Optimal classical and quantum real and complex dimension witness

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We find the minimal number of independent preparations and measurements certifying the dimension of a classical or quantum system limited to d states, optionally reduced to the real subspace. As a dimension certificate, we use the linear independence tested by a determinant. We find the sets of preparations and measurements that maximize the chance to detect larger space if the extra contribution is very small. We discuss the practical application of the test to certify the space logical operations on a quantum computer.

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I. INTRODUCTION

Few-state systems have become standard building blocks in current classical and quantum technologies. In particular two-state (bit) classical logic is the base of computers and information transfer. Qubits (quantum two-state systems) are basic logical elements of quantum computers. To increase the quality of classical and quantum computation and communication, these systems need precise certification. For instance, the contribution of external states to qubit operations can lead to systematic errors, accumulating in long operation circuits and difficult to correct.

To certify that the number of classical or quantum states is limited, one can use a dimension witness (the dimension is the number of states). The usual construction of the witness is based on a two-stage protocol, the initial preparation and final measurement [1], which are taken from several respective possibilities and are independent of each other. Importantly, the preparation phase must be completed before the start of the measurement. Such early witnesses were based on linear inequalities, tested experimentally [2–5], but they could not detect, e.g., small contributions from other states. In the latter case, it would be better to use a nonlinear witness [6]. A completely robust witness must be based on equality, i.e., a quantity which is exactly zero up to a certain dimension and can be nonzero above [7,8].

A good witness test is the linear independence of the specific outcome probability p(y|x) for the preparation x and measurement y by a suitable determinant [7,8]. In previous works, a witness of dimension d needed 2k preparations and k measurements, with $d \le k$ for the classical system and $d^2 \le k$ for the quantum system. Equality-based tests, like the Sorkin equality [9] in the three-slit experiment [10–12] testing Born's rule [13], belong to a family of precision tests of quantum

mechanics, benchmarking our trust in fundamental quantum models and their actual realizations.

Here we show that the number of preparations can be reduced to k + 1, preserving the properties of the witness, i.e., being zero for $k \ge d$, (d+1)d/2, d^2 for classical, real, and complex quantum systems, respectively. The real quantum system is described by a Hilbert subspace of only real vectors, which occur, e.g., when the Hamiltonian is purely imaginary and the unitary operations become real rotations in real space [14]. The witness is essentially a determinant of the matrix with entries p(y|x) and an extra row of ones. The construction of the witness allowed us to analyze both its extremal violation by additional states and minimal deviations. The extremal examples for a bit, trit, or qubit can be described in the hybrid analytical-numerical form, while only the numerical form can be used for qutrits and higher dimensions. This analysis should help us to estimate the bounds in practical tests of the dimension and in the effort to eliminate parasitic states.

II. DIMENSION CERTIFICATE

We consider the standard prepare and measure scenario with a binary (yes or no or 1 or 0) outcome (Fig. 1). The state is prepared in one of *m* possibilities represented by Hermitian matrices $0 \leq \hat{X}_1, \ldots, \hat{X}_m$, $\operatorname{Tr} \hat{X}_j = 1$. The probability of the measurement of an outcome of 1 (yes) is applied out of kpossibilities $p(y_i|x_j) \equiv p_{ij} = \text{Tr}\hat{Y}_i\hat{X}_k$ for the measurement operators $0 \leq \hat{Y}_1, \dots, \hat{Y}_k \leq \hat{1}$. If the system is classical, with d states, then $p_{ij} = \sum_{a} q_{ia}r_{aj}$, with a = 1, ..., d and r describing the transfer probabilities from the prepared state to the classical *d*-dimensional register, while *q* is the transfer probability from the register to the measurement outcome. The quantum states and measurements can be either real or fully complex. The real register of a *d*-level quantum state consists of (d + 1)d/2 Gell-Mann basis matrices with all zeros except a single 1 on the diagonal or a symmetric off-diagonal pair of two 1's, and the complex register is enlarged by (d-1)d/2antisymmetric matrices with entries (i, -i).

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FIG. 1. Preparation and measurement scenario; the state is prepared as x and measured by y to give an outcome of either 1 or 0.

Main theorem. Suppose a witness of dimension d, $W(\{p_{ii}\})$, is always equal to zero for a system of dimension \leq d. Then the minimal number of measurements is $k = d^2$ and k = (d + 1)d/2 in the complex and real spaces, respectively, while the minimal number of prepared states is m = k + 1.

Proof. We set $k = d^2$ and k = (d + 1)/2 in the complex and real spaces, respectively. Then each operator \hat{Y}_i has k independent entries, while \hat{X}_j has k-1 independent entries (the trace is 1). If either the number of measurements is k' < k or the number of preparations is m < k + 1, then the number of all p_{ij} is k'm, and the dimension of available space is not smaller, either k'k or m(k-1), meaning that p_{ij} are essentially independent.

On the other hand, setting m = k + 1 and $\hat{Y}_{k+1} = \hat{1}$ (the auxiliary always-yes measurement, which is actually not performed, meaning $p_{k+1,j} = 1$ to get a $(k+1) \times (k+1)$ matrix of p_{ij} , we can define the witness

$$W_k = \det p. \tag{1}$$

Note that the determinant can be reduced to a $k \times k$ matrix without changing its value, subtracting, e.g., the last column from each previous one, i.e.,

$$p_{ij} \to p_{ij} - p_{i,k+1},\tag{2}$$

to make it equivalent to the previous one, with all odd preparations being identical [7]. In our way, the number of preparations is reduced from 2k to k + 1. Nevertheless, the original $(k + 1) \times (k + 1)$ form is better suited for the analysis of the extremal cases. Now, $W_k = 0$ for $d \leq k$ classically, $(d+1)d/2 \leq k$ in the real quantum case, and $d^2 \leq k$ in the complex quantum case. The determinant is a sum of signed products of permuted elements of every column. This means that the given column or row can occur only once in a single product. Therefore, whenever the prepared state \hat{X}_i is a convex combination of pure states, the determinant is also a convex combination of the cases with \hat{X}_i replaced by the pure states. Looking for the extreme case, one can reduce the search to pure states. For the measurement \hat{Y}_i the situation is a bit different; the search can be reduced to projections but not necessarily to one dimension. Because of the always-yes measurement, it suffices to consider the maximal dimension of the projection space up to d/2.

