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Descriptors of dimensionality for $n \times n$ density matrices

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Abstract By using the recently introduced parametrization of an n-dimensional density matrix in terms of the indices of population asymmetry and the intrinsic coherences, we define descriptors in both integer and continuous forms of the effective dimension that take place for a complete description of a density matrix, thus providing accurate information beyond the rank of the density matrix. The concepts of dimensional folding, hidden dimensional purity, and dimensional entropy are introduced and discussed in view of the new approach presented. The results are applicable to any physical system represented by a density matrix, such as n-level quantum systems, qutrits, sets of interacting pencils of radiation, classical polarization states, and to transformations of density matrices, as occurs with quantum channels.

1 Introduction

Density matrices play a key role in quantum mechanics [1–3] as well as in the treatment of classical mixed states, i.e., states that can be expressed as a convex sum of classical pure states [4–6]. An important example in the classical context is the normalized polarization matrix and its representation in terms of the polarization matrices of fully polarized (pure) states [7]. Regarding the dimensional structure of a system represented by a density matrix $\boldsymbol{\rho}$, it is well known that there are two integer parameters that play key roles, namely the dimensions n of $\boldsymbol{\rho}$ (i.e., the number of rows and files of $\boldsymbol{\rho}$), and $r = \text{rank}\boldsymbol{\rho}$, with $1 \leq r \leq n$. Since through an appropriate change of the complex basis used to represent the system $\boldsymbol{\rho}$, the $m = n - r$ last files and columns of the transformed density matrix can always be converted to zero, one may be tempted to interpret r as the minimum number dimensions required for a complete description, without loss of physical information, of $\boldsymbol{\rho}$. Nevertheless, through a more detailed analysis it will be shown that such a minimum number of dimensions is given by an integer number k (hereafter called the *true dimension* of $\boldsymbol{\rho}$) satisfying $r \leq k \leq n$. Moreover, a new parameter describing, in a continuous manner, the closeness of the state to the determined true dimension can be defined.

In this paper, novel quantities and concepts describing the dimensionality properties of n-dimensional density matrices are introduced and interpreted in terms of the population asymmetry exhibited by the considered physical system. The fact that some of these notions have proven to be fruitful for the study of polarization density matrices in three-dimensional (3D) optical systems, supports their generalization to nD density matrices. Despite the fact that this work focuses on general systems described by density matrices, the results have direct applications in the analysis concerning, e.g., sets of n interacting pencils of radiation [8–10], classical optical coherence [11, 12], qutrits, or any mixed n-state quantum system (n-level systems). Furthermore, the research of the features of quantum channels as transformers of density matrices [13–16] can also potentially benefit from the formalism.

After a brief summary of the theoretical framework necessary to develop the formulation of the problem, the concepts of dimensionality index and effective dimension are introduced as natural generalizations of their versions for 3D polarimetric systems [17–19]. Then, it is shown that the dimensionality index is identical to the degree of population asymmetry introduced recently [20], which broadens their physical interpretation and significance. On the basis of such developments, the concepts of dimensional folding, hidden dimensional purity, and dimensional entropy are defined and discussed.

2 Theoretical background

Consider a classical nD system whose state is characterized by a set of n random variables v_i ($i = 1, \ldots, n$) that can be arranged into a unit complex vector $\hat{\mathbf{v}} = v_1, \ldots, v_n)^{\mathrm{T}}$, where the superscript "T" indicates transpose. The ensemble averages $\rho_{ij} = \left\langle v_i v_j^* \right\rangle (i, j = 1, 2, \ldots, n)$ over the sample realizations $v_i v_j^*$ provide all the second-order measurable quantities associated with $\hat{\mathbf{v}}$ and constitute the

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elements of the corresponding density matrix, defined as $\boldsymbol{\rho} = \langle \hat{\mathbf{v}} \otimes \hat{\mathbf{v}}^{\dagger} \rangle$, where $\otimes$ stands for the Kronecker product and the dagger indicates conjugate transpose. Except for variables obeying Gaussian statistics, higher-order moments are in general necessary for a complete description of the stochastic classical system; nevertheless, for many problems the second-order description is sufficient in practice (as occurs frequently in polarization optics). In quantum physics, density matrices arise naturally in the description of statistical mixtures of pure states [21].

