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New Dual Views of the Generalized Degree of Purity

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Abstract: Several approaches and descriptors have been proposed to characterize the purity of coherency or density matrices describing physical states, including the polarimetric purity of 2D and 3D partially polarized waves. This work introduces two new interpretations of the degree of purity: one derived from statistics and another from algebra. In the first one, the degree purity is expressed in terms of the mean and standard deviation of the eigenvalue spectrum of the density or coherency matrix of the corresponding state. The second one expresses the purity in terms of two specific measures obtained by decomposing the coherency matrix as a sum of traceless symmetric, anti-symmetric and scalar matrices. These two approaches offer better insights into the purity measure. Furthermore, interesting relations with existing quantities in polarization optics are described.

The degree of polarimetric purity is an invariant dimensionless quantity that characterizes the closeness of a polarization state of a wave to a pure state and is related to the Von Neumann entropy [1]. The polarimetric purity of a plane wave characterized by the second-order statistics (i.e., the covariance matrix) is uniquely described by the degree of polarization. However, such a two-dimensional (2D) formalism is only applicable when the electric field of the wave fluctuates in a fixed plane. This assumption is typical in optical and radar polarimetric measurements. Therefore, one must consider all the components to describe the general state of wave polarization. Starting from Samson [2], and Barakat [3], several different concepts have been proposed in the literature to describe the 3D *degree of polarization* [4–9].

As a generalization to n-dimensions of the degree of polarization for 3D random light fields established by Setälä et al. [7], the *degree of purity*, P_{nD} [10–12] for the $n \times n$ Hermitian and positive semi-definite coherency matrix $\mathbf{\Phi}$ is defined as,

$$P_{nD} = \left\{ \frac{1}{n-1} \left[\frac{n[\mathrm{tr}\,(\mathbf{\Phi}^2)]}{(\mathrm{tr}\,\mathbf{\Phi})^2} - 1 \right] \right\}^{1/2} \tag{1}$$

where $\mathrm{tr}\,\mathbf{\Phi}$ is the trace of $\mathbf{\Phi}$. Besides the general application of this concept to coherency or density matrices representing n-level systems, the interest from the point of view of optics was pointed out by Barakat [13] when dealing with systems composed of n partially coherent pencils of radiation (not necessarily interfering at a given point), with potential application to optical quantum channels [14].

The degree of purity is an invariant dimensionless quantity satisfying, $0 \leq P_{nD} \leq 1$. The minimum value $P_{nD} = 0$ corresponds to a state whose n variables are second-order uncorrelated. In contrast, the maximum value $P_{nD} = 1$ corresponds to a statistically pure state. The degree of purity can take values between the two limits depending on the second-order correlations between the n variables involved.

In this work, we propose two new approaches to express the degree of purity, P_{nD}. In the first approach, we utilize the definition of the mean and standard deviation of real positive eigenvalues of Hermitian positive semi-definite matrices [15, 16]. In the second approach, we use elementary concepts from vector calculus and align them with a matrix decomposition procedure following certain notions from Lie algebra [17]. Finally, we establish the parity of the two approaches to compute the degree of purity of the n-dimensional state considered. This work provides simple and elegant expressions of the degree of purity using well-known and meaningful statistical and algebraic representations. The two distinct approaches offer deeper insights into the purity measure.

1. Approach I: Coefficient of Variation

In the first approach, let us consider the algebraic mean (m) and the standard deviation (s) of the real positive eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ for a $n \times n$ coherency matrix $\mathbf{\Phi}$ that are defined using a simple function of the trace of the matrix and the trace of its square [15] as,

$$m = \frac{1}{n}\,\mathrm{tr}(\mathbf{\Phi}) = \frac{1}{n}\sum_{j=1}^{n}\lambda_j, \text{ and} \tag{2}$$

$$s^2 = \frac{1}{n}\left[\sum_{j=1}^{n}\lambda_j^2 - \frac{1}{n}\left(\sum_{j=1}^{n}\lambda_j\right)^2\right] = \frac{\mathrm{tr}\,(\mathbf{\Phi}^2) - (\mathrm{tr}\,\mathbf{\Phi})^2/n}{n} = \frac{\mathrm{tr}(\mathbf{\Phi}^2)}{n} - m^2. \tag{3}$$

In the cases of coherency matrices representing 2D and 3D polarization states, m is proportional to the intensity via the scale coefficient $1/n$. When dealing with coherency matrices associated with Mueller matrices (4D), m represents the mean intensity coefficient (transmittance or reflectance for incident unpolarized light) scaled by $1/4$. In the general case of nD density matrices m becomes simply $m = 1/n$.

