

Supplementary Document for the article:
“Multi-stage tomography based on eigenanalysis
for high-dimensional dense unitary processes
in gate-based quantum computers”

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Abstract

This Supplementary Document contains additional information for the associated article defined in its title.

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1 Connections between our QPT methods and classical signal processing

As stated in Section 1 of the associated paper, the type of QPT approaches proposed in this paper has connections with works that were previously reported in the classical domain. These connections may be defined as follows. QPT may be considered as the quantum version of so-called (classical) system identification [1]. The latter classical problem consists of estimating the parameter values of a transform from the input to

the output of a system. That system may have multiple inputs, so that it then performs a combination of them. In the classical framework, such a combination is called a mixture. The classical problem then considered in the literature is therefore also referred to as mixture identification and it especially includes blind mixture identification, or BMI [2–5]. This terminology should be used with care when also considering the quantum domain, because the above classical “mixtures” have nothing to do with the “statistical mixtures”, i.e. “mixed states”, faced in the quantum domain and used in our paper. Only considering previous works in the *classical* domain at this stage of our discussion, the above-mentioned BMI has a close relationship with source separation, especially including blind source separation, or BSS [3, 4, 6–10]. BSS does not focus on identifying the transform performed by the above, i.e. direct, system itself, but mainly on deriving an estimate of the inverse of that transform, so as to apply it to the outputs of the above direct system and to thus restore the unknown source signals that form the input of the direct system. This relationship between BMI and BSS even appears in the name of the well-known SOBI method [11], which stands for “Second-Order Blind Identification”, whereas it is claimed to be a BSS method. The term “Second-Order” here refers to the fact that this method applies to random signals and uses the statistical properties of the measured signals, more precisely their usual second-order statistical parameters that consist of their covariance matrices involving different time delays between signals.

So far, we especially discussed how SOBI-like methods and the methods proposed in the present paper are connected in terms of the nature of data processing problems that they address. These two types of methods also have relationships in terms of the approaches that they use to solve the considered problems. More precisely, in classical BSS/BMI, when the transform performed by the direct system is linear (and memoryless) and its identification is performed by using the above-mentioned second-order statistics of the output signals of the direct system, an equation similar to (A1) is obtained [5, 11–14]. That classical counterpart of the structure of (A1) was already exploited to perform classical BSS/BMI by means of several methods based on eigen-decomposition. The real-valued version of the basic structure of (A1) was first used in [5, 12] together with a required modified form of this equation (a related approach also appears in [14]). It was then extended in [11], by combining it with more than one modified form of this equation, to obtain a more robust method. Another version [13] aims at extending that type of approach from the standard case of stationary time-domain source signals to nonstationary time-domain sources. That version eventually uses complex-valued signals (whereas the mixing transform remains real-valued) because one moves to the Fourier domain.

2 Creating a mixed state that has a diagonal density matrix

The algorithm proposed in Section 2.1 of the associated paper uses an input density matrix ρ_1 that is diagonal. It should be noted that, when one considers that one is able to create a pure state, then, creating the type of state considered here is not a problem, as will now be shown. We here consider the approach initially used by von

Neumann in [15] to define a statistical mixture: such a state is expressed as being composed of a set of pure states, each of them being associated with a probability of occurrence. Then, to create experimental data corresponding to the state defined by the diagonal density matrix ρ_1 , one just has to repeatedly, randomly, select one of the pure states that form the considered basis of the state space, moreover selecting the k th basis state with a probability that is equal to the k th value on the diagonal of ρ_1 . This simplicity of implementation is worth noting because, in contrast, the authors of [16, 17] consider that using a mixed input state is too complex (maybe because they have non-diagonal density matrices in mind), so that they choose to restrict themselves to pure states, which has the drawback of requesting many such multiqubit input states, as opposed to only two multiqubit input states in the complete approach that we here start to describe (namely the mixed state with a density matrix ρ_1 considered here, and then the pure state $|\Psi_1\rangle$ in Section 2.2 of the associated paper. Beyond their relationship based on considering (A1), our approach and the one in [16] are therefore quite different.