From a formal point of view, a given $n \times n$ matrix $\boldsymbol{\rho}$ can be considered a density matrix if and only if $\boldsymbol{\rho}$ is a trace-normalized nonnegative definite Hermitian matrix, i.e., $\mathrm{tr}\boldsymbol{\rho} = 1$ where "tr" stands for the trace, $\boldsymbol{\rho} = \boldsymbol{\rho}^{\dagger}$, and the n eigenvalues of $\boldsymbol{\rho}$ are real and nonnegative. The density matrix can always be diagonalized as $\boldsymbol{\rho} = \mathbf{U3U}^{\dagger}$ (spectral theorem [22]), where $\mathbf{U}$ is the unitary matrix whose columns are the orthonormal eigenvectors of $\boldsymbol{\rho}$, whereas $\boldsymbol{\Lambda} = \mathrm{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is the diagonal matrix whose diagonal elements are the eigenvalues of $\boldsymbol{\rho}$, which are taken in decreasing order, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Due to the trace normalization, the eigenvalues satisfy $\lambda_1 + \lambda_2 + \ldots + \lambda_n = 1$. When $\boldsymbol{\rho}$ has a single nonzero eigenvalue ($\lambda_1 > 0$, $\lambda_2 = \ldots = \lambda_n = 0$), the state is said to be pure and the matrix is denoted by $\boldsymbol{\rho}_p$, which constitutes a limiting case of the general mixed states. On the other hand, maximally mixed states ($\lambda_1 = \lambda_2 = \ldots = \lambda_n = 1/n$) are represented by the identity matrix $\mathbf{I}$ scaled by $1/n$ and denoted as $\boldsymbol{\rho}_u = \mathrm{I}/\boldsymbol{n}$.

An overall measure of the degree of purity of a state $\boldsymbol{\rho}$ is given by [23–25]

$$P_{nD}^2 = \frac{1}{n-1}\left(n\mathrm{tr}\boldsymbol{\rho}^2 - 1\right) = \frac{1}{n-1}\sum_{\substack{i,j=1 \\ i<j}}^{n}\left(\lambda_i - \lambda_j\right)^2, \tag{1}$$

which satisfies $0 \leq P_{nD} \leq 1$ and reaches its extremal values $P_{nD} = 1$ and $P_{nD} = 0$ for pure and maximally mixed states, respectively. While P_{nD} is a global measure of the purity of the state represented by $\boldsymbol{\rho}$, detailed quantitative information on the structure of purity is given by the $n-1$ indices of purity (hereafter IP), defined in analogy to the indices of polarimetric purity (IPP) as [25]

$$P_k = \sum_{j=1}^{k}\lambda_j - k\lambda_{k+1}, \qquad 1 \leq k \leq n-1. \tag{2}$$

In comparison with other possible alternative sets of $n-1$ parameters obtained as linear functions of λ_i, the IP has the hierarchical property that they obey the nested inequalities $0 \leq P_1 \leq \ldots \leq P_{n-1} \leq 1$. The expression for P_{nD} in terms of the IP is [25]

$$P_{nD}^2 = \frac{n}{n-1}\sum_{k=1}^{n-1}\frac{P_k^2}{k(k+1)}. \tag{3}$$

This relation is obtained by using the expressions of the eigenvalues λ_i of $\boldsymbol{\rho}$ in terms of the IP (see Eq. (36) of Ref. [25]) and then applying them to the latter form of P_{nD} in Eq. (1).

