j'k']$ are in E and if $[ijk] \neq [i'j'k']$, then at most one of the equations $i = i'$, $j = j'$ and $k = k'$ holds. (This implies that there are no nontrivial orthogonality relations.) Then the set of E-points for these states is convex.*

Proof. Let $\lambda_l^{(a)I}$ and $\lambda_l^{(a)II}$ be the eigenvalues of the states with the specified nonzero coefficients. Let $A_{ijk} \equiv |c_{ijk}|^2$ and write $A_{ijk} = A_{ijk}^I$ and A_{ijk}^{II} for these states. Then, for any $\lambda_l^{(a)}$ given by

$$
\lambda_l^{(a)} = \alpha \lambda_l^{(a)I} + (1 - \alpha) \lambda_l^{(a)II}
$$

with $0 \leq \alpha \leq 1$ for all a and l, a corresponding state is obtained by letting

$$
A_{ijk} = \alpha A_{ijk}^I + (1 - \alpha) A_{ijk}^{II}
$$

for all $[ijk]$. $\square$

IX.   CONSTRUCTION OF THE SET S

We have constructed states with some E-points in the convex set S in Proposition 10 and Lemma 30. We will start constructing states with their E-points in outlying subregions of S. First we divide the region S into two: one region S_1 that satisfies

$$
P_8 \equiv 2\lambda_2^{(2)} + \lambda_3^{(2)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} - 2\lambda_2^{(1)} - \lambda_3^{(1)} \leq 0 \tag{64}
$$

and the other which satisfies $P_8 \geq 0$. The only corner point of S with $P_8 < 0$ is $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$ which has $P_8 = -1/4$. The corner points satisfying $P_8 = 0$ are

$$[O, O, O], \; [B, B, O], \; [A, A, O], \; [A, O, A],$$
$$[A, B, A], \; \left[0\frac{1}{3}\frac{2}{3}, B, 0\frac{1}{3}\frac{2}{3}\right], \; \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right], \; \left[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right]. \tag{65}$$

Using this observation, we show that the set S_1 consists of three simplices.

Lemma 33. *The subset of S satisfying $P_8 \leq 0$, i.e the convex set S_1, consists of the three simplices C_1, C_2 and C_3 with the following five E-points being corner points of all three simplices:*

$$[O, O, O], \; [B, B, O], \; [A, A, O], \; \left[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right], \; \left[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}\right],$$

and with the additional corner points for each simplex given by

$$C_1 \; : \; [A, B, A], \; \left[0\frac{1}{3}\frac{2}{3}, B, 0\frac{1}{3}\frac{2}{3}\right];$$
$$C_2 \; : \; [A, O, A], \; [A, B, A];$$
$$C_3 \; : \; [A, O, A], \; \left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right].$$

Proof. Since the E-point $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$ is the only E-point satisfying $P_8 < 0$, the boundary hyperplanes of S_1 are $P_8 = 0$ and those of S that contain $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$. The latter are $\lambda_1^{(1)} = 0$, $\lambda_2^{(1)} = \lambda_3^{(1)}$, $\lambda_1^{(2)} = \lambda_2^{(2)}$, $\lambda_1^{(3)} = 0$, (2) with $(abc) = (231)$, (3) with $(abc) = (132)$, (6) with $(abc) = (132)$ and (7) with $(abc) = (132)$. It is enough to show that $C_1 \cup C_2 \cup C_3$ is bounded by these hyperplanes.

Let us define the following functions:

$$\begin{aligned} P_9 &\equiv 2\lambda_1^{(1)} + \lambda_2^{(1)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} - 2\lambda_1^{(2)} - \lambda_2^{(2)}, \\ P_{10} &\equiv \lambda_2^{(1)} - \lambda_2^{(2)} - \lambda_2^{(3)}. \end{aligned} \tag{66}$$

Then the boundary hyperplanes of the simplex C_1 can be given as follows, where the E-point listed with each boundary hyperplane is the one which is not on the hyperplane:

$$\begin{aligned} &[O, O, O] \; : \; (7), (abc) = (132); \quad [B, B, O] \; : \; \lambda_1^{(1)} = 0; \\ &[A, A, O] \; : \; \lambda_1^{(2)} = \lambda_2^{(2)}; \quad \left[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] \; : \; \lambda_1^{(3)} = 0; \\ &\left[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}\right] \; : \; P_8 = 0; \quad [A, B, A] \; : \; (3), (abc) = (132); \\ &\left[0\frac{1}{3}\frac{2}{3}, B, 0\frac{1}{3}\frac{2}{3}\right] \; : \; P_9 = 0. \end{aligned}$$

Those for C_2 are

$$\begin{aligned} &[O, O, O] \; : \; \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, B, O] \; : \; \lambda_1^{(1)} = 0; \\ &[A, A, O] \; : \; \lambda_1^{(2)} = \lambda_2^{(2)}; \quad \left[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] \; : \; \lambda_1^{(3)} = 0; \\ &\left[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}\right] \; : \; P_8 = 0; \quad [A, O, A] \; : \; P_9 = 0; \\ &[A, B, A] \; : \; P_{10} = 0. \end{aligned} \tag{67}$$

