Generating pseudo-random quantum states: On the overparametrized method

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The numerical generation of pseudo-random quantum states is an important procedure for investigations in quantum information science. In general, this endeavor requires from the beginning some kind of parametrization for the density matrices. The overparametrized method can be used to create pseudo-random positive semidefinite matrices with unit trace from pseudo-randomly produced general complex matrices in a simple way that is friendly for numerical implementations. In this article we first discuss a relevant issue related to the possible domains that may be used for the real and imaginary parts of the elements of such general complex matrices. Afterwards the problem of a too fast concentration of measure in the quantum state space that appears in this parametrization is reported. Our results show that care must be taken when using this method and also that it is not in general a sensible choice if one wants a reasonably fair sampling in the space of density matrices.

I. INTRODUCTION

About three decades ago Paul Benioff, Richard Feynman, and others scientists [1–4] envisaged a computer whose basic constituents could be in a complex quantum superposition state. In the last few years we have been witnessing astonishing theoretical and experimental developments in quantum computing and quantum simulation [5–7], and also in others subareas of quantum information science [8–11], with experimental implementations already going beyond the best present classical capabilities [12]. These are the first sights of what will turn out to be a revolution in our science and technology [13, 14]. Nevertheless, before that can in fact becomes a reality, we still have much to understand concerning quantum systems with many degrees of freedom. One important tool for accomplishing this task is the generation of pseudo-random quantum states (pRQS) [15–24], which will have an analogous role to that that pseudo-random numbers have in classical stochastic theories [25–28]. The parametrization of quantum states [15, 29, 30] is the initial step towards generating them numerically and is the main topic of this article.

In the next subsections we briefly review two such parametrizations, the standard method and the overparametrized method (OPM), and comment on how they can be used to generate pRQS numerically. The remainder of the article is dedicated to investigate some issues regarding the OPM. In Sec. II we discuss unwanted physical consequences of the ranges used in the literature so far for the real and imaginary parts of the elements of the general complex matrices involved in this method and present a simple solution for this problem. In Sec. III we report an important drawback of the OPM regarding its use for random sampling in the quantum state space: its too fast concentration of measure. A summary of the article is presented in Sec. IV.

A. The standard method for generating pseudo-random quantum states

The states of a $d$–level quantum system are described, in the most general scenario, by a density matrix $\rho$ [31, 32], which is a positive semidefinite matrix (notation: $\rho \geq 0$) with unit trace ($\text{Tr}(\rho) = 1$). Any such matrix can be written in the form of a spectral decomposition:

$$
\rho = \sum_{j=1}^{d} r_j |r_j\rangle\langle r_j|,
$$

with the real eigenvalues of $\rho$ being nonnegative ($r_j \geq 0$ for all $j = 1,\cdots,d$) and summing up to one ($\sum_{j=1}^{d} r_j = 1$). That is to say, $\{r_j\}_{j=1}^{d}$ is a probability distribution [25, 28]. The eigenvectors of $\rho$, $\{|r_j\rangle\}_{j=1}^{d}$, form an orthonormal basis for the vector space $\mathbb{C}^d$, i.e., $\langle r_j | r_k \rangle = \delta_{jk}$ and $\sum_{j=1}^{d} |r_j\rangle\langle r_j| = I_d$, where $I_d$ is the $d \times d$ identity matrix. Here we use the standard notation of Dirac for vectors and, for a generic matrix $A$, we denote $A^\dagger$ as its adjoint (conjugate transpose). Thus the row matrix $|r_j\rangle$ is the conjugate transpose of the column matrix $\langle r_j|$.

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Let us look over the number of real parameters needed for a complete description of an arbitrary density matrix. In order to describe the probability distribution \( \{ r_j \}_{j=1}^d \), the eigenvalues of \( \rho \), we need \( d - 1 \) real numbers. Besides, as any two bases for the vector space \( \mathbb{C}^d \) are connected by an unitary matrix \( U \) (i.e., \( UU^\dagger = \mathbb{I}_d \)), one can write

\[
|r_j\rangle = U|c_j\rangle,
\]

for \( j = 1, \ldots, d \), with \( \{|c_j\rangle\}_{j=1}^d \) being the standard computational basis. Therefore the bases \( \{|r_j\rangle\}_{j=1}^d \) is completely determined by \( U \). Once \( d^2 \) real parameters are needed to specify completely an arbitrary unitary matrix \( U \) with dimensions \( dxd \), it follows that \( d^2 + d - 1 \) real parameters are sufficient for a thorough description of any density matrix.

From the last two paragraphs, we see that the numerical generation of a pRQS (using the density matrix as written in Eq. (1)) can be cast in terms of the creation of a pseudo-random discrete probability distribution (pRDPD) [30, 33] and of a pseudo-random unitary matrix (pRU) [29, 34–36]. More details about numerical implementations of pRDPDs can be found in Ref. [37]. From the several possibilities available, in this article we choose the Hurwitz parametrization for generating pRUs. For a comprehensive exposition of this method see Ref. [35]. It is worthwhile observing that this approach for generating pRQS is used here as a benchmark for our analysis of the OPM, that shall be introduced in the next subsection and will be studied in the remainder of the article.