Another concept that must be taken into account to formulate the results of this work is the intrinsic density matrix described below. Given an nD density matrix $\boldsymbol{\rho}$, there always exists a proper orthogonal matrix $\mathbf{Q}$ ($\mathbf{Q}^{\mathrm{T}} = \mathbf{Q}^{-1}$, $\det \mathbf{Q} = +1$) that allows one to perform the diagonalization of the real part $\mathrm{Re}\boldsymbol{\rho}$ of $\boldsymbol{\rho}$, $\mathbf{Q}^{\mathrm{T}}(\mathrm{Re}\boldsymbol{\rho})\,\mathbf{Q} = \mathrm{diag}\,(a_1, a_2, \ldots, a_n) = \mathbf{A}$. Observe that, since the orthogonal transformation $\mathbf{Q}^{\mathrm{T}}\boldsymbol{\rho}\,\mathbf{Q}$ of $\boldsymbol{\rho}$ has always the form of a density matrix, their diagonal elements $(a_1, a_2, \ldots, a_n)$, which coincide with the eigenvalues of the symmetric matrix $\mathrm{Re}\boldsymbol{\rho}$, are necessarily nonnegative, showing that $\mathrm{Re}\boldsymbol{\rho}$ has the formal character of a density matrix. Without loss of generality, the convention $a_1 \geq a_2 \geq \ldots \geq a_n$ (with $\mathrm{tr}\boldsymbol{\rho} = a_1 + a_2 + \ldots + a_n = 1$) is taken, so that $(a_1, a_2, \ldots, a_n)$ are the ordered (real, nonnegative) eigenvalues of $\mathrm{Re}\boldsymbol{\rho}$ and referred to as intrinsic populations [20].

The orthogonal transformation $\mathbf{Q}^{\mathrm{T}}(\mathrm{Re}\boldsymbol{\rho})\,\mathbf{Q}$ can always be formally interpreted as a proper rotation of the original nD Cartesian reference frame $X_1X_2\ldots X_n$, used for the representation of $\mathrm{Re}\boldsymbol{\rho}$ in the associated nD real space, to the *intrinsic reference frame* $X_{1O}X_{2O}\ldots X_{nO}$ [20] for which the real part of the density matrix takes the diagonal form $\mathbf{A}$. By denoting $k = \mathrm{rank}\,(\mathrm{Re}\boldsymbol{\rho}) = \mathrm{rank}\,\mathbf{A}$, the diagonal matrix $\mathbf{A}$ can be expressed as $\mathbf{A} = \mathrm{diag}\,(a_1, a_2, \ldots, a_k, 0, \ldots 0)$, with $a_1 \geq a_2 \geq \ldots \geq a_k > 0$ and $a_{k+1} = a_{k+2} = \ldots = a_n = 0$. Note that, as is well known in matrix algebra, $\mathbf{Q}$ is not unique when some diagonal elements of $\mathbf{A}$ are equal, i.e., some eigenvalues of $\mathrm{Re}\boldsymbol{\rho}$ are degenerate. This fact does not affect the developments performed below.

By applying the orthogonal transformation represented by $\mathbf{Q}$ to the entire density matrix $\boldsymbol{\rho}$, we get its associated *intrinsic density matrix* [20, 26]

$$\boldsymbol{\rho}_O = \mathbf{Q}^{\mathrm{T}}\boldsymbol{\rho}\,\mathbf{Q} = \mathbf{A} + i\,\frac{1}{2}\mathbf{N}, \quad \left[\mathbf{A} = \mathbf{Q}^{\mathrm{T}}(\mathrm{Re}\boldsymbol{\rho})\,\mathbf{Q}, \quad \mathbf{N} = 2\mathbf{Q}^{\mathrm{T}}(\mathrm{Im}\boldsymbol{\rho})\,\mathbf{Q}\right], \tag{4}$$

where $\mathbf{N}$ is an antisymmetric real matrix, $\mathbf{N}^{\mathrm{T}} = -\mathbf{N}$, whose off-diagonal elements n_{ij} are called the intrinsic coherences. The terms populations and coherences are used by analogy to the names employed commonly in quantum mechanics, but we apply them to any kind of quantum or classical state represented by a density matrix. Thus, any density matrix, $\boldsymbol{\rho}$, has an associated intrinsic density matrix, $\boldsymbol{\rho}_O$, which represents the same state as $\boldsymbol{\rho}$, but referenced with respect to the associated intrinsic reference frame (real and Euclidean) defined from $\boldsymbol{\rho}$ via $\mathrm{Re}\boldsymbol{\rho}$.