Those for C_3 are

$$\begin{aligned} &[O, O, O] \; : \; \lambda_2^{(1)} = \lambda_3^{(1)}; \quad [B, B, O] \; : \; \lambda_1^{(1)} = 0; \\ &[A, A, O] \; : \; \lambda_1^{(2)} = \lambda_2^{(2)}; \quad \left[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] \; : \; (2), (abc) = (231); \\ &\left[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}\right] \; : \; P_8 = 0; \quad [A, O, A] \; : \; (6), (abc) = (132); \\ &\left[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}\right] \; : \; P_{10} = 0. \end{aligned} \tag{68}$$

The E-point $[0\frac{1}{3}\frac{2}{3}, B, 0\frac{1}{3}\frac{2}{3}]$ is the only corner point of C_1, C_2 or C_3 with $P_9 < 0$, and all other corner points of C_1 satisfy $P_9 = 0$. Hence all E-points in C_1 satisfy $P_9 \le 0$. The E-point $[A, \frac{1}{6}\frac{1}{6}\frac{2}{3}, \frac{1}{6}\frac{1}{6}\frac{2}{3}]$ is the only E-point of C_1, C_2 or C_3 with $P_{10} > 0$, and all other corner points of C_3 satisfy $P_{10} = 0$. Hence all E-points in C_3 satisfy $P_{10} \ge 0$. All corner points of C_2 satisfy $P_9 = P_{10} = 0$ except $[A, O, A]$ with $P_9 = 1$ and $P_{10} = 0$ and $[A, B, A]$ with $P_9 = 0$ and $P_{10} = -1/3$. Hence all E-points in C_2 satisfy $P_9 \ge 0$ and $P_{10} \le 0$. Thus, the intersections $C_1 \cap C_2$ and $C_2 \cap C_3$ are hyperplanes $P_9 = 0$ and $P_{10} = 0$, respectively. The corner points of these boundary hyperplanes are

$$P_9 : [A, B, A], \left[A, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}, 0\tfrac{1}{4}\tfrac{3}{4}\right], \left[A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right], [A, A, O], [B, B, O], [O, O, O];$$
$$P_{10} : [A, O, A], \left[A, \tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{2}, 0\tfrac{1}{4}\tfrac{3}{4}\right], \left[A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right], [A, A, O], [B, B, O], [O, O, O].$$

Thus, the simplices C_1, C_2 and C_3 are glued together at these boundaries, and all other boundaries are boundaries of the convex set S_1. Hence $S_1 = C_1 \cup C_2 \cup C_3$. $\qquad\square$

Now we construct states with their E-points in the simplices C_1, C_2 and C_3.

Lemma 34. *There is a state with any E-point in $S_1 = C_1 \cup C_2 \cup C_3$.*

Proof. Since $C_2 \subset S_0$, there is a state with any E-point in C_2 due to Proposition 10. Next we construct a state with any E-point in the simplex C_1. From the list (67) we see that the boundary obtained by omitting $[A, B, A]$ is

$$\lambda_2^{(2)} + \lambda_3^{(2)} + \lambda_2^{(3)} + \lambda_1^{(3)} - \lambda_2^{(1)} - \lambda_3^{(1)} = 0. \tag{69}$$

This suggests that the states may be constructed by using Lemma 31 after letting $(\lambda_1^{(1)}, \lambda_2^{(1)}) \rightarrow (\lambda_2^{(1)}, \lambda_3^{(1)})$ and $(\lambda_1^{(2)}, \lambda_2^{(2)}) \rightarrow (\lambda_2^{(2)}, \lambda_3^{(2)})$. This is allowed since the only inequalities among $\lambda_i^{(a)}$ that we need for this lemma to hold are $\lambda_2^{(a)} \ge \lambda_1^{(a)}$ for $a = 1, 2$. For an E-point satisfying equality (69), we have, using the notation of this lemma,

$$\begin{aligned}
r^2 &= \lambda_2^{(2)} + \lambda_3^{(2)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_2^{(1)} - \lambda_3^{(1)} = 0, \\
a^2 &= \lambda_2^{(1)} + \lambda_3^{(1)} - \lambda_2^{(2)} - \lambda_3^{(2)} - \lambda_1^{(3)} = \lambda_2^{(3)} \ge 0, \\
s^2 - \lambda_3^{(2)} &= \lambda_2^{(1)} + \lambda_3^{(1)} - \lambda_1^{(3)} - \lambda_2^{(3)} - \lambda_3^{(2)} = \lambda_2^{(2)} \ge 0
\end{aligned}$$

and $f^2 = \lambda_1^{(3)}$. Hence we have $r^2 \le \lambda_2^{(2)} \le \lambda_3^{(2)} \le s^2$. We also have

$$a^2 - f^2 - 2r^2 = \lambda_2^{(3)} - \lambda_1^{(3)} \ge 0.$$

The possible range of $\lambda_3^{(1)} - \lambda_2^{(1)}$ is

$$|\lambda_2^{(3)} - \lambda_1^{(3)} - \lambda_3^{(2)} + \lambda_2^{(2)}| \le \lambda_3^{(1)} - \lambda_2^{(1)} \le \lambda_2^{(3)} - \lambda_1^{(3)} + \lambda_3^{(2)} - \lambda_2^{(2)}.$$