In the case of trace-normalized nD coherency matrices (density matrices), the quantity $\mathrm{tr}\,(\mathbf{\Phi}^2)$ is usually called the purity parameter, with $m \leq \mathrm{tr}\,(\mathbf{\Phi}^2) \leq 1$. Where the maximum is realized uniquely by pure states, while the minimum corresponds to maximally mixed states. Note that, in contrast to such a definition of purity, the degree of purity P_{nD} is defined in such a manner that its minimum is zero. Thus, when applied to a nD density matrix, s^2 takes the form $s^2 = m(\mathrm{tr}\,(\mathbf{\Phi}^2) - m)$.

Using these two quantities, we propose a new expression for the degree of purity as,

$$P_{nD} = \frac{s}{\sqrt{n-1}\,m}. \tag{4}$$

One can easily observe that for $n = 2$, and $n = 3$, the expressions for the degree of purity given in equation (1) can be related as [16],

$$P_{2D} = \left\{\frac{2[\mathrm{tr}\,(\mathbf{\Phi}^2)]}{(\mathrm{tr}\,\mathbf{\Phi})^2} - 1\right\}^{1/2} = s/m \tag{5}$$

$$P_{3D} = \left\{\frac{1}{2}\left[\frac{3[\mathrm{tr}\,(\mathbf{\Phi}^2)]}{(\mathrm{tr}\,\mathbf{\Phi})^2} - 1\right]\right\}^{1/2} = s/\sqrt{2}m \tag{6}$$

The proposed expression given in equation (4) is physically intuitive as it directly relates the measure of polarimetric purity to the coefficient of variation (i.e., s/m) of the eigenvalues of a $n \times n$ coherency matrix. The coefficient of variation is a standard metric often used to analyze the signal-to-noise ratio in images acquired by radar remote sensing sensors and optical systems (e.g., coherence tomography).

It has been shown in [2, 11, 12] that the degree of purity could also be expressed as a symmetric quadratic mean of all the relative differences between pairs of eigenvalues, λ's of $\mathbf{\Phi}$ as,

$$P_{nD}^2 = \frac{1}{n-1}\sum_{\substack{i,j=0\\ i<j}}^{n} p_{ij}^2, \quad p_{ij} = \frac{\lambda_i - \lambda_j}{\operatorname{tr}\mathbf{\Phi}}. \tag{7}$$

From this definition, one can show that the standard deviation of the eigenvalues spectrum can be expressed as,

$$s = \frac{1}{n}\sqrt{\sum_{\substack{i,j=0\\ i<j}}^{n} (\lambda_i - \lambda_j)^2}. \tag{8}$$

Therefore, along with $m = \operatorname{tr}(\mathbf{\Phi})/n$, the expression given in equation (7) demonstrates its equivalency with the proposed expression given in (4) for the degree of purity.

The set of positive semi-definite matrices is closed under addition and non-negative scaling. Such a set is called a convex cone [18]. It has a particular structure with the identity matrix that forms the central direction. Specific kinds of symmetries exist around this central direction. The position of each matrix in the cone depends strongly on its eigenvalues and, therefore, on its rank. When the rank of a symmetric positive semi-definite matrix decreases, its angle with the identity matrix increases, therefore, rank-1 matrices are farthest from the identity matrix, and all form a fixed angle with that matrix.

In $\mathbb{R}^{n\times n}$ (i.e., the set of square matrices of order n), the Frobenius inner product between two matrices $\mathbf{A}$ and $\mathbf{B}$ is defined as, $\langle \mathbf{A}, \mathbf{B}\rangle_{\mathrm{F}} = \operatorname{tr}(\mathbf{A}^{\mathrm{T}}\mathbf{B})$. This inner product then allows us to define the cosine of the angle between two matrices in $\mathbb{R}^{n\times n}$ as, $\cos(\mathbf{A}, \mathbf{B}) = \langle \mathbf{A}, \mathbf{B}\rangle_{\mathrm{F}}/(\|\mathbf{A}\|_{\mathrm{F}}\|\mathbf{B}\|_{\mathrm{F}})$. The cone of symmetric and positive definite matrices (SPD) in this inner product space contains a rich geometrical structure. In this context, the angle that any SPD matrix forms with the identity axis, i.e., $\alpha\mathbf{I}_n$, for $\alpha > 0$, depicts an important geometrical property that one can use to characterize the degree of purity.