As with the definition of the IP from the λ_i of $\boldsymbol{\rho}$, a set of $n-1$ indices of population asymmetry (IPA) are defined from the a_i of $\mathbf{A}$ as [20]

$$M_k = \sum_{j=1}^{k} a_j - k\,a_{k+1}, \quad 1 \le k \le n-1. \tag{5}$$

The IPA satisfies the nested inequalities $0 \le M_1 \le M_2 \ldots \le M_{n-1} \le 1$ and provides detailed information on the structure of population asymmetry of the state represented by $\boldsymbol{\rho}$. States with full population symmetry ($a_1 = a_2 = \ldots = a_n = 1/n$) are characterized by $M_1 = M_2 = \ldots = M_{n-1} = 0$, while the maximal population asymmetry ($a_1 = 1$, $a_2 = \ldots = a_n = 0$) is expressed by $M_1 = M_2 = \ldots = M_{n-1} = 1$.

According to Eq. (4), two complementary contributions to purity arise naturally from the population asymmetry (derived from $\mathbf{A}$) and from the coherence asymmetry (derived from $\mathbf{N}$), respectively, in such a manner that the degree of purity can be expressed as [20] ($n > 1$ assumed)

$$P_{nD}^2 = P_p^2 + \frac{n}{2(n-1)} P_c^2, \quad \left[0 \le P_p \le 1,\ 0 \le P_c \le 1\right] \tag{6}$$

where the degree of population asymmetry, P_p, and the degree of coherence asymmetry, P_c, are defined as

$$P_p^2 = \frac{1}{n-1}\left(n\mathrm{tr}\mathbf{A}^2 - 1\right) = \frac{n}{n-1}\sum_{k=1}^{n-1}\frac{M_k^2}{k(k+1)}, \quad P_c^2 = \frac{1}{2}\|\mathbf{N}\|_{\mathrm{F}}^2 = \sum_{\substack{i,j=1 \\ i<j}}^{n} |n_{ij}|^2, \tag{7}$$

where $\|\mathbf{N}\|_{\mathrm{F}}$ denotes the Frobenius norm. Clearly, purity is related to the population and coherence asymmetries of the structure of $\boldsymbol{\rho}$; the greater the asymmetry, the closer the state is to a pure state, while the greater the symmetry, the closer the state is to a maximally mixed state.

3 True dimension and effective dimension of a density matrix

To show the origin and motivation of the general approach described below, let us first consider the particular case of a 3×3 density matrix $\boldsymbol{\rho}_m = (1/2)\,\mathbf{U}\mathrm{diag}\,(1,\ 1,\ 0)\,\mathbf{U}^{\dagger}$ (with a double degenerate nonzero eigenvalue and $\mathrm{rank}\boldsymbol{\rho}_m = 2$) whose associated intrinsic density matrix is of the form

$$\boldsymbol{\rho}_{mO} = \mathbf{Q}^{\mathrm{T}}\boldsymbol{\rho}_m\,\mathbf{Q} = \begin{pmatrix} a_1 & -in_3/2 & in_2/2 \\ in_3/2 & a_2 & -in_1/2 \\ -in_2/2 & in_1/2 & a_3 \end{pmatrix}, \quad [0 < a_3 \le a_2 \le a_1] \tag{8}$$

so that $k(\boldsymbol{\rho}_m) = \mathrm{rank}\,(\mathrm{Re}\boldsymbol{\rho}_m) = 3$. The matrix $\boldsymbol{\rho}_m$ is the middle component (hence the subscript m) or the so-called the *discriminating* component in the characteristic decomposition [7, 27] of the 3×3 polarization matrix and its detailed general structure can be found in [28] dealing with nonregularity of polarization states. Note that, since qutrit states are represented by 3×3 density matrices [29, 30], the concept of discriminating density matrices $\boldsymbol{\rho}_m$ [20] can be applied to certain kind of qutrit states. In analogy to the fact that discriminating polarization states cannot be considered as two-dimensional polarization states embedded in the 3D representation [27], qutrits with associated density matrices of the form $\boldsymbol{\rho}_m$ (with $k(\boldsymbol{\rho}_m) = 3$) cannot be considered as qubits embedded in qutrit structures.