These are equivalent to the following three inequalities if Eq. (69) is satisfied: inequality (5) with $(abc) = (231)$, inequality (6) with $(abc) = (132)$ and inequality (7) with $(abc) = (132)$. Hence these are all satisfied by the corner points satisfying (69). For $[A, B, A]$, we find $r^2 = 1/6$, $a^2 = 1/3$, $s^2 - \lambda_3^{(2)} = 1/6$, and $a^2 - f^2 - 2r^2 = 0$. Thus, $|2r^2 + f^2 - a^2 \pm \lambda_3^{(2)} - \lambda_2^{(2)}| = 0$, and the condition

$$|a^2 - f^2 - 2r^2 - \lambda_3^{(2)} + \lambda_2^{(2)}| \le \lambda_3^{(1)} - \lambda_2^{(1)} \le a^2 - f^2 - 2r^2 + \lambda_3^{(2)} - \lambda_2^{(2)}$$

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is satisfied by $[A, B, A]$. Therefore, by Lemma 31 all E-points in C_1 have corresponding states.

The construction of states with their E-points in C_3 is similar. We note that the boundary of C_3 obtained by omitting $[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}]$ is

$$\lambda_1^{(1)} + \lambda_3^{(1)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_1^{(2)} - \lambda_3^{(2)} = 0. \tag{70}$$

This suggests that we can apply Lemma 31 with $\lambda_2^{(1)} \leftrightarrow \lambda_3^{(1)}$, $\lambda_2^{(3)} \leftrightarrow \lambda_3^{(3)}$ and then with $(1) \to (2) \to (3) \to (1)$. For an E-point satisfying (70) we have, using the notation of this lemma,

$$\begin{aligned}
r^2 &= \lambda_1^{(1)} + \lambda_3^{(1)} + \lambda_1^{(3)} + \lambda_2^{(3)} - \lambda_1^{(2)} - \lambda_3^{(2)} = 0, \\
a^2 &= \lambda_1^{(2)} + \lambda_3^{(2)} - \lambda_1^{(3)} - \lambda_2^{(3)} - \lambda_1^{(1)} = \lambda_3^{(1)}, \\
s^2 - \lambda_2^{(3)} &= \lambda_1^{(2)} + \lambda_3^{(2)} - \lambda_1^{(1)} - \lambda_3^{(1)} - \lambda_2^{(3)} = \lambda_1^{(3)}
\end{aligned}$$

and $f^2 = \lambda_1^{(1)}$. So these are all nonnegative on the E-points satisfying (70). For $[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}]$ we find $r^2 = 1/6$, $f^2 = 0$, $a^2 = 1/3$, $s^2 - \lambda_2^{(3)} = 0$. For the E-points satisfying (70) we have $a^2 - f^2 - 2r^2 = \lambda_3^{(1)} - \lambda_1^{(1)} \geq 0$. For $[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}]$ we have $a^2 - f^2 - 2r^2 = 0$. Then, for C_3 to be realized by the states constructed here it is sufficient to have

$$|2r^2 + f^2 - a^2 + \lambda_2^{(3)} - \lambda_1^{(3)}| \leq \lambda_3^{(2)} - \lambda_1^{(2)} \leq -2r^2 - f^2 + a^2 + \lambda_2^{(3)} - \lambda_1^{(3)} \tag{71}$$

for all corner points. This is satisfied by $[A, B, \frac{1}{6}\frac{1}{6}\frac{2}{3}]$ since $\lambda_2^{(3)} - \lambda_1^{(3)} = \lambda_3^{(2)} - \lambda_1^{(2)} = 0$. For the E-points satisfying (70), Equation (71) is equivalent to inequality (4) with $(abc) = (123)$, inequality (6) with $(abc) = (132)$ and

$$2\lambda_3^{(1)} + \lambda_1^{(1)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} \geq 2\lambda_1^{(2)} + \lambda_3^{(2)}.$$

This inequality can readily be verified by using inequality (3) with $(abc) = (231)$ and $\lambda_3^{(1)} \geq 1/3 \geq \lambda_1^{(2)}$. $\qquad \square$

Thus, we have constructed a state with any E-point in S with an additional condition $P_8 \leq 0$. Since the intersection of S and the hyperplane $P_8 = 0$ is the 5-dimensional convex set with corner points (65), the convex subset of S with the condition $P_8 \geq 0$ are those of S excluding $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$. By symmetry we can construct a state with any E-point in S satisfying

$$2\lambda_2^{(c)} + \lambda_3^{(c)} + 2\lambda_1^{(b)} + \lambda_2^{(b)} - 2\lambda_2^{(a)} - \lambda_3^{(a)} \leq 0 \tag{72}$$

for any (abc). Thus, our next task is to construct a state with any E-point in S with additional conditions

$$2\lambda_1^{(b)} + \lambda_2^{(b)} + 2\lambda_2^{(c)} + \lambda_3^{(c)} - 2\lambda_2^{(a)} - \lambda_3^{(a)} \geq 0 \tag{73}$$

for all (abc). This set of E-points is the convex set with all the corner points inherited from S except for $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$ and those obtained by qutrit permutations from it. Let us denote this set by S_2. From the construction of S_1 it is clear that inequalities (2), (3), (6) and (7) are redundant once we impose (73). We give a more straightforward proof of this fact.

