A Transformational Property of

2-Dimensional Density Matrices

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Introduction. This note derives from recent work related to decoherence models described by Zurek[1] and Albrecht.[2] In both models a qubit $\mathcal{S}$ interacts with a high-dimensional system $\mathcal{E}$—the "environment." The dynamically evolved state of $\mathcal{S}$ is described by a 2×2 hermitian matrix, the reduced density matrix $\mathbb{R}_{\mathcal{S}}$. The following discussion was motivated by issues that arose in that connection.

Structure of the characteristic polynomial. Let $\mathbb{D}$ be diagonal

$$\mathbb{D} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

and let its characteristic polynomial be denoted $p(x) \equiv \det(\mathbb{D} - x\mathbb{I})$. Obviously

$$\begin{aligned} p(x) &= (\lambda_1 - x)(\lambda_2 - x) \\ &= x^2 - (\lambda_1 + \lambda_2)x + \lambda_1\lambda_2 \\ &= x^2 - (\lambda_1 + \lambda_2)x + \tfrac{1}{2}\big[(\lambda_1 + \lambda_2)^2 - (\lambda_1^2 + \lambda_2^2)\big] \\ &= x^2 - T_1 x + \tfrac{1}{2}(T_1^2 - T_2) \end{aligned} \tag{1}$$

where $T_n \equiv \mathrm{tr}\,\mathbb{D}^n$. More than fifty years ago I had occasion to develop—and have many times since had occasion to use—a population of trace formulæ of which (1) is a special instance.[3]Remarkably, the formulæ in question pertain to *all* square matrices, and so in particular does (1): the diagonality assumption can be dispensed with. For *any* 2×2 $\mathbb{M}$ we have

$$p(x) = x^2 - T_1 x + \tfrac{1}{2}(T_1^2 - T_2) \quad \text{with} \quad T_n \equiv \mathrm{tr}\,\mathbb{M}^n \tag{2}$$

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[1] W. H. Zurek, "Environment-induced superselection rules," Phys. Rev. D **26**, 1862-1880 (1982); M. Schlosshauer, *Decoherence & the Quantum-to-Classical Transition* (2008), §2.10.

[2] A. Albrecht, "Investigating decoherence in a simple model," Phys. Rev. D **46**, 5504-5520 (1992).

[3] See, for example, "A mathematical note: Algorithm for the efficient evaluation of the trace of the inverse of a matrix" (December 1996), where (1) appears as illustrative equation (12).

from which it follows in particular that for any such $\mathbb{M}$

$$\det \mathbb{M} = \tfrac{1}{2}(T_1^2 - T_2) \tag{3}$$

Application to density matrices. Density matrices are positive-definite hermitian matrices with unit trace, and *vice versa*. Hermiticity insures that the eigenvalues of such a matrix $\mathbb{R}$ are real, positive definiteness

$$(\alpha|\mathbb{R}|\alpha) > 0 \quad : \quad \text{all column vectors } |\alpha)$$

requires that they be non-negative, and since they are required to sum to unity each must fall within the unit interval: $0 \le \lambda_1, \lambda_2 \le 1$. From this condition it follows that

$$0 \le \lambda_i^2 \le \lambda_i \le 1 \quad \text{with } \lambda_i^2 = \lambda_i \text{ iff } \lambda_i = 0 \text{ else } 1$$

From $\lambda_1 + \lambda_2 = 1$ is follows moreover that if one λ vanishes the other must be unity. We therefore have

$$\text{tr}\,\mathbb{R} = 1 \quad \text{and} \quad 0 < \text{tr}\,\mathbb{R}^2 \le 1 \ : \ \begin{cases} \text{mixed cases} \\ \text{pure cases} \end{cases}$$

