Geometry of density states

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We reconsider the geometry of pure and mixed states in a finite quantum system. The ranges of eigenvalues of the density matrices delimit a regular simplex (Hypertetrahedron $T_N$) in any dimension $N$; the polytope isometry group is the symmetric group $S_{N+1}$, and splits $T_N$ in chambers, the orbits of the states under the projective group $PU(N+1)$. The type of states correlates with the vertices, edges, faces, etc. of the polytope, with the vertices making up a base of orthogonal pure states. The entropy function as a measure of the purity of these states is also easily calculable; we draw and consider some isentropic surfaces. The Casimir invariants acquire then also a more transparent interpretation.

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I. INTRODUCTION

Pure states $\pi$ in Quantum Mechanics are described by rays in a Hilbert space $\mathcal{H}$, or equivalently as unidimensional subspaces. As such, they can be identified with orthogonal projectors of unit trace (so for $k$-dimensional subspaces they will have trace $k$); denoting by $End\,\mathcal{V}$ the linear operators of a vector space $\mathcal{V}$, we have

$$\{\text{space of pure states}\} \approx \{\pi \in End\,\mathcal{H} | \pi = \pi^\dagger, \quad Tr[\pi] = 1, \quad \pi^2 = \pi\}$$

To include mixed states $\rho$, it is enough (von Neumann) to relax idempotency ($\pi^2 = \pi$, so Spectrum $\pi = \{1,0\}$) to mere positivity, $\rho \geq 0 \iff \text{Spec } \rho \geq 0$, which implies $0 \leq \mu_i \leq 1$ for $\mu_i \in \text{Spec } \rho$. Hence

$$\{\text{space of pure/mixed states}\} \approx \{\rho \in End\,\mathcal{H} | \rho = \rho^\dagger, \quad Tr[\rho] = 1, \quad \rho \geq 0\}$$

So the pure states are extremal, as $\rho^2 \leq \rho$, and one can write the mixed states as incoherent addition of pure ones,

$$\rho = \sum p_i \pi_i, \quad \sum p_i = 1, \quad p_i \geq 0$$

For finite quantum systems ($\mathcal{H} \to \mathcal{V}$, dim $V = N < +\infty$) the geometry of these states has been studied lately from different points of view, as it is pertinent to quantum information and other modern applications. For example, in [1] the nature of the space of pure states, namely the projective spaces $CP^{N-1}$, is stressed, as they are rank-one symmetric spaces; in [2] the mixed states are related to a coherence vector $\vec{n}$, lying in a subset of euclidean space, determined by the values of Casimir invariants for the group $SU(N)$. [3] studies the stratification of general states under the projective group

$$PU(N) = U(N)/U(1) = SU(N)/Z_n$$

in relation to a (in general not regular) foliation by Kähler manifolds, similar to the orbits of the (co-)adjoint representation of $SU(N)$, that is, the Kirillov-Souriau method. The geometry of the $N = 3$ case had been studied sometime ago also by Michel [4] in relation to $SU(3)$ as a flavor group.

In this report we would like to complete the above descriptions in several ways. In particular, we elaborate on an idea in [3], showing that the set of eigenvalues $\mu_i$ of the density operator $\rho$, $\mu_i \in \text{Spec } \rho$, coincides precisely with the points of a solid simplex (the hypertetrahedron $T_N$), the simplest regular polytope. The natural isometry group, the full symmetric group $S_{N+1}$, corresponds, of course, to a (finite) Coxeter group, that is, the Weyl group of the Lie algebra $A_N$ of the group $SU(N+1)$: the unit trace in our case is traded for the traceless character of (anti-)hermitian matrices describing $A_N$. The orbit space $T_N/S_{N+1}$ is still an (irregular) hypertetrahedron, of size $1/(N+1)!$ of the previous regular one, behaves like the Weyl chambers, and describes precisely the orbits of our states under the projective group, each point being just an orbit. The type of orbits, as classified by the little groups, is in correspondence with the combinatorial elements of the simplices, namely vertices, edges, faces and so on, and also with the partitions of the number $N$.