III. MAXIMAL NONZERO VALUE

The relevant question about the dimension witness is how nonzero it is, which allows determining whether the system has the desired dimension. First of all, there always exists a classical maximum, by linearity obtained for p_{ij} equal to 0 or 1, known as the Hadamard determinant. The general upper bound is $(k+1)^{(k+1)/2}/2^k$ but is not reached for particularly low values of k, for which the maximum can be found using

TABLE I. The classical maximum of W_k equivalent to a maximal determinant of the $k \times k$ matrix with entries of 0 or 1.

k	1	2	3	4	5	6	7	8	9
maxW _k	1	1	2	3	5	9	32	56	144

algebraic methods [15–17], as summarized in Table I. Second, for a classical system, the maximum is achieved immediately when d > k, taking the initial classical state m = 1, $r_{m1} = 1$ and 0 otherwise, and $q_{im} = p_{ij}$ for a given p (a maximal example is given in Table II). Third, the above classical maximum is also obtained for a quantum state with d > k, using analogous reasoning. The nontrivial bounds are for a quantum system such that $d^2 > k \ge d$. Due to the antisymmetry of the determinant, the bounds are always symmetric.

A special case is k + 1 = (d + 1)d/2 and $k + 1 = d^2$ for real and complex quantum states of dimension d, respectively. In these cases the determinant can be written as a product of determinants of separate square matrices for the preparations \hat{X}_i and measurements \hat{Y}_i so that (a) the maximum can be determined separately for x and y and (b) the same maximum is reached if either preparations or measurements are rotated by an arbitrary orthogonal (unitary) matrix in the real (complex) case, i.e., $\hat{X}_i \to \hat{R}\hat{X}_i\hat{R}^T$ or $\hat{X}_i \to \hat{U}\hat{X}_i\hat{U}^{\dagger}$. The maximum $W_2 = (3/4)^{3/2} \simeq 0.65$ in both real and com-

plex qubit space is reached by

$$\mathbf{x}_{1} = (0, 0, 1),$$

$$\mathbf{x}_{2} = (\sqrt{3}/2, 0, -1/2),$$

$$\mathbf{x}_{3} = (-\sqrt{3}/2, 0, -1/2)$$

$$(3)$$

(i.e., the vertices of the equilateral triangle) and $y_1 = (0, 0, 1)$, y = (1, 0, 0) using the Bloch sphere notation

$$2\hat{Y} = \hat{1} + \mathbf{y} \cdot \hat{\boldsymbol{\sigma}}, \ 2\hat{X} = \hat{1} + \mathbf{x} \cdot \hat{\boldsymbol{\sigma}}, \tag{4}$$

with $|\mathbf{y}| = |\mathbf{x}| = 1$; standard Pauli matrices $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$, where $\hat{\sigma}_1 = |1\rangle\langle 2| + |2\rangle\langle 1|$, $\hat{\sigma}_2 = i|2\rangle\langle 1| - i|1\rangle\langle 2|$, and $\hat{\sigma}_3 = i|2\rangle\langle 1| - i|1\rangle\langle 2|$ $|1\rangle\langle 1| - |2\rangle\langle 2|$; and $\hat{1} = |1\rangle\langle 1| + |2\rangle\langle 2|$.

For a complex qubit, the maximum $W_3 = 2\sqrt{3}/9 \simeq 0.38$ is achieved for

$$y_{1} = (1, 0, 0), y_{2} = (0, 1, 0), y_{3} = (0, 0, 1),$$

$$x_{1} = (1, 1, 1)/\sqrt{3},$$

$$x_{2} = (1, -1, -1)/\sqrt{3},$$

$$x_{3} = (-1, -1, 1)/\sqrt{3},$$

$$x_{4} = (-1, 1, -1)/\sqrt{3},$$

(5)

i.e., axes for y and the vertices of the regular tetrahedron for *x*.

For higher k and d, the search for the maximum of the determinant-based dimension witness becomes an arduous task if tackled only from the analytic point of view, although it is always some algebraic number. That is why we shall resort to numerical computations in order to maximize the determinant of the corresponding $(k + 1) \times (k + 1)$ matrix. Therefore, approximate or heuristic methods are required in

TABLE II. Binary matrices $(k + 1) \times (k + 1)$ (without the last row of 1's) with the maximal W_k given in Table I. They reduce to a $k \times k$
determinant; for example, the last (not shown) row is subtracted from those rows with 1 in the first column, reversing the sign of those rows.