In mixed cases the spectral decomposition of $\mathbb{R}$ reads

$$\mathbb{R}_{\text{mixed}} = \lambda_1 |r_1)(r_1| + \lambda_2 |r_2)(r_2|$$

where $|r_1)$ and $|r_2)$ are orthonormal eigenvectors, while in pure cases the spectral decomposition trivializes:

$$\mathbb{R}_{\text{pure}} = 1\,|r_1)(r_1| + 0\,|r_2)(r_2| = |r_1)(r_1|$$

The characteristic polynomials of 2-dimensional density matrices have the structure

$$p(x) = x^2 - x + \tfrac{1}{2}(1 - T_2)$$

which gives

$$\lambda_\pm = \tfrac{1}{2}\big[1 \pm \sqrt{2T_2 - 1}\big] \tag{4}$$

The invariable reality of $\lambda_\pm$ implies that in all cases

$$\tfrac{1}{2} \le T_2 \le 1$$

(which sharpens the condition $0 < \text{tr}\,\mathbb{R}^2 \le 1$ stated above): maximal mixing arises at the lower bound (where the eigenvalues become equal and the spectrum degenerate), purity at the upper bound. Finally, (3) has become

$$\det \mathbb{R} = \tfrac{1}{2}(1 - T_2) \tag{5}$$

Transformations that preserve both $\mathbf{T}_1$ and $\mathbf{T}_2$. The most general 2-dimensional density matrix can be written

$$\mathbb{R} = \begin{pmatrix} p_1 & re^{+i\varphi} \\ re^{-i\varphi} & p_2 \end{pmatrix}$$

of which the eigenvalues are

$$\begin{aligned} \lambda_\pm &= \tfrac{1}{2}\Big[(p_1+p_2) \pm \sqrt{4r^2 + (p_1-p_2)^2}\Big] \\ &= \tfrac{1}{2}\Big[1 \pm \sqrt{4r^2 + (p_1-p_2)^2}\Big] \end{aligned} \tag{6}$$

while

$$\det \mathbb{R} = p_1 p_2 - r^2 \tag{7}$$

Comparison of (6) witn (4) supplies

$$T_2 = 2r^2 + 1 + \tfrac{1}{2}\big[(p_1-p_2)^2 - 1\big] \tag{8.1}$$

while comparison of (7) with (5) supplies

$$T_2 = 2r^2 + 1 - 2p_1p_2 \tag{8.2}$$

The equivalence of equations (8) follows from

$$\tfrac{1}{2}\big[(p_1-p_2)^2 - 1\big] = \tfrac{1}{2}\big[(p_1-p_2)^2 - (p_1+p_2)^2\big] = -2p_1p_2 \tag{9}$$

We are interested in transformations

$$\mathbb{R} = \begin{pmatrix} p_1 & re^{+i\varphi} \\ re^{-i\varphi} & p_2 \end{pmatrix} \longrightarrow \tilde{\mathbb{R}} = \begin{pmatrix} p_1+a & s \\ s & p_2-a \end{pmatrix}$$

that preserve T_2 (the preservation of T_1 has been prearranged). This—by (5)—is equivalent to asking for transformations that preserve $\det\mathbb{R}$. We proceed stepwise. STEP 1: Trivially

$$\det\begin{pmatrix} p_1 & re^{+i\varphi} \\ re^{-i\varphi} & p_2 \end{pmatrix} = \det\begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix}$$

STEP 2: Show by (*Mathematica*-assisted) calculation that

$$\det\begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix} = \det\begin{pmatrix} p_1+a & r+s \\ r+s & p_2-a \end{pmatrix}$$

if $s = -r \pm \sqrt{r^2 + a(p_2-p_1) - a^2} \equiv -r \pm R$. STEP 3: Observe that trivially

$$\det\begin{pmatrix} p_1+a & \pm R \\ \pm R & p_2-a \end{pmatrix} = \det\begin{pmatrix} p_1+a & \pm Re^{+i\vartheta} \\ \pm Re^{-i\vartheta} & p_2-a \end{pmatrix}$$

The net implication is that the matrices

$$\tilde{\mathbb{R}}(a,\vartheta) = \begin{pmatrix} p_1 + a & e^{+i\vartheta}\sqrt{r^2 + a(p_2 - p_1) - a^2} \\ e^{-i\vartheta}\sqrt{r^2 + a(p_2 - p_1) - a^2} & p_2 - a \end{pmatrix}$$

are—for all a and all ϑ—tracewise (and $\therefore$ determinantally) identical[4] to $\mathbb{R}$, and give back $\mathbb{R}$ as a special case:

$$\tilde{\mathbb{R}}(0,\varphi) = \mathbb{R}$$

The previous $\pm$ has been absorbed into the definition of ϑ, and the unit trace presumption entails $p_1 + p_2 = 1$.

