Beyond the density operator and $Tr(\rho \hat{A})$: Exploiting the higher-order statistics of random-coefficient pure states for quantum information processing

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Two types of states are widely used in quantum mechanics, namely (deterministic-coefficient) pure states and statistical mixtures. A density operator can be associated with each of them. In this paper, we address a third type of states, that we previously introduced in a more restricted framework. These states generalize pure ones by replacing each of their deterministic ket coefficients by a random variable. We therefore call them Random-Coefficient Pure States, or RCPS. We here analyze their properties and their relationships with both types of usual states. We show that RCPS contain much richer information than the density operator and mean of observables that we associate with them. This occurs because the latter operator only exploits the second-order statistics of the random state coefficients, whereas their higher-order statistics contain additional information. That information can be accessed in practice with the multiple-preparation procedure that we propose for RCPS, by using second-order and higher-order statistics of associated random probabilities of measurement outcomes (we also discuss our single-preparation procedure). Exploiting these higher-order statistics opens the way to a very general approach for performing advanced quantum information processing tasks. We illustrate the relevance of this approach with a generic example, dealing with the estimation of parameters of a quantum process and thus related to quantum process tomography. This parameter estimation is performed in the non-blind (i.e. supervised) or blind (i.e. unsupervised) mode. For the considered type of measurements, we show that this problem cannot be solved by using only the density operator ρ of an RCPS and the associated mean value $Tr(\rho \hat{A})$ of the operator \hat{A} that corresponds to the considered physical quantity. In contrast, we succeed in solving this problem by exploiting a fourth-order statistical parameter of state coefficients, in addition to second-order statistics. Numerical tests validate this result and show that the proposed method yields accurate parameter estimation for the considered number of state preparations.

I. INTRODUCTION

Two types of states are widely used in quantum mechanics, namely pure states (with deterministic coefficients: see below) and mixed states, i.e. statistical mixtures, the latter being a superset of the former. Due to our needs for new classes of quantum information processing (QIP) methods, in [1] we introduced a third approach, based on the concept that we then called "random pure states", and that is hereafter more precisely referred to as Random-Coefficient Pure States and abbreviated as RCPS.

We previously used these RCPS to perform various QIP tasks based on blind adaptation/estimation, i.e. unsupervised quantum machine learning [2]. These tasks are Blind Quantum Source Separation (BQSS, introduced in [1]; see also e.g. [2–4]), Blind Quantum Process Tomography (BQPT, introduced in [5]; see also e.g. [6]), Blind Hamiltonian Parameter Estimation (BHPE, introduced in [2]) and other QIP tasks [2]. Beyond the above practical QIP methods, we started to investigate more fundamental aspects of RCPS in [7]: we showed how these states can be physically implemented and we briefly commented about their relationship with the concept of density operator. We addressed the latter topic in a much more detailed way very recently in [8]. This especially showed that, starting from an RCPS, one can associate a density operator with it.

In this paper, we proceed much further in the investigation of RCPS. In Section II, we first provide a general definition of these states, beyond their specific versions considered in our above-mentioned application-driven papers. We then analyze various features of these states and show their potential for QIP, as compared with more standard approaches. We especially explain how one may try to handle RCPS by adapting the standard practice in quantum mechanics, which is based on defining other states (namely mixed ones) by a density operator ρ and using the mean value $\text{Tr}(\rho \hat{A})$ of a physical quantity (i.e. observable) A represented by an operator \hat{A} . We prove that this standard approach does not allow one to access all the information that is present in an RCPS. That information can indeed be accessed, by using measurements and the associated statistics of the moduli of the random ket coefficients of that state. A major result of this paper is thus that certain QIP tasks cannot be carried out

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by only resorting to the standard approach to quantum mechanics, whereas they can be performed by exploiting the higher-order statistics of the random coefficients of an RCPS. In Section III, we illustrate this phenomenon with a generic example, dealing with non-blind or blind quantum parameter estimation and related to (B)QPT and (B)HPE. In Section IV, we focus on the discrete version of RCPS and analyze their connections with usual mixed states, as defined by von Neumann. Relationships with other works from the literature, that are more or less connected with RCPS and their higher-order statistics, are then discussed in Section V. Finally, we draw conclusions from this investigation in Section VI.

