IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **44** (2011) 335301 (19pp) doi:10.1088/1751-8113/44/33/335301

Numerical shadow and geometry of quantum states

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Received 22 April 2011, in final form 27 June 2011
Published 21 July 2011
Online at stacks.iop.org/JPhysA/44/335301

Abstract

The totality of normalized density matrices of dimension N forms a convex set $\mathcal{Q}_N$ in $\mathbb{R}^{N^2-1}$. Working with the flat geometry induced by the Hilbert–Schmidt distance, we consider images of orthogonal projections of $\mathcal{Q}_N$ onto a two-plane and show that they are similar to the numerical ranges of matrices of dimension N. For a matrix A of dimension N, one defines its numerical shadow as a probability distribution supported on its numerical range $W(A)$, induced by the unitarily invariant Fubini–Study measure on the complex projective manifold $\mathbb{C}P^{N-1}$. We define generalized, mixed-state shadows of A and demonstrate their usefulness to analyse the structure of the set of quantum states and unitary dynamics therein.

PACS numbers: 02.10.Yn, 02.30.Tb, 03.67.−a

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Investigation of the geometry of the set of quantum states remains a subject of current scientific interest in view of possible applications in the theory of quantum information processing. The set Ω_N of pure quantum states belonging to an N-dimensional complex Hilbert space $\mathcal{H}_N$ is known to be equivalent to the complex projective space, $\Omega_N = \mathbb{C}P^{N-1}$, of $2N-2$ real dimensions. However, as this set is embedded into the (N^2-1)-dimensional set $\mathcal{Q}_N$ of density matrices of dimension N by a nonlinear constraint, $\rho = \rho^2$, the geometric structure of the set of mixed quantum states is rather involved [1, 2]. The only simple case corresponds to the one-qubit system, $N = 2$.

The set Ω_2 of $N = 2$ pure states forms the *Bloch sphere*, $\mathbb{C}P^1 = S^2$, with respect to the standard Hilbert–Schmidt metric. The 3-disc inside the sphere, often called the *Bloch ball*, represents the set $\mathcal{Q}_2$ of one-qubit mixed states. In this simple case, any projection of this set onto a plane forms an ellipse, which can be degenerated to an interval. In the case of $N = 3$, the eight-dimensional set $\mathcal{Q}_3$ of one-qutrit mixed states is neither a polytope nor an ellipsoid [3–5], and the set $\Omega_3 = \mathbb{C}P^2$ of its extremal states is connected and has four real dimensions.

Due to the high dimensionality of the problem, our understanding of the geometry of the set $\mathcal{Q}_N$ of mixed states is still rather limited. This set forms a convex body which contains an in-ball of radius $r_N = \sqrt{1/N(N-1)}$ and can be inscribed into an out-sphere of radius $R_N = (N-1)r_N = \sqrt{(N-1)/N}$ [2]. Some information on the subject can be gained by studying the two-dimensional cross-sections of $\mathcal{Q}_N$ as demonstrated in [6–8] for $N = 3$ and $N = 4$. Another option is to investigate projections of this set into a plane—such an approach was advocated for $N = 3$ in [9]. As the set $\mathcal{Q}_N$ of quantum states is convex, also its cross-sections and projections inherit convexity.

In this work, we study the general structure of a two-dimensional projection of the set $\mathcal{Q}_N$ of mixed states. A bridge between the geometry of the set of quantum states and the notion of numerical range used in operator theory is established. For any operator A, acting on the complex Hilbert space $\mathcal{H}_N$, one defines its *numerical range* [10, 11] (also called *field of values*) as a subset of the complex plane which contains expectation values of A among arbitrary normalized pure states

$$W(A) = \{z : z = \langle\psi|A|\psi\rangle,\ |\psi\rangle \in \mathcal{H}_N,\ \langle\psi|\psi\rangle = 1\}. \tag{1}$$

We analyse the set of orthogonal projections of the set $\mathcal{Q}_N$ onto a 2-plane and prove that it is equivalent to the set of all possible numerical ranges of complex matrices of dimension N. Numerical ranges of normal matrices of dimension N correspond to orthogonal projections of the set $\mathcal{C}_N$ of classical states—the $(N-1)$-dimensional simplex $\Delta_{N-1} \subset \mathbb{R}^{N-1}$.

Further information on the structure of the set of quantum states of a dimension N can be obtained by studying the *numerical shadow* [12–14] of various matrices of dimension N. For any operator A acting on $\mathcal{H}_N$, one defines a probability distribution $P_A(z)$ on the complex plane, supported in the numerical range $W(A)$:

$$P_A(z) := \int_{\Omega_N} \mathrm{d}\mu(\psi)\delta(z - \langle\psi|A|\psi\rangle). \tag{2}$$

Here, $\mu(\psi)$ denotes the unique unitarily invariant (Fubini–Study) measure on the set Ω_N of N-dimensional pure quantum states. In other words, the shadow P of matrix A at a given point z characterizes the likelihood that the expectation value of A among a random pure state is equal to z.

The distribution $P_A(z)$ is naturally associated with a given matrix A, and some of its properties were described in [13]. In this work, we advocate a complementary approach and show that investigating the shadows of several different complex matrices A of a fixed dimension N contributes to our understanding of the structure of the entire set $\mathcal{Q}_N$ of quantum states. In a sense, the choice of a matrix A corresponds to the selection of the plane, onto which the set of quantum states is projected.

This paper is organized as follows. In section 2, we fix the notation and introduce necessary concepts. A link between two-dimensional projections of the set of quantum states of a given dimension N and the set of possible numerical ranges of matrices of dimension N is presented in section 3. In section 4, we analyse different classes of numerical shadows of matrices of small dimension $N = 2, 3, 4$. Unitary dynamics of a pure quantum state in the background of numerical shadow is presented in section 5. Section 6 is devoted to the mixed-state numerical shadow, which corresponds to a projection of the full set $\mathcal{Q}_N$ of density matrices onto a plane. The case of a large dimension, $N \gg 1$, is treated in section 7 jointly with the shadow of random matrices. Finally, in section 8, we provide some concluding remarks and summarize the contribution of this paper.

2. Classical and quantum states

Let $p = \{x_1, x_2, \ldots, x_N\}$ be a normalized probability vector, so $x_i \geqslant 0$ and $\sum_{i=1}^N x_i = 1$. Such a vector represents a *classical state*, and the set $\mathcal{C}_N$ of all classical states forms an $(N-1)$-dimensional regular simplex $\Delta_{N-1} \subset \mathbb{R}^{N-1}$. There exist exactly N *classical pure states*, which correspond to the corners of the simplex. All other classical states can be expressed by a convex combination of pure states and are called *mixed*. Typical mixed states are characterized by the full rank and they form the entire interior of the probability simplex.

In quantum theory, one describes a physical system with N distinguishable states by elements of a complex Hilbert space $\mathcal{H}_N$ of dimension N. Its elements represent pure quantum states, $|\psi\rangle \in \mathcal{H}_N$. Quantum states are assumed to be normalized, $||\psi||^2 = \langle\psi|\psi\rangle = 1$, so they belong to the sphere of dimension $2N-1$. Since one identifies two states, which differ by a global phase only, $|\psi\rangle \sim |\phi\rangle = \mathrm{e}^{-\alpha}|\psi\rangle$, the set of all pure quantum states Ω_N, which act on $\mathcal{H}_N$, is equivalent to the complex projective space $\Omega_N = \mathbb{C}P^{N-1}$ [2].

In analogy to the classical case, one also defines mixed quantum states (density matrices) by a convex combination of projectors onto pure states, $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, where $p_i > 0$ and $\sum_i p_i = 1$. Let us denote the set of all density matrices of dimension N by $\mathcal{Q}_N$. It contains all density operators which are positive and normalized:

$$\mathcal{Q}_N = \{\rho : \mathcal{H}_N \to \mathcal{H}_N, \rho^* = \rho, \rho \geqslant 0, \mathrm{Tr}\,\rho = 1\}. \tag{3}$$

Since density operators are Hermitian and normalized, this set is $N^2 - 1$ dimensional. It includes the set of classical states, $\mathcal{Q}_N \supset \mathcal{C}_N = \Delta_{N-1}$, as well as the set of pure quantum states, $\mathcal{Q}_N \supset \Omega_N = \mathbb{C}P^{N-1}$. We will work with the geometry implied by the Hilbert–Schmidt norm of a matrix, $|A|_{\mathrm{HS}} := \sqrt{\mathrm{Tr}(A^*A)}$, and the Hilbert–Schmidt distance in the space of matrices,

$$d_{\mathrm{HS}}(A, B) := |A - B|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}(A-B)(A-B)^*}. \tag{4}$$

It will also be convenient to define a real inner-product by setting the polar identity

$$\langle A, B\rangle = \tfrac{1}{4}|A+B|_{\mathrm{HS}}^2 - \tfrac{1}{4}|A-B|_{\mathrm{HS}}^2 = \tfrac{1}{2}[\mathrm{Tr}(A^*B + B^*A)]. \tag{5}$$

If $A^* = A$ and $B^* = B$, then $\langle A, B\rangle = \mathrm{tr}\,AB$.