Trace invariance implies—by (2)—that of the characteristic polynomial, whence of the eigenvalues (6), which by (9) can be written

$$\lambda_\pm = \tfrac{1}{2}\Big[1 \pm \sqrt{1 - 4(p_1 p_2 - r^2)}\,\Big]$$

and give $\lambda_+\lambda_- = p_1 p_2 - r^2 = \det \mathbb{R}(a,\vartheta)$. Positive semi-definiteness (which presumes reality) is seen to require

$$0 \le 1 - 4(p_1 p_2 - r^2) \le 1$$

The first inequality $1 - 4p_1p_2 \le 4r^2$ poses no constraint upon r^2, since p_1p_2 ranges on $[0, \frac{1}{4}]$ as $\{p_1, p_2\}$ partition the unit interval, giving $0 \le 1 - 4p_1p_2$. The second inequality can be written $r^2 \le p_1p_2$, which entails

$$-r_{\max} \le r \le +r_{\max} \quad \text{with} \quad r_{\max} = \sqrt{p_1 p_2} = \text{geometric mean} \le \tfrac{1}{2}$$

We note that while spectral positivity implies $\lambda_+\lambda_- = \det \mathbb{R} > 0$, the converse is not true: $\det \mathbb{R} > 0$ would result if both eigenvalues were *negative*. It is, therefore, somewhat accidental that in the present context the spectral positivity condition *can* be formulated $\det \mathbb{R} = p_1p_2 - r^2 > 0$.

Spectral stability does not imply stability of the eigenvectors, though preservation of hermiticity ensures that the eigenvectors (except in spectrally degenerate cases) do remain orthogonal. I propose to describe the normalized eigenfunctions of $\tilde{\mathbb{R}}(a,\vartheta)$. But those turn out to be fairly intricate, and their structure not at all obvious, so I will take a moment to describge how those results were obtained.

The (unnormalized) symbolic eigenvectors supplied by *Mathematica* are of the asymmetric form

$$e_1 = \begin{pmatrix} x_1 \\ 1 \end{pmatrix}, \quad e_2 = \begin{pmatrix} x_2 \\ 1 \end{pmatrix} \tag{10.1}$$

[4] I understand this phrase to mean "T_1 and T_2-preserving."

But orthonormal vectors in complex 2-space can invariably be displayed[5]

$$u_1 = e^{i\,\xi_1}\cdot\begin{pmatrix}\cos\alpha\\ +\sin\alpha\cdot e^{i\beta}\end{pmatrix},\quad u_2 = e^{i\,\xi_2}\cdot\begin{pmatrix}\sin\alpha\\ -\cos\alpha\cdot e^{i\beta}\end{pmatrix}$$

We observe that if in u_2 we flip the elements and change a sign we obtain a vector proportional to u_1 (and *vice versa*). So as an alternative to (10.1) we have

$$f_1 = \begin{pmatrix}1\\ -x_2\end{pmatrix},\quad f_2 = \begin{pmatrix}1\\ -x_1\end{pmatrix} \tag{10.2}$$

Sums of eigenvectors are eigenvectors, so we obtain the symmetrized pair

$$g_1 = \begin{pmatrix}1+x_1\\ 1-x_2\end{pmatrix},\quad g_1 = \begin{pmatrix}1+x_2\\ 1-x_1\end{pmatrix} \tag{10.3}$$

That $g_1 \perp g_2$ is seen to follow from $e_1 \perp e_2 \Longleftrightarrow 1+\bar{x}_1x_2 = 0 = 1+\bar{x}_2x_1$. The norms of g_1 and g_2 are given by

$$\begin{aligned}|g_1| &= \sqrt{2+(x_1+\bar{x}_1)-(x_2+\bar{x}_2)+(\bar{x}_1x_1+\bar{x}_2x_2)}\\ |g_2| &= \sqrt{2-(x_1+\bar{x}_1)+(x_2+\bar{x}_2)+(\bar{x}_1x_1+\bar{x}_2x_2)}\end{aligned}$$