II. DEFINITION AND FEATURES OF RANDOM-COEFFICIENT PURE STATES (RCPS)

A. Definition of an RCPS

First considering the classical framework, the following concepts should be kept in mind. Beyond a scalar deterministic (i.e. fixed) value X, a random variable (RV) may be defined as a function **X** whose scalar value $X(\alpha)$ depends on an outcome α of the considered probability space Ω . That outcome α is randomly drawn and, once selected, it completely defines the corresponding (complex or real) value $X(\alpha)$ of **X**. One may thus e.g. model an experiment where a die is cast, each of its faces corresponds to an outcome α , and the user's numerical gain $X(\alpha)$ associated with each given face α in a game is fixed. More generally, a random vector is a vector whose components are RV, i.e. all their values are fixed by the considered single outcome α .

Now moving to the quantum framework, the simplest states considered in the literature, called pure states, are deterministic: such a state may be defined as a ket

$$|\psi\rangle = \sum_{k=0}^{d-1} c_k |k\rangle \tag{1}$$

where the kets $|k\rangle$ form an orthonormal basis of the considered *d*-dimensional space (with $d = 2^Q$ for Q qubits) and the corresponding complex-valued coefficients c_k are fixed for a given state $|\psi\rangle$. In our above-mentioned papers, we extended that concept to *random-coefficient* pure states, or RCPS. Such a state may be defined as a ket

$$|\psi\rangle = \sum_{k=0}^{d-1} \mathbf{c}_{\mathbf{k}} |k\rangle \tag{2}$$

where the complex-valued coefficients $\mathbf{c}_{\mathbf{k}}$ are RV, i.e. they depend on a randomly drawn outcome α . Once a single α has been selected, all corresponding coefficient values $c_k(\alpha)$ are fixed, as in a classical random vector. A given outcome α thus yields a fixed, i.e. deterministiccoefficient, pure state

$$|\psi(\alpha)\rangle = \sum_{k=0}^{d-1} c_k(\alpha) |k\rangle.$$
(3)

Such RCPS $|\psi\rangle$ and their realizations $|\psi(\alpha)\rangle$ can actually be faced in practice. For instance, in [7], we showed how to create an RCPS for a single electron spin 1/2, placed in a Stern-Gerlach device with a randomly drawn direction for the magnetic field. A second example is introduced here for quantum communications. In this scenario, the receiver gets a pure state with coefficient values that he does not know in advance, because he does not know which data were used by the emitter to prepare the pure state that he sent. The receiver may then describe the coefficients of the received pure state with RV c_k .

Whatever the considered RCPS, the coefficients $c_k(\alpha)$ of each state realization (3) have the same constraints as those of usual, i.e. deterministic-coefficient, pure states (1): the state $|\psi(\alpha)\rangle$ is normalized, so that

$$\sum_{k=0}^{d-1} |c_k(\alpha)|^2 = 1 \tag{4}$$

and $|\psi(\alpha)\rangle$ is defined up to a global phase factor, so that $c_0(\alpha)$ may be restricted to a real non-negative value $r(\alpha)$. In particular, setting d = 2 in the above equations, an RCPS of a single qubit reads

$$|\psi\rangle = \mathbf{r}|0\rangle + \sqrt{1 - \mathbf{r}^2} e^{i\phi}|1\rangle \tag{5}$$

where \mathbf{r} and $\boldsymbol{\phi}$ are real-valued RV and \mathbf{r} is non-negative.

B. RCPS preparation and measurements

Information about deterministic-coefficient or randomcoefficient pure states can be extracted by means of measurements. For a given deterministic-coefficient pure state (1) or (3), one may first use measurements in the computational basis $\{|k\rangle\}$, which e.g. consists of measuring the s_z spin component for an electron spin 1/2whose state is expressed in the standard basis. The results of these measurements have a random nature, but their possible values and the probabilities of these values are fixed for a given deterministic-coefficient pure state: for state (3), the probability of the result associated with the basis vector $|k\rangle$ is

$$p_k(\alpha) = |c_k(\alpha)|^2.$$
(6)

Estimates of these probabilities may be obtained, especially by preparing K copies of $|\psi(\alpha)\rangle$, performing one (possibly multiqubit) measurement per copy and computing the sample frequencies of all possible measurement results over all these state copies [9, 10].