In the set Ω_N of quantum pure states, one defines the Fubini–Study measure μ_{FS}, which is induced by the Haar measure on $U(N)$ and is invariant with respect to unitary transformations. In the case of one-qubit states, this measure corresponds to the uniform distribution of points on the Bloch sphere S^2.

In practice, to generate pure states at random according to the measure μ_{FS}, it is sufficient to uniformly generate points at the sphere S^{2N-1}. One may also select an arbitrary column (or row) of a random unitary matrix U distributed according to the Haar measure. It directly gives the set of N coefficients of the random state in a given basis, $|\psi\rangle = \sum_{i=1}^N c_i|i\rangle$. For instance, choosing the first column of U, we set $c_i = U_{i,1}$ for $i = 1, \ldots, N$. Alternatively, one may generate N independent complex random numbers z_i and renormalize them, $c_i = z_i/\sqrt{\sum_i |z_i|^2}$, to obtain the desired distribution [15, 3].

In this work, we will use the following.

Proposition 1. *Let* $|\psi\rangle \in \Omega_N$ *be a random pure state of dimension N distributed according to the Fubini–Study measure. If one represents it in an arbitrary fixed basis,* $|\psi\rangle = \sum_{i=1}^{N} c_i|i\rangle$*, then the squared absolute values of the coefficients,* $p_i = |c_i|^2$*, form a probability vector distributed uniformly in the probability simplex* Δ_{N-1}.

This is equivalent to the known statement (see e.g. [2]) that the only constraint on the components of a single column of a random unitary matrix U distributed according to the Haar measure is the normalization condition $P(U_{11},\ldots U_{N1}) \sim \delta\big(1-\sum_{i=1}^{N}|U_{i1}|^2\big)$. This fact directly implies

Corollary 2. *For any quantum state* ρ *define a classical state* $p = \mathrm{diag}(\rho)$*, so* $p_i = \rho_{ii}$*. Then, the Fubini–Study measure on the set* Ω_N *of quantum pure states induces by this mapping the uniform measure in the classical probability simplex* Δ_{N-1}.

In the case of $N = 2$, the Fubini–Study measure covers uniformly the Bloch sphere S^2. Working with the standard polar coordinates, (r, θ, φ), we write the element of the volume of the unit sphere as $\mathrm{d}S = \mathrm{d}\varphi \sin\theta d\theta = \mathrm{d}\varphi d(\cos\theta)$. The polar angle θ is defined with respect to the axis z, so the projection of a point of the sphere at this axis reads $z = \cos\theta$. Hence, the Fubini–Study measure implies the uniform distribution $d(\cos\theta) = \mathrm{d}z$ along the one-dimensional set Δ_1 of $N = 2$ classical states.

3. Numerical range as a projection of the set of quantum states

The set $\Omega_N = \mathbb{C}P^{N-1}$ of pure states of dimension N forms the set of extremal points in $\mathcal{Q}_N$. Any mixed state $\rho \in \mathcal{Q}_N$ can thus be decomposed into a convex mixture of projectors $|\psi\rangle\langle\psi|$. The expectation value of an operator A among a pure state reads $\langle\psi|A|\psi\rangle = \mathrm{Tr}\rho A$. Taking into account the convexity of $W(A)$, the standard definition (1) of the numerical range of A can therefore be rewritten as [16]

$$W(A) = \{z : z = \mathrm{Tr}\rho A,\ \rho \in \mathcal{Q}_N\}. \tag{6}$$

This expression suggests a possible link between the numerical range and the structure of the set, the $\mathcal{Q}_N$. Usually one studies the numerical range $W(A)$ for a given A [11]. Here, we propose to fix the dimension N and consider the set of all possible numerical ranges of matrices A of this dimension to analyse the geometry of quantum states. More precisely, we establish the following facts.

Proposition 3. *Let* $\mathcal{C}_N$ *denote the set of classical states of dimension N, which forms the regular simplex* Δ_{N-1} *in* $\mathbb{R}^N$*. Then, for each normal matrix A (such that* $AA^* = A^*A$*) of dimension* N*, there exists an affine rank 2 projection P of the set* $\mathcal{C}_N$ *whose image is congruent to the numerical range* $W(A)$ *of the matrix A. Conversely for each rank 2 projection* P*, there exists a normal matrix A whose numerical range* $W(A)$ *is congruent to the image of* $\mathcal{C}_N$ *under projection P.*

Proposition 4. *Let* $\mathcal{Q}_N$ *denote the set of quantum states dimension N embedded in* $\mathbb{R}^{N^2}$ *with respect to the Euclidean geometry induced by the Hilbert–Schmidt distance. Then, for each (arbitrary) matrix A of dimension* N*, there exists an affine rank 2 projection P of the set* $\mathcal{Q}_N$ *whose image is congruent to the numerical range* $W(A)$ *of the matrix A. Conversely for each rank 2 projection* P*, there exists a matrix A whose numerical range* $W(A)$ *is congruent to the image of* $\mathcal{Q}_N$ *under projection P.*

To prove the above propositions, we will need an abstract lemma concerning the real inner-product Euclidean spaces.

Lemma 5. *Suppose $u_1, u_2, v_0 \in V$, where V is an Euclidean vector space (with the inner product $\langle\cdot,\cdot\rangle$ and norm $|x| = \langle x, x\rangle^{1/2}$), $v_0 \neq 0$ and* $\dim(\mathrm{span}\{u_1, u_2, v_0\}) \geqslant 2$. *Then, there exist real numbers $\alpha > 0, \gamma_1, \gamma_2$ such that the vectors*

$$v_1 := \frac{1}{\alpha}(u_1 + \gamma_1 v_0), \qquad v_2 := \frac{1}{\alpha}(u_2 + \gamma_2 v_0) \tag{7}$$

are normalized and orthogonal:

$$|v_1|^2 = 1 = |v_2|^2, \qquad \langle v_1, v_2\rangle = 0. \tag{8}$$

Proof. Let $u_i' = u_i - \frac{\langle u_i, v_0\rangle}{|v_0|^2} v_0$, $i = 1, 2$. By hypothesis $|u_1'|^2 + |u_2'|^2 > 0$. For $i = 1, 2$ set $c_i := |v_0|\gamma_i + \frac{\langle u_i, v_0\rangle}{|v_0|}$ so that $v_i = \frac{1}{\alpha}\left(u_i' + \frac{c_i}{|v_0|}v_0\right)$. The desired equations become

$$|u_1'|^2 + c_1^2 = \alpha^2, \qquad |u_2'|^2 + c_2^2 = \alpha^2, \qquad \langle u_1', u_2'\rangle + c_1 c_2 = 0. \tag{9}$$

Eliminating coefficient α, we arrive at a quadratic equation for c_1^2 or c_2^2. Set

$$d = (|u_1'|^2 - |u_2'|^2)^2 + 4\langle u_1', u_2'\rangle^2;$$

then,

$$c_1^2 = \tfrac{1}{2}(|u_2'|^2 - |u_1'|^2) + \tfrac{1}{2}\sqrt{d}, \tag{10}$$

$$c_2^2 = \tfrac{1}{2}(|u_1'|^2 - |u_2'|^2) + \tfrac{1}{2}\sqrt{d}, \tag{11}$$

$$\mathrm{sign}(c_1 c_2) = -\mathrm{sign}\langle u_1', u_2'\rangle, \tag{12}$$

$$\alpha = \left(\tfrac{1}{2}(|u_1'|^2 + |u_2'|^2) + \tfrac{1}{2}\sqrt{d}\right)^{1/2}. \tag{13}$$

Recall $|u_1'|^2 + |u_2'|^2 > 0$ by hypothesis; thus, $\alpha > 0$. There are generally two solutions differing only in the signs of c_1 and c_2. If $\langle u_1', u_2'\rangle = 0$, then $\sqrt{d} = ||u_1'|^2 - |u_2'|^2|$, and one of the three following cases apply:

(1) $|u_1'| > |u_2'| \geqslant 0, c_1 = 0, c_2 = \pm\sqrt{|u_1'|^2 - |u_2'|^2}, \alpha = |u_1'|$;
(2) $|u_2'| > |u_1'| \geqslant 0, c_1 = \pm\sqrt{|u_2'|^2 - |u_1'|^2}, c_2 = 0, \alpha = |u_2'|$;
(3) $|u_1'| = |u_2'| > 0, c_1 = 0, c_2 = 0, \alpha = |u_1'|$. □

Note that formulae (10) and (11) for c_1 and c_2 allow us to obtain the constants γ_1 and γ_2, which enter equation (7). The scaling factor $\alpha = 1$ if and only if $\langle u_1', u_2'\rangle^2 = (1 - |u_1'|^2)(1 - |u_2'|^2)$, $|u_1'|^2 \leqslant 1$ and $|u_2'|^2 \leqslant 1$.