For example for $N = 2$ the set of pure states is the 2-sphere $S^2 = CP^1$, the set of all states is the three dimensional Bloch ball $B^3$ of unit radius, with boundary being the pure states, the simplex is just the closed segment $[-1, 1]$, the Weyl group $Z_2$ is reflection in the middle, and the chamber is the half-segment $I/Z_2 = [0, 1]$ with 0 the most mixed states (called mixMax or $mM$ henceforth), and with 1 indicating the (sphere of) pure states. In this simplest (and nonrepresentative) case there is only one stratum, i.e. one type of orbit (namely 2-spheres), besides of course the fix point $mM$ or 0; the (single)
Casimir $I_2$ just labels the radius of these spheres $S_r$, $0 < r \leq 1$. The $mM$ state corresponds to partition $[2]$, the rest to $[1^2]$, as stratum orbits $\approx U(2)/U(1)^2$.

The Casimir invariants $I_l$ admit a double interpretation, as an homogeneous system of generators of the center of the enveloping algebra of Lie group, or in our case, as the symmetrization functions (Newton) over the roots of the spectral equation for the density operator. We elaborate here the considerations of \[2\], based on the pioneer work of Biedenharn \[3\].

In this picture it is also clear how to compute the entropy $\eta$ of these mixed states, where $\eta(\rho) = - \text{Tr} \log(\rho)$. This varies between $\eta = \log N$ for the $mM$ state to $\log 1 = 0$ for pure states. We include some graphs showing the entropy for some boundary lines on the "chambers" of the orbit space, as well as some isentropic surfaces in the general case. Each case $N$ includes, in a precise sense, all the previous ones, $n < N$.

We stress also the action of the projective isometry group $PU(N + 1) \subset SO((N + 1)^2 - 1)$ as the group acting effectively in the space of states, in the sense of the characterization of geometries (F. Klein): in the transformation $\rho \rightarrow U \rho U^\dagger$ the effective group acting $PU = U/U(1)$: the kernel of the $U$ action is $U(1)$, and even $SU$ acts with kernel $Z_n$; the explanatory diagram is

$$
Z_n \rightarrow SU(N) \rightarrow PSU(N)
\downarrow
U(1) \rightarrow U(N) \rightarrow PU(N)
\downarrow
U(1) =: U(1)
$$

The organization of the paper is as follows. In Sect. 2 we establish notation and show several properties of our objects needed later. In Sect. 3 we recall the situation for qubits ($N=2$), qutrits ($N=3$), and $N=4$, incorporating the new observations of above and suggesting generalizations to higher dimensions. Then Sect. 4 deals with the general theory for arbitrary $N$: we exhibit explicitly the polytope, the Weyl quotient ("chamber"), the types of states, the Casimir invariants and discuss the entropy function, and also some cases of isentropic surfaces.

Other considerations (including mention of omissions) are in our final Sect. 5.

II. GENERAL DESCRIPTION AND PROPERTIES OF MIXED STATES

In this Section we summarize important results of \[2\] to \[4\]. Let $\mathcal{S}$ be set of $N$-dimensional density matrices $\rho$, and let $\mathcal{P} \subset \mathcal{S}$ the subset of pure states, $\pi$, with $\pi^2 = \pi$. The conditions

$$
\rho = \rho^\dagger, \quad \text{Tr}[\rho] = 1
$$

are respectively linear and affine, so the whole set of solutions of the equation is like a real vector space of dim $N^2-1$. The positivity condition $\rho > 0$, though, is a convex condition, and selects a nonlinear submanifold $\mathcal{S}$ of $R^{N^2-1}$ (which is closed as the spectral restriction is really $0 \leq \mu_i \leq 1$), of the same dimension, with $\mathcal{P}$ as the extremals of the convex set (not the boundary, in general: we know of course that $\mathcal{P} = CP^{N-1}$, so dim $\mathcal{P} = 2N - 2 \leq N^2 - 1$ for large $N$). In the set of hermitian traceless matrices $\{h\}$ one introduces the definite scalar product

$$
< h_1, h_2 > := (1/2) \text{Tr}[h_1 h_2]
$$

and therefore there exists an orthonormal base $\lambda_1, \lambda_2, \ldots, \lambda_{N^2-1}$ with properties

$$
\lambda_i = \lambda_i^\dagger, \quad \text{Tr}[\lambda_i] = 0, \quad \text{Tr}[\lambda_i^2] = 2.
$$

So the general density matrix can be written as

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

where the factor $\sqrt{N(N-1)/2}$ guarantees that pure states, $\pi^2 = \pi$ have norm $|n| = 1$; see \[2\] for details; $\vec{n}$ is called the coherence vector.