Now consider a random-coefficient pure state $|\psi\rangle$ defined by (2). For any given basis vector $|k\rangle$, the probability $p_k(\alpha)$ depends on the randomly drawn outcome α ,

so that this type of probability itself becomes randomvalued! It defines an RV, that is denoted as $\mathbf{p}_{\mathbf{k}}$ and that may be expressed as

$$\mathbf{p}_{\mathbf{k}} = |\mathbf{c}_{\mathbf{k}}|^2. \tag{7}$$

For instance, for the single-qubit RCPS (5), this yields

$$\mathbf{p_0} = \mathbf{r}^2 \tag{8}$$

$$\mathbf{p_1} = 1 - \mathbf{r}^2 = 1 - \mathbf{p_0}.$$
 (9)

Measurements may be used in a two-level procedure to extract information about an RCPS defined by (2). At the higher level, N values of the set of coefficients $\{c_0(\alpha), \ldots, c_{d-1}(\alpha)\}$ associated with an outcome α are randomly drawn. This yields N deterministic-coefficient states $|\psi(\alpha)\rangle$ defined by (3). Then, at the lower level, for each such state $|\psi(\alpha)\rangle$, one uses K copies of $|\psi(\alpha)\rangle$ to estimate all $p_k(\alpha)$ as described above for deterministiccoefficient pure states. For any index k, the overall set of N estimates of $p_k(\alpha)$ thus obtained yields an estimate of the statistical distribution (i.e. law) of the RV \mathbf{p}_k . One may then e.g. derive the corresponding histogram, which is an estimate of the probability density function (pdf) of \mathbf{p}_k .

The above procedure involves randomness at *two* levels, instead of one level for usual (i.e. deterministiccoefficient) pure states: a) in the selection of the set of coefficients $\{c_0(\alpha), \ldots, c_{d-1}(\alpha)\}$, i.e. in the selection of an outcome α , and b) in the result provided by a single (possibly multiqubit) measurement performed for a given, i.e. deterministic-coefficient, state. In our previous papers, we first called that approach the "Repeated Write/Read" or RWR approach, with "write" referring to state preparation and "read" referring to measurements (see e.g. [1, 3]). We then called it the "multiplepreparation" (per state $|\psi(\alpha)\rangle$) approach [2], as opposed to the "single-preparation approach" that we later proposed in [2, 6, 11] and that is considered in Section IV.

We stress that the multiple-preparation approach requires what we call "segmented data", in the following sense: to use an RCPS with the above procedure, in the overall set of NK prepared states defined above, one should know which subset composed of K prepared states corresponds to a given state value $|\psi(\alpha)\rangle$, in order to estimate each corresponding value $p_k(\alpha)$ as a sample frequency over only that subset. That segmentation is typically performed by successively preparing the K copies corresponding to the first drawn state $|\psi(\alpha)\rangle$, then the K copies corresponding to the second drawn state, and so on, with a known value K. The case of "unsegmented data" is discussed in Section IV.

As stated above, from the point of view of someone aiming at using an RCPS (i.e. at reading it in our RWR procedure), the outcomes α are considered to be randomly drawn. How they are drawn, and therefore which statistical distributions are obtained for these outcomes and for the set of coefficients $\{c_0(\alpha), \ldots, c_{d-1}(\alpha)\}$, depends on the considered application. For instance, in the above-mentioned communication scenario, the receiver is the "reader" of our RWR procedure, whereas the emitter is the "writer", who prepares the states to be sent to the receiver. The emitter may know the statistical distribution of the states he prepares, especially because the coefficients of the emitted ket may be defined by classical RV that may have known statistical distributions. Then, when the emitted ket is transferred through the considered quantum channel to define the received ket, the statistical distribution of the ket coefficients is altered by that channel. Similar considerations apply to the quantum parameter estimation problem discussed in Section III, where the method used for drawing the considered RV is described.