(1	0),	$\begin{pmatrix} 1\\ 0 \end{pmatrix}$	0 1	0) 0)), (1 0 0	0 1 0	0 0 1	$\begin{pmatrix} 1\\1\\1 \end{pmatrix}$,	$\begin{pmatrix} 1\\ 0\\ 0\\ 0 \\ 0 \end{pmatrix}$	0 1 0 0	0 0 1 0	0 0 0 1	$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$,		0 1 0 0 0	0 0 1 0 0	1 1 1 1 0	1 1 0 1	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$
		$\begin{pmatrix} 1\\0\\0\\1\\0\\1 \end{pmatrix}$	1	1 1 0 0 1 0	0 1 1 0 0 1	1 0 1 1 0 0	0 1 0 1 1 0	0 0 1 1 1 1	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$	$ \begin{array}{c} \begin{pmatrix} 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1\\ 1 \end{array} $	0 1 0 1 0 1 0	1 0 1 1 0 0	0 0 1 1 0 0 1	1 1 0 0 0 0	0 1 0 0 1 0 1	$ \begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{array} $	$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$,			
	$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$	0 1 1 0 0 1 0	$ \begin{array}{c} 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 1 \end{array} $	$ \begin{array}{c} 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{array} $	0 0 1 0 1 1 1 0	1 0 0 1 0 1 1 1	1 0 0 1 0 1	() 1 () () 1 () 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$), ($\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	$ \begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{array} $	0 1 0 0 0 0 1 0 1	0 0 1 0 0 1 0 1 0 0 1 0 0 1	0 0 0 0 1 1 1 0 1 0 1 0 1 0 1 0		0 1 0 1 1 0 1 0	$ \begin{array}{c} 1 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{array} $	$ \begin{array}{c} 1\\ 1\\ 1\\ 1\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\$	

practice to find the optimal states. The most successful statistical method to date, the one we employ, is the stochastic model of *simulated annealing* [18], that is, the Metropolis Monte Carlo algorithm with a fixed temperature T at each state of the annealing schedule. Other methods exist which are not of a statistical nature, such as the downhill or amoeba or gradient methods [19], which involve finite differences when considering the corresponding function in terms of all real variables involved.

The optimization is taken over the states x_1, \ldots, x_{k+1} and measurements y_1, \ldots, y_k , which are real or complex unit vectors in \mathbb{R}^d and \mathbb{C}^d , depending on the particular instance (e.g., d = 2 refers to qubits, d = 3 corresponds to qutrits, and so on). For d = 4, 5 we add a second set of vectors y'_1, \ldots, y'_k (and a third one, y'', for d = 6) and Gram-Schmidt orthogonalize it to y, covering all possible dimensions of the projection space in a single run. With a proper parametrization, the problem consists of finding the supremum of the determinant (1). Initially, the temperature is set to the high value T_0 , which implies that the domain of possible values for the variables Ω is broadly spread. Finishing one cycle means visiting all the variables in Ω one after the other. After that, we compute W_k , which is the cost function. Then, the cycle starts anew with a different temperature T_1 (we choose the temperature to decrease as $T_{s+1} = r T_s$, r = 1/4, with s being the number of runs). As the temperature drops, the domain Ω_s continuously decreases until we reach the desired precision $(10^{-9} \text{ in our case})$; that is, the algorithm terminates when some stopping criterion is met. The details of the algorithms, their use, and the results are given in Appendix A.

The numerical results are presented in Table III. We found a few remarkable features: (i) The maximum needs the maximal dimension of the projection space, i.e., 2 for d = 4, 5and 3 for d = 6. (ii) For d close to k, the real and complex cases give the same maximum, so that the witness cannot distinguish them. (iii) For some maxima the corresponding states and measurements are surprisingly regular (e.g., heptagonal symmetry for k = 7, d = 5 in the complex case), and the maximum is rational, while others are almost completely irregular (e.g. k = 5, d = 3 complex). (iv) The value increases with d but not always with k.

IV. DETECTION OF HIGHER DIMENSION

The most practical application of the determinant-based witness is the diagnostic test of a finite-dimensional quantum system. Suppose the system is designed to be a perfect *d*-level state and we want to check it with high accuracy. A possible contribution from an imaginary part (for a real state) or a higher level (a complex state) is expected to be small, so even a small nonzero value of W_k would detect this. Making a decomposition,

$$\hat{Y}_{i} = \hat{Y}_{i}^{0} + \delta \hat{Y}_{i}, \ \hat{X}_{j} = \hat{X}_{j}^{0} + \delta \hat{X}_{j}, \tag{6}$$

with \hat{Y}^0 and \hat{X}^0 restricted to a *d*-dimensional Hilbert space (real or complex) and only (small) deviations $\delta \hat{Y}$ and $\delta \hat{X}$ in the imaginary or higher-dimensional states. To detect higher (imaginary) states one must use the witness for $k \ge (d^2 + d)/2$ (real case) or $k \ge d^2$ (complex case) because lower *k* will give a nonzero value even for clean *d* levels. The Jacobi identity implies in the lowest perturbative order

$$W_k \simeq \operatorname{Tr}(\delta p \operatorname{Adj} p^0),$$
 (7)

where Adj *p* is the adjoint matrix of $p_{ij}^0 = \text{Tr}\hat{Y}_i^0\hat{X}_j^0$ and $\delta p_{ij} = \text{Tr}\delta\hat{Y}_i\delta\hat{X}_j$. For k > (d+1)d/2 or $k > d^2$ all the minors in the zeroth order are zero, so the optimal choice is k = (d+1)d/2, d^2 . Moreover, as stressed earlier for this particular *k*, the values of the minors do not depend on the basis of *x* or *y*. To maximize the witness with respect to a potential higher-space contribution one has to maximize the minors. In particular, if a single preparation and measurement are suspected, we simply maximize the corresponding minor, taking the determinant with $k \to k - 1$ whose maximum we have already discussed.

The practical application of the test requires *N* repetitions of $k^2 + k$ experiments for all values of *i* and *j*, with $p_{ij} \rightarrow N_{ij}/N$ for N_{ij} positive results. Assuming independence between experiments, the variance of W_k in the null case (a perfect *d*-level state) can then be estimated as

$$N\langle W_k^2 \rangle \simeq \sum_{ij} p_{ij} (1 - p_{ij}) (\text{Adj } p)_{ji}^2.$$
(8)

k	2r	2c	3r	3c	4r	4c	5r	5c	6r	6c
1	1									
2	0.65		1							
3	0	0.38	0.84		2					
4	0	0	0.60	0.63	1.87		3			
5	0	0	0.42	0.46	1.78		3.14		6	
6	0	0	0	0.33	1.61	1.68	3.40		5.04	
7	0	0	0	0.23	1.41	1.64	3.51	3.72	6.05	6.18
8	0	0	0	0.15	1.30	1.47	3.65	3.79	7.49	7.50
9	0	0	0	0	1.29	1.39	3.77	3.84	10.14	10.34

TABLE III. The quantum maximum of W_k for the $(k + 1) \times (k + 1)$ matrix for a *d*-dimensional system, either real (r) or complex (c). An empty cell means the value is the nearest number to the left in the row.