Proposition 11. *Inequalities (2), (3), (6) and (7) follow from inequalities (1), (4), (5) and (73).*

Proof. Inequalities (6) and (7) follow immediately from inequality (73) by noting that $\lambda_2^{(b)} \geq \lambda_1^{(b)}$ and $\lambda_3^{(c)} \geq \lambda_2^{(c)}$, respectively. Inequality (5) is equivalent to

$$2\lambda_3^{(a)} + \lambda_2^{(a)} \leq 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_3^{(c)} + \lambda_2^{(c)}.$$

By adding this and inequality (73) and dividing by three we obtain inequality (3). Inequality (1) is equivalent to

$$2\lambda_3^{(a)} + \lambda_1^{(a)} \leq 2\lambda_2^{(b)} + \lambda_1^{(b)} + 2\lambda_3^{(c)} + \lambda_1^{(c)}.$$

On the other hand, inequality (73) is equivalent to

$$2\lambda_1^{(a)} + \lambda_3^{(a)} \leq 2\lambda_1^{(b)} + \lambda_2^{(b)} + 2\lambda_1^{(c)} + \lambda_3^{(c)}.$$

By adding these inequalities together and dividing by three we obtain inequality (2). $\qquad\square$

We observe that among the corner points of S_2 (in fact of S) the E-point $[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}]$ is the only E-point which violates the inequality

$$\tilde{P}_9 \equiv 2\lambda_1^{(2)} + \lambda_2^{(2)} + 2\lambda_1^{(3)} + \lambda_2^{(3)} - 2\lambda_1^{(1)} - \lambda_2^{(1)} \geq 0.$$

It has $\tilde{P}_9 = -1/3$. The E-points which satisfy $\tilde{P}_9 = 0$ are

$$[O, O, O], \; [A, A, O], \; [A, O, A], \; [B, O, B],$$
$$[B, B, O], \; [B, A, A], \; \left[B, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right], \; \left[B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A\right].$$

These E-points are the corner points of the convex subset of S_2 with the additional condition $\tilde{P}_9 \leq 0$ as we will show below.

Lemma 35. *Let S_3 be the convex subset of S_2 obtained by imposing an additional inequality $\tilde{P}_9 \leq 0$. Then $S_3 = D_1 \cup D_2 \cup D_3$ where D_1, D_2 and D_3 are simplices. The following E-points are the corner points of all three simplices:*

$$\left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right], \; [O, O, O], \; [B, B, O], \; [B, O, B], \; [B, A, A].$$

The additional corner points of each simplex are as follows:

$$\begin{aligned}
D_1 &: [A, A, O], \; \left[B, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right]; \\
D_2 &: [A, A, O], \; [A, O, A]; \\
D_3 &: [A, O, A], \; \left[B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A\right].
\end{aligned} \tag{74}$$

Proof. Since the E-point $[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}]$ is the only E-point satisfying $\tilde{P}_9 < 0$, the boundary hyperplanes of S_3 are $\tilde{P}_9 = 0$ and the boundary hyperplanes of S_2 that contain $[B, \frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}]$. The latter are $\lambda_1^{(1)} = \lambda_2^{(1)}$, $\lambda_2^{(1)} = \lambda_3^{(1)}$, $\lambda_1^{(2)} = 0$, $\lambda_1^{(3)} = 0$, (73) with $(abc) = (231)$, (73) with $(abc) = (321)$, (1) with $(abc) = (123)$, (5) with $(abc) = (123)$ and (5) with $(abc) = (132)$. It is enough to show that $D_1 \cup D_2 \cup D_3$ is bounded by these hyperplanes. We define

$$\begin{aligned}
Q_1 &\equiv \lambda_2^{(1)} - \lambda_1^{(1)} - \lambda_2^{(2)} + \lambda_1^{(2)} + \lambda_2^{(3)} - \lambda_1^{(3)}, \\
Q_2 &\equiv \lambda_2^{(1)} - \lambda_1^{(1)} + \lambda_2^{(2)} - \lambda_1^{(2)} - \lambda_2^{(3)} + \lambda_1^{(3)}.
\end{aligned}$$