We recall also two related properties of the group $SU(N)$; first, the square of the adjoint representation contains the adjoint BOTH in the symmetric and in the antisymmetric part (for $N=2$ the first is missing), and second, consequently, this induces two algebras in the space of matrices (corresponding to the coefficients $f_{ijk}$ and $d_{ijk}$ of Gell-Mann; of course, the $f$'s correspond to the Lie algebra structure); for details see \[4\].

Now the group $PU(N)$ is acting in the set of states $\mathcal{S}$ as $\rho \rightarrow U \rho U^{-1}$. If the eigenvalues of $\rho$ are different, the little group is $U(1)^{N-1}$, and then the generic orbit is $PU(N)/U(1)^{N-1}$, of dimension $N(N-1)$. This is a Kähler manifold, as are all orbits of the adjoint of any simple Lie group (we notice that $N(N-1)$ is even); in particular this space is called a (complex) flag manifold, with structure (as homogeneous space),

$$
\mathcal{F}\mathcal{L}_C(N) = PU(N)/U(1)^{N-1} = U(N)/U(1)^N.
$$

The other extreme contains the pure states, with little group $U(N-1)$; these most critical orbits have dimension $2(N-1)$, as we said above. There is always naturally a single most-mixed state, $O$ (or $mM$), with $\vec{n} = 0$: this is the fixed point under the $PU$ action, and it is unique. Orbits in state space with conjugate little groups form what is called a stratum (see e.g. \[4\]), and in fact for a compact group (as is our case) acting "nicely" in some space $X$ the number of strata is finite; we shall see that it coincides with the number of types of states and also naturally with the partitions of $N$.

We define the entropy $\eta = \eta(\rho)$ of a state $\rho$ as the expectation value of the operator $H = -\log(\rho) > 0$ (von Neumann; notice $\rho \leq 1$, so $\log(\rho)$ is negative); recalling
that in the density formalism $<A>=\text{Tr}(\rho A)$, we have, with $\mu_i \in \text{Spec } \rho$,
\[
\eta(\rho) = -\text{Tr} \rho \log(\rho) = \log(\prod \mu_i^{-\mu_i}).
\]

This varies, as said, between $\log N$ and $\log 1=0$: the mM state is the most disordered, and the pure states are the most ordered: we shall see also the $N$ case reproduces the entropy function for all previous cases $n < N$, and therefore there must be several manifolds of mixed states isentropic, with the same value for the entropy: we shall provide some examples.

As for the Casimir invariants, we define them from the spectral equation for the density operator as the coefficients of the powers, i.e.:
\[
\rho^N - (\text{Tr}\rho)\rho^{N-1} + I_2\rho^{N-2} - I_3\rho^{N-3} + \ldots (-1)^N \text{det}\rho = 0
\]

where $I_1 = \text{Tr}(\rho) \equiv 1$, (the first Casimir). They determine the spectrum up to a permutation, e.g.
\[
I_2 = \sum_{i<j} \mu_i \mu_j,
\]
and $I_n = \prod \mu_i = \mu_1 \ldots \mu_N$

These operators can be expressed also as traces of powers of representative matrices, as for example
\[
I_2 = (1/2)[(\text{Tr}\rho)^2 - \text{Tr}(\rho^2)]; \text{ so it's zero iff } \rho \text{ is pure.}
\]
\[
I_3 = (1/6)[(\text{Tr}\rho)^3 + 2\text{Tr}(\rho^3) - 3\text{Tr}(\rho)\text{Tr}(\rho^2)].
\]

There are also several inequalities assuring all Casimirs are nonnegative, etc.