This lemma implies the following.

Corollary 6. *Suppose $E \subset \{x \in V : \langle x, v_0\rangle = 1\}$ and $u_1, u_2 \in V$ define a linear map $\Phi : E \to \mathbb{C}$ by $x \mapsto \langle x, u_1\rangle + \mathrm{i}\langle x, u_2\rangle$. Unless $u_1, u_2 \in \mathbb{R}v_0$ in which case Φ is constant, the map Φ is isometrically isomorphic to an orthogonal projection followed by a similarity transformation (dilation and translation).*

Proof. By lemma 5, there exist orthonormal vectors $v_i = \frac{1}{\alpha}(u_i + \gamma_i v_0)$ for $i = 1, 2$ and $\alpha > 0$. Let $V_0 = \mathrm{span}\{v_1, v_2\}$. The orthogonal projection onto V_0 is given by $\pi x := \langle x, v_1\rangle v_1 + \langle x, v_2\rangle v_2$ and this is the general form of a rank 2 orthogonal projection.

The linear map $\theta : a_1 v_1 + a_2 v_2 \mapsto a_1 + \mathrm{i}a_2$ is an isometry $V_0 \to \mathbb{C}$. If $x \in E$, then $\langle v_0, x\rangle = 1$ and

$$\theta(\alpha\pi x - (\gamma_1 v_1 + \gamma_2 v_2)) = \theta \sum_{i=1}^{2} (\langle u_i + \gamma_i v_0, x\rangle - \gamma_i) v_i = \theta \sum_{i=1}^{2} \langle u_i, x\rangle v_i = \phi x. \tag{14}$$

□

Now we are ready to prove the main result of this paper, namely propositions 3 and 4.

3.1. Normal matrices

Proof of proposition 3. Let A be a normal matrix of dimension N with eigenvalues $\{\lambda_1, \ldots, \lambda_N\}$. With respect to an orthonormal basis of eigenvectors of A, one has $\sum_{i,j=1}^{N} \overline{\psi_i} A_{ij} \psi_j = \sum_{i=1}^{N} \lambda_i |\psi_i|^2$ and the numerical range W_A is the image of the simplex $\Delta_{N-1} := \left\{t \in \mathbb{R}^N : t_i \geqslant 0 \forall i, \sum_{i=1}^{N} t_i = 1\right\}$ under the map

$$\Phi : t \longmapsto \sum_{i=1}^{N} t_i \,\mathrm{Re}\,\lambda_i + \mathrm{i} \sum_{i=1}^{N} t_i \mathrm{Im}\,\lambda_i = \langle t, u_1\rangle + \mathrm{i}\langle t, u_2\rangle, \tag{15}$$

where $t \in \Delta_{N-1}$ and $(u_1)_i = \mathrm{Re}\,\lambda_i$, $(u_2)_i = \mathrm{Im}\,\lambda_i$ for $1 \leqslant i \leqslant N$. If $A \neq c\mathbb{1}$ (multiple of the identity, the eigenvalues are all equal), then lemma 5 and corollary 6 apply with $v_0 = (1, \ldots, 1)$, which completes the proof of proposition 3. □

3.2. Non-normal matrices

Proof of proposition 4. The set $\mathcal{Q}_N$ of quantum states (3) contains Hermitian operators ρ which can be diagonalized, $\rho = UDU^*$. Here, U is unitary while D is a diagonal matrix with $d_{ii} \geqslant 0$ and $\sum_{i=1}^{N} d_{ii} = 1$.

Consider any matrix A of dimension N and write $\mathrm{Tr}\,\rho A = \mathrm{Tr}\,\rho A_1 + \mathrm{i}\,\mathrm{Tr}\,\rho A_2$ with $A_1 = \frac{1}{2}(A + A^*)$ and $A_2 = \frac{1}{2\mathrm{i}}(A - A^*)$. Lemma 5 and corollary 6 apply now to the map

$$\Phi : \rho \longmapsto \mathrm{Tr}\,\rho A_1 + \mathrm{i}\,\mathrm{Tr}\,\rho A_2 \tag{16}$$

of the set $\mathcal{Q}_N$ onto the numerical range $W(A)$ with V representing the linear space of complex matrices of dimension N (or the real subspace of Hermitian matrices), the real inner product (5), and $v_0 = I$, $u_1 = A_1$, $u_2 = A_2$ provided $A \neq c\mathbb{1}$.

Thus, we have shown that for any matrix A, its numerical range $W(A)$ is equal to an orthogonal projection of the set of density matrices. To show the converse, we may read formulae (7) backwards: the projection of $\mathcal{Q}_N$ is determined by two orthonormal Hermitian matrices V_1 and V_2, which then satisfy $|V_1|_{\mathrm{HS}} = |V_2|_{\mathrm{HS}} = 1$ and $\mathrm{Tr}(V_1 V_2) = 0$. Set $A = V_1 + \mathrm{i}V_2$, which now gives the required matrix such that $W(A)$ is equal to the desired projection. In this way, a link between numerical ranges of generic matrices of dimension N and projections of the set $\mathcal{Q}_N$ onto a two-plane is established and proposition 4 is proved.

□

To obtain explicit formulae for the similarity transformation corresponding to an arbitrary matrix A of dimension N, define three traceless matrices

$$B = A - \frac{\mathrm{Tr}\,A}{N} I, \qquad B_1 = \frac{1}{2}(B + B^*), \qquad B_2 = \frac{1}{2\mathrm{i}}(B - B^*). \tag{17}$$

The latter two represent vectors in the Hilbert–Schmidt space and correspond to u_1', u_2' in lemma 5 Making use of the Hilbert–Schmidt norm, we compute the required coefficients for a given traceless matrix B:

$$d = \operatorname{Tr} B^2 \operatorname{Tr} B^{*2} = |\operatorname{Tr} B^2|^2, \qquad \alpha = \left(\tfrac{1}{2}\operatorname{Tr}(BB^*) + \tfrac{1}{2}|\operatorname{Tr} B^2|\right)^{1/2}, \tag{18}$$

$$c_1^2 = -\tfrac{1}{4}(\operatorname{Tr} B^2 + \operatorname{Tr} B^{*2}) + \tfrac{1}{2}|\operatorname{Tr} B^2|, \qquad c_2^2 = \tfrac{1}{4}(\operatorname{Tr} B^2 + \operatorname{tr} B^{*2}) + \tfrac{1}{2}|\operatorname{Tr} B^2|, \tag{19}$$

and $\operatorname{sign}(c_1c_2) = -\operatorname{sign}\langle u_1', u_2'\rangle = -\operatorname{sign}(\operatorname{Im}\operatorname{Tr} B^2)$.

4. Numerical shadow and quantum states

The projectors $|\psi\rangle\langle\psi|$ onto pure states form extremal points of the set $\mathcal{Q}_N$ of quantum states; hence, the shape of a projection of the set Ω_N of pure states onto a given plane coincides with the shape of the projection of the set of density matrices on the same plane. As shown in the previous section, this set is equal to the numerical range $W(A)$ of a matrix A of dimension N, which determines the projection.

However, the differences appear if one studies not only the support of the projection but also the corresponding probability measure. A measure $P_A(z)$ determined by the numerical shadow (2) is induced by the Fubini–Study measure on the set Ω_N of the pure state. Thus, the standard numerical shadows of various matrices of dimension N can be interpreted as a projection of the complex projective space, $\Omega_N = \mathbb{C}P^{N-1}$, onto a plane. Before discussing in detail the cases of low dimensions, let us present here some basic properties of the numerical shadow [13] (also called the *numerical measure* [14]).