3 A variant for the first part of single-stage QPT methods

We here again consider the first part of single-stage QPT methods. As in the variant that we proposed in Section 2.1 of the associated paper for that first part, we here use a mixed input state, represented by the density matrix ρ_1 . However, for the sake of generality, this matrix is here not any more constrained to be diagonal. It is still Hermitian and therefore unitarily diagonalizable. In the version considered here, as in Section 2.1 of the associated paper, we request all its eigenvalues to be different. That input density matrix ρ_1 is here requested to be known (i.e. fixed a priori or estimated from copies of that state, so that this variant is supervised or semi-supervised).

Using the same properties of eigendecomposition as in Section 2.1 of the associated paper, we consider all unitarily diagonalized forms of ρ_1 that have the following properties:

1. The eigenvalues are in a known order along the diagonal of ρ_1 . Without loss of generality, we hereafter consider the case when they are in decreasing order.
2. All eigenvectors have unit norm.

All these eigendecompositions of ρ_1 may be expressed as

$$\rho_1 = U_{I1} \rho_{I1D} U_{I1}^\dagger \quad (1)$$

where U_{I1} and ρ_{I1D} are respectively a unitary matrix and a diagonal matrix associated with that first input of the considered process.

Starting from a given ρ_1 , the first step of the algorithm proposed in the present section consists of determining one (arbitrary) of these decompositions (1) meeting the above-defined conditions. This is performed by 1) running an eigendecomposition algorithm, then 2) reordering the values in the matrix obtained for ρ_{I1D} if they are not directly provided in decreasing order by the considered eigendecomposition algorithm,

3) reordering the columns of the matrix obtained for U_{I1} accordingly and 4) dividing these columns by their norms if the considered practical eigendecomposition algorithm is not guaranteed to yield unit-norm vectors. Thus, we especially get a known value U_{I1} (which contains indeterminacies consisting of a phase factor separately for each of its columns). U_{I1} is used in the second part of this version of our algorithm: see Section 5 of the present document.

Besides, using (1), Equation (A1) may be expressed as

$$\rho_2 = U_g \rho_{I1D} U_g^\dagger \quad (2)$$

where the global unitary matrix

$$U_g = U U_{I1} \quad (3)$$

includes the effect of the eigendecomposition of ρ_1 , in addition to the considered process U .

Formally, (2) addresses exactly the same problem as in Section 2.1 of the associated paper (see (A1) with a diagonal ρ_1), but now with a diagonal input density matrix ρ_{I1D} and a process U_g (that is also unitary). We can therefore apply the algorithm and results of Section 2.1 of the associated paper to this reformulated problem, i.e., briefly, we diagonalize $\hat{\rho}_4$ and we then reorder the eigenvalues (in the same order as in ρ_{I1D}) and associated normalized eigenvectors. This guarantees that the algorithm of Section 2.1 of the associated paper here provides an estimate $\hat{U}_2$ that restores U_g up to a phase factor for each of its columns, with (A2) here replaced by

$$\hat{U}_2 = U_g D_\phi \quad (4)$$

$$= U U_{I1} D_\phi \quad (5)$$

where D_ϕ is again a diagonal matrix that contains unknown phase factors $e^{\phi_1}, \dots, e^{\phi_d}$ on its main diagonal.

As opposed to the basic version of the first step defined in Section 2.1 of the associated paper, the estimate $\hat{U}_2$ here contains the effect of U_{I1} in addition. The second part of the method must then be modified accordingly, as compared with its basic version defined in Section 2.2 of the associated paper. A solution to this problem is provided in Section 5 of the present document.