For large *N* this equation allows us to estimate how perfect the qubit (or any *d*-dimensional system) is. For d = 2 (complex), we numerically found the constraint $\langle W_4^2 \rangle \leq 1/6N$, saturated by preparations and measurements given by

$$\mathbf{x}_{1} = \mathbf{x}_{2} = (0, 0, -1), \ \mathbf{x}_{3} = (2\sqrt{2}/3, 0, 1/3),$$

$$\mathbf{x}_{4,5} = (-\sqrt{2}/3, \pm \sqrt{2/3}, 1/3),$$

$$\mathbf{y}_{1} = (0, 0, 1), \ \mathbf{y}_{2} = (1, 0, 0),$$

$$\mathbf{y}_{3,4} = (-1/2, \pm \sqrt{3}/2, 0),$$
(9)

using the notation (4). If the measured deviation squared is of the order of the variance, then we cannot claim the higher state contribution. For larger W_k formula (7) will reveal the estimated magnitude of the deviation. As a side remark, this protocol applies also classically for k = d to test contributions from higher classical states.

Generalization of the above protocol to higher k is possible but more complicated. For instance, if $k = d^2 + 1$ or d(d + 1)/2, the deviation is of higher order,

$$W_k = \sum_{ij,i'j'} \operatorname{sgn}(j'-j) \delta p_{ij} \delta p_{i'j'} M_{jj',ii'} (-1)^{i+j+i'+j'}, \quad (10)$$

where i < i', $j \neq j'$, and $M_{jj',ii'}$ is the minor obtained by removing columns *i*, *i'* and rows *j*, *j'*. On the other hand, the variance in the null case (qubit) is

$$N^2 \langle W_k^2 \rangle \simeq \sum_{ij,i'j'} p_{ij} p_{i'j'} (1 - p_{ij}) (1 - p_{i'j'}) M_{jj',ii'}^2.$$
(11)

Equation (11) shows that detection of nonzero W_k for a given number of repetitions N for $k = d^2 + 1$ or d(d + 1)/2 + 1 has the same confidence level as for d^2 and d(d + 1)/2 for small deviations δp .

As examples, for a qubit or qutrit we can take pure states $\hat{X}_{j}^{0} = |x_{j}\rangle\langle x_{j}|$ and $\hat{Y}_{i}^{0} = |y_{i}\rangle\langle y_{i}|$, and the smallest deviations should have the forms $\delta\hat{X}_{j} = |x'_{j}\rangle\langle x_{j}| + |x_{j}\rangle\langle x'_{j}|$ and $\delta\hat{Y}_{i} = |y'_{i}\rangle\langle y_{i}| + |x_{i}\rangle\langle y'_{i}|$ with some small vectors $|x'_{j}\rangle$ and $|y'_{i}\rangle$ being either just purely imaginary (for a real-state test) or in higher-level space (for a complex-state test). Let us consider a test of a qubit $\hat{X}_{i}^{0} = \hat{Y}_{i}^{0}$ defined by (4) with

$$\mathbf{x}_1 = -\mathbf{x}_2 = (1, 0, 0), \ \mathbf{x}_3 = (0, 1, 0), \mathbf{x}_4 = (0, 0, 1) = -\mathbf{x}_5,$$
 (12)

which gives

$$4W_4 = \sum_{i=1,2} (\delta p_{i1} + \delta p_{i2} - \delta p_{i4} - \delta p_{i5})$$
(13)

and $\langle W_4^2 \rangle \simeq 1/16N$. Certainly, our proposal does not exclude other choices, and the potential higher-level contributions can occur in different operations. One should remember that the test can only falsify the assumed dimension since obtaining $W_k = 0$ (within the error bounds) can happen in an accidental configuration.

V. DISCUSSION

An equality-based dimension witness with an optimal number states and measurements can help in efficient diagnostics of the working Hilbert space of supposed quantum systems. Deviations from zero can reveal the influence of parasitic states. By testing various sets of preparations, one should quantify them and take measures to eliminate them. The witness can be generalized to various suboptimal configurations, e.g., combinations of more preparations and/or measurements. In any case, the applicability of this scheme can depend on the actual physical system and conjectured contributions from extra states. Even more generally, the witness can, in principle, test any dimension-limited subalgebra of the Hilbert space. At high dimensions, it becomes problematic to find maximal W_k , which is essential to estimate the sensitivity of the witness to extra space contributions.