(1) By construction, the distribution $P_A(z)$ is supported on the numerical range of $W(A)$ and it is normalized, $\int_{W(A)} P_A(z)\, \mathrm{d}^2z = 1$.
(2) The (numerical) shadow is unitarily invariant, $P_A(z) = P_{UAU^*}(z)$. This is a consequence of the fact that the integration measure $\mathrm{d}\mu(\psi)$ is unitarily invariant.
(3) For any normal operator A acting on $\mathcal{H}_N$, such that $AA^* = A^*A$, its shadow covers the numerical range $W(A)$ with the probability corresponding to a projection of a *regular* N-simplex of classical states $\mathcal{C}_N$ (embedded in $\mathbb{R}^{N-1}$) onto a plane.
(4) For a non-normal operator A acting on $\mathcal{H}_N$, its shadow covers the numerical range $W(A)$ with the probability corresponding to an orthogonal projection of the complex projective manifold $\Omega_N = \mathbb{C}P^{N-1}$ onto a plane.
(5) For any two operators A and B acting on $\mathcal{H}_N$, the shadow of their tensor product does not depend on the order

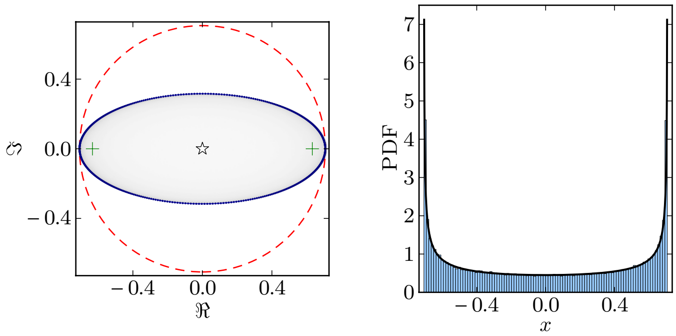
$$P_{A\otimes B}(z) = P_{B\otimes A}(z). \tag{20}$$

To show this property define a unitary swap operator S which acts on a composite Hilbert space and interchanges the order in the tensor product, $S(|z\rangle \otimes |y\rangle) = |y\rangle \otimes |z\rangle$. Thus, $\langle x|A \otimes B|x\rangle = \langle x|S^*B \otimes AS|x\rangle$, and since S is unitary it does not influence the numerical shadow induced by the unitarily invariant Fubini–Study measure on complex projective space.

4.1. *One-qubit states, $N = 2$*

The analysis of the numerical shadow is particularly simple in the case of matrices of dimension $N = 2$. The spectrum of the operator A consists of two complex numbers, $\sigma(A) = \{\lambda_1, \lambda_2\}$.

In the case of a normal matrix A, the numerical range $W(A)$ forms the closed interval $[\lambda_1, \lambda_2]$, and the numerical shadow $P_A(z)$ covers this interval uniformly [13].



(*a*) Shadow of matrix $A_0^{(2)}$ (*b*) Cross-section for $\Im = 0$

Figure 1. Projection of the set Ω_2 of one-qubit states generated by the numerical shadows of operators of dimension $N = 2$: (*a*) numerical shadow of generic matrix $A_0^{(2)}$ with an elliptical support. Eigenvalues are denoted with crosses and the dashed circle of radius $R_2 = \sqrt{2}/2$ denotes the diameter of the Bloch ball. Numerically obtained histogram is plotted in black, and the analytical plot is blue. The plot is made for the matrix translated in such a way that its trace ($\star$) is equal to zero and suitably rescaled. (*b*) Histogram of the cross-section of the shadow supported in the interval $[-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]$; the solid line represents a probability density function of the arcsine distribution $P(x) = (\pi\sqrt{\frac{1}{2} - x^2})^{-1}$.

If the matrix A is non-normal, the numerical range forms an elliptical disc with λ_1, λ_2 as focal points and minor axis, $d = \sqrt{\mathrm{Tr} AA^* - |\lambda_1|^2 - |\lambda_2|^2}$. For a simple proof of this 1932 result of Murnaghan [17], see the note by Li [18]. In this generic case, the numerical shadow is given by the probability distribution obtained by the projection of the hollow Bloch sphere of one-qubit pure states onto a plane [13]. In particular, the cross-section of the numerical shadow supported in an interval $x \in [0, 1]$ is given by the arcsine distribution, $P(x) = 1/(\pi\sqrt{x(1-x)})$. The non-normal case is shown in figure 1, obtained for a matrix

$$A_0^{(2)} = a_0 \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}.$$

For simplicity, we have selected the centred matrix such that $\mathrm{Tr} A = 0$ so that one has $B = A$ in equation (17). The normalization constant $a_0 = \sqrt{2/5}$ is chosen in such a way that the scaling constant defining the projection in (18) is set to unity, $\alpha = 1$, so the shadow of the set of quantum states is shown in its 'natural size': the distance between both eigenvalues, $l = 2a_1 = \sqrt{2}$, is equal to the diameter of the Bloch ball, $2R_2 = \sqrt{2}$.

4.2. One-qutrit states, $N = 3$

The structure of the numerical range for $N = 3$ was analysed in detail by Keeler *et al* [19]. The numerical range of a matrix A of dimension $N = 3$ with the spectrum $\lambda_1, \lambda_2, \lambda_3$ forms

(a) a compact set of an 'ovular' shape with three eigenvalues in its interior;
(b) a compact set with *one* flat part—e.g. the convex hull of a cardioid;
(c) a compact set with *two* flat parts—e.g. the convex hull of an ellipse and a point outside it;
(d) triangle: for any *normal* matrix A its numerical range is equal to the triangle spanned by the spectrum, $W(A) = \Delta(\lambda_1, \lambda_2, \lambda_3)$. In the latter case, the numerical shadow can be verbally interpreted as the shadow of the set $\mathcal{C}_3$ of $N = 3$ classical states—a uniformly covered equilateral triangle Δ_2.

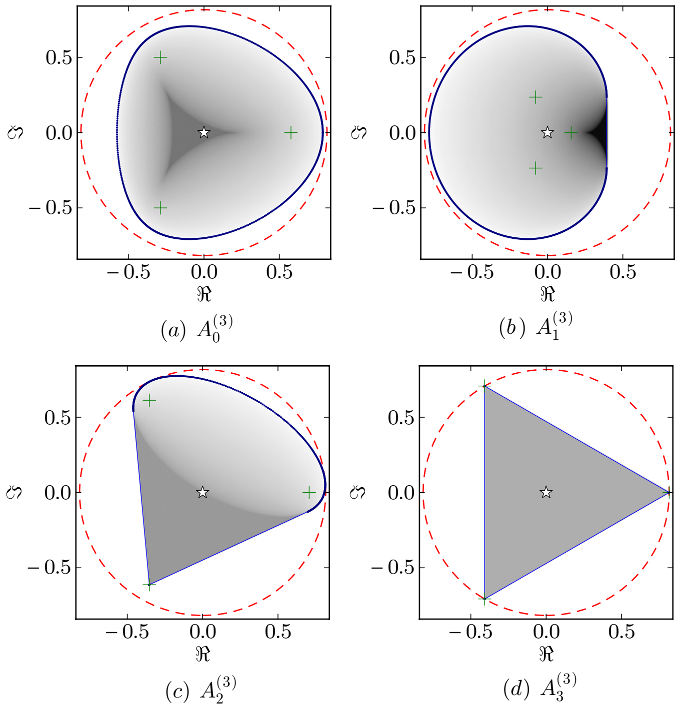


Figure 2. Projections of the set Ω_3 of one-qutrit states generated by the numerical shadows of operators of dimension $N = 3$; (*a*) a generic matrix $A_0^{(3)}$ with an oval-like numerical shadow, (*b*) $A_1^{(3)}$ with one flat part of the boundary ∂W of the numerical range, (*c*) $A_2^{(3)}$ a simple sum with two flat parts of ∂W, (*d*) a diagonal normal matrix $A_3^{(3)}$ with the numerical range equal to the triangle of eigenvalues, represented by (+). The dashed circle of radius R_3 represents the projection of the sphere in which Ω_3 is inscribed. All plots are made for matrices translated in such a way that their trace ($\star$) is equal to zero and suitably rescaled.