4 A variant for the second part of single-stage QPT methods

In the framework of single-stage QPT methods that include a first part as defined in Section 2.1 of the associated paper, we here again consider the associated second part, that aims at estimating the phase factors $e^{i\phi_1}, \dots, e^{i\phi_d}$, by using a second input state of the considered process. The method that we proposed in Section 2.2 of the associated paper for that second part uses a pure input state defined by a ket $|\Psi_1\rangle$. However, a mixed input state having a density matrix ρ_5 may be used instead, as will

now be shown. As $|\Psi_1\rangle$ in Section 2.2 of the associated paper, the input density matrix ρ_5 is here supposed to be initially known (supervised case) or estimated by using part of the available copies of that state (semi-supervised case).

The input state ρ_5 yields a state ρ_6 at the output of the considered process, and these two states have the same relationship as in (A1). In practice, what is available, thanks to QST, is an estimate $\hat{\rho}_8$ of ρ_6 , here again after it has been pre-processed, if required, so as to be Hermitian and to have unit trace. Thus, up to estimation errors, $\hat{\rho}_8$ meets the condition

$$\hat{\rho}_8 = U \rho_5 U^\dagger. \quad (6)$$

Then, knowing $\hat{\rho}_8$ and $\hat{U}_2$ obtained in the first part of our algorithm (see Section 2.1 of the associated paper), the next step of our algorithm here consists of combining them to form

$$\rho_9 = \hat{U}_2^\dagger \hat{\rho}_8 \hat{U}_2. \quad (7)$$

This may be seen as the extension, to a mixed state, of the quantity (A3) in the variant of the present method that uses a pure input state instead: for the latter type of state, $\hat{\rho}_8$ reduces to

$$\hat{\rho}_8 = |\hat{\Psi}_2\rangle\langle\hat{\Psi}_2| \quad (8)$$

and the state $|\Psi_3\rangle$ considered in Section 2.1 of the associated paper corresponds to $\rho_9 = |\Psi_3\rangle\langle\Psi_3|$. Combining the latter expression with (A3) and using (8), the resulting expression of ρ_9 is fully compatible with its extension (7) to an arbitrary mixed input state considered here.

Combining (6), (7) and (A2), with U unitary, yields

$$\rho_9 = D_\phi^* \rho_5 D_\phi. \quad (9)$$

This shows that a diagonal matrix ρ_5 cannot be used in this approach, because all three matrices in the right-hand term of (9) are then diagonal, so that D_ϕ^* and D_ϕ cancel out and (9) reduces to

$$\rho_9 = \rho_5 \quad (10)$$

and ρ_9 does not yield any information about the phase factors in D_ϕ . This is not surprising because all the information that can be extracted with a diagonal input density matrix was already extracted by using such a matrix in the first part of our algorithm (see Section 2.1 of the associated paper). We therefore consider a non-diagonal matrix ρ_5 hereafter.

Whatever the input density matrix ρ_5 , denoting ρ_{kl} its elements, (9) yields (again up to estimation errors)

$$\rho_9 = \begin{bmatrix} \rho_{11} & \rho_{12}e^{i(\phi_2-\phi_1)} & \dots & \rho_{1d}e^{i(\phi_d-\phi_1)} \\ \dots & & & \dots \end{bmatrix}. \quad (11)$$

Therefore, we consider a value of ρ_5 that is arbitrary except that all the elements of its first row are nonzero (this method may be adapted to the case when another row only has nonzero elements). The next step of our algorithm consists of computing the quantity

$$[\rho_9]_{1\bullet} \oslash [\rho_5]_{1\bullet}. \quad (12)$$

where $[\cdot]_{1\bullet}$ represents the row vector equal to the first row of the considered matrix (i.e. row 1 and all columns, or “columns $\bullet$ ”). Thanks to (11), we have

$$[\rho_9]_{1\bullet} \odot [\rho_5]_{1\bullet} = \left[1, e^{i(\phi_2 - \phi_1)}, \dots, e^{i(\phi_d - \phi_1)}\right] \quad (13)$$

and hence

$$\text{diag}([\rho_9]_{1\bullet} \odot [\rho_5]_{1\bullet})^* = e^{i\phi_1} D_\phi^*. \quad (14)$$