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APPENDIX A: NUMERICAL SEARCH FOR THE MAXIMUM

Our basic algorithm to find the maximum of W_k (1) is as follows:

- 1 initial set of states $\{x_i\}$ and observables $\{y_i\}$ given
- 2 $T \leftarrow T_0$

3 repeat until stopping criterion is met

4	repeat (k, d) times	
5	orientate all unit vectors	
6	move to the next term within the set	
7	endrepeat	
8	set the matrix p	
9	compute W_k	
10	$T_{s+1} \leftarrow r T_s$	
11	endrepeat	
12	return the supremum of W_k	(A1)

The number of updates (k, d) depends on the way the states are parametrized (k is the number of x_i states, and d is their dimension)

In order to illustrate the dynamics of the numerical analysis we shall reproduce the numerics of the case k = 4 and a ququart (a four-level system, d = 4) for two cases, namely, \hat{Y}_j are (i) only one-dimensional projections $|y_j\rangle\langle y_j|$ and (ii) two-dimensional projections $|y_j^{(1)}\rangle\langle y_j^{(1)}| + |y_j^{(2)}\rangle\langle y_j^{(2)}|$. In this last case, $|y_j^{(1)}\rangle$ and $|y_j^{(2)}\rangle$ ought to be orthogonal, so we must implement a Gram-Schmidt orthogonalization process. In both instances, we must maximize the absolute value of the determinant of the matrix p_{ij} with $p_{ij} = \langle x_i | \hat{Y}_j | x_i \rangle$ for i < 5and $p_{5j} = 1$

In principle, for d = 4 the general parametrization for a complex ray x_i requires $2 \times 4 = 8$ real numbers, which reduce to 6 after normalization and a global phase, which is irrelevant for the computation of p_{ij} . However, this number can be lowered a bit further after some rotations (unitary operations). Thus, we shall have

$$\begin{aligned} x_1 &= [1, 0, 0, 0], \\ x_2 &= [\cos A(1), \sin A(1), 0, 0], \\ x_3 &= [\cos A(2) \cos A(3), e^{iA(4)} \sin A(2) \cos A(3), \\ &\sin A(3), 0], \\ x_4 &= [\sin A(5) \sin A(6) \cos A(7), \\ &e^{iA(8)} \sin A(5) \sin A(6) \sin A(7), \\ &e^{iA(9)} \sin A(5) \cos A(6), \cos A(5)], \\ x_5 &= [\sin A(10) \sin A(11) \cos A(12), \\ &e^{iA(13)} \sin A(10) \sin A(11) \sin A(12), \\ &e^{iA(14)} \sin A(10) \cos A(11), \\ &e^{iA(15)} \cos A(10)]. \end{aligned}$$

The additional $\{y_1, y_2, y_3, y_4\}$ follow the general expression of state x_5 in (A2), adding a total of 39 angles, such that $A(j) \in [0, 2\pi)$ for j = 1-39. Similarly, for the case of two projectors, we have a total of 63 angles, that is, $A(j) \in [0, 2\pi)$ for j = 1-63.

In Fig. 2 we depict the evolution of the value of $|W_k|$ versus each individual determinant evaluation over the set of $A(j) \in [0, 2\pi)$, j = 1-39 angles. The evolution of $|W_k|$ is bounded from above by the value 0.936442615, which, upon identification of the corresponding states $\{x_i, y_j\}$, easily leads to



FIG. 2. Plot of the evolution of the maximum determinant for k = 5, d = 4 and one projector for the measurement during the simulated annealing computation. See text for details.

the analytic result $W_k = 2^{11}/3^7$. Likewise, the evolution of the value of $|W_k|$ for the case of two projectors is shown in Fig. 3, returning the maximum value $W_k = 2^{12}/3^7 \simeq 1.87288523$.

Other instances are tackled exactly in the same vein, changing only the number of variables, which requires further computational effort.

APPENDIX B: SPECIAL CASES WITH THE HALF-ANALYTIC REPRESENTATION

For k = 2 and k = 3 and a qubit we can use the Bloch representation (4), writing

$$p_{ij} = (1 + \mathbf{y}_i \cdot \mathbf{x}_j)/2, \tag{B1}$$

so by a quick algebra we get

$$W_2 = [(\mathbf{x}_1 - \mathbf{x}_3) \times (\mathbf{x}_2 - \mathbf{x}_3)] \cdot (\mathbf{y}_1 \times \mathbf{y}_2)/4,$$
(B2)
$$W_3 = [\mathbf{x}_1 - \mathbf{x}_4, \mathbf{x}_2 - \mathbf{x}_4, \mathbf{x}_3 - \mathbf{x}_4][\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3]/8,$$



FIG. 3. Plot of the evolution of the maximum determinant for k = 5, d = 4 and two projectors for the measurement during the simulated annealing computation. See text for details.

where $[a, b, c] = a \cdot (b \times c)$ is the mixed product. Now with $|x_j| = |y_i| = 1$ we quickly find that the maximum is achieved if y_i are the two or three axes while $|(x_1 - x_3) \times (x_2 - x_3)|/2$ is the area of the triangle and $[x_1 - x_4, x_2 - x_4, x_3 - x_4]/6$ is the volume of the tetrahedron with vertices x_j . To get the largest volume, the triangle (tetrahedron) inscribed in a circle (sphere) of radius 1 must be regular. A simple argument is that the area (volume) can always be increased by moving an apex to the diameter perpendicular to the opposite side (face), making the edges adjacent to the apex equal.

For other cases we can guess the partial symmetry of the states and measurement configurations.

For k = 3 and a qutrit, the optimal case (real and complex) is

$$|x_{j}\rangle = a\cos\frac{2\pi j}{3}|1\rangle + a\sin\frac{2\pi j}{3}|2\rangle) + b|3\rangle,$$

$$|y_{j}\rangle = q\cos\frac{2\pi j}{3}|1\rangle + q\sin\frac{2\pi j}{3}|2\rangle + r|3\rangle$$
(B3)

for j = 1, 2, 3, and $|x_4\rangle = |3\rangle$, with $a^2 + b^2 = q^2 + r^2 = 1$, gives $W_3 = (27/32)(4br + aq)^2(3q^2 - 2)a^4q^2$. The naive choice a = q = 1 gives 27/32, but the actual maximum 0.8447648009582842 = 1.0012 × 27/32 is higher for a = 0.993819, q = 0.996329.