The four classes of $N = 3$ numerical ranges are illustrated in figure 2. It shows the numerical shadow supported on the corresponding numerical range, obtained for

$$A_0^{(3)} = a_0 \begin{bmatrix} 1 & 1 & 1 \\ 0 & \omega_3 & 1 \\ 0 & 0 & \omega_3^2 \end{bmatrix}, \qquad A_1^{(3)} = a_1 \begin{bmatrix} 5-3\mathrm{i} & 0 & 6 \\ 0 & 5+3\mathrm{i} & 6 \\ -6 & -6 & -10 \end{bmatrix},$$
$$A_2^{(3)} = a_2 \begin{bmatrix} 1 & 1 & 0 \\ 0 & \omega_3 & 0 \\ 0 & 0 & \omega_3^2 \end{bmatrix}, \qquad A_3^{(3)} = a_3 \begin{bmatrix} 1 & 0 & 0 \\ 0 & \omega_3 & 0 \\ 0 & 0 & \omega_3^2 \end{bmatrix}.$$

The symbol ω_k denotes the kth root of unity, so $\omega_3 = \exp(\mathrm{i}2\pi/3)$. As before, the matrices are chosen to be traceless, so $B = A$ in (17) and the shadows are centred. Furthermore, the normalization constants are designed to ensure that the scaling constant in equation (18) in every case is set to unity, $\alpha = 1$, so the figure shows images of the set of quantum states in its natural size. For instance, in the case of the diagonal matrix $A_3^{(3)}$, the prefactor reads $a_3 = \sqrt{2/3}$, so that the eigenvalues are located at the distance $\sqrt{2/3}$ from the origin. This is just the radius R_3 of the sphere in which the set $\mathcal{Q}_3$ is inscribed.

The study of the geometry of the numerical range was initiated by Kippenhahn [20] and later developed by Fiedler [21] and Gutkin [22]. In recent papers [23, 24], the differential topology and projection aspects of the numerical range were investigated. In particular, it was shown [23] that the numerical range of a generic matrix A of dimension 3 pertains to the class (a) above, as the boundary of $W(A)$ does not contain intervals. Critical lines inside the range, analysed in [23, 24], were shown to influence the structure of the numerical shadow [13]. Thus, we may now relate the critical lines with the geometry of complex projective spaces projected onto a plane.

In the one-qutrit case $N = 3$ obtained probability distributions can be interpreted as images of the set of pure states $\Omega_3 = \mathbb{C}P^2$ on the plane. Although it is not so simple to imagine the structure of the complex projective space [25], some experience is gained by studying numerical shadows of various non-normal matrices of dimension 3.

4.3. Four-level systems, $N = 4$

Various shapes of the numerical range for matrices of dimension $N = 4$ correspond to various projections of the set $\mathcal{Q}_4$ of quantum states of dimension 4. As in the case of the qutrit, we analyse numerical shadows of traceless matrices normalized such that the scaling constant α is set to unity.

Even though several results on the geometry of the numerical range for $N = 4$ are available [26, 27], a complete classification of numerical ranges in this case is still missing. To provide an overview of the possible structure of the numerical shadow, we analysed the following matrices of dimension 4:

$$A_0^{(4)} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & \mathrm{i} & 1 & 1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}, \quad A_1^{(4)} = \begin{bmatrix} \mathrm{i} & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 1-\mathrm{i} & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad A_2^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & \mathrm{i} & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix},$$

$$A_3^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & \mathrm{i} & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}, \quad A_4^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}, \quad A_5^{(4)} = \begin{bmatrix} \mathrm{i} & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 1-\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$A_6^{(4)} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & \mathrm{i} & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}, \quad A_7^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}, \quad A_8^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{bmatrix}.$$

Numerical shadows of these representatives of each class of $N = 4$ matrices are shown in figure 3. The pictures can be interpreted as projections of the six-dimensional complex projective space $\mathbb{C}P^3$ onto a plane. Making use of formula (18), we find that the normalization constant for the last example $A_8^{(4)}$ reads $a_8 = 1/\sqrt{2}$. Thus, the diameter of the shadow, $2a_4 = \sqrt{2}$, coincides in this case with the Hilbert–Schmidt distance between any two orthogonal pure states in $\mathcal{Q}_4$. The dashed circle of radius $R_4 = \sqrt{3}/2$ represents the projection of the sphere into which the set $\mathcal{Q}_4$ can be inscribed.

5. Unitary dynamics projected inside the numerical shadow

As the numerical range and the numerical shadow give us an opportunity to observe the structure of the space of quantum states, it is possible to apply these tools to investigate quantum

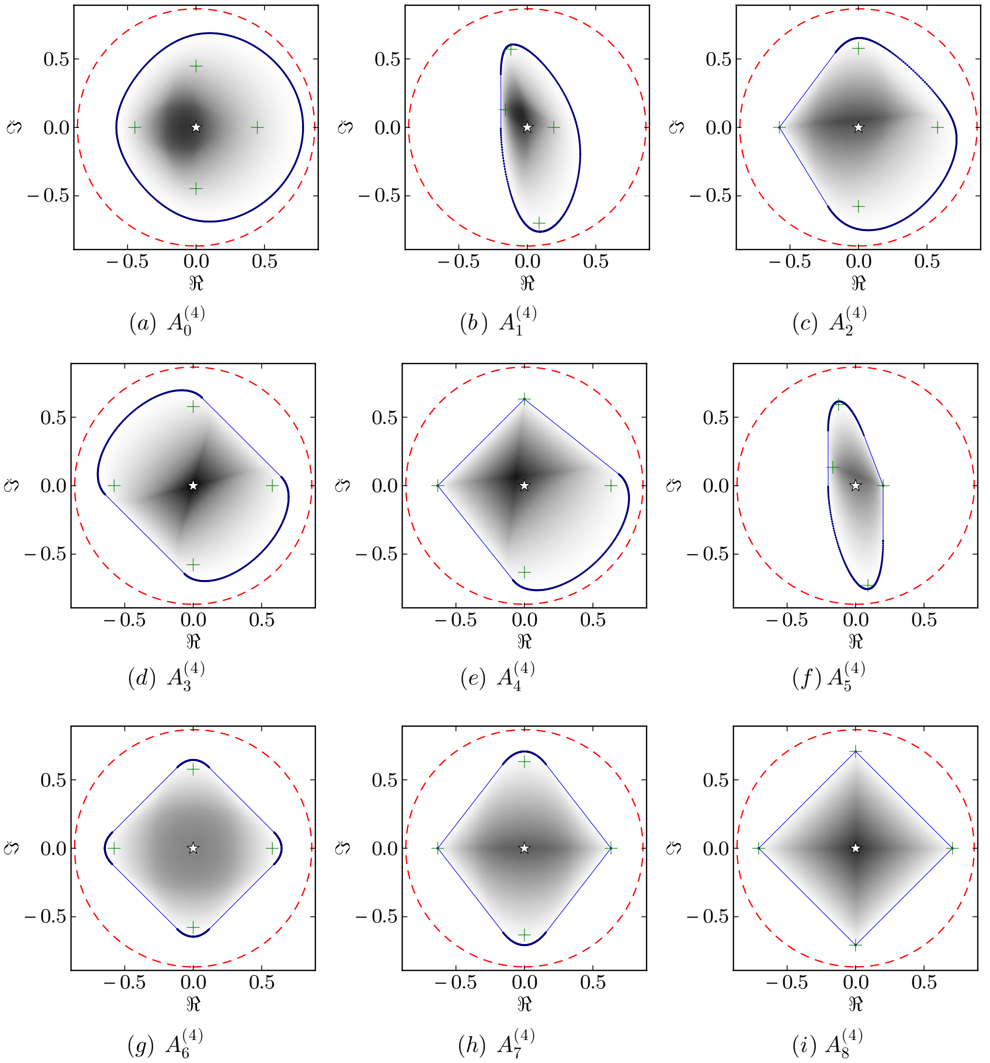


Figure 3. Projections of the set Ω_4 of $N = 4$ quantum states emerging as numerical shadows of appropriately normalized operators of dimension 4: (*a*) a generic matrix $A_0^{(4)}$ with a an oval-like numerical range $W(A)$, (*b*) $A_1^{(4)}$ with one flat part of the boundary ∂W of the numerical range, (*c*) $A_2^{(4)}$ being a simple sum $3 \oplus 1$ with two flat parts of ∂W, (*d*) $A_3^{(4)}$ a simple sum $2 \oplus 2$ with two flat parts of ∂W, (*e*) $A_4^{(4)}$ three flat parts of ∂W connected with corners and one oval-like part, (*f*) $A_5^{(4)}$ three flat parts of ∂W with only one corner and two oval-like parts, (*g*) $A_6^{(4)}$ a simple sum $2 \oplus 2$, with four flat parts of ∂W, (*h*) $A_7^{(4)}$ pair of flat parts of ∂W connected with a corner connected with two oval-like parts, (*i*) a diagonal normal matrix $A_8^{(4)}$ with the numerical range W equal to the convex hull of eigenvalues denoted by (+). All plots are made for matrices translated in such a way that their trace ($\star$) is equal to zero and suitably rescaled.

dynamics. A unitary time evolution of a quantum system is governed by the Hamiltonian operator H (i.e. a self-adjoint operator representing the total energy of the system), which leads to $U(t) = \exp(-\mathrm{i}Ht)$.