If the 2×2 restricted form $\boldsymbol{\rho}_{m(2\times2)} = \mathbf{U}_{(2\times2)}\mathrm{diag}\,(1,\ 1)\,\mathbf{U}_{(2\times2)}^{\dagger}$ of $\boldsymbol{\rho}_m$ is taken, the specific information determining $\mathbf{U}$ is lost, and therefore $\boldsymbol{\rho}_{mO}$ cannot be recovered from $\boldsymbol{\rho}_{m(2\times2)}$. This shows that, in general, given a density matrix satisfying $k > r = \mathrm{rank}\,\boldsymbol{\rho}$, its $r \times r$ restricted version $\boldsymbol{\rho}_{(r\times r)}$ obtained by eliminating then n-r rows-columns associated with zero eigenvalues of the original $\boldsymbol{\rho}$ does not allow for recovering the complete information held by $\boldsymbol{\rho}$.

From a general point of view, let us now consider the ranks of $\boldsymbol{\rho}$ and $\mathrm{Re}\boldsymbol{\rho}$ denoted by $r = \mathrm{rank}\,\boldsymbol{\rho}$ and $k = \mathrm{rank}\,(\mathrm{Re}\boldsymbol{\rho})$, and observe that condition $k \ge r$ is necessarily satisfied (proven in the Appendix). Furthermore, looking at the possible representations of the state $\boldsymbol{\rho}$, the number of dimensions that take place in the problem is the true dimension k (and not r). In fact, when a number q of intrinsic populations are zero, a restricted version of the density matrix can be used by removing $n - k = q$ (and not $n - r$) rows and columns from $\boldsymbol{\rho}_O$. It is important to note that, when a given intrinsic population is zero, the intrinsic correlations appearing in the associated row-column necessarily vanish, which justifies the above analysis based on intrinsic populations only.

Thus, k constitutes an integer descriptor of the true physical dimensions involved in the representation of the state. Situations of this kind have been studied in the context of polarization optics, leading to new and fruitful concepts like nonregularity and the structure of spin vectors of polarization states [28–32]. It is also important to keep in mind that states satisfying $a_1 = a_2 = \ldots = a_n = 1/n$, whose density matrices will be denoted by $\boldsymbol{\rho}_{Au}$, are not necessarily maximally mixed states since such states can exhibit certain amount of correlation asymmetry, regardless of their full population symmetry. It should be stressed that the 3×3 approach developed in previous papers under the scope of polarization optics, whose generalization is dealt with in this work, can entirely be applied to qutrit states and density matrices representing 3-level quantum states in general.

The true dimension, k, of a state, provides a discrete measure which does not reflect, in a continuous functional manner, the dimensional features of a state. Thus, we next introduce the dimensionality index, d, of the state $\boldsymbol{\rho}$ as

$$d^2 = \frac{1}{(n-1)} \sum_{\substack{i,j=1 \\ i<j}}^{n} \left(a_i - a_j\right)^2, \quad n > 1 \tag{9}$$

which is the mean square average of the differences between all pairs of intrinsic populations and takes values in the range $0 \leq d \leq 1$. Thus, d is defined as a generalization of the dimensionality index of random light fields ($n = 3$) introduced for the first time in [17]. States with a single nonzero intrinsic population ($a_1 = 1$, maximal population asymmetry) are characterized uniquely by $d = 1$. These states are necessarily pure, while the converse is not generally true. An example of a pure state with $d < 1$ is a circularly polarized state in optics [17]. The lower limit $d = 0$ is reached, uniquely, by states $\boldsymbol{\rho}_{Au}$ exhibiting maximal population symmetry. In addition, by using the relation $a_1 + a_2 + \ldots + a_n = 1$ in the expression of P_p in Eq. (7), it is straightforward to show that in fact $P_p = d$. Thus, the dimensionality index is a proper measure of the degree of population asymmetry and also a measure of the Frobenius distance between the state $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_{Au}$.