For k = 4 and a real qutrit, we take

$$\begin{aligned} |x_1\rangle &= |1\rangle, \\ |x_{2,3}\rangle &= \frac{-|1\rangle \pm \sqrt{3}|2\rangle}{2}, \ |x_{4,5}\rangle = \frac{-|1\rangle \pm \sqrt{3}|3\rangle}{2}, \\ |y_{1,2}\rangle &= a|1\rangle \pm b|2\rangle, \ |y_{3,4}\rangle = q|1\rangle \pm r|3\rangle, \end{aligned}$$
(B4)

with $a^2 + b^2 = q^2 + r^2 = 1$, aq = 1/2. Then, $W_4 = 27\sqrt{5/4 - z}(7/4 - z)/8$ for $z = a^2 + q^2$. From maximization we get z = 9/8 and $W_4 = 27\sqrt{2}/64 \simeq 0.5966213466261494$.

When searching for the maximum for a complex qutrit, the numerical analysis shows that the maximal case lies in a particular subset of all possibilities given by projection onto

$$\begin{aligned} |x_{j}\rangle &= a|1\rangle + b\omega^{j}|2\rangle + c\omega^{2j}|3\rangle, \ |x_{4}\rangle &= |1\rangle, \ |x_{5}\rangle = |2\rangle, \\ |y_{j}\rangle &= q|1\rangle + \omega^{j}r|2\rangle + \omega^{2j}s|3\rangle, \ |y_{4}\rangle &= |1\rangle \end{aligned} \tag{B5}$$

for j = 1, 2, 3, with $a, b, c, p, q, r \in [-1, 1], a^2 + b^2 + c^2 = q^2 + r^2 + s^2 = 1$. Then

det
$$p = 27c^2(s^2 - r^2)(aqbr + brcs + csaq)^2$$
, (B6)

and maximizing over two spheres gives approximately 0.6319201017558774. For a ququart (a four-level system) the maximum is larger, and we can distinguish two cases, \hat{Y} , as only one-dimensional projections and up to two-dimensional projections. In both cases we take

$$\sqrt{3}|x_j\rangle = \sqrt{3}|y_1\rangle = \pm |1\rangle \pm |2\rangle \pm |3\rangle$$
 (B7)

for j = 1, 2, 3, 4, taking the cases with an even number of minus signs (again, vertices of a regular tetrahedron) and $|x_5\rangle = |4\rangle$. Then for $\hat{Y}_j = |y_j\rangle\langle y_j|$ we get det $= 2^{11}/3^7 \simeq 0.94$, while for $\hat{Y}_j = |y_j\rangle\langle y_j| + |4\rangle\langle 4|$ we get $W_4 = 2^{12}/3^7 \simeq 1.872885230909922$.

For k = 5, we can maximize det with a real qutrit, with x and y being in the independent bases, with

$$|x_{3a+b}\rangle = [|a\rangle + (-1)^b \phi |a+1\rangle]/\sqrt{\phi+2}$$
 (B8)

for a = 0, 1, 2 and $0 \equiv 3, b = 1, 2$, and the golden ratio $\phi = (1 + \sqrt{5})/2$, i.e., (pairs of) vertices of a regular icosahedron, while

$$|y_j\rangle = \alpha[\cos(2\pi j/5)|1\rangle + \sin(2\pi j/5)|2\rangle] + \sqrt{1 - \alpha^2}|3\rangle.$$
(B9)

We have to maximize $(t - 1)(3t - 2)t^3$, $\alpha = t^2$, which has the derivative $t^2(15t^2 - 20t + 6)$ with the nontrivial roots $t = (10 \pm \sqrt{10})/15$. The larger $W_5 = (25 + 34\sqrt{10})2^5/5^33^4 \simeq 0.4188205525198219$ is for +.

A complex qutrit gives a larger maximum 0.457413503 in the real 10-parameter family of vectors

$$|y_{1}\rangle = |1\rangle, |x_{j}\rangle = a_{j}|1\rangle + b_{j}|2\rangle,$$

$$|x_{34}\rangle = f|1\rangle + g|2\rangle \pm h|3\rangle,$$

$$|x_{56}\rangle = f'|1\rangle + g'|2\rangle \pm ih'|3\rangle,$$

$$|y_{23}\rangle = q|1\rangle + r|2\rangle \pm s|3\rangle,$$

$$|y_{45}\rangle = q'|1\rangle + r'|2\rangle \pm is'|3\rangle$$

(B10)

for j = 1, 2, with $a_j^2 + b_j^2 = f^2 + g^2 + h^2 = q^2 + r^2 + s^2 = f'^2 + g'^2 + h'^2 = q'^2 + r'^2 + s'^2$ (two circles and four spheres).

For a ququart, the maximum is found for two-dimensional \hat{Y}_i (real and complex). We take

$$|x_{12}\rangle = a|1\rangle \pm b|3\rangle,$$

$$|x_{34}\rangle = a|3\rangle \pm b|4\rangle),$$

$$|x_{56}\rangle = (|2\rangle \pm |4\rangle)/\sqrt{2},$$

(B11)

and $\hat{Y}_j = |y_j\rangle\langle y_j| + |y'_j\rangle\langle y'_j|,$

$$|y_1\rangle = |y_2\rangle = (|1\rangle + |2\rangle)/\sqrt{2}, |y_3\rangle = |1\rangle,$$

$$|y_{45}\rangle = s|2\rangle \pm c|4\rangle,$$

$$|y'_{12}\rangle = (|3\rangle \pm |4\rangle)/\sqrt{2},$$

$$|y'_{345}\rangle = |3\rangle,$$

(B12)

with $a^2 = (5 + \sqrt{5})/10$, $b^2 = (5 - \sqrt{5})/10$, and $c = \cos(\pi/5) = (1 + \sqrt{5})/4$, $s = \sin(\pi/5) = \sqrt{(5 - \sqrt{5})/8}$. Then

$$W_5 = (1 + 1/\sqrt{5})^{5/2}/\sqrt{2} \simeq 1.78162618305857.$$
 (B13)