It is by this strategy that I have (with major assistance by *Mathematica*) constructed (and checked) the eigenvectors reported below:

In the context that motivated this discussion the off-diagonal elements of $\tilde{\mathbb{R}}(a,\vartheta)$ are real; indeed, the constrants which we have been motivated to impose upon $\{p_1,p_2,a\}$ render *all* elements real, so we can dispense with all allusions to the complex conjugates of variables. Introducing these auxiliary definitions

$$\begin{aligned}p = p_1 &\quad\text{so}\quad p_2 = 1-p\\ A(a) &= \sqrt{r^2+a(1-2p)-a^2} &&= \sqrt{r^2+a(p_2-p_1)-a^2}\\ B(a) &= \tfrac{1}{2}-p-a &&= \tfrac{1}{2}(p_2-p_1)-a\\ C &= \tfrac{1}{2}\sqrt{1+4r^2-4p(1-p)} &&= \tfrac{1}{2}\sqrt{1+4(r^2-p_1p_2)}\\ & &&= \tfrac{1}{2}\sqrt{2T_2-1}\end{aligned}$$

we look to the eigenvalues/vectors of the matrix

$$\mathbb{R}(a) = \begin{pmatrix}p_1+a & A(a)\\ A(a) & p_2-a\end{pmatrix}$$

which by design has the property that $T_1 \equiv \text{tr}\,\mathbb{R}(a) = 1$ and

$$T_2 \equiv \text{tr}\,\mathbb{R}^2(a) = \text{tr}\begin{pmatrix}p_1 & r\\ r & p_2\end{pmatrix}^2 = 2r^2+p_1^2+p_2^2 = 1+2(r^2-p_1p_2)\quad:\quad\text{all } a$$

The eigenvalues are

$$\lambda_1 = \tfrac{1}{2}-C\quad\text{and}\quad\lambda_2 = \tfrac{1}{2}+C$$

[5] See *Advanced Quantum Topics* (2000), Chapter 1, page 5.

which are seen to supply $\lambda_1 + \lambda_2 = 1 = T_1$ and

$$\lambda_1^2 + \lambda_2^2 = \tfrac{1}{2} + \tfrac{1}{2}C^2 = 1 + 2(r^2 - p_1 p_2) = T_2$$

—as anticipated. The (unnormalized) eigenvectors are

$$g_1 = \begin{pmatrix} A - B - C \\ A + B - C \end{pmatrix} \quad \text{and} \quad g_2 = \begin{pmatrix} A - B + C \\ A + B + C \end{pmatrix}$$

In confirmation of orthogonality we (with *Mathematica*'s assistance) verify that

$$(A - B)^2 - C^2 + (A + B)^2 - C^2 = 2(A^2 + B^2 - C^2) = 0$$

The respective norms are

$$\begin{aligned} |g_1| &= \sqrt{2[(A - C)^2 + B^2]} \\ &= 2\sqrt{(C - A)C} \qquad \star \\ |g_2| &= \sqrt{2[(A + C)^2 + B^2]} \\ &= 2\sqrt{(C + A)C} \qquad \star \end{aligned}$$

where the equations marked $\star$ follow from the previously-remarked circumstance that the definitions of A, B and C entail $A^2 + B^2 - C^2 = 0$.

In the case $a = 0$ we have

$$\begin{aligned} A(0) &= r \\ B(0) &= \tfrac{1}{2} - p & &= \tfrac{1}{2}(p_2 - p_1) \\ C &= \tfrac{1}{2}\sqrt{1 + 4r^2 - 4p(1 - p)} & &= \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)} \end{aligned}$$

$$\mathbb{R}(0) = \mathbb{R} = \begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix}$$