### III. THE SIMPLEST CASES

For $N=1$ we have just a single point, a pure state, as $CP^0 = \text{point}$, with entropy $\log(1)=0$. For $N=2$ the density matrix can be written as
\[
\rho = (1/2)(1 + \vec{\sigma} \cdot \vec{x});
\]
we have $\vec{x} \in B^3$ ball (radius 1) with the 2-dim boundary sphere $S^2 = CP^1$ of pure states. The set of eigenvalues $\{(1+z)/2,(1-z)/2\}$ or $(x,y)$ with $x+y=1$ makes up a segment $I$ in fig 1 where $P_1$ is e.g. the state $[0,-1]$, mM is $[1/2,1/2]$, and $P_2$ is $[1,0]$. The crucial but trivial point now is that under the symmetry $Z_2$: $(x,y) \rightarrow (y,x)$ the states are equivalent, so the segment $I$ becomes just the half-segment $[0,1]$; that is, the mM state $0$, the mixed states $0 < x < 1$ and the (representative of) pure state(s) $P$, $x=1$. In this case $PU(2) = SU(2)/Z_2 = SO(3)$, so the orbits are just spheres, and $x$ in the half-segment means just the radius of them. There are only two strata, the fixed point (little group $SO(3)$) and the rest, little group $SO(2)=U(1)$. The strata correspond to the two partitions namely $U(2)/U(2) = \{\text{Point}\} = mM$ is $[2]$ and $U(2)/U(1)^2 = PU(2)/U(1) = CP^1$ is the partition $[1^3] = [1,1,1]$. The entropy is a smooth function from $\log(2)=0.693$ (for the mM state) to $\log(1)=0$ for the pure one (fig 2); we shall see that the entropy function of the $N$ case always contains that of the $n < N$ previous cases.

There is only a Casimir, the quadratic one, with
\[
I_2 = [(1+z)/2][(1-z)/2] = xy = x(1-x),
\]
which lies between $1/4$ and zero.

One can also use an "angle" picture [2], namely with $z = \cos \theta$, $0 \leq \theta \leq \pi$, $x = \cos^2 \theta/2$, $y = \sin^2 \theta/2$. The (quadratic) Casimir is now $(1/4) \sin^2 \theta$. The entropy in terms of angle variables is
\[
\eta(\theta) = -\cos^2(\theta/2) \log[\cos^2(\theta/2)] - \sin^2(\theta/2) \log[\sin^2(\theta/2)].
\]

For $N=3$ we have $\rho = (1/3)(1 + \sqrt{3} \vec{n} \cdot \vec{\lambda})$, where the $\lambda$'s are e.g. the Gell-Mann matrices. Choosing $\lambda_3$ and $\lambda_8$ diagonal, we get, with $n = (0,0,a,0,0,0,0,b)$ and
\[
\rho_{\text{diag}} = \frac{1}{3} \left( \begin{array}{ccc} 1 + \sqrt{3}a + b & 0 & 0 \\ 0 & 1 - \sqrt{3}a + b & 0 \\ 0 & 0 & 1 - 2b \end{array} \right)
\]
as $\rho_{\text{diag}} = (1 + \sqrt{3}(a\lambda_3 + b\lambda_8))/3$. Hence positivity implies $-1 \leq b \leq 1/2$, and one gets a regular triangle "upside down" inscribed in the circle of radius one (fig 2).

Notice the three vertices $P_{1,2,3}$; 3 edges $l_{1,2,3}$, and the three interior lines (heights) $h_{1,2,3}$ with intersection points $Q_{1,2,3}$. The figure is identical to the so-called Fano plane, related (among other things) to the octonion multiplication rule [6] and to the projective plane $F_2P^2$, with automorphisms the simple group $PSL_3(2)$ of 168 elements [7]. This is another test of the relation of $SU(3)$ with octonions!

Under the action of the symmetry group, now $S_3$ with 6 elements, isomorphic to the dihedral group $D_3$ (the isometry of the regular n-gon is $D_n$), the fundamental domain or chamber is a little rectangular triangle (there
are six of them), 1/6 in area of the big one; we select one of them as $\triangle OQP$ as in fig. 3 Here $O$ is the mixMax state, $P$ the pure, $Q$ intermediate, i.e., $\eta(O)=\log(3)$, $\eta(Q)=\log(2)$, $\eta(P)=\log(1)=0$.