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First we note that all E-points in D_1 satisfy $Q_1 \leq 0$ and $Q_2 \geq 0$, all E-points in D_2 satisfy $Q_1 \geq 0$ and $Q_2 \geq 0$, and all E-points in D_3 satisfy $Q_1 \geq 0$ and $Q_2 \leq 0$. Let us list the boundaries of each simplex together with the E-point omitted to obtain each boundary 5-simplex:

$$
\begin{aligned}
D_1 \ : \ & \left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right] \ : \ \tilde{P}_9 = 0; \ [O, O, O] \ : \ \lambda_2^{(1)} = \lambda_3^{(1)}; \\
& [B, O, B] \ : \ (73), (abc) = (321); \ [B, B, O] \ : \ \lambda_1^{(2)} = 0; \\
& [B, A, A] \ : \ (5), (abc) = (132); \ [A, A, O] \ : \ \lambda_1^{(1)} = \lambda_1^{(2)}; \\
& \left[B, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] \ : \ Q_1 = 0;
\end{aligned}
$$

$$
\begin{aligned}
D_2 \ : \ & \left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right] \ : \ \tilde{P}_9 = 0; \ [O, O, O] \ : \ \lambda_2^{(1)} = \lambda_3^{(1)}; \\
& [B, O, B] \ : \ \lambda_1^{(3)} = 0; \ [B, B, O] \ : \ \lambda_1^{(2)} = 0; \\
& [B, A, A] \ : \ (1), (abc) = (123); \ [A, A, O] \ : \ Q_2 = 0; \\
& [A, O, A] \ : \ Q_1 = 0;
\end{aligned}
$$

$$
\begin{aligned}
D_3 \ : \ & \left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right] \ : \ \tilde{P}_9 = 0; \ [O, O, O] \ : \ \lambda_2^{(1)} = \lambda_3^{(1)}; \\
& [B, O, B] \ : \ \lambda_1^{(3)} = 0; \ [B, B, O] \ : \ (73), (abc) = (231); \\
& [B, A, A] \ : \ (5), (abc) = (123); \ [A, O, A] \ : \ \lambda_1^{(1)} = \lambda_1^{(2)}; \\
& \left[B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A\right] \ : \ Q_2 = 0;
\end{aligned}
$$

Thus, the simplices D_1 and D_2 are glued together at the common boundary $Q_1 = 0$ with corner points $[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}]$, $[O, O, O]$, $[B, O, B]$, $[B, B, O]$, $[B, A, A]$ and $[A, A, O]$, and D_2 and D_3 at $Q_2 = 0$ with corner points $[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}]$, $[O, O, O]$, $[B, O, B]$, $[B, B, O]$, $[B, A, A]$ and $[A, O, A]$. The other boundaries are all boundary hyperplanes of S_3. Hence, $S_3 = D_1 \cup D_2 \cup D_3$. $\square$

Next we construct states which have E-points in this region.

Lemma 36. *There is a state with any E-point in S_3.*

Proof. Note that states with their E-points in D_2 have been constructed by Lemma 30. In order to construct states with their E-points in D_1 we consider the following PNCs: $c_{333}, c_{113}, c_{223}, c_{121}, c_{231}, c_{322}, c_{132}$. Since there are no nontrivial orthogonality relations, the set of E-points obtained from these coefficients is convex by Lemma 32. Hence it suffices to construct the corner points of D_1 using this set. This can be done as follows (with $A_{ijk} \equiv |c_{ijk}|^2$) :

$$
\begin{aligned}
& \left[B, 0\tfrac{1}{3}\tfrac{2}{3}, 0\tfrac{1}{3}\tfrac{2}{3}\right] \ : \ A_{132} = A_{223} = A_{333} = 1/3; \\
& [O, O, O] \ : \ A_{333} = 1; \\
& [B, O, B] \ : \ A_{333} = A_{231} = A_{132} = 1/3; \\
& [B, B, O] \ : \ A_{333} = A_{113} = A_{223} = 1/3; \\
& [B, A, A] \ : \ A_{132} = A_{223} = 1/3, \ A_{322} = A_{333} = 1/6; \\
& [A, A, O] \ : \ A_{333} = A_{223} = 1/2; \\
& \left[B, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] \ : \ A_{121} = A_{132} = 1/6, \ A_{333} = A_{223} = 1/3.
\end{aligned}
$$

The simplex D_3 is obtained from D_1 by the qutrit permutation $(2) \leftrightarrow (3)$. $\square$

Thus, we have constructed states with their E-points in the convex subset of S_2 satisfying $\tilde{P}_9 \leq 0$. By symmetry we can construct states with their E-points in S_2 if they satisfy

$$P_9^{(abc)} \equiv 2\lambda_1^{(b)} + \lambda_2^{(b)} + 2\lambda_1^{(c)} + \lambda_2^{(c)} - 2\lambda_1^{(a)} - \lambda_2^{(a)} \leq 0$$

for some (abc). Let us denote the convex subset of S_2 satisfying $P_9^{(abc)} \geq 0$ for all (abc) by S_4. Our task is now reduced to constructing states with their E-points in S_4. The corner points of S_4 are those of S excluding $[A, \frac{1}{4}\frac{1}{4}\frac{1}{2}, 0\frac{1}{4}\frac{3}{4}]$ and $[B, 0\frac{1}{3}\frac{2}{3}, 0\frac{1}{3}\frac{2}{3}]$ and those obtained by qutrit permutations from them. The following lemma, which allows us to reduce the convex set S_4 further by removing $[A, A, A]$ from the corner points, can be proved by using Proposition 10.