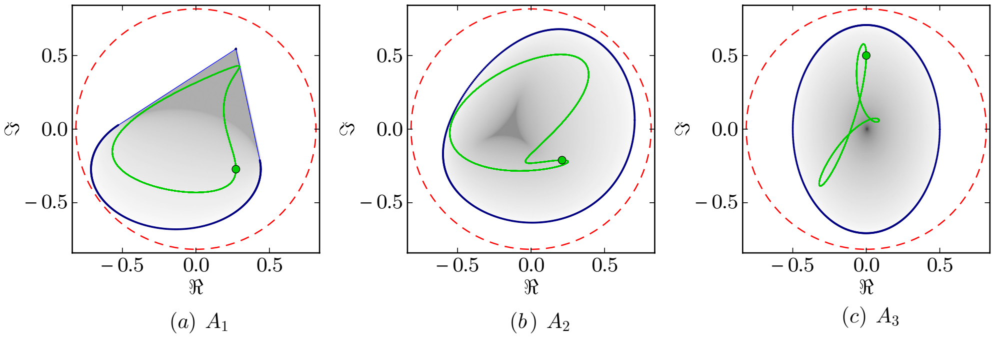


Figure 4. Shadow of the operators A_1, A_2 and A_3 of dimension 3 serves as a background for the trajectory representing the unitary dynamics defined by $U = \exp(-\mathrm{i}Ht)$ with H given by (21) with the initial state $|\phi(0)\rangle$ (marked by a circle in the picture). All plots are made for matrices translated in such a way that their trace is equal to zero and suitably rescaled.

Note that eigenvalues of the Hamiltonian determine the cyclicity of the trajectory. The trajectory is periodic iff eigenvalues of the Hamiltonian are commensurable. The period in this case is given by the least common multiple of the eigenvalues.

Let us consider a three-level system (qutrit). For concreteness, we choose the Hamiltonian

$$H = \begin{bmatrix} -1 & -1-\mathrm{i} & 1 \\ -1+\mathrm{i} & 0 & 1+\mathrm{i} \\ 1 & 1-\mathrm{i} & 1 \end{bmatrix} \tag{21}$$

and select an initial pure state of the system as $|\psi(0)\rangle = |0\rangle \in \mathcal{H}_3$. The state of the system at some specific time t is described by the transformed state $|\psi(t)\rangle = U(t)|\psi(0)\rangle$.

In order to use the numerical shadow to study the time evolution of the system, one needs to choose an arbitrary 3×3 non-Hermitian matrix. To get some information on the dynamics in the space of pure states of a qutrit and to observe it from different points of view, we selected the following matrices:

$$A_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & \mathrm{i} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad A_2 = \begin{bmatrix} 0 & 1 & 1 \\ 0 & \mathrm{i} & 1 \\ 0 & 0 & -1 \end{bmatrix}, \qquad A_3 = \begin{bmatrix} \mathrm{i} & 0 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \end{bmatrix}. \tag{22}$$

For each of these auxiliary matrices, the quantum dynamics can now be visualized as a trajectory in the complex plane defined by a parametric equation

$$z(t) := \langle\psi(t)|A|\psi(t)\rangle = \langle\psi(0)|A'|\psi(0)\rangle, \tag{23}$$

where the unitarily transformed matrix reads $A' = U^*AU = \mathrm{e}^{\mathrm{i}Ht} A\, \mathrm{e}^{-\mathrm{i}Ht}$. The time evolution of the initial state $|\psi(0)\rangle = (1, 0, 0)^T \in \mathcal{H}_3$ generated by the Hamiltonian (21) is shown in figure 4 from three different perspectives determined by matrices (22).

5.1. Identical trajectories

For given matrix A and Hermitian matrix H, a unitary time evolution induces a path in the numerical range Λ_A given by

$$\langle\xi|\, \mathrm{e}^{-\mathrm{i}Ht} A\, \mathrm{e}^{\mathrm{i}Ht} |\xi\rangle, \qquad t \in \mathbb{R}, \tag{24}$$

for a given starting point $|\xi\rangle$. In the mixed state scenario, the trajectory is given by

$$\operatorname{tr} \rho\, \mathrm{e}^{-\mathrm{i}Ht} A\, \mathrm{e}^{\mathrm{i}Ht}, \qquad t \in \mathbb{R}, \tag{25}$$

for a given starting point ρ.

The question one may pose is: under what conditions for two different starting points ρ_0 and ρ_1 trajectories on the numerical range of A are identical:

$$\operatorname{tr} \rho_0 \, \mathrm{e}^{-\mathrm{i}Ht} A \, \mathrm{e}^{\mathrm{i}Ht} = \operatorname{tr} \rho_1 \, \mathrm{e}^{-\mathrm{i}Ht} A \, \mathrm{e}^{\mathrm{i}Ht}, \qquad t \in \mathbb{R}. \tag{26}$$

To convince yourself that such a situation may occur, consider the daily rotation of the earth around its axis. Choosing two initial points at the same meridian on opposite sides of the equator (say close to Cairo and Durban in Africa), we see that the trajectories they generate after projecting onto the equatorial plane do coincide. This is because the dynamics, both initial points and the kind of the projection, are chosen in a special way and satisfy certain constraints. To characterize these constraints in a general setting, we start with the following definitions.

For a given matrix A, let $X_A = \{B \in M_N^H(\mathbb{C}) : \operatorname{tr} B = 0, \operatorname{tr} BA = 0\}$. We also define the set H_A:

$$H_A = \{H \in M_N^H(\mathbb{C}) : \forall t > 0, B \in X_A \text{ we have } \mathrm{Ad}_{\mathrm{e}^{\mathrm{i}Ht}}(B) \in X_A\}, \tag{27}$$

where Ad is the adjoint mapping given by $\mathrm{Ad}_C(B) = CBC^{-1}$.

Now we can state the fact concerning identical trajectories.

Lemma 7. *Trajectories* $\operatorname{tr} \rho_0 \, \mathrm{e}^{-\mathrm{i}Ht} A \, \mathrm{e}^{\mathrm{i}Ht}$ *and* $\operatorname{tr} \rho_1 \, \mathrm{e}^{-\mathrm{i}Ht} A \, \mathrm{e}^{\mathrm{i}Ht}$ *for* $t \in \mathbb{R}$ *are identical if and only if* $\rho_0 - \rho_1 \in X_A$ *and* $H \in H_A$.

Proof. For $H \in H_A$, we have $\operatorname{tr} \mathrm{Ad}_{\mathrm{e}^{\mathrm{i}Ht}}(B) \in X_A = 0$ for all $B \in X_A$ and since $\rho_0 - \rho_1 \in X_A$, $\operatorname{tr}[\mathrm{e}^{\mathrm{i}Ht}(\rho_0 - \rho_1) \, \mathrm{e}^{-\mathrm{i}Ht} A] = 0$. Conversely, it easy to see that $\rho_0 - \rho_1 \in X_A$ and, as the trajectories are supposed to be equivalent, we have $\operatorname{tr}[(\rho_0 - \rho_1) \, \mathrm{e}^{-\mathrm{i}Ht} A \, \mathrm{e}^{\mathrm{i}Ht}] = 0$ for $t \in \mathbb{R}$. Any $B \in X_A$ can be written as the difference of quantum states and thus $H \in H_A$. □

The definition of H_A is somehow complicated; here we put the reasoning which presents it in a simpler form. We have the property $\mathrm{Ad}_{e^C} = \mathrm{e}^{\mathrm{ad}_C}$, where $\mathrm{ad}_C(B) = [C, B]$ (see e.g. [35]). Using this property, we can state the following lemma.

Lemma 8. *The Hermitian matrix H is an element of* H_A*, if and only if for all* $B \in X_A$*, we have* $\mathrm{ad}_{\mathrm{i}H}(B) \in X_A$.