In terms of the eigenvalues of $\rho$, $O$ is $(1/3, 1/3, 1/3)$, $P$ is $(1, 0, 0)$, $Q$ is $(1/2, 1/2, 0)$; recall that the order is immaterial. The line $OQ$ is type $h(xxy, x \geq y)$; the line $QP$ is type $l(xy0, x \geq y \geq 0)$, and this line reproduces the $N=2$ case, with $Q$ seen as the mM state.

The line $OP$ is type $h$, with $(xxy, x \geq y)$. Note all the statements are order-invariant! In fact in the large triangle the line $PQ$ is a single line! Notice also the boundary lines in the big triangle unite pure states, so they have 0 in the spectrum. Each line represents the three embeddings of $SU(2)$ in $SU(3)$, called by Gell-Mann $u$, $v$ and $w$ spin. It becomes a single line in the little triangle, line $PQ$.

Note the set of generic states (little group $U(1)^2$) is 6-dimensional, open and dense; therefore, the representatives are bi-dimensional (2+6=8=dim $SU(3)$). The critical states (two equal eigenvalues, little group $U(2)$) are the two lines emanating from $O$, but $O$ is the fixed point, with isotropy just $PU(3)$ itself. The three partitions of $[3]$ are: $mM = U(3)/U(3)$ is $[3]$, $U(3)/U(1) \times U(2) = CP^2$ and $U(3)/U(1)^3$, which is the flag manifold. Notice also the little triangle is rectangular, NOT regular.

The Casimir invariants now are two, quadratic and cubic. They are

$$ I_2 = \mu_1\mu_2 + \mu_2\mu_3 + \mu_3\mu_1, \quad I_3 = \mu_1\mu_2\mu_3, $$ (17)

The quadratic Casimir is zero for the pure state, the cubic zero for pure state also and on the boundary line $QP$. We have:

|   | $I_2$ | $I_3$ |
|---|---|---|
| $O$ | 1/3 | 1/27 |
| $P$ | 1/4 | 0 |
| $Q$ | 0 | 0 |

There is an inequality between $I_2$ and $I_3$, because the cubic equation has to have real roots; see [2].

One can also parameterize the states with two angles $[2]$, with e.g.

$$ x = \sin^2 \theta/2 \cos^2 \phi/2, \quad y = \sin^2 \theta/2 \sin^2 \phi/2, \quad z = \cos^2 \theta/2 $$ (18)

The entropy of the $(xyz)$ state, with $x + y + z = 1$, is $\log(x^{-x} y^{-y} z^{-z})$. Fig 4 shows the entropy surface. It varies from $\log(3)$ at $O$ to $\log(2)$ at $Q$ to $\log(1)=0$ at $P$. Fig 5 shows the isentropic lines over the triangle. The point $R$ on line $OP$ with $\eta(R) = \log(2)$ is $x y y = .768, .116, .116$.

We have come now to the $N = 4$ case. The general state with $\lambda_1, \ldots \lambda_{15}$ is

$$ \rho = \frac{1}{4}(1 + \sqrt{6} \mathbf{n} \cdot \tilde{\lambda}). $$ (19)

We take $\lambda_{15}$ as

$$ \lambda_{15} = \frac{1}{\sqrt{6}} \text{diag}\{1, 1, 1, -3\}, $$ (20)
which gives the diagonal density matrix

\[ \rho \approx \frac{1}{4} \begin{pmatrix} 1 + \sqrt{6}a + \sqrt{2}b + c & 0 & 0 \\ 0 & 1 - \sqrt{6}a + \sqrt{2}b + c & 0 \\ 0 & 0 & 1 - 2\sqrt{2}b + c \end{pmatrix} \] (21)

in particular \( c \leq \frac{1}{3} \). The figure is now a regular tetrahedron inscribed in \( S^2 \). Again, the action of the 24 elements of the \( S_4 \) group generates the little rectangular tetrahedron as quotient (fig 6).

In the eigenvalue notation \((xyzu)\), \( x + y + z + u = 1 \), the coordinates of the vertices are:
- \( O \) is \((1/4, 1/4, 1/4, 1/4)\); \( mM \) state=\( U(4)/U(4) \), partition \([4]\).
- \( P \) is \((1, 0, 0, 0)\); pure state=\( U(4)/[U(1) \times U(3)] \), partition \([3,1]\).
- \( Q_A \) is \((1/2, 1/2, 0, 0)\); nongeneric mixed state=\( U(4)/U(2)^2 \), partition \([2,2]\).
- \( Q_F \) is \((1/3, 1/3, 1/3, 0)\); nongeneric mixed state=\( U(4)/[U(1) \times U(3)] \), partition \([3,1]\).