The next step of our algorithm therefore consists of computing

$$\hat{U}_5 = \hat{U}_2 \text{diag}([\rho_9]_{1\bullet} \odot [\rho_5]_{1\bullet})^* \quad (15)$$

$$= \hat{U}_2 \text{diag}\left(\left[\hat{U}_2^\dagger \hat{\rho}_8 \hat{U}_2\right]_{1\bullet} \odot [\rho_5]_{1\bullet}\right)^* \quad (16)$$

where (16) results from (7) and defines the complete processing performed in this second part of our algorithm, starting from the estimate $\hat{U}_2$ of U obtained in the first part of the algorithm and combining it with the density matrices ρ_5 and $\hat{\rho}_8$ used in that second part.

Combining (15), (14) and (A2) yields

$$\hat{U}_5 = e^{i\phi_1} U \quad (17)$$

i.e. $\hat{U}_5$ succeeds in restoring U (once again, up to a global phase factor that has no physical consequences and up to the estimation errors that were mentioned above but implicit in the above equations).

5 Another variant for the second part of single-stage QPT methods

In the framework of single-stage QPT methods, we here again consider the case when the first part is defined as in Section 3 of the present document. We present an associated solution for the second part of the method, using a pure input state defined by a ket $|\Psi_1\rangle$. $|\Psi_1\rangle$ is requested to be known, i.e. fixed a priori (supervised case) or estimated from a subset of its copies (semi-supervised case).

Starting with the same approach as in Section 2.2 of the associated paper, this here again yields the output ket estimate (A5). Our algorithm then computes $|\Psi_3\rangle$ defined by (A3), as in Section 2.2 of the associated paper, but now with $\hat{U}_2$ that meets (5). Combining (5) with (A3) and (A5) and considering that U is unitary (hence $U^\dagger U = I$), we get

$$|\Psi_3\rangle = e^{i\theta} D_\phi^* |\Psi_4\rangle \quad (18)$$

where we introduce

$$|\Psi_4\rangle = U_{I1}^\dagger |\Psi_1\rangle \quad (19)$$

which is a known quantity. Comparing (18) with (A6) shows that $|\Psi_4\rangle$ here replaces the ket $|\Psi_1\rangle$ used in the method of Section 2.2 of the associated paper (which is coherent with the fact that the latter method is a reduced form of the present one, for

the case when ρ_1 is diagonal and hence U_{I1} is the identity matrix). The remainder of the present method is then derived by modifying the end of the method of Section 2.2 of the associated paper accordingly: here using

$$\hat{U}_5 = \hat{U}_2 \text{diag}(|\Psi_3\rangle \otimes |\Psi_4\rangle) U_{I1}^\dagger \quad (20)$$

it may be shown in the same way as in Section 2.2 of the associated paper that we here again get (A7), i.e. $\hat{U}_5$ here again succeeds in restoring U , up to a global phase factor (and again up to estimation errors).

6 Pseudo-codes of the EQPT3 and EQPT4 two-stage QPT methods

The pseudo-codes of our EQPT3 and EQPT4 two-stage QPT methods are respectively provided in Algorithm 1 and Algorithm 2 of the present document.

7 Fluctuation model for density matrix estimation

In Section 5 of the associated paper, we presented the statistical model that we used in our tests to represent the fluctuations that may be faced when estimating a ket with a QST algorithm. We hereafter describe a corresponding model for the estimation of density matrices. Whereas we eventually apply it to mixed states, we first build it by considering a pure state, to make it compatible with the model used for ket estimation in Section 5 of the associated paper. We therefore consider a pure state represented by the density matrix

$$\rho = |\psi\rangle\langle\psi|. \quad (21)$$

Denoting c_k each actual component of $|\psi\rangle$ and ϵ_k the additive random complex-valued error made when estimating it, each actual element of the density matrix ρ reads

$$\rho_{k\ell} = c_k c_\ell^* \quad (22)$$

and its estimated version may be expressed as

$$\hat{\rho}_{k\ell} = (c_k + \epsilon_k)(c_\ell + \epsilon_\ell)^* \quad (23)$$

$$= c_k c_\ell^* + c_k \epsilon_\ell^* + \epsilon_k c_\ell^* + \epsilon_k \epsilon_\ell^*. \quad (24)$$