Lemma 37. *The convex subset of S_4 satisfying*

$$Q_3 \equiv 1 + \lambda_1^{(1)} - \lambda_2^{(1)} + \lambda_1^{(2)} - \lambda_2^{(2)} + \lambda_1^{(3)} - \lambda_2^{(3)} \leq 0 \tag{75}$$

is a simplex with the following corner points:

$$[A, A, A], \; [O, A, A], \; [A, O, A], \; [A, A, O], \; [B, A, A], \; [A, B, A], \; [A, A, B].$$

There is a state with any E-point in this simplex.

Proof. It is straightforward to check that $Q_3 > 0$ for any corner point of S_4 not listed here. We have $Q_3 = -1/2$ for $[A, A, A]$ and $Q_3 = 0$ for the other E-points in the list. The simplex with the corner points given here is bounded by the hyperplane $Q_3 = 0$ and the boundary hyperplanes of S_4 that contain $[A, A, A]$, which are $\lambda_1^{(a)} = 0$ and $\lambda_2^{(a)} = \lambda_3^{(a)}$, $a = 1, 2, 3$. Hence, this simplex is the subset of S_4 with the condition (75). All E-points in this simplex can be realized by quantum states by Proposition 10 since it is a subset of S_0. $\square$

Thus, our task is further reduced to constructing the convex set S_5 whose corner points are those of S_4 excluding $[A, A, A]$. The following proposition almost accomplishes this task.

Proposition 12. *There is a state with any E-point in the convex set $S_6^{(1)}$ bounded by hyperplanes with the same corner points as S_5 excluding $[O, A, A]$.*

Proof. Consider the following set of PNCs:

$$\{c_{333}, c_{113}, c_{131}, c_{223}, c_{232}, c_{211}, c_{321}, c_{312}, c_{122}\}.$$

Note that this set is invariant under the qutrit permutation $(2) \leftrightarrow (3)$. Note also that there are no nontrivial orthogonality relations to be satisfied. Hence, the set of the E-points realized by the states considered here is convex by Lemma 32. Therefore all we need to do is find the values of $A_{ijk} = |c_{ijk}|^2$ for each corner point of S_5 except for $[O, A, A]$. This can

be done as follows:

$$
\begin{aligned}
&[O, O, O] \ : \ A_{333} = 1; \\
&[B, B, B] \ : \ A_{333} = A_{113} = A_{133} = \cdots = A_{122} = 1/9; \\
&[B, A, B] \ : \ A_{333} = A_{223} = A_{131} = A_{232} = A_{321} = A_{122} = 1/6; \\
&[A, B, B] \ : \ A_{333} = A_{223} = A_{211} = A_{232} = A_{321} = A_{312} = 1/6; \\
&[B, B, O] \ : \ A_{333} = A_{113} = A_{223} = 1/3; \\
&[O, B, B] \ : \ A_{333} = A_{312} = A_{321} = 1/3; \\
&[B, A, A] \ : \ A_{333} = A_{122} = 1/3, \ A_{232} = A_{223} = 1/6; \\
&[A, B, A] \ : \ A_{333} = A_{232} = 1/6, \ A_{312} = A_{223} = 1/3; \\
&[A, A, O] \ : \ A_{333} = A_{223} = 1/2; \\
&[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}] \ : \ A_{211} = A_{232} = A_{223} = 1/6, \ A_{333} = 1/2; \\
&[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}] \ : \ A_{223} = A_{122} = A_{321} = 1/6, \ A_{333} = 1/2; \\
&[A, B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}] \ : \ A_{211} = A_{312} = 1/6, \ A_{333} = A_{223} = 1/3; \\
&[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, B, A] \ : \ A_{333} = A_{312} = 1/3, \ A_{223} = A_{122} = 1/6; \\
&[B, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A] \ : \ A_{122} = A_{113} = 1/6, \ A_{333} = A_{232} = 1/3.
\end{aligned}
$$

The E-points which are obtained from these by the qutrit permutation $(2) \leftrightarrow (3)$ can also be obtained by letting $A_{ijk} \to A_{ikj}$ in this list. □

There are two convex sets $S_6^{(2)}$ and $S_6^{(3)}$ where all corner points of S_5 are realized except $[A, O, A]$ and except $[A, A, O]$, respectively, which are constructed similarly. Therefore all simplices whose corner points are also corner points of S_5 can be realized except those with all three E-points $[O, A, A]$, $[A, O, A]$ and $[A, A, O]$ as corner points. This observation can be used to finish the construction of states with their E-points in S_5.

Proposition 13. *There is a state with any E-point in S_5.*

Proof. Any E-point X in the set S_5 can be represented as

$$
X = \sum_s \alpha_s Y_s, \tag{76}
$$

where Y_s are the corner points of S_5 and where the α_s are nonnegative and satisfy $\sum_s \alpha_s = 1$. If the coefficients α_s for the corner points $[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}]$, $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}]$ and $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A]$ are zero, then the corresponding E-point is realized by a state by Proposition 10. Also, if the coefficient α_s for $[A, A, O]$, $[A, O, A]$ or $[O, A, A]$ vanishes, then, the corresponding E-point is realized by Proposition 12 and the remark following it.