Let ψ denote the angle between $\mathbf{\Phi}$ and the identity matrix $\mathbf{I}_n$ in the space of $n\times n$ matrices. Analogously, we can express this angle between the vector of eigenvalues, $\lambda_1, \lambda_2, \ldots, \lambda_n$, and the equiangular line formed by the vector of the diagonal elements of $\mathbf{I}_n$ as [15],

$$\psi = \cos^{-1}\left(\operatorname{tr}\mathbf{\Phi}/\sqrt{n[\operatorname{tr}(\mathbf{\Phi}^2)]}\right) \tag{9}$$

therefore, using ψ we can also express the degree of purity as,

$$P_{nD} = \frac{\tan\psi}{\sqrt{n-1}} \tag{10}$$

which immediately establishes that $\tan\psi = s/m$. A simple calculation shows that,

$$\tan\psi = \frac{\sqrt{1-\cos^2\psi}}{\cos\psi} \tag{11}$$

$$= \left[\frac{n[\operatorname{tr}(\mathbf{\Phi}^2)]}{(\operatorname{tr}\mathbf{\Phi})^2} - 1\right]^{1/2}. \tag{12}$$

Thus, one can easily relate equation (12) to the part of the expression of P_{nD} given in equation (1), providing an additional geometric interpretation of the degree of purity.

2. Approach II: Direct Sum Decomposition

In the second approach, let us decompose the $n \times n$ coherency matrix $\mathbf{\Phi}$ as,

$$\mathbf{\Phi} = \mathbf{\Phi}_1 + \mathbf{\Phi}_2 + \mathbf{\Phi}_3 \tag{13}$$

where,

$$\mathbf{\Phi}_1 = \frac{(\mathbf{\Phi} + \mathbf{\Phi}^*)}{2} - \frac{\mathrm{tr}(\mathbf{\Phi})}{n}\mathbf{I}_n, \quad \text{(Traceless symmetric matrix)} \tag{14}$$

$$\mathbf{\Phi}_2 = \frac{(\mathbf{\Phi} - \mathbf{\Phi}^*)}{2}, \quad \text{(Anti-symmetric matrix)} \tag{15}$$

$$\mathbf{\Phi}_3 = \frac{\mathrm{tr}(\mathbf{\Phi})}{n}\mathbf{I}_n, \quad \text{(Scalar matrix)} \tag{16}$$

where $\mathbf{I}_n$ is the $n \times n$ identity matrix and $\mathbf{\Phi}^*$ is the conjugate of $\mathbf{\Phi}$. Dennis [19] has addressed such a decomposition by the orthogonal transformation of the 3×3 coherency matrix. However, the scalar part (i.e., $\mathbf{\Phi}_3$) is not separated from the tensor part (i.e., $\mathbf{\Phi}_1 + \mathbf{\Phi}_3$) to make it traceless for geometrical convenience. Note that $\mathbf{\Phi}_1$ and $\mathbf{\Phi}_2$, by themselves, do not represent physical states because they are not positive-semidefinite Hermitian matrices.

On the one hand, we can consider this representation as a direct sum decomposition of the Lie algebra $\mathfrak{gl}(n)$. It is known from the literature [17] that the sub-algebra of traceless matrices is the Lie algebra $\mathfrak{sl}(n)$ of the $SL(n)$ group (i.e., the special linear group). The anti-symmetric matrices form the Lie algebra $\mathfrak{so}(n)$ of the $SO(n)$ group (i.e., the special orthogonal group).

On the other hand, we can interpret using elementary property from vector calculus that the symmetric, trace-free derivative operation relates formally to that of a *shear* [20]. Mathematically this operation is represented by the matrix, $\mathbf{\Phi}_1$, which one can imagine as the gradient of a vector field in an arbitrary direction. However, the anti-symmetric matrix, $\mathbf{\Phi}_2$ represents pure rotation (i.e., the curl operator).

Using the traceless symmetric matrix, $\mathbf{\Phi}_1$, let us first define the quantity

$$P_{ns} = \frac{\sqrt{\frac{n}{n-1}}\,\|\mathbf{\Phi}_1\|_{\mathrm{F}}}{\mathrm{tr}(\mathbf{\Phi})} \tag{17}$$

where $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm of the matrix. It is remarkable that this quantity is identical to the *degree of population asymmetry*, P_p proposed independently by Gil [21] while describing the structure of purity of a density matrix. In earlier work, Dennis [19] interpreted the traceless part as a measure of the departure of the inertia tensor (defined by $\Re(\mathbf{\Phi})$, i.e., the real part of $\mathbf{\Phi}$) from isotropy.