We aim at building an *approximation* of that quantity that, as with the “noisy ket model” of Section 5 of the associated paper, yields a noisy model of the density matrix that is expressed as the sum of the actual density matrix and of a term that represents fluctuations that are consistent with those of the random model used in Section 5 of the associated paper for kets. To this end, we first note that, in (24), the first term, namely $c_k c_\ell^*$, is nothing but the actual value (22), whereas all other terms are the random fluctuations. We aim at deriving an approximation of these terms, that only depends on 1) the actual value (22), 2) a single random variable ϵ_R for the real part

Input : a) Estimate $\hat{\rho}_4$ of output density matrix ρ_2 (provided by QST and obtained for input density matrix (A8) with the diagonal values defined in (A9)). b) Estimate $\hat{\rho}_8$ of output density matrix ρ_6 (provided by QST and obtained for input density matrix (A10) with the diagonal values defined in (A9)). c) Estimate $|\hat{\Psi}_2\rangle$ of output ket $|\Psi_2\rangle$ (provided by QST and obtained for all components of input ket $|\Psi_1\rangle$ equal to $1/\sqrt{d}$).

Output: Estimate $\hat{U}_5$ of quantum process matrix U .

```

begin
  /* Exploit  $\hat{\rho}_4$ : */
  Eigendecomposition: derive 1) a diagonal matrix  $D_4$  that contains the eigenvalues of  $\hat{\rho}_4$  in an
  arbitrary order and 2) a matrix  $V_4$  whose columns are eigenvectors of  $\hat{\rho}_4$  in the same order as
  eigenvalues;
  Reorder the eigenvalues in  $D_4$  in nonincreasing order and apply the same permutation to the
  columns of  $V_4$  to create the matrix  $\hat{U}_2$ ;
  /* Exploit  $\hat{\rho}_8$ : */
  Eigendecomposition: derive 1) a diagonal matrix  $D_8$  that contains the eigenvalues of  $\hat{\rho}_8$  in an
  arbitrary order and 2) a matrix  $V_8$  whose columns are eigenvectors of  $\hat{\rho}_8$  in the same order as
  eigenvalues;
  Reorder the eigenvalues in  $D_8$  in nonincreasing order and apply the same permutation to the
  columns of  $V_8$  to create the matrix  $\hat{U}_3$ ;
  /* Combine  $\hat{U}_2$  and  $\hat{U}_3$ : */
  for  $m_1 = 1$  to  $d_2$  do
    for  $m_2 = 1$  to  $d_2$  do
      Set column of  $\hat{U}_4$  with index equal to  $((m_1 - 1)d_1 + m_2)$ : Set it to first vector
      provided by CCA of 1) the set of columns of  $\hat{U}_2$  with indices  $((m_1 - 1)d_1 + n_1)$  with
       $n_1 \in \{1, \dots, d_1\}$  and 2) the set of columns of  $\hat{U}_3$  with indices  $((m_2 - 1)d_1 + n_2)$ 
      with  $n_2 \in \{1, \dots, d_1\}$ ;
      /* If the CCA tool does not provide unit-norm vectors, then do it: */
      Divide above column of  $\hat{U}_4$  by its norm;
    end
  end
  Find decomposition of  $\hat{U}_4$  as  $\hat{U}_4 = V\Sigma W^\dagger$  with SVD;
   $\hat{U}_{4u} = VW^\dagger$ ;
  /* Exploit  $|\hat{\Psi}_2\rangle$ : */
   $|\Psi_3\rangle = \hat{U}_{4u}^\dagger |\hat{\Psi}_2\rangle$ ;
   $\hat{U}_5 = \hat{U}_{4u} \text{diag}(|\Psi_3\rangle \otimes |\Psi_1\rangle)$ ;
end

```

Algorithm 1: EQPT3: third Eigenanalysis-based QPT algorithm (composed of two stages). This version is for the case when the QST algorithm provides estimates that meet the known properties of the actual quantities. Otherwise, see text.

of the fluctuations and 3) a single random variable ϵ_I for the imaginary part of the fluctuations.