While the index d is defined as a relative measure constrained to the range $0 \leq d \leq 1$, the *effective dimension*, D, of a state $\boldsymbol{\rho}$ is defined as

$$D = n - (n-1)d \tag{10}$$

which takes continuous values in the range $1 \leq D \leq n$ and allows for distinguishing among different physical situations with equal true dimensions in terms of their closeness to the possible values of k. We remark that in the context of polarization optics D has been called the polarimetric dimension [17] but here the term effective dimension is invoked for the general case. States with maximal population asymmetry (smallest effective dimension) are characterized by $D = 1$, while $D = n$ is achieved uniquely by states $\boldsymbol{\rho}_{Au}$ with maximal population symmetry (largest effective dimension). Therefore, the real parameter D provides a continuous and more accurate characterization for the effective dimensionality of $\boldsymbol{\rho}$ than that given by the integer parameter k. The ability of D to characterize the dimensionality of optical evanescent waves and tightly focused beams has been described in previous works [19, 31, 33].

4 Dimensional folding

When a given density matrix $\boldsymbol{\rho}$ satisfies $k > r$ we may say that a number $f = k - r$ of dimensions of the state represented by $\boldsymbol{\rho}$ are folded. More precisely, despite that $\boldsymbol{\rho}$ has r nonzero eigenvalues, the state cannot be represented through an $r \times r$ density matrix, but instead such a representation necessitates a $k \times k$ density matrix. Since both the true dimension and the effective dimension of $\boldsymbol{\rho}$ are determined by the eigenvalues of $\mathrm{Re}\boldsymbol{\rho}$ (and not by the eigenvalues of $\boldsymbol{\rho}$), this phenomenon corresponds to states with $D > r$, which means that the effective dimension is larger than the rank r of $\boldsymbol{\rho}$. Hence, the minimum number of dimensions to describe both $\mathrm{Re}\boldsymbol{\rho}$ and $\boldsymbol{\rho}$ is k and not r. States exhibiting dimensional folding ($k > r$) are characterized by any of the two following equivalent properties: (1) $D > r$, and (2) the number of IPA equal to 1 ($n - k - 1$) is smaller than the number of IP with value 1 ($n - r - 1$).

A good example of a dimensionally folded state is given by the incoherent superposition of two pure polarization states whose polarization planes (the planes where their corresponding polarization ellipses lie) are different. Contrary to what could be expected at first sight, polarization states of this kind ($r = 2$) cannot be represented by 2×2 polarization density matrices, but must be represented by 3×3 ones. Another physical example is a system composed of n interacting pencils of radiation [8–10]. Generally, the notion of dimensional folding can be applied to any density matrix whose representation with respect to an nD Euclidean space is physically significant.

5 Hidden dimensional purity

The notion of purity of a density matrix $\boldsymbol{\rho}$ is closely linked to that of dimensional folding and, in general, to the dimensional structure of $\boldsymbol{\rho}$. The present section is devoted to the analysis and quantification of the part of the purity that corresponds to the extra dimensions that, being relevant to the problem under study, are not considered in the representation of $\boldsymbol{\rho}$.

Prior to address the general approach, and in order to exemplify the problem, it is worth to recall that hidden dimensional purity occurs, for instance, for 2D polarization states of light, whose usual 2D representation does not reflect the fact that all physical polarization states are realized in the 3D Euclidean space. Indeed, the 2D degree of polarization $P_{2\mathrm{D}}$ could even take its minimum value $P_{2\mathrm{D}} = 0$ regardless of the fact that such states satisfy $P_{3\mathrm{D}} \geq 1/2$ [34, 35]. In other words, the 2D representation of a polarization state leaves hidden the fact that a half of the purity, i.e., the indicated threshold $1/2$ for $P_{3\mathrm{D}}$, comes from dismissing the additional third real dimension involved in the complete description of the state.

We next introduce the notion of hidden dimensional purity, which is linked to the dimensionality properties of a state that is represented by an mD density matrix, where m is smaller than the actual dimensions n in which the state is described by an nD

density matrix. This procedure is equivalent to discarding a number $q = n - m$ of the IP of the true nD system having maximal values $P_{n-1} = P_{n-2} = \ldots = P_{n-q} = 1$, which implies that a considerable part of the purity of the state is contained in the hidden q dimensions.