There are six lines joining vertices, as follows

| \( OP \) | \( OQ_A \) | \( OQ_F \) | \( Q_A P \) | \( Q_A Q_F \) | \( Q_F P \) |
|--------|--------|--------|--------|--------|--------|
| Length | 1 \( \sqrt{3} \) | 1/3 \( \sqrt{2}/3 \) | \( \sqrt{2}/3 \) \( \sqrt{2}/3 \) | \( 2\sqrt{2}/3 \) |
| Spectrum | \( x > yyy \) \( xx > yy \) \( xxx > y \) \( xy00 \) \( xx > y0 \) \( yy > x0 \) |
| Type | \([3,1]\) | \([2,2]\) | \([3,1]\) | \([2,1,1]\) | \([2,1,1]\) | \([2,1,1]\) |

There are four faces; we describe just two here:

- \( OPQ_A \) \( PQQ_A \)
- Spectrum \( xyzz \) \( xy00 \)
- Type \([2,1,1]\) \([1,1,1,1]\)

Finally, there are five types of orbits:

| Spectrum | 1/4, 1/4, 1/4, 1/4 | \( xxx, 1 - 3x \) | \( xyyy \) | \( xyzz \) | \( xyzu \) |
|----------|-----------------|-----------------|--------|--------|--------|
| Representative | \( mM = O \) | \( mM = O \) | \( V = 1000 \) | \( V = 6 \) | Pure states \( \approx CP^2 \) |
| dim | 0 | 6 | 8 | 10 | \( U(4)/[U(1) \times U(3)] \) |
| character | Fixed point | Pure states \( \approx CP^2 \) | \( U(4)/U(4) \) | \( U(4)/U(2)^2 \) | \( U(4)/[U(2) \times U(1)^2] \) |
| G/H | \( U(4)/U(4) \) | \( U(4)/U(4) \) | \( U(4)/U(4) \) | \( U(4)/U(2)^2 \) | \( U(4)/[U(2) \times U(1)^2] \) |
| Interior | | | | | \( U(4)/U(1)^4 \) |
| Generic (Flag manifold) | | | | | \( U(4)/U(1)^4 \) |

IV. GENERALIZATION

The density matrix for an \( N \) level system is given by

\[ \rho = \frac{1}{N} \left( 1 + \sqrt{\frac{N(N-1)}{2}} \bar{n} \cdot \bar{x} \right) \] (22)

where the \( \lambda \)'s are \( N^2 - 1 \) Hermitian traceless \( N \times N \) matrices with square 2; \( N - 1 \) of them can be diagonalized simultaneously; let us call them \( \lambda_3, \lambda_8, \lambda_{15}, ..., \lambda_{N^2-1} \).
Then the density matrix is given by

\[
\rho = \frac{1}{N} \begin{pmatrix}
1 + \sqrt{\frac{N(N-1)}{2}}(a + b/\sqrt{3} + c/\sqrt{6} + \ldots + z/\sqrt{2(N-1)}) & 0 & 0 & 0 \\
0 & 1 + \sqrt{\frac{N(N-1)}{2}}(-a + b/\sqrt{3} + \ldots) & 0 & 0 \\
0 & 0 & \ldots & \ldots \\
0 & 0 & \ldots & 1 - (N-1)z
\end{pmatrix}
\]

(23)

So again, \(-1 \leq z \leq 1/(N-1)\); the ranges of eigenvalues always give us a regular simplex or solid hypertetrahedron \(T_N\), because there are \(N+1\) orthogonal pure states in \(CP^N\), symmetrically distributed in the \(S^{N-1}\) sphere of unit radius. The hyperfaces of the polytope delimit the range. The center corresponds to the \(mM\) state, which remains invariant under \(U(N+1)\) or \(PU(N+1)\).