The values of T_1 and T_2 are unchanged (that was the whole point of this exercise!) and so also therefore do the values of λ_1 and λ_2. The eigenvectors become

$$g_{01} = \begin{pmatrix} r - \tfrac{1}{2}(p_2 - p_1) - \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)} \\ r + \tfrac{1}{2}(p_2 - p_1) - \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)} \end{pmatrix}$$

$$g_{02} = \begin{pmatrix} r - \tfrac{1}{2}(p_2 - p_1) + \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)} \\ r + \tfrac{1}{2}(p_2 - p_1) + \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)} \end{pmatrix}$$

with norms

$$|g_{01}| = 2\sqrt{\left(-r + \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)}\right)\tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)}}$$

$$|g_{02}| = 2\sqrt{\left(+r + \tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)}\right)\tfrac{1}{2}\sqrt{1 + 4(r^2 - p_1 p_2)}}$$

In the trivial case $r = a = 0$ the preceding results give

$$\begin{aligned} A_0(0) &= r \\ B_0(0) &= \tfrac{1}{2} - p & &= \tfrac{1}{2}(p_2 - p_1) \\ C_0 &= \tfrac{1}{2}\sqrt{1 - 4p(1 - p)} & &= \tfrac{1}{2}\sqrt{1 - 4p_1 p_2} \\ &= \tfrac{1}{2}(1 - 2p) \end{aligned}$$

$$\mathbb{R}_0(0) = \mathbb{R}_0 = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}$$

The eigenvalues become

$$\begin{aligned} \lambda_1 &= \tfrac{1}{2} - \tfrac{1}{2}(1-2p) = p \qquad \equiv p_1 \\ \lambda_2 &= \tfrac{1}{2} + \tfrac{1}{2}(1-2p) = 1 - p = p_2 \end{aligned}$$

as, of course, they must. The eigenvectors become

$$g_{001} = \begin{pmatrix} -\frac{1}{2}(1-2p) - \frac{1}{2}(1-2p) \\ +\frac{1}{2}(1-2p) - \frac{1}{2}(1-2p) \end{pmatrix} = \begin{pmatrix} p_1 - p_2 \\ 0 \end{pmatrix}$$

$$g_{002} = \begin{pmatrix} -\frac{1}{2}(1-2p) + \frac{1}{2}(1-2p) \\ +\frac{1}{2}(1-2p) + \frac{1}{2}(1-2p) \end{pmatrix} = \begin{pmatrix} 0 \\ p_1 - p_2 \end{pmatrix}$$

of which the predicted norms are

$$\begin{aligned} |g_{001}| &= 2\sqrt{\tfrac{1}{2}(1-2p)\cdot\tfrac{1}{2}(1-2p)} = (1-2p) = p_1 - p_2 \\ |g_{002}| &= \text{ditto} \end{aligned}$$

as again they must be.

Rotational aspects of the problem. Transformations that map density matrices to density matrices (*i.e.,* which preserve hermiticity, unit trace and positivity) have come to be called "operations," and can in general be accomplished by Kraus processes

$$\mathbb{R} \longrightarrow \mathbb{R}' = \sum_k \mathbb{A}_k \mathbb{R} \mathbb{A}_k{}^+ \quad \text{where} \quad \sum_k \mathbb{A}_k{}^+ \mathbb{A}_k = \mathbb{I}$$

We have been concerned with an operation that in the 2-dimensional case preserves not only T_1 but also T_2 (and therefore the spectrum). Kraus processes invariably preserve T_1 but typcally do *not* preserve $\{T_2, T_3, \ldots\}$ unless the set of Kraus matrices $\{\mathbb{A}_1, \mathbb{A}_2, \ldots, \mathbb{A}_n\}$ contains but a single member, when we have

$$\mathbb{R} \longrightarrow \mathbb{R}' = \mathbb{A}\,\mathbb{R}\,\mathbb{A}^+ \quad \text{where} \quad \mathbb{A}^+\mathbb{A} = \mathbb{I}, \text{ so } \mathbb{A} \text{ is } \textit{unitary}$$

Such unitary similarity transformations do in any dimension preserve the traces of *all* powers of $\mathbb{R}$.