The quantification of the hidden dimensional purity when the system is represented with $n - 1$ dimensions instead of n can be performed through the following expression, Eq. (43) of [25], that links the consecutive degrees of purity P_{nD} and $P_{(n-1)D}$ with P_{n-1} (the largest IP in the nD representation)

$$P_{nD}^2 = \frac{n(n-2)}{(n-1)^2} P_{(n-1)D}^2 + \frac{1}{(n-1)^2} P_{n-1}^2. \tag{11}$$

When the last dimension n is ignored, this is equivalent to set all elements of the n-th row and column of the density matrix to zero, which in turn corresponds to $P_{n-1} = 1$, in which case

$$P_{nD}^2 = \frac{n(n-2)}{(n-1)^2} P_{(n-1)D}^2 + \frac{1}{(n-1)^2} \Rightarrow P_{nD} \geq \frac{1}{n-1}, \tag{12}$$

and the lost dimensional purity is quantified in $1\big/(n-1)$.

For a given $\boldsymbol{\rho}$, the recursive application of Eq. (11) leads to the expression that relates the nD degree of purity P_{nD}, the mD degree of purity P_{mD} (with $1 < m < n$), and the last $q - 1$ indices of purity

$$P_{nD}^2 = \frac{n(m-1)}{(n-1)m} P_{mD}^2 + \frac{n}{n-1} \sum_{l=m}^{n-1} \frac{P_l^2}{l(l+1)}. \tag{13}$$

Consequently, when the last $q = n - m$ dimensions are hidden, in which case $P_l = 1$ ($l = m, \ldots, n-1$), the corresponding hidden dimensional purity, P_h, is

$$P_h^2 = \frac{n}{n-1} \sum_{l=m}^{n-1} \frac{1}{l(l+1)} = \frac{q}{(n-1)m}, \tag{14}$$

so that

$$P_{nD}^2 = \frac{n(m-1)}{(n-1)m} P_{mD}^2 + P_h^2 \Rightarrow P_{nD} \geq P_h. \tag{15}$$

6 Dimensional entropy

The von Neumann entropy of a system represented by a density matrix has proven to be a very fruitful concept, which motivates the introduction of a similar, but complementary, quantity obtained from $\boldsymbol{\rho}$ via the associated real density matrix $\mathrm{Re}\boldsymbol{\rho}$. Obviously, both quantities have different physical meanings.

As we have seen, the detailed information on the true dimensionality of a state represented by a given density matrix is provided either by the dimensionality index d or by the effective dimension D, which are defined in terms of the (ordered) intrinsic populations a_i ($i = 1, 2, \ldots, n$). This fact suggests the introduction of a quantity akin to the conventional von Neumann entropy, which is expressed in terms of the eigenvalues of the density matrix. In particular, we define the *dimensional entropy* of a state represented by $\boldsymbol{\rho}$ as the following entropy-like measure of the information provided by $\boldsymbol{\rho}$ regarding effective dimensionality (and hence population asymmetry, because of its essential link to D):

$$S_D(\boldsymbol{\rho}) = S(\mathrm{Re}\boldsymbol{\rho}) = S(\mathbf{A}) = -\mathrm{tr}(\mathbf{A} \ln \mathbf{A}) = -\sum_{i=1}^{n} (a_i \ln a_i). \tag{16}$$

Note that the fact that $\mathrm{Re}\boldsymbol{\rho}$ has the mathematical structure of a density matrix justifies the above definition of the dimensional entropy in terms of the eigenvalues a_i of $\mathrm{Re}\boldsymbol{\rho}$. Thus, as with the conventional concept of von Neumann entropy, $S_D(\boldsymbol{\rho})$ is limited by $0 \leq S_D(\boldsymbol{\rho}) \leq \ln n$, with its maximum value $S_D(\boldsymbol{\rho}) = \ln n$ corresponding to states with maximal population symmetry ($d = 0$, $D = n$), while its minimum $S_D(\boldsymbol{\rho}) = 0$ is reached by 1D states ($d = 1$, $D = 1$), i.e., states with maximal population asymmetry, which constitutes a particular category of pure states. In general, the larger is the effective dimension the more disordered the state is regarding the physical dimensions and the larger is the dimensional entropy.