Proof. If $\mathrm{ad}_{\mathrm{i}H}(B) \in X_A$ for all $B \in X_A$, then by iterating we have that $\mathrm{ad}_{\mathrm{i}H}^k(B) \in X_A$ for $k = 0, 1, \ldots$. Since X_A is a linear space, we obtain

$$\mathrm{Ad}_{\mathrm{e}^{\mathrm{i}tH}}(B) = \sum_{k=0}^{\infty} \frac{t^k}{k!} \mathrm{ad}_{\mathrm{i}H}^k(B) \in X_A. \tag{28}$$

On the other hand if $\mathrm{Ad}_{\mathrm{e}^{\mathrm{i}tH}}(B) \in X_A$, then using the fact that

$$\mathrm{i}[H, B] = \lim_{t \to 0} \frac{\mathrm{e}^{\mathrm{i}Ht} B \, \mathrm{e}^{-\mathrm{i}Ht} - B}{t}, \tag{29}$$

and the continuity of the function $X \mapsto \operatorname{tr} XA$, we obtain the result. □

Note that the condition $\mathrm{i}[H, B] \in X_A$ can be stated as $\operatorname{tr} H[A, B] = 0$; this follows from the cyclicity of trace. The linear space X_A is a real $(N^2 - 1 - d(A))$-dimensional space, where $d(A) = \dim(\{\Re(A), \Im(A)\})$, where $\Re(A) = \frac{1}{2}(A + A^*)$ and $\Im(A) = \frac{1}{2\mathrm{i}}(A - A^*)$. Thus, in the generic case, X_A has dimension $N^2 - 3$. The set H_A forms a real subspace of Hermitian matrices orthogonal to the sum of two real subspaces ($\mathrm{ad}_{\mathrm{i}\,\Re(A)}(X_A)$ and $\mathrm{ad}_{\mathrm{i}\,\Im(A)}(X_A)$)):

$$H_A = (\mathrm{ad}_{\mathrm{i}\,\Re(A)}(X_A) \cup \mathrm{ad}_{\mathrm{i}\,\Im(A)}(X_A))^{\perp}, \tag{30}$$

where $^{\perp}$ denotes the orthogonal component in the real space of Hermitian matrices.

6. Mixed-state numerical shadow

The standard numerical shadow (2) of matrix A is defined by choosing randomly a pure state $\rho = |\psi\rangle\langle\psi|$ with respect to the unitarily invariant, natural measure on the set of pure states, and taking the expectation value $\mathrm{Tr} A\rho$. However, one may also consider an expression analogous to (6) and use it with a different measure in the set $\mathcal{Q}_N$ of mixed states. More precisely, we introduce the *mixed-state numerical shadow* of A with respect to a measure μ:

$$P_A^\mu(z) := \int_{\mathcal{Q}_N} \mathrm{d}\mu(\rho)\delta(z - \mathrm{Tr}\,\rho A). \tag{31}$$

The measure μ defined on the set $\mathcal{Q}_N$ of mixed states of dimension N is supposed to be unitarily invariant. For instance, we will use the family of *induced measures* μ_K obtained by taking a random pure state $|\xi\rangle \in \mathcal{H}_N \otimes \mathcal{H}_K$ and generating a mixed state by partial trace over the K-dimensional subsystem, $\rho = \mathrm{Tr}_K|\xi\rangle\langle\xi|$. Since the pure states $|\xi\rangle$ are generated randomly, the unitary matrices determining the eigenvectors of ρ are distributed according to the Haar measure on $U(N)$. The probability distribution of the eigenvalues λ_i of the random mixed state ρ of dimension N obtained in this way reads

$$P_{N,K}(\lambda) = C_{N,K}\,\delta\left(1 - \sum_{i=1}^N \lambda_i\right)\prod_{i=1}^N \lambda_i^{K-N}\prod_{i<j}(\lambda_i - \lambda_j)^2. \tag{32}$$

It is assumed here that $K \geqslant N$ and the normalization constants $C_{N,K}$ are given in [28]. In the symmetric case, $K = N$, the above formula simplifies and the measure μ_N coincides with the flat Hilbert–Schmidt measure, induced by the metric (4). In the opposite case $K < N$, the joint probability density function is given by (32) with exchanged parameters $N \leftrightarrow K$.

Consider now a pure state $|\xi\rangle$ on the bi-partite $N \times K$ system. It can be represented in its Schmidt decomposition [2]:

$$|\xi\rangle = \sum_{i=1}^{\min\{N,K\}} \sqrt{\lambda_i}\,|e_i\rangle \otimes |f_i\rangle, \tag{33}$$

where $\{|e_i\rangle\}_{i=1}^N$ is an orthonormal basis in $\mathcal{H}_N$ while $\{|f_i\rangle\}_{i=1}^K$ is an orthonormal basis of $\mathcal{H}_K$. Taking a partial trace of the projector $|\xi\rangle\langle\xi|$ over the K-dimensional system, we see that the spectrum of the resulting mixed state ρ coincides with the set of the Schmidt coefficients $\{\lambda_i\}$ of the pure state $|\xi\rangle$. Thus, formula (32) describes the distribution of the Schmidt coefficients of a pure state $|\xi\rangle$ drawn randomly according to the uniform distribution on the sphere S^{NK-1}. By construction of the Schmidt decomposition of a random state $|\xi\rangle$, the vectors $|e_i\rangle$ and $|f_i\rangle$ can be considered as columns of the unitary matrix in $U(N)$ and $U(K)$, respectively, distributed according to the Haar measure on the unitary group. A simple calculation shows that

$$\begin{aligned}\langle\xi|(A \otimes \mathbb{1}_K)|\xi\rangle &= \sum_{i,j=1}^{\min\{N,K\}} \sqrt{\lambda_i\lambda_j}\langle e_i|A|e_j\rangle\langle f_i|f_j\rangle \\ &= \sum_{i=1}^{\min\{N,K\}} \lambda_i\langle e_i|A|e_i\rangle = \sum_{i=1}^{\min\{N,K\}} \lambda_i(U^\dagger AU)_{i,i},\end{aligned} \tag{34}$$

where U is a unitary matrix distributed according to the Haar measure on $U(N)$.

These considerations imply that the shadow of $A \otimes \mathbb{1}_K$ is a mixture of diagonal elements of A in a random basis, given by the sum $\sum_{i=1}^{\min\{N,K\}} \lambda_i(U^\dagger AU)_{i,i}$. As before, U stands for a random unitary matrix of dimension N while the joint probability distribution function of the

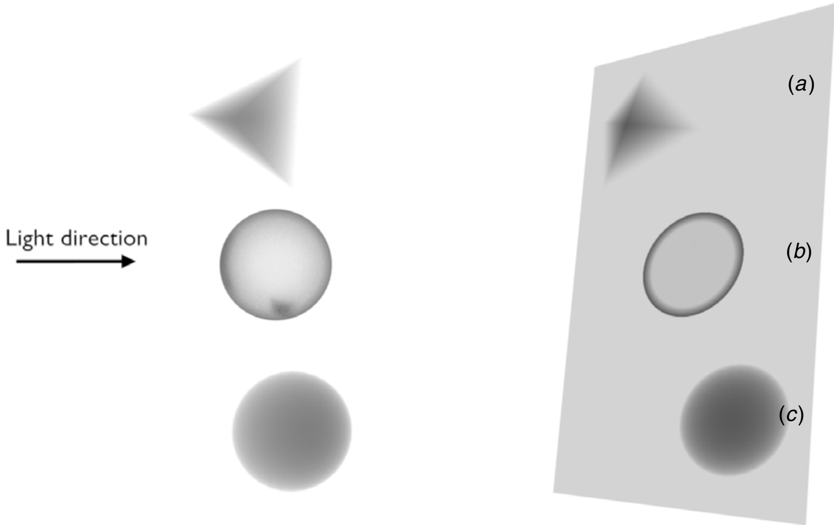


Figure 5. Sketch of a projections onto a two-plane of (*a*) the set $\mathcal{C}_4 = \Delta_3$ of $N = 4$ classical states onto the quadrangle formed by the numerical range W of a normal matrix A of dimension 4; (*b*) the set $\Omega_2 = S^2$ of one-qubit pure quantum states onto a disc formed by the numerical range of a non-normal Jordan matrix J_2 of dimension 2; (*c*) a mixed-state numerical shadow of J_2, corresponding to the projection of the full three-dimensional Bloch ball onto a plane, is equal to the standard, pure-state shadow of an extended matrix $J_2 \otimes \mathbb{1}_2$. The picture is plotted using perspective.

coefficients λ_i is given by (32). This proves that the mixed states shadow of A with respect to the induced measure μ_K coincides with the standard numerical shadow of the extended operator $A \otimes \mathbb{1}_K$:

$$P_A^{\mu_K}(z) = P_{A\otimes\mathbb{1}_K}(z) = P_{\mathbb{1}_K\otimes A}(z). \tag{35}$$

The last equality follows from property (20). In the most important case, $K = N$, the induced measure μ_N is equivalent to the Euclidean (flat) measure in $\mathbb{R}^{N^2-1}$, corresponding to the Hilbert–Schmidt distance (4). Thus, the projection of the 'full' set $\mathcal{Q}_N$ of mixed quantum states on the plane determined by a given matrix A of dimension N is equivalent to the standard shadow of an extended operator $A \otimes \mathbb{1}_N$. In the case of $N = 2$, this is visualized in figure 5(*c*), in which the shadow of the full Bloch ball $\mathcal{Q}_2$ can be compared with the shadow of the hollow Bloch sphere $\Omega_2 = S^2$, displayed in figure 5(*b*).