Hermiticity-preservation is by itself sufficient to ensure that the orthonormal eigenbasis $\{|f_j) : j = 1, 2, \ldots, n\}$ defined by $\mathbb{R}'$ is a unitary transform of the eigenbasis $\{|\,e_i) : i = 1, 2, \ldots, n\}$ defined by $\mathbb{R}$—this even when $\mathbb{R} \longrightarrow \mathbb{R}'$ is *not* unitary; we have

$$(f_j| = \sum_i (f_j|e_i)(e_i| \equiv \sum_i U_{ji}(e_i|$$

where

$$\sum_i (f_j|e_i)(e_i|f_k) = (f_j|f_k) = \delta_{jk} \Longrightarrow \sum_i U_{ji}\bar{U}_{ik} = \delta_{jk}$$
$$\Downarrow$$
$$\mathbb{U}\mathbb{U}^+ = \mathbb{I}$$

We have been working in a context in which the eigenvectors are (to within an irrelevant complex phase factor) real-valued, so our $\mathbb{U}$-matrix is in fact a simple 2×2 rotation matrix. And the transformations that have concerned us preserve not only orthonormality but also T_2 (whence both eigenvalues). We conclude that the operation

$$\begin{aligned} \mathbb{R} &= \begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix} \\ &\downarrow \\ \mathbb{R}(a) &= \begin{pmatrix} p_1 + a & \sqrt{r^2 + a(p_2 - p_1) - a^2} \\ \sqrt{r^2 + a(p_2 - p_1) - a^2} & p_2 - a \end{pmatrix} \\ &= \begin{pmatrix} p_1 + a & A(a) \\ A(a) & p_2 - a \end{pmatrix} \end{aligned} \tag{11.1}$$

contemplataed on page 4 amounts to no more nor less than a simple rotational transformation

$$\begin{aligned} \mathbb{R} &= \begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix} \\ &\downarrow \\ \mathbb{R}(\alpha) &= \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix} \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \\ &= \begin{pmatrix} p_1\cos^2\alpha + p_2\sin^2\alpha + r\sin 2\alpha & \frac{1}{2}(p_2 - p_1)\sin 2\alpha + r\cos 2\alpha \\ \frac{1}{2}(p_2 - p_1)\sin 2\alpha + r\cos 2\alpha & p_1\sin^2\alpha + p_2\cos^2\alpha - r\sin 2\alpha \end{pmatrix} \end{aligned} \tag{11.2}$$

which, we observe, gives back $\mathrm{tr}\,\mathbb{R}(\alpha) = p_1 + p_2 = 1$ and $\mathrm{tr}\,\mathbb{R}^2(\alpha) = p_1^2 + p_2^2 + 2r^2$ for all values of α.

Remarkably, the matrix elements $\{p_1, p_2, r\}$ enter linearly into (11.2), but non-linearly into (11.1). Consistency must hinge on the $\{p_1, p_2, r\}$-dependence of α. I show now how this comes about.

Working from either of the diagonal conditions

$$p_1\cos^2\alpha + p_2\sin^2\alpha + r\sin 2\alpha = p_1 + a$$
$$p_2\cos^2\alpha + p_1\sin^2\alpha - r\sin 2\alpha = p_2 - a$$

we write $\tau \equiv \tan\alpha$ and use $\sin^2\alpha = \tau^2/(1+\tau^2)$, $\cos^2\alpha = 1/(1+\tau^2)$ to obtain

$$(a + p_1 - p_2)\tau^2 - 2r\tau + a = 0 \tag{12.1}$$

of which the solutions are

$$\tau_\pm \equiv \tan\alpha_\pm = \frac{r \pm \sqrt{r^2 + a(p_2 - p_1) - a^2}}{a - (p_2 - p_1)} = \frac{r \pm A(a)}{a - (p_2 - p_1)}$$