An interesting alternative definition of the dimensional entropy is given by the normalized form

$$\hat{S}_D(\boldsymbol{\rho}) = \hat{S}(\mathrm{Re}\boldsymbol{\rho}) = \hat{S}(\mathbf{A}) = -\mathrm{tr}\big(\mathbf{A} \log_n \mathbf{A}\big) = -\sum_{i=1}^{n} \big(a_i \log_n a_i\big) \tag{17}$$

where $\hat{S}_D(\boldsymbol{\rho})$ is then constrained to the interval $0 \leq \hat{S}_D(\boldsymbol{\rho}) \leq 1$ regardless of the value of n, with the maximum $\hat{S}_D(\boldsymbol{\rho}) = 1$ corresponding to full population symmetry.

7 Conclusions

In this work, we examined the structural characterization of nD density matrices with emphasis on dimensionality properties. By considering the intrinsic populations of such matrices, we extended the concepts of dimensionality index and effective dimension established for 3D polarization states in optics to generic physical systems in n dimensions. We further introduced the notion of dimensional folding which occurs when the number of nonzero eigenvalues of the density matrix is less than that of nonzero intrinsic populations, i.e., the dimensions needed to describe the state exceeds the rank of the density matrix. We also put forward the property we call hidden dimensional purity which characterizes the amount of purity in dimensions not taken into account in the representation of the state. Finally, we presented the notion of dimensional entropy as a measure for the effective dimensionality associated with a density matrix. The results of this work apply to the description of classical or quantum mixed states of any dimensionality.

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Appendix

To prove that $k \geq r$, let us first observe that, from the very definition of the intrinsic density matrix $\boldsymbol{\rho}_O = \mathbf{Q}^{\mathrm{T}}\,\boldsymbol{\rho}\,\mathbf{Q}$ associated with $\boldsymbol{\rho}$, it follows that the last $n-k$ rows and columns of both $\boldsymbol{\rho}_O$ and $\mathbf{A}$ are zero (see Eq. (4)). On the other hand, the last $n-r$ diagonal elements of the eigenvalue matrix $\boldsymbol{\Lambda} = \mathbf{U}^{\dagger}\boldsymbol{\rho}\mathbf{U}$ are zero, which makes it obvious that the last $n-r$ rows and columns of $\boldsymbol{\Lambda}$ are zero. In fact, since density matrices have the mathematical structure of trace-normalized covariance matrices, the elements ρ_{Oij} ($i,\ j = 1, \ldots, n$) of $\boldsymbol{\rho}_O$ can be parameterized as $\rho_{Oii} = \sigma_i^2$ (diagonal elements, with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_k > 0$ and $\sigma_{k+1} = \sigma_{k+2} = \ldots = \sigma_n = 0$), and $\rho_{Oij} = \rho_{Oij}^{*} = i\sigma_i\sigma_j v_{Oij}$ (off-diagonal elements), so that for all zero diagonal elements of $\boldsymbol{\rho}_O$, the corresponding adjacent rows and columns are necessarily zero.

Thus, if the inequality $k < r$ were satisfied, this would imply that the unitary (orthogonal) similarity transformation $\mathbf{Q}^{\mathrm{T}}\,\boldsymbol{\rho}\,\mathbf{Q} = \boldsymbol{\rho}_O$ has a number greater than $n-r$ of last zero rows and columns, which is incompatible with $\mathrm{rank}\boldsymbol{\rho}_O = \mathrm{rank}\boldsymbol{\rho} = r$.

Depending on the values of the off-diagonal elements of $\boldsymbol{\rho}_O$ (which are determined by matrix $\mathbf{N}$), k can be either equal or greater than r. Regarding this point, it is worth recalling, for instance, the fact that, for any given $\boldsymbol{\rho}$, there always exist an orthogonal matrix $\mathbf{Q}_E$ such that all diagonal elements of the transformed density matrix $\mathbf{Q}_E^{\mathrm{T}}\boldsymbol{\rho}\mathbf{Q}_E$ are nonzero, including the case that all diagonal elements are equal [36].

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