For a real and complex ququint (d = 5) and the case of single projections $\hat{Y}_j = |y_j\rangle \langle y_j|$, we take the vertices of a 5-cell (a generalization of a tetrahedron in four dimensions) in space 1234

$$|x_{1}\rangle = |4\rangle, |x_{6}\rangle = |5\rangle,$$

$$|x_{2}\rangle = [\sqrt{5}(|1\rangle + |2\rangle + |3\rangle) - |4\rangle]/4,$$

$$|x_{3}\rangle = [\sqrt{5}(|1\rangle - |2\rangle - |3\rangle) - |4\rangle]/4,$$

$$|x_{4}\rangle = [\sqrt{5}(|2\rangle - |3\rangle - |1\rangle) - |4\rangle]/4,$$

$$|x_{5}\rangle = [\sqrt{5}(|3\rangle - |1\rangle - |2\rangle) - |4\rangle]/4,$$
 (B14)

and $|y_j\rangle = |x_j\rangle$, giving $W_5 = 5^5 3^4 / 2^{18}$.

The case of double projections $\hat{Y}_j = |y_j\rangle \langle y_j| + |y'_j\rangle \langle y'_j|$ for

$$|x_{j}\rangle = a|1\rangle + \cos\frac{2\pi j}{3}b|2\rangle + \sin\frac{2\pi j}{3}b|3\rangle,$$

$$|y_{j}\rangle = q|1\rangle - \cos\frac{2\pi}{3}r|2\rangle - \sin\frac{2\pi j}{3}r|3\rangle,$$

$$|y_{j}'\rangle = \sin\frac{2\pi j}{3}|2\rangle - \cos\frac{2\pi j}{3}|3\rangle,$$

$$|x_{4}\rangle = |y_{4}\rangle = |4\rangle, |x_{5}\rangle = |y_{5}\rangle = |5\rangle,$$

$$|x_{6}\rangle = |y_{4}'\rangle = |y_{5}'\rangle = |1\rangle$$

(B15)

for j = 1, 2, 3, with $a^2 + b^2 = q^2 + r^2 = 1$. Then $W_5 = (27/32)b^4q^2(2+q^2)(4ar+bq)^2$. Maximizing with respect to *b* at constant *c* and *a* gives the condition

$$c^{2} = \frac{(8 - 12b^{2})^{2}}{(8 - 12b^{2})^{2} + 9b^{2}(1 - b^{2})}.$$
 (B16)

Inserting it into the formula, we get

$$W_5 = \frac{6^4 b^6 (3b^2 - 2)^2 (32 - 93b^2 + 69b^4)}{(64 - 183b^2 + 135b^4)^3},$$
 (B17)

whose maximum 3.144615108566082 is for the largest root of

$$2048 - 12032b^2 + 26409b^4 - 25668b^6 + 9315b^8 = 0.$$
(B18)

For k = 6, 7 and d = 3 the complex case gives the respective maxima 0.330364646,0.225213334. For k = 6 and d = 4 in the real and complex cases we got 1.61439616 and 1.68093981, respectively, with two-dimensional \hat{Y} . For d = 5 in the real case we get 3.39847186, and the complex case is the same. In this case the maximum is realized for

$$|x_{12}\rangle = a|1\rangle \pm b|2\rangle,$$

$$|x_{34}\rangle = a|1\rangle \pm b|3\rangle,$$

$$|x_{56}\rangle = a|1\rangle \pm b|4\rangle,$$

$$|x_7\rangle = |5\rangle,$$

(B19)

with $a^2 + b^2 = 1$, while $\hat{Y}_i = |y_i\rangle\langle y_i| + |y'_i\rangle\langle y'_i|$, with

$$|y_{12}\rangle = c|1\rangle \pm d|1\rangle, |y'_{12}\rangle = |3\rangle,$$

$$|y_{34}\rangle = c|1\rangle \pm d|3\rangle, |y'_{34}\rangle = |4\rangle,$$

$$|y_{56}\rangle = c|1\rangle \pm d|4\rangle, |y'_{56}\rangle = |2\rangle,$$

(B20)

with $c^2 + d^2 = 1$ giving $W_6 = 512a^3b^7c^3d^3[3a^2c^2 + (1 + d^2)b^2](c^2 + d^4)$. The maximum is 3.3984718576415207 for *a* being the root of the equation,

$$0 = -1 + 5a^{2} + 24a^{4} - 296a^{6} + 1480a^{8} - 5088a^{10} + 11392a^{12} - 14336a^{14} + 8192a^{16},$$
(B21)

 $a^2 = 0.3016492773799042$. For d = 6 we get the same maximum in the real and complex case for states

$$|x_1\rangle = a|1\rangle + b|2\rangle, |x_{23}\rangle = a|1\rangle + \frac{b}{2}(-|2\rangle \pm \sqrt{3}|2\rangle),$$
$$|x_4\rangle = a|1\rangle + b|4\rangle, |x_{56}\rangle = a|1\rangle + \frac{b}{2}(-|4\rangle \pm \sqrt{3}|5\rangle),$$
$$|x_7\rangle = |6\rangle,$$
(B22)

while
$$\hat{Y}_{j} = |y_{j}\rangle\langle y_{j}| + |y_{j}'\rangle\langle y_{j}'| + |6\rangle\langle 6|$$
, with
 $|y_{1}\rangle = |3\rangle, |y_{23} = |3\rangle/2 \pm \sqrt{3}|2\rangle/2,$ (B23)
 $|y_{4}\rangle = |5\rangle, |y_{23} = |5\rangle/2 \pm \sqrt{3}|4\rangle/2,$
 $|y_{1}'\rangle = c|1\rangle + d|2\rangle, |y_{23}'\rangle = c|1\rangle + \frac{d}{2}(-|2\rangle \pm \sqrt{3}|2\rangle),$
 $|y_{4}'\rangle = c|1\rangle + d|4\rangle, |y_{56}'\rangle = c|1\rangle + \frac{d}{2}(-|4\rangle \pm \sqrt{3}|5\rangle)$

for $a^2 + b^2 = c^2 + d^2 = 1$, giving

$$W_{6} = \frac{3^{6}}{2^{10}}b^{6}c^{2}(1+d^{2})(2+c^{2}+2a^{2}-5a^{2}c^{2})$$
$$\times [c^{4}+98a^{2}d^{2}(c^{2}-a^{2})-2a^{2}c^{2}+a^{4}+343a^{4}d^{2}$$
$$-16abc^{3}d-16a^{3}bcd(17d^{2}-1)], \qquad (B24)$$

giving the numerical maximum 5.0467662420644475.