Working on the other hand from either of the (identical) off-diagonal conditions

$$\tfrac{1}{2}(p_2-p_1)\sin 2\alpha + r\cos 2\alpha = A(a)$$

we use $\sin 2\alpha = 2\tau/(1+\tau^2)$, $\cos 2\alpha = (1-\tau^2)/(1+\tau^2)$ to obtain

$$(A+r)\tau^2 + (p_2-p_1)\tau + (A-r) = 0 \tag{12.2}$$

where again $A = A(a) = \sqrt{r^2 + a(p_2-p_1) - a^2}$. Notice that the equations (12) impose distinct quadratic conditions on τ. The solutions of (12.2) are

$$\begin{aligned}\hat{\tau}_\pm &= \frac{\pm(p_2-p_1) - \sqrt{4r^2 + (p_2-p_1)^2 - 4A^2}}{2(r+A)}\\ &= \frac{\pm(p_2-p_1) - \big((p_2-p_1)-2a\big)}{2(r+A)}\\ &= \begin{cases} \dfrac{a}{r+A} \\[2ex] \dfrac{(p_2-p_1)-a}{r+A}\end{cases}\end{aligned}$$

We have interest only in the *simultaneous* solution of (12.1) and (12.2). With *Mathematica*'s assistance we survey the possibilities, with the following results:

$$\begin{aligned}\tau_+ &= \hat{\tau}_+ &&: \text{true}\\ \tau_+ &= \hat{\tau}_- &&: \text{false}\\ \tau_- &= \hat{\tau}_+ &&: \text{false}\\ \tau_- &= \hat{\tau}_- &&: \text{false}\end{aligned}$$

The implication is that

$$\tau \equiv \tan\alpha = \frac{a}{r + \sqrt{r^2 + a(p_2-p_1) - a^2}} \tag{13}$$

To check the accuracy or this result, we insert the implied evaluations of

$$\sin\alpha = \frac{\tau}{1+\tau^2} \quad \text{and} \quad \cos\alpha = \frac{1}{1+\tau^2}$$

into (11.2) and, according to *Mathematica*, do in fact recover

$$\mathbb{R}(\alpha) = \begin{pmatrix} \dfrac{p_1+a}{\sqrt{r^2+a(p_1-p_2)-a^2}} & \dfrac{\sqrt{r^2+a(p_1-p_2)-a^2}}{p_2-a}\end{pmatrix}$$

Concluding remarks. Let the characteristic polynomial of an n-dimensional square matrix $\mathbb{M}$ be written

$$\det(\mathbb{M} - x\mathbb{I}) = c_0x^n + c_1x^{n-1} + \cdots + c_{n-1}x^1 + c_n$$

By the Cayley-Hamilton theorem $c_0\mathbb{M}^n + c_1\mathbb{M}^{n-1} + \cdots + c_{n-1}\mathbb{M} + c_n\mathbb{I} = \mathbb{O}$, so

$$\mathbb{M}^{n+1} = -(1/c_0)\Big\{c_1\mathbb{M}^n + c_2\mathbb{M}^{n-1}\cdots + c_{n-1}\mathbb{M}^2 + c_n\mathbb{M}\Big\}$$

of which the trace reads

$$T_{n+1} = -(1/c_0)\Big\{c_1T_n + c_2T_{n-1} + \cdots + c_{n-1}T_2 + c_nT_1\Big\}$$

It is known,[3,6] moreover, that the coefficients $\{c_0, c_1, \ldots, c_n\}$ can be developed as multinomials in the low-order traces $\{T_0, T_1, \ldots, T_n\}$; specifically (look again to (2))

$$\begin{aligned}
c_0 &= (-)^n 1\\
c_1 &= (-)^{n-1}T_1\\
c_2 &= (-)^{n-2}\tfrac{1}{2!}\big[T_1^2 - T_2\big]\\
c_3 &= (-)^{n-3}\tfrac{1}{3!}\big[T_1^3 - 3T_1T_2 + 2T_3\big]\\
&\;\;\vdots\\
c_k &= (-)^{n-k}\tfrac{1}{k!}\begin{vmatrix}
T_1 & T_2 & T_3 & T_4 & \cdots & \cdots & T_k\\
1 & T_1 & T_2 & T_3 & \cdots & \cdots & T_{k-1}\\
0 & 2 & T_1 & T_2 & \cdots & \cdots & T_{k-2}\\
0 & 0 & 3 & T_1 & \cdots & \cdots & T_{k-3}\\
\vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots\\
0 & 0 & 0 & 0 & \cdots & (k-1) & T_1
\end{vmatrix} \quad : \quad 1 \le k \le n\\
&\;\;\vdots\\
c_n &= \det\mathbb{M} = \text{trace-wise development of the determinant}
\end{aligned}$$