### B. The overparametrized method

The basic motivational idea for this method comes from the simple observation that, for any complex matrix \( A = (A_{jk}) \), we have: \( \langle \psi | A^\dagger A | \psi \rangle = ||A|\psi||^2 = |||\phi|||^2 \geq 0 \), where \( |\psi\rangle \) is any vector of \( \mathbb{C}^d \) and \( |||\phi||| := \sqrt{\langle \phi | \phi \rangle} \) is the Euclidean norm of the vector \( |\phi\rangle \in \mathbb{C}^d \). That is to say, for a general complex matrix \( A \), the matrix \( A^\dagger A \) is guaranteed to be positive semidefinite (\( A^\dagger A \geq 0 \)). Thus, if \( A \) is normalized, i.e., if we define

\[
A := \frac{A}{||A||_2},
\]

it is possible to write a valid density operator as:

\[
\rho = A^\dagger A.
\]

Above \( ||A||_2 := \sqrt{\langle A | A \rangle} \) is the Hilbert-Schmidt norm of \( A \), with \( \langle A | B \rangle := \text{Tr}(A^\dagger B) \) being the Hilbert-Schmidt inner product between the matrices \( A \) and \( B \) [32].

The simple formula for \( \rho \) in Eq. (4) has found some applications in quantum information science [15, 30]. Once the complete description of a general complex \( dxd \) matrix \( A \) requires \( 2d^2 \) real parameters, one notes that this parametrization, despite being simple and friendly for numerical implementations, uses more real numbers than needed. Thus it is dubbed as the overparametrized method. The numerical generation of pRQS via this method is further explained in the next section.

### II. AN ISSUE REGARDING THE DOMAINS OF \( \text{Re}(A_{jk}) \) AND \( \text{Im}(A_{jk}) \)

Let us start our analysis of the production of pRQS via the overparametrized method by considering the simplest quantum system, a two-level system also known as quantum bit, or qubit for short. The advantage of using this system as our starting point is that it can be visualized in the \( \mathbb{R}^3 \). For that purpose we simply need to write a density operator \( \rho \) using the 2x2 identity matrix \( \mathbb{I}_2 \) and the Pauli matrices \( \sigma_j \) (\( j = 1, 2, 3 \)) as a basis:

\[
\rho = 2^{-1} \left( \mathbb{I}_2 + \sum_{j=1}^3 x_j \sigma_j \right),
\]

where \( x_j = \text{Tr}(\rho \sigma_j) \) is the value of the component of the system’s “polarization” in the direction \( j = 1, 2, 3 \equiv x, y, z \). The real numbers \( (x_1, x_2, x_3) \equiv (x, y, z) \) are used as the Cartesian coordinates in \( \mathbb{R}^3 \). Enforcing the \( \rho \) in Eq. (5) to be a density matrix leads to the following restrictions: \(-1 \leq x_j \leq 1 \) and \( \sum_{j=1}^3 x_j^2 \leq 1 \). Therefore the points \( (x_1, x_2, x_3) \) must be in a ball with radius equal to one and centered in \((0, 0, 0)\), known as the Bloch’s ball (BB).

There are several functions one may be interested in when working in quantum information science. Some relevant examples are quantum state tomography [38], quantum discord [39], quantum coherence [40, 41], and quantum channel capacities [42]. All of these quantities can, in general, be defined using distance measures in the
quantum state space (the vector space formed by density matrices). For our purposes in this article, the Hilbert-Schmidt distance (HSD) fits well. The HSD between two density matrices $\rho$ and $\zeta$ is defined as the Hilbert-Schmidt norm of their subtraction \cite{31,32}:

$$d_{hs}(\rho, \zeta) := \|\rho - \zeta\|_2. \quad (6)$$

If $\lambda_j$ are the real eigenvalues of the Hermitian matrix $\rho - \zeta$, then

$$d_{hs}(\rho, \zeta) = \sqrt{\text{Tr}((\rho - \zeta)^\dagger(\rho - \zeta))} = \sqrt{\sum_{j=1}^{d} \lambda_j^2}. \quad (7)$$

For the calculations involved in this article, the Mersenne Twister method \cite{43} is used as the pseudo-random number generator (pRNG) and the LAPACK subroutines \cite{44} are utilized for computing eigenvalues. With these tools at hand, when the standard method described in Sec. I A is applied for generating one-qubit pRQS, the distribution of such states in the Bloch’s ball and the histogram for the probability of the possible values of HSD are those shown in the upper green panel of Fig. 1. It is worth mentioning that the higher density of states observed closer to the center of
this figure can be understood by noticing that the direction in \( \mathbb{R}^3 \) defined by \( U \) is random and that \( r_1 \) and \( r_2 = 1 - r_1 \) are uniformly distributed in the interval \([0, 1]\).