Suppose that the coefficient for $[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}]$ is $\alpha_1^{(1)}$ and that for $[O, A, A]$ is $\alpha_2^{(1)}$ for an E-point X in (76). Note that

$$
2\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] + [O, A, A] = [A, A, O] + [A, O, A] + [O, B, B].
$$

Suppose that $\alpha_1^{(1)} \geq 2\alpha_2^{(1)}$. Then

$$
\begin{aligned}
\alpha_1^{(1)}\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] + \alpha_2^{(1)}[O, A, A] \ = \ &(\alpha_1^{(1)} - 2\alpha_2^{(1)})\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}\right] \\
&+ \alpha_2^{(1)}\left\{[A, A, O] + [A, O, A] + [O, B, B]\right\}.
\end{aligned}
$$

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Thus, the E-point X can be reexpressed in such a way that the coefficient for $[O, A, A]$ vanishes. On the other hand, if $\alpha_1^{(1)} \leq 2\alpha_2^{(1)}$, then we can write

$$\alpha_1^{(1)} \left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3} \right] + \alpha_2^{(1)} [O, A, A] = \left(\alpha_2^{(1)} - \tfrac{1}{2}\alpha_1^{(1)} \right) [O, A, A]$$
$$+ \tfrac{1}{2}\alpha_1^{(1)} \left\{ [A, A, O] + [A, O, A] + [O, B, B] \right\}.$$

Hence, the E-point X can be reexpressed in such a way that the coefficient for $\left[A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3} \right]$ vanishes. By symmetry the same conclusions can be made for the case where the coefficients for both $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}]$ and $[A, O, A]$ are nonzero or where those for both $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A]$ and $[A, A, O]$ are nonzero.

Let the coefficients for $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}]$ and $[\tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, \tfrac{1}{6}\tfrac{1}{6}\tfrac{2}{3}, A]$ be $\alpha_1^{(2)}$ and $\alpha_1^{(3)}$, respectively, and those for $[A, O, A]$ and $[A, A, O]$ be $\alpha_2^{(2)}$ and $\alpha_2^{(3)}$, respectively, for the E-point X. If $\alpha_1^{(a)} \geq 2\alpha_2^{(a)}$ for some a, then the E-point X can be reexpressed in such a way that one of the coefficients $\alpha_2^{(a)}$ vanishes. Then by Proposition 12 we can conclude that E-point X has a corresponding state. If $\alpha_1^{(a)} < 2\alpha_2^{(a)}$ for all a, then by successively applying the argument above to each qutrit, we can make $\alpha_1^{(a)}$ vanish for all a. (Note that the coefficients $\alpha_2^{(a)}$ never decrease in this process.) Then by Proposition 10 the E-point X has a corresponding state. $\qquad\square$

X. CONCLUDING REMARK

It is surprising that there is a very simple condition on the RDMs for the n-qubit pure quantum state [1, 2] for all n. The analogous condition for the qutrit system has turned out to be more complicated as shown in this paper. Nevertheless, the result, Theorem 1, has some structure, and it is probable that there is a proof simpler than the one given here. It is natural to investigate the corresponding problem for the n-qudit pure quantum system for all n. There are two features in our result which may be true in the general case. One is that the set of the allowed E-points is convex. The other is that the boundaries of this set are hyperplanes in the space of E-points. We conclude this paper by a proposition which suggests that the boundaries are indeed hyperplanes in the n-qudit case.

An n-qudit quantum state is given by

$$|\Psi\rangle \equiv \sum_{1 \leq i_1, i_2, \dots, i_n \leq d} c_{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{77}$$

with $\sum_{i_1, i_2, \dots, i_n} |c_{i_1 i_2 \cdots i_n}|^2 = 1$, where $|1\rangle$, $|2\rangle$,...,$|d\rangle$ form an orthonormal basis. As before we assume that the RDMs are diagonal. Let $\lambda_i^{(a)}$ be the ith smallest eigenvalue of the RDM for the ath qudit. We regard the set of these eigenvalues as a point in the $n(d-1)$-dimensional Euclidean space parametrized by $\lambda_i^{(a)}$, $1 \leq i \leq d-1$, $1 \leq a \leq n$ and call this set an E-point as before. It is convenient to define the lattice E-point $L_{i_1 i_2 \dots i_n}$ as the E-point given by $\lambda_{i_a}^{(a)} = 1$ and, as a result, $\lambda_i^{(a)} = 0$ if $i \neq i_a$. Note that these E-points do not correspond to a physical state unless $i_1 = i_2 = \cdots = i_n = d$ because they do not satisfy the conditions $\lambda_i^{(a)} \leq \lambda_j^{(a)}$ for $i < j$. For a given set N of n-tuples we define V_N to be the convex set whose elements λ are the E-points given as

$$\lambda = \sum_{[i_1 i_2 \cdots i_n] \in N} A_{i_1 i_2 \cdots i_n} L_{i_1 i_2 \cdots i_n},$$

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where $0 \leq A_{i_1 i_2 \cdots i_n} \leq 1$ and $\sum_{[i_1 i_2 \cdots i_n] \in N} A_{i_1 i_2 \cdots i_n} = 1$. The following lemma is useful in proving our proposition.