One can show that P_{ns} is invariant under unitary transformation. In particular, P_{3s} can be considered as the degree of polarization of the real part of the partially polarized 3×3 intrinsic coherency matrix, $\Re(\mathbf{\Phi})$ [22]. Moreover, it is interesting to note that we can relate P_{ns} to the components of polarimetric purity (CPP) proposed in previous papers [23, 24] i.e., the *degree of linear polarization*, P_ℓ, for 2D and 3D cases, and the *degree of directionality*, P_d, for the 3D case as,

$$P_{2s}^2 = P_\ell^2, \tag{18}$$

$$P_{3s}^2 = \frac{3}{4}P_\ell^2 + \frac{1}{4}P_d^2. \tag{19}$$

Thus, one can notice from equation (19) that for the 3D case, P_{3s} involves not only the *degree of linear polarization*, P_ℓ, but also the *degree of directionality*, P_d, which measures the stability of the plane that contains the polarization ellipse, or equivalently, a measure of closeness of the state represented by $\mathbf{\Phi}$ to that of a 2D state [24]. In a similar way, this can be further extended for $n > 3$. However, one needs an appropriate physical interpretation of such extension to higher dimensions.

Further, using the anti-symmetric matrix, $\mathbf{\Phi}_2$, we express the *degree of circular polarization* for 2D and 3D states exactly as defined by Gil [24] as,

$$P_c = \frac{\sqrt{2}\|\mathbf{\Phi}_2\|_{\mathrm{F}}}{\mathrm{tr}(\mathbf{\Phi})}. \tag{20}$$

This quantity measures all contributions to circular polarization and is also invariant under unitary transformation. However, for $n > 3$, the number of correlation parameters exceeds the dimensions (n) and therefore P_c cannot be considered as the absolute value of a vector immersed in n dimensions. Therefore, Gil [21] calls this parameter as the degree of correlation asymmetry for general coherency (or density) matrices.

Finally, in agreement with the corresponding result obtained in Eq. (20) of [21], we express the degree of purity by combining the degree of population asymmetry (17) and the degree of correlation asymmetry (20), as,

$$P_{nD} = \sqrt{P_{ns}^2 + \frac{n}{2\,(n-1)}P_c^2}. \tag{21}$$

Furthermore, one can relate the degree of purity for 2D and 3D cases to the three CPP parameters using equations (18), and (19), and equation (20) as,

$$P_{2D} = \sqrt{P_{2s}^2 + P_c^2} \tag{22}$$

$$= \sqrt{P_\ell^2 + P_c^2}, \tag{23}$$

and

$$P_{3D} = \sqrt{P_{3s}^2 + \frac{3}{4}P_c^2} \tag{24}$$

$$= \sqrt{\frac{3}{4}P_\ell^2 + \frac{1}{4}P_d^2 + \frac{3}{4}P_c^2}. \tag{25}$$

In previous works [24, 25], the relationships of P_{2D} and P_{3D} with the CPP parameters have been shown explicitly. Therefore, as shown in [26, 27], P_{3s} coincides with the so-called *polarimetric dimension index*, and provides fractional contributions from both P_ℓ and P_d, whereas P_{2s} provides pure contribution from P_ℓ. Using the derivation proposed in Sheppard et al., [22], we can show that,

$$P_L^2 = \frac{3}{4}P_\ell^2 + \frac{1}{4}P_d^2 - \frac{1}{4}P_c^2 \tag{26}$$

$$= P_{3s}^2 - \frac{1}{4}P_c^2, \tag{27}$$

where P_L is defined in [22] as the degree of *total linear polarization*, i.e., the contribution from both the purely polarized and mixed state.

Now, expanding P_{ns}, and P_c in the expression of P_{nD} given in equation (21) in terms of the

Frobenius norm and the matrix trace, we find that,

$$P_{nD}^2 = \left(\frac{n}{n-1}\right)\left[\frac{\|\mathbf{\Phi}_1\|_F^2 + \|\mathbf{\Phi}_2\|_F^2}{(\mathrm{tr}\,\mathbf{\Phi})^2}\right] \tag{28}$$

$$= \left(\frac{n}{n-1}\right)\left[\frac{ns^2}{n^2m^2}\right], \tag{29}$$

and therefore,

$$P_{nD} = \frac{s}{\sqrt{n-1}\,m}. \tag{30}$$

which is coincident with equation (4).

Hence, we suitably verify the equivalence among the two approaches for the expression of the *generalized degree of purity*, P_{nD}.

In summary, these two approaches offer distinctive perspectives of the degree of purity fundamentally stemming from concepts well studied in statistics and algebra. Note that while proposing these two approaches, we come across a few new quantities and some relations with existing polarization indices widely reported in the literature. The proposed viewpoint can be an ideal starting point for further advanced studies about the structures of physical states described through coherency or density matrices, as is the case of polarization states.

3. Disclosures.

The authors declare no conflicts of interest.

4. Data availability.

No data were generated or analyzed in the presented research.

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