As a simple approximation, we separately consider the real and imaginary parts of the fluctuations and then just add them in our final approximate model. The real part is handled as follows. The random variable ϵ_R takes both ϵ_k and ϵ_ℓ of (24) into account. Therefore, it represents an error for a ket component and it is drawn with the same statistics as the fluctuations of a ket component of Section 5 of the associated paper, i.e. it is real-valued and uniformly drawn over the range $[-w/2, w/2]$. In other words, to obtain a simple model, both ϵ_k and ϵ_ℓ are here replaced by ϵ_R in (24) (without taking their possible statistical independence into account). Then, to express this real-valued part of the fluctuation model only with respect to $\rho_{k\ell}$ in addition to ϵ_R , as explained above, we ignore the phases of c_k and c_ℓ^* in the second and third terms of (24) and we replace both of them with $\sqrt{|\rho_{k\ell}|}$, based on (22). The resulting

Input : a) Estimate $\hat{\rho}_4$ of output density matrix ρ_2 (provided by QST and obtained for input density matrix (A8) with the diagonal values defined in (A9)). b) Estimate $\hat{\rho}_8$ of output density matrix ρ_6 (provided by QST and obtained for input density matrix (A10) with the diagonal values defined in (A9)). c) Estimate $|\hat{\Psi}_2\rangle$ of output ket $|\Psi_2\rangle$ (provided by QST and obtained for all components of input ket $|\Psi_1\rangle$ equal to $1/\sqrt{d}$).

Output: Estimate $\hat{U}_5$ of quantum process matrix U .

```

begin
  /* Exploit  $\hat{\rho}_4$ : */
  Eigendecomposition: derive 1) a diagonal matrix  $D_4$  that contains the eigenvalues of  $\hat{\rho}_4$  in an
  arbitrary order and 2) a matrix  $V_4$  whose columns are eigenvectors of  $\hat{\rho}_4$  in the same order as
  eigenvalues;
  Reorder the eigenvalues in  $D_4$  in nonincreasing order and apply the same permutation to the
  columns of  $V_4$  to create the matrix  $\hat{U}_2$ ;
  /* Exploit  $\hat{\rho}_8$ : */
  Eigendecomposition: derive 1) a diagonal matrix  $D_8$  that contains the eigenvalues of  $\hat{\rho}_8$  in an
  arbitrary order and 2) a matrix  $V_8$  whose columns are eigenvectors of  $\hat{\rho}_8$  in the same order as
  eigenvalues;
  Reorder the eigenvalues in  $D_8$  in nonincreasing order and apply the same permutation to the
  columns of  $V_8$  to create the matrix  $\hat{U}_3$ ;
  /* Combine  $\hat{U}_2$  and  $\hat{U}_3$ : */
  for  $m_1 = 1$  to  $d_2$  do
    for  $m_2 = 1$  to  $d_2$  do
      Set column of  $\hat{U}_4$  with index equal to  $((m_1 - 1)d_1 + m_2)$ : Set it to first vector
      provided by CCA of 1) the set of columns of  $\hat{U}_2$  with indices  $((m_1 - 1)d_1 + n_1)$  with
       $n_1 \in \{1, \dots, d_1\}$  and 2) the set of columns of  $\hat{U}_3$  with indices  $((m_2 - 1)d_1 + n_2)$ 
      with  $n_2 \in \{1, \dots, d_1\}$ ;
      /* If the CCA tool does not provide unit-norm vectors, then do it: */
      Divide above column of  $\hat{U}_4$  by its norm;
    end
  end
  /* Exploit  $|\hat{\Psi}_2\rangle$ : */
   $|\Psi_3\rangle = \hat{U}_4^\dagger |\hat{\Psi}_2\rangle$ ;
   $\hat{U}_{5p} = \hat{U}_4 \text{diag}(|\Psi_3\rangle \otimes |\Psi_1\rangle)$ ;
  Find decomposition of  $\hat{U}_{5p}$  as  $\hat{U}_{5p} = V\Sigma W^\dagger$  with SVD;
   $\hat{U}_5 = V W^\dagger$ ;
end