For k = 7 and d = 4 in the real and complex cases, we get $W_7 = 1.41149223$ and 1.63898287, respectively (twodimensional \hat{Y}). For d = 5 in the real and complex cases (two-dimensional \hat{Y}) we get 3.50557203 and $7^7/2^{13}3^3 =$ 3.723338939525463, respectively. In the latter case the states read $|x_8\rangle = |5\rangle$, while the rest are, in the basis $|1\rangle$, $|2\rangle$, $|3\rangle$, $|4\rangle$,

$$\begin{aligned} |x_{j}\rangle &= \frac{\hat{U}^{j}}{2} \begin{pmatrix} 1\\1\\1\\1 \end{pmatrix}, \quad \hat{U} = \begin{pmatrix} 1 & 0 & 0 & 0\\0 & \zeta & 0 & 0\\0 & 0 & \zeta^{2} & 0\\0 & 0 & 0 & \zeta^{4} \end{pmatrix}, \\ \hat{Y}_{j} &= \hat{U}^{j} \begin{pmatrix} 1/2 & \xi & \xi & \xi\\-\xi & 1/2 & \xi & -\xi\\-\xi & -\xi & 1/2 & \xi\\-\xi & \xi & -\xi & 1/2 \end{pmatrix} \hat{U}^{\dagger j} \end{aligned} (B25)$$

for $\zeta = \exp(2\pi i/7)$ and $\xi = i/2\sqrt{3}$. Then, due to the Gauss identity

$$1 + 2(\zeta + \zeta^2 + \zeta^4) = i\sqrt{7}$$
 (B26)

we obtain

$$|\langle x_i | x_j \rangle|^2 = \begin{cases} 1 & \text{for } i = j, \\ 1/8 & \text{for } i \neq j \text{ and } i, j < 8, \\ 0 & \text{otherwise,} \end{cases}$$
(B27)

 $\operatorname{Tr} \hat{Y}_j \hat{Y}_i = 5/6 \text{ for } i \neq j, \text{ and }$

$$p_{ji} = \langle x_i | \hat{Y}_j | x_i \rangle$$

$$= \begin{cases} 1 & \text{for } j = 8, \\ 0 & \text{for } i = 8 \text{ and } j < 8, \\ 1/2 & \text{for } i = j < 8, \\ \frac{1}{2} + \frac{\sqrt{7}}{4\sqrt{3}} & \text{for } i, j < 8 \text{ and } j - i = 1, 2, 4 \text{ mod } 7, \\ \frac{1}{2} - \frac{\sqrt{7}}{4\sqrt{3}} & \text{otherwise.} \end{cases}$$

(B28)

For d = 6 in the real and complex cases, we get 6.05145518 and 6.17876168.

We can maximize W_8 with a complex qutrit with x and y with optimal x,

$$|x_{3a+b}\rangle = (|a\rangle + e^{i\alpha_a}\omega^b |a+1\rangle)/\sqrt{2}$$
(B29)

for $\omega = e^{2\pi i/3} = (i\sqrt{3} - 1)/2$, a = 0, 1, 2, b = 1, 2, 3, and $|0\rangle \equiv |3\rangle$ with free angles α_a , and optimal *y*,

$$|y_j\rangle = \sqrt{5/6}|y'_j\rangle + \sqrt{1/6}|3\rangle, \tag{B30}$$

with y'_i defined in $|1\rangle$, $|2\rangle$ space,

$$|y'_{j}\rangle = i\sqrt{1/3}|1\rangle + \omega^{j}\sqrt{2/3}|2\rangle \tag{B31}$$

for $j = 1, 2, 3, |y'_4\rangle = |1\rangle$, and $|y'_{j+4}\rangle = -|y'_j\rangle$. Then the maximum is $W_8 = 5^5/3^4 2^8 \simeq 0.1507040895061728$.

For d = 4 in the real and complex cases, $W_8 = 1.2962761$ and 1.47025989, while for d = 5 in the real and complex cases $W_8 = 3.64938453$ and 3.79495481 and for d = 6 in the real and complex cases 7.48985655 and 7.49786979, respectively.

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The next nontrivial case is k = 9, which discriminates between a qutrit and ququart. For instance, taking $\hat{Y}_{j-1} = \hat{X}_j$ with

$$|x_{j}\rangle = |j\rangle, \ j = 1-4,$$

$$2|x_{j}\rangle = \sum_{m=1}^{4} i^{mj} |m\rangle, \ j = 5-8,$$

$$2|x_{9}\rangle = |1\rangle + |2\rangle - |3\rangle - 4\rangle,$$

$$2|x_{10}\rangle = |1\rangle - |2\rangle - |3\rangle + |4\rangle,$$
(B32)

we get $W_9 = 1/8$. However, the numerical maximum for d = 4 is $W_9 = 1.28868526$ and 1.39037781 for the real and complex cases, respectively. For d = 5 we get, respectively, 3.76568067 and 3.83579182, and for d = 6, we get 10.1361814 and 10.3359304.

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