Let us consider the same kind of calculation, but applying now the overparametrized method for generating the pRQS. For that purpose the pRNG can be utilized for the sake of obtaining pRNs for generating the real,

\[
\text{Re}(A_{jk}) =: A_{jk}^r,
\]

and imaginary,

\[
\text{Im}(A_{jk}) =: A_{jk}^i,
\]

parts of the matrix elements of \( A = (A_{jk}) \). The first issue we want to deal with here is with regard to the domains that one may use for those numbers. For instance, we can follow Refs. [15] and [30] and generate the matrix elements \( A_{jk} \) using

\[
A_{jk}^r, A_{jk}^i \in [0, 1].
\]

As shown at the right hand side of the gray panel at the middle of Fig. 1, the probability distribution for the HSD obtained in this way is, to some extent, qualitatively similar to that obtained using the standard method. This may lead to the impression that our choice for the domain of the matrix elements is fine. However, a rapid inspection of the distribution of states in the Bloch’s ball obtained using the OPM with \( A_{jk}^r, A_{jk}^i \in [0, 1] \) reveals a misfortune. Even though the polarization in the \( y \) and \( z \) directions have approximately equal chance to be positive or negative, only positive values for the polarization in the \( x \) direction are generated.

We notice that a simple solution for this problem is generating the matrix elements \( A_{jk} \) with

\[
A_{jk}^r, A_{jk}^i \in [-1, 1].
\]

With this change, for this case, the distribution of states in the BB becomes even more uniform than that that we get using the standard method, as shown in the pink panel at the bottom of Fig. 1. We want to emphasize already at this point that increasing the range of values for \( A_{jk}^r \) and \( A_{jk}^i \) does not causes any significant modification of the results that shall reported in the next section.

\section*{III. TOO FAST CONCENTRATION OF MEASURE IN THE OVERPARAMETERIZED METHOD}

In the previous section we showed that the application of the OPM with the real and imaginary parts of \( A_{jk} \) generated in the interval \([-1, 1]\) yields an uniform distribution of one-qubit pseudo-random density matrices. This encouraging result leads naturally to the question of if such a scheme can be applied successfully also for high-dimensional quantum systems. In this section we investigate this question answering it in the negative.

It is known for some time now that, in high-dimensional spaces, random variables tend to concentrate around their mean values [45]. In the last few years, this phenomenon of concentration of measure, that is formalized in Levy’s Lemma, has gained great importance and utility in quantum information science (see for instance Ref. [46] and references therein).

Notwithstanding, as shown in the gray panel at the bottom of Fig. 2, the OPM leads to a too fast concentration of measure for the HSD in the quantum state space as the system’s dimension \( d \) increases. Note that such a concentration of measure is much more slow in our benchmarking method: the standard method with the Hurwitz’s parametrization for unitary matrices. It is worth mentioning that, in part, the shift in the probability distribution for the HSD observed with the standard method (upper green panel in Fig. 2) can be understood as being due to the fact that as \( d \) increases the same number of points will be spread in a bigger space, diminishing thus the chance for closer pairs of configurations to be generated.

\section*{IV. CONCLUDING REMARKS}

In this article we studied the numerical generation of pseudo-random quantum states with particular emphasis on the overparametrized method. After using a qubit system to identify and solve a problem related to the domains of the matrix elements used so far in the literature in implementations of the OPM, we considered its possible application for high-dimensional quantum systems. In this last scenario, we showed the OPM is not an appropriate choice since it leads to a too rapid concentration of measure that will prevent any fair random sampling of states even for quantum systems with moderate dimension. An interesting problem that remains for future investigations is with regard to the possible explanation of these numerical results in a more visual-analytical manner.
Figure 2: (color online) Probability distribution for the different possible values of the Hilbert-Schmidt distance for one million pairs of quantum states generated using the standard method (green panel above) or generated via the overparametrized method with $A^i_{jk}, A^j_{ik} \in [-1,1]$ (gray panel below). We see that, in contrast to what happens in the standard method, there is a too fast concentration of measure in the OPM as the system’s dimension $d$ increases. We observe that although only even values of $d$ are shown in this figure, the mentioned effect is smooth and gradual.

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[1] P. Benioff, The computer as a physical system: A microscopic quantum mechanical hamiltonian model of computers as represented by Turing machines, J. Stat. Phys. 22, 563 (1980).
[44] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, *LAPACK Users’ Guide*, 3rd Ed. (Society for Industrial and Applied Mathematics, Philadelphia, 1999).

[45] M. Ledoux, The concentration of measure phenomenon, Mathematical Surveys and Monographs of the American Mathematical Society **89** (2001).

[46] P. Hayden, Concentration of measure effects in quantum information, Proceedings of Symposia in Applied Mathematics **68**, 3 (2010).