```

Algorithm 2: EQPT4: fourth Eigenanalysis-based QPT algorithm (composed of two stages). This version is for the case when the QST algorithm provides estimates that meet the known properties of the actual quantities. Otherwise, see text.

approximate model for the real part of fluctuations, corresponding to the real part of the last three terms of (24), is thus equal to $2\sqrt{|\rho_{k\ell}|}\epsilon_R + \epsilon_R^2$.

As explained above, the imaginary part of fluctuations is handled in the same way and just added to the above real part. As an overall result, the complete approximate noisy model for any density matrix element reads

$$\hat{\rho}_{k\ell} = \rho_{k\ell} + 2\sqrt{|\rho_{k\ell}|}\epsilon_R + \epsilon_R^2 + i \left(2\sqrt{|\rho_{k\ell}|}\epsilon_I + \epsilon_I^2 \right). \quad (25)$$

We again stress that this model contains approximations but meets the required constraints: it allows one to create a “noisy” version $\hat{\rho}_{k\ell}$ of a given “noiseless” density matrix element $\rho_{k\ell}$ by just drawing a sample of each of the random variables ϵ_R and ϵ_I , whose statistics are defined in a way which is qualitatively consistent with those of the random variable used in Section 5 of the associated paper for deriving a “noisy” version of a ket component. This then mainly allows us to compare the

performance of several QPT methods with the *same* (relevant) fluctuation statistics. This qualitative relevance of our simplified model is thus sufficient for our needs. This is to be contrasted with, e.g., the situation when one would consider a given physical system and one would have to develop a model of it that is as accurate as possible.

Appendix A Copy of equations of the associated paper also used in this Supplementary Document

$$\rho_2 = U \rho_1 U^\dagger \quad (\text{A1})$$

$$\hat{U}_2 = U D_\phi. \quad (\text{A2})$$

$$|\Psi_3\rangle = \hat{U}_2^\dagger |\hat{\Psi}_2\rangle, \quad (\text{A3})$$

$$|\hat{\Psi}_2\rangle = e^{i\theta} |\Psi_2\rangle \quad (\text{A4})$$

$$= e^{i\theta} U |\Psi_1\rangle. \quad (\text{A5})$$

$$|\Psi_3\rangle = e^{i\theta} D_\phi^* |\Psi_1\rangle \quad (\text{A6})$$

$$\hat{U}_5 = e^{i\theta} U \quad (\text{A7})$$

$$\rho_1 = \begin{bmatrix} r_1 & 0 & \dots & & 0 \\ & \ddots & & & \\ & & r_1 & & \\ & & & r_2 & \\ & & & & \ddots \\ & & & & & r_2 \\ & & & & & & \ddots \\ & & & & & & & 0 \\ 0 & \dots & & & & & & r_{d_2} \end{bmatrix} \quad (\text{A8})$$

$$r_k = \frac{2(d_2 - k + 1)}{d(d_2 + 1)} \quad k \in \{1, \dots, d_2\}. \quad (\text{A9})$$

$$\rho_5 = \begin{bmatrix} r_1 & 0 & \dots & & 0 \\ & \ddots & & & \\ & & r_{d_2} & & \\ & & & r_1 & \\ & & & & \ddots \\ & & & & & r_{d_2} \\ & & & & & & \ddots \\ 0 & & & & & & & \ddots \end{bmatrix}. \quad (\text{A10})$$

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