Lemma 38. *Consider a state of the form (77) with the eigenvalues $\Lambda_i^{(a)}$, $i = 1, ..., d$, $a = 1, ..., n$, such that $c_{i_1 i_2 \cdots i_n} \neq 0$ only if $[i_1 i_2 \ldots i_n] \in N$. Then the corresponding E-point $\Lambda \equiv (\Lambda_i^{(a)})$ is in V_N.*

Proof. An E-point $\lambda \equiv (\lambda_i^{(a)})$ in V_N is given by

$$\lambda_i^{(a)} = \sum_{(j_1, j_2, \ldots, j_n) \in N} A_{j_1 j_2 \ldots j_n} \delta_{j_a i} ,$$

where $0 \leq A_{j_1 j_2 \ldots j_n} \leq 1$ and $\sum_{[i_1 i_2 \ldots i_n] \in N} A_{i_1 i_2 \ldots i_n} = 1$. These are the formulae for $\lambda_i^{(a)}$ for the state (77) if we make the identification $A_{i_1 i_2 \cdots i_n} = |c_{i_1 i_2 \cdots i_n}|^2$. $\quad\square$

Proposition 14. *Let U be an open set in the $d(n-1)$-dimensional space of E-points. Suppose that the eigenvalues are not degenerate in U. Suppose further that an E-point $\lambda \equiv (\lambda_i^{(a)})$ has a corresponding state if and only if $f(\lambda) \geq 0$, where f is a function with a continuous and nonzero gradient and that the hypersurface $f(\lambda) = 0$ is connected. Then this hypersurface is part of the hyperplane V_N for some set of n-tuples N.*

Proof. Suppose that a state with $\lambda_i^{(a)} = \Lambda_i^{(a)}$ is in U and on the boundary so that $f(\Lambda) = 0$, where $\Lambda \equiv (\Lambda_i^{(a)})$, and that both $c_{i_1 i_2 \cdots i_n}$ and $c_{i'_1 i'_2 \cdots i'_n}$ are nonzero for this state. We consider the variation

$$\delta c_{i_1 i_2 \cdots i_n} = \alpha c_{i'_1 i'_2 \cdots i'_n} , \quad \delta c_{i'_1 i'_2 \cdots i'_n} = -\overline{\alpha} c_{i_1 i_2 \cdots i_n}$$

with all other $\delta c_{I_1 I_2 \cdots I_n}$ vanishing. Then the variation of the function f is given by

$$\begin{aligned}
\delta f &= \sum_{a=1}^{n} \sum_{i=1}^{d-1} \left.\frac{\partial f}{\partial \lambda_i^{(a)}}\right|_{\lambda = \Lambda} \delta \lambda_i^{(a)} \\
&= \sum_{a=1}^{n} \left.\left[\frac{\partial f}{\partial \lambda_{i_a}^{(a)}} - \frac{\partial f}{\partial \lambda_{i'_a}^{(a)}}\right]\right|_{\lambda = \Lambda} \cdot 2\mathrm{Re}\left(\alpha c_{i'_1 i'_2 \cdots i'_n} \overline{c_{i_1 i_2 \cdots i_n}}\right) ,
\end{aligned}$$

where we have defined $\partial f / \partial \lambda_d^{(a)} = 0$ for all a, because there are no degenerate eigenvalues. For δf to be nonnegative for all α we must have

$$\sum_{a=1}^{n} \left.\frac{\partial f}{\partial \lambda_{i_a}^{(a)}}\right|_{\lambda = \Lambda} = \sum_{a=1}^{n} \left.\frac{\partial f}{\partial \lambda_{i'_a}^{(a)}}\right|_{\lambda = \Lambda} . \tag{78}$$

Define a linear function F by

$$F(\lambda) = \sum_{a=1}^{n} \sum_{i=1}^{d-1} \left.\frac{\partial f}{\partial \lambda_i^{(a)}}\right|_{\lambda = \Lambda} \lambda_i^{(a)} .$$

Then Eq. (78) implies that $F(L_{i_1 i_2 \cdots i_n})$ must be the same for all $[i_1 i_2 \ldots i_n] \in \tilde{N}$, where $\tilde{N}$ is the set of n-tuples such that $c_{i_1 i_2 \cdots i_n} \neq 0$ for the given state. Let this value be v. Then the equation $F(\lambda) = v$ determines a hyperplane containing all lattice E-points $L_{i_1 i_2 \cdots i_n}$ such

that $[i_1 i_2 \ldots i_n] \in \tilde{N}$. This implies that the convex set $V_{\tilde{N}}$ is contained in a hyperplane. Thus, $V_{\tilde{N}} \subset V_N$ with $\tilde{N} \subset N$, where V_N is a hyperplane. Hence, by Lemma 38 we find $\Lambda \in V_{\tilde{N}} \subset V_N$. Thus, all E-points on $f(\lambda) = 0$ are on a hyperplane V_N for some N. Since there are only a finite number of such hyperplanes, and since the connected hypersurface $f(\lambda) = 0$ has a tangent hyperplane everywhere, this hypersurface must coincide with a single hyperplane V_N. $\square$

Acknowledgments

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