The relevant implication is that high-order traces can be described (recursively) in terms of leading-order traces

$$T_p = f_p(T_1, T_2, \ldots, T_n) \quad : \quad p > n$$

And therefore that transformations $\mathbb{M} \longrightarrow \mathbb{M}'$ which preserve leading-order traces automatically preserve *all* traces, and have therefore the form

$$\mathbb{M} \longrightarrow \mathbb{M}' = \mathbb{S}\,\mathbb{M}\,\mathbb{S}^{-1}$$

It follows, moreover, that the eigenvalues of $\mathbb{M}$ are—since they can evidently be developed as algebraic functions

$$\lambda_k(T_1, T_2, \ldots, T_n) \quad : \quad k = 1, 2, \ldots n$$

of the leading-order traces—are invariant under such transformations.

[6] See also "Some applications of an elegant formula due to V. F. Ivanoff," Notes for a seminar presented 28 May 1969 to the Applied Math Club at Portland State University, expecially page 14.

We have been concerned in these pages with a 2-dimensional problem. Our objective was to describe transformations $\mathbb{M} \longrightarrow \mathbb{M}'$ which preserve the properties characteristic of density matrices (hermiticity, positivity and unit trace) and additionally preserve T_2, which is conventionally used to quantify the "degree of mixedness."[7] In two dimensions the invariance of T_1 and T_2 has been seen to imply the invariance of the characteristic polynomial (whence of the spectrum), of traces of *all* orders, and that

$$\mathbb{M} \longrightarrow \mathbb{M}' = \mathbb{S}\,\mathbb{M}\,\mathbb{S}^{-1} \quad \text{with} \quad \mathbb{S} \text{ unitary} \tag{14}$$

If—as we have, for expository reasons been content to assume—the elements of $\mathbb{M}$ are real then "unitary" becomes "rotational." Elements of $\mathbb{S} \in O(2)$ are identified by a single parameter α. At (11.1) we encountered an alternative one-parameter construction

$$\begin{pmatrix} p_1 & r \\ r & p_2 \end{pmatrix} \longrightarrow \begin{pmatrix} p_1 + a & A \\ A & p_2 - a \end{pmatrix}$$

where the specific structure of A was forced by the required invarinace of T_2. At (13) we describe the relationship between the parametrs α and a.

In $n = 3$ dimensions the invariance of T_1 and T_2 does *not* enforce the invariance of T_3 or of higher order traces. Transformations of type (14) describe now only a *subset* of the possibilities (which is to say: if $n = 3$ then T_2-preserving transformations can, in general, *not* be presented as instances of (14)), and

$$\begin{pmatrix} p_1 & r & s \\ r & p_2 & t \\ s & t & p_3 \end{pmatrix} \longrightarrow \begin{pmatrix} p_1 + a_1 & A & B \\ A & p_2 + a_2 & C \\ B & C & p_3 + a_3 \end{pmatrix} \quad : \quad \begin{cases} p_1 + p_2 + p_3 = 1 \\ a_1 + a_2 + a_3 = 0 \end{cases}$$

poses a much more difficult analytical problem than the one treated here; the elements of $\mathbb{S} \in O(3)$ are 3-parameter objects, but additional parameters enter into the construction of $\{A, B, C\}$. As n advances beyond 3 the problem becomes progressively more intractable.

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[7] The defining properties ensure that every density matrix can be written

$$\mathbb{R} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \quad : \quad \text{all } \lambda_i \in [0,1] \text{ and } \textstyle\sum \lambda_1 = 1$$

from which it follows that

$$T_1 = 1 \geq T_2 \geq T_3 \geq \cdots \geq T_n$$

where all inequalities become equalities if and only if $\mathbb{R}$ refers to a pure mixture. This means that the traces $T_{k>2}$ serve as well (if less conveniently than) T_2 to quantify "degree of mixedness."