The (full) symmetry group is \(S_{N+1}\), of course (arbitrary permutation of vertices etc.); this divides \(T_N\) in \(N!\) rectangular, irregular little hypertetrahedra. In any of them we have \(O\), the \(mM\) state; \(P\), the vertex; and \(N-1\) \(Q\)'s, from \(Q_F\) (center of the hyperface) to \(Q_A\) (center of the edge uniting, in \(T_N\), \(P\) with another vertex \(V'\)).

Notice in this picture some elements are interior in the original, regular polytope, others are at the boundary (extremal); for example, the cell which does not contain the \(O = mM\) is in the boundary, but the others are interior; similar for other elements: faces, edges, etc.

The calculation of the Casimir invariants starting from eq. (23) is mechanical and trivial. Some general results are

\[I_N = \text{det} \rho = 0 \text{ for a boundary state} \] (24)

because of a zero eigenvalue. Also
\[I_{N-1} = 0 \text{ for a boundary edge state} \] (25)

because of two zero eigenvalues, etc. Besides

\[I_j(mM \text{ state}) = \binom{N}{j} \frac{1}{N^j} \] (26)

because all the eigenvalues are equal to \(1/N\).

Let us discuss the entropy in this general situation; the formula

\[\eta(\rho) = \log(\Pi \mu_i^{-\mu_i}), \sum \mu_i = 1 \] (27)

can be applied without any difficulty; again, we just include some results

\[\eta(O) = \log N > \eta(\rho) > \log(P) = \log 1 = 0 \] (28)

for \(O \neq \rho \neq P\). Besides for \(A = \text{edge}, F = \text{face}\), we have

\[\eta(Q_A) = \log 2, \quad \eta(Q_F) = \log 3, \quad \ldots, \quad \eta(Q_{cell}) = \log(N-1) \] (29)

where \(Q_A\) is in the boundary edge, \(Q_F\) in the boundary face, \(Q_{cell}\) in the boundary cell, the \((N-1)\)-polytope. There are plenty of isentropic surfaces, which we refrain to make explicit, as we already established them in the \(N = 3\) case. See also [2].

V. FINAL REMARKS

Our purpose in this work has been to describe the eigenvalue set and the orbit space of density matrices in a finite quantum system. The picture is

\[
\{\text{set of states}\} \leftrightarrow \text{solid hypertetrahedron } T_N \quad \{\text{orbit space}\} = T_N/S_{N+1} \leftrightarrow \text{rectangular nonregular small } h\text{-tetrahedron } t_N
\]

(30) \hspace{1cm} (31)

where \(t_N = \{\text{set of density states}\} / PU(N)\).

The actual geometry of mixed states, out of the \(N = 1, 2\) cases, is rather involved [3] and we have not pretended to improve on it. There is also the interesting problem of finding maps between density states, positive/strictly positive, untouched also here; see e.g. the recent work [9].

The geometry of the complex flag manifolds \(U(N)/U(1)^N\) is very rich; we remark here only one result

\[U(3)/U(1)^2 := Fl_{C}(3) = SU(3)/U(1)^2 \sim CP^1 \circ CP^2 \]

(32)

where the twisted product \(\circ\) is similar to the used in \[10\] to express the homology of Lie groups.

The \(N = 3\) case reminds one of the 3-dim Jordan algebras: the action of \(SU(3)\) on the 3 x 3 hermitian traceless matrices is similar to the action of the exceptional group \(F_4\) on the exceptional Jordan octonionic algebra; indeed, the Moufang plane \(OP^2\) is \(F_4/Spin(9)\) (Borel, 1950), whereas our \(CP^2\) is \(SU(3)/U(2)\). In fact, the two cases are related, as the following beautiful chain of groups show

\[
\begin{array}{ccc}
SU(3) & Spin(8) & E_6 \\
\times & a \swarrow & d \uparrow \\
SO(3) & G_2 & F_4
\end{array}
\]

(33)
where $a \equiv \text{Aut}$ leads to the fixes sets (i.e. $E_6 \to F_4$, $\text{Spin}(8) \to G_2$ and $SU(3) \to SO(3)$), and $t$ (triality) and $d$ (duality) means to relate $\text{Spin}(8)$ with $F_4$ and $SU(3)$ with $G_2$. That is, $F_4 \approx \text{Spin}(8)$ plus the 3 8-dim representations and $G_2 \approx SU(3)$ plus $3$ and $\bar{3}$.

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