Note that for $K = 1$, the induced measure μ_1 is supported on the set Ω_N of pure states only and coincides with the Fubini–Study measure, so formula (31) with $\mu = \mu_1$ reduces to the standard definition (2) of the pure-state numerical shadow.

7. Large *N* limit and random matrices

It is instructive to analyse the numerical shadow of a random matrix in the limit of large matrix dimension N. Let us consider two cases of the problem: the shadow of a random density matrix σ generated according to the induced measures [28] and the shadow of random unitary matrix U distributed with respect to the Haar measure on $U(N)$.

The numerical shadow of the random matrix which is distributed with unitarily invariant measure is related to the distribution of its arbitrary diagonal element in a fixed basis. In this section, we consider the measures induced by partial trace and the Haar measure on the unitary group, which are unitarily invariant. Let us begin with the following.

Lemma 9. *Let A be a random square matrix of dimension N distributed according to a unitarily invariant measure. Let $|x\rangle$ be a random pure state of dimension N generated according to the Fubini–Study measure on $\Omega_N = \mathbb{C}P^{N-1}$. Then, the expectation value has the same distribution as the matrix element $A_{1,1}$:*

$$P(\langle x|A|x\rangle) = P(A_{1,1}). \tag{36}$$

Proof. Since $|x\rangle$ is a random pure state, $|x\rangle \sim U|0\rangle$, where $|0\rangle$ is an arbitrary fixed state while U is a random unitary matrix of dimension N. Now we write

$$P(\langle x|A|x\rangle) = P(\langle 0|U^{\dagger}AU|0\rangle) = P(A_{1,1}). \tag{37}$$

The last equality follows from invariance of the distribution $P(A)$ with respect to unitary transformations. □

7.1. Shadow of random quantum state

Consider a random density matrix σ of dimension N generated with respect to the Hilbert–Schmidt measure μ_{HS}, so that its eigenvalues λ_i are distributed according to equation (32) with $K = N$ [28]. The diagonal elements of σ are of the form

$$\sigma_{ii} = \frac{\sum_{j=i}^{N}\left(\xi_{ij}^2 + \eta_{ij}^2\right)}{\sum_{j,k=1}^{N}\left(\xi_{jk}^2 + \eta_{jk}^2\right)}, \tag{38}$$

where ξ_{ij} and η_{ij} are independent, identically distributed random variables with normal distribution $\mathcal{N}(0, 1)$. The basic properties of the Gamma distribution $\Gamma(a, b)$ [29] imply that

$$\sigma_{ii} = \frac{G_1}{G_1 + G_2}, \tag{39}$$

where G_1 and G_2 are stochastically independent variables distributed according to the Gamma distribution $\Gamma(N, 2)$ and $\Gamma(N(N-1), 2)$, respectively. Therefore, the diagonal elements of a random matrix σ generated according to the measure μ_{HS} are described by the Beta distribution with parameters $\{N, N(N-1)\}$.

The same reasoning can also be used for a general class of induced measures (32) parametrized by the dimension K of the auxiliary subsystem. In this case, the diagonal elements of a density matrix $\sigma \in \mathcal{Q}_N$ generated with respect to the measure $\mu_{N,K}$ are distributed according to the Beta distribution with parameters $\{K, K(N-1)\}$.

Using the above reasoning and lemma 9, we get the following.

Proposition 10. *The numerical shadow of a random matrix σ generated with respect to the induced measure $\mu_{N,K}$ is given by the Beta distribution with parameters $\{K, K(N-1)\}$, which can be expressed in terms of the Beta function*

$$P_{\sigma}(r) = \frac{1}{B(K, K(N-1))}(1-r)^{K-1}r^{K(N-1)-1}, \qquad 0 \leqslant r \leqslant 1. \tag{40}$$

7.2. Random unitary matrices

Let us now consider a random unitary matrix U distributed according to the Haar measure.

Proposition 11. *The numerical shadow of a Haar random unitary matrix is supported in the unit disc. This distribution is invariant with respect to rotations, and* $|\langle x|U|x\rangle|^2$ *is distributed according to the Beta distribution with parameters* $\{1, N-1\}$.

Proof. Random unitary matrix distributed with the Haar measure can be generated using the QR decomposition of matrices pertaining to the Ginibre ensemble [30]. The QR factorization can be realized by a Gram–Schmidt orthogonalization procedure. Then, the element $U_{1,1}$ of the generated unitary matrix reads

$$U_{1,1} = \frac{A_{1,1}}{\sqrt{\sum_{i=1}^{N} |A_{i,1}|^2}}, \tag{41}$$

where A is a non-Hermitian random matrix from the Ginibre ensemble. Therefore,

$$|U_{1,1}|^2 = \frac{\xi_{1,1}^2 + \eta_{1,1}^2}{\sum_{i=1}^{N}\left(\xi_{i,1}^2 + \eta_{i,1}^2\right)}, \tag{42}$$

where ξ_{ij} and η_{ij} are independent, identically distributed random variables with normal distribution $\mathcal{N}(0, 1)$. Thus, $|U_{1,1}|^2$ has the Beta distribution with parameters $\{1, N-1\}$ and using lemma 9, we arrive at the desired result. □

8. Concluding remarks

Our study may be briefly summarized by the following observation. The *numerical shadow* of a normal operator acting on $\mathcal{H}_N$ reflects the structure of the set of (mixed) classical states, which belong to the probability simplex Δ_{N-1}, while investigation of numerical shadows of *non-normal operators* provides information about the set $\mathcal{Q}_N$ of quantum states of dimension N.

In particular, we have shown that the set of orthogonal projections of the set $\mathcal{Q}_N$ of density matrices onto a two-plane is equivalent, up to shift and rescaling, to the set of all possible numerical ranges $W(A)$ of matrices of dimension N. The numerical shadow of A forms a probability distribution on the plane, supported in $W(A)$, which corresponds to the 'shadow' of the complex projective space $\mathbb{C}P^{N-1}$ covered uniformly according to the Fubini–Study measure, and projected onto the plane. Another probability distribution in $W(A)$ is obtained if one projects onto this plane the entire convex set $\mathcal{Q}_N$ of density matrices. If this set is covered uniformly with respect to the Hilbert–Schmidt (Euclidean) measure, an explicit expression for this distribution is derived. In this way, the analysis of numerical ranges and numerical shadows of matrices of a fixed dimension N contributes to our understanding of the intricate geometry of the set $\mathcal{Q}_N$ of quantum states [2].

The numerical range [31] and its generalizations [32, 16] found several applications in various problems of quantum information theory. In analogy to the *product numerical range*, defined for spaces with a tensor product structure [33], one can introduce the numerical shadow restricted to the subset of separable (product) states or the set of maximally entangled states [12]. Analysing such restricted numerical shadows for operators of a composite dimension NM, one may thus investigate the geometry of the selected set of separable (maximally entangled) quantum pure states. Such an approach is advocated in a forthcoming publication [34].

Acknowledgments

The authors thank G Auburn and S Weis for fruitful discussions. Work by J Holbrook was supported in part by an NSERC of Canada research grant. Work by P Gawron was supported by the Polish Ministry of Science and Higher Education (MNiSW) under the grant no N519 442339, JAM was supported by MNiSW under the project no IP2010 052270, ZP was supported by MNiSW under the project no IP2010 033470, while KŻ acknowledges support by MNiSW grant number N202 090239. They would also like to thank S Opozda for his help with the preparation of 3D models.

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