The ket coefficients $\mathbf{c}_{\mathbf{k}}$ in (2) may be expressed in polar form as

$$\mathbf{c}_{\mathbf{k}} = \mathbf{r}_{\mathbf{k}} e^{i\boldsymbol{\phi}_{\mathbf{k}}} \tag{10}$$

as also illustrated by the simplified single-qubit form in (5). The measurements in the computational basis considered so far only allow one to access (i.e. estimate) the modulus parameters $\mathbf{r}_{\mathbf{k}}$, since (7) yields

$$\mathbf{p}_{\mathbf{k}} = (\mathbf{r}_{\mathbf{k}})^2. \tag{11}$$

This also appears in the simplified single-qubit form in (8)-(9). Besides, measurements in bases other than the computational basis (see p. 22 of [12], and [13]) provide information about the phase parameters $\phi_{\mathbf{k}}$, since one thus estimates the squared modulus of linear combinations of the coefficients $\mathbf{c}_{\mathbf{k}}$. This e.g. corresponds to measuring s_x spin components for electron spins 1/2 whose overall state is expressed in the standard basis, as detailed in [13]. In the present paper we only consider measurements in the computational basis, whereas other types of measurements for RCPS will be addressed in future papers.

The very general and major result obtained so far in this paper is that the RCPS framework with measurements in the computational basis makes it possible to access (estimates of) the above-defined probabilities $\mathbf{p}_{\mathbf{k}}$, that are RV, and this then makes it possible to exploit all their statistics, e.g. to perform QIP tasks. The remainder of this paper shows the wealth provided by these statistics. This will be especially appreciated by contrasting the capabilities thus reached with those of the restricted approach to RCPS that is obtained by using only the standard tools of quantum mechanics. Therefore, we first define that restricted approach hereafter.

C. The density operator associated with an RCPS

In Chapter IV of his famous book [14], von Neumann first considers (deterministic-coefficient) pure states and claims (p. 295): "we succeeded in reducing all assertions of quantum mechanics to the statistical formula ...",

where that formula defines the expectation (i.e. mean value) of a physical quantity A and reads

$$E\{A\}_{|\psi\rangle} = \langle \psi | \hat{A} | \psi \rangle \tag{12}$$

with our notations, including those defined in Section I, and where $E\{.\}$ stands for expectation, here calculated for the considered state $|\psi\rangle$. Then considering mixed states (p. 296), von Neumann further claims that the density operator "characterizes the mixture of states just described completely, with respect to its statistical properties" and von Neumann then provides a formula that defines the expectation of A for a mixed state and that here reads

$$E\{A\}_{\rho} = \operatorname{Tr}(\rho \hat{A}) \tag{13}$$

with the above-defined notations.

Whereas the latter claim refers to the usual mixed states ρ considered by von Neumann, one may wonder whether, for our RCPS too, one only has to consider the mean of a physical quantity A and whether it can still be expressed as $\text{Tr}(\rho \hat{A})$. This leads to the preliminary question: starting from and RCPS, can one associate a density operator ρ with it? To this end, one should keep in mind that, for a deterministic-coefficient pure state (1), we have

$$\rho = |\psi\rangle\langle\psi| \tag{14}$$

so that the elements of the corresponding density matrix read

$$\rho_{k\ell} = c_k c_\ell^* \tag{15}$$

where * stands for complex conjugate, and k and ℓ range from 0 to (d-1) as in (1). Therefore, as explained in [7, 8]. with an RCPS defined by (2), one can associate a density matrix whose elements read

$$\rho_{k\ell} = E\{\mathbf{c_k}\mathbf{c_\ell}^*\}.\tag{16}$$

In particular, its diagonal elements read

$$\rho_{kk} = E\{|\mathbf{c}_{\mathbf{k}}|^2\} = E\{\mathbf{p}_{\mathbf{k}}\}.$$
(17)

If \hat{A} is diagonal, $\text{Tr}(\rho \hat{A})$ only depends on these diagonal elements ρ_{kk} of ρ .

Eq. (17) shows that the diagonal of the density matrix only allows one to access very limited information about the RV $\mathbf{c_k}$ and $\mathbf{p_k}$. The quantity in (17) may first be seen as a *second-order* statistical parameter of $\mathbf{c_k}$, whose classical counterpart is often called the "mean power" when considering its extension to a random signal instead of an RV [15–20]. For a real-valued RV $\mathbf{c_k}$, this parameter $E\{\mathbf{c_k}^2\}$ is also the second-order (non-centered) moment of this RV (for a complex-valued $\mathbf{c_k}$, Eq. (17) therefore corresponds to the second-order moment of the RV $|\mathbf{c_k}|$). Eq. (17) may also be seen as the *first-order* moment (i.e. expectation) of $\mathbf{p_k}$. The off-diagonal elements (16) of the density matrix may yield additional information, but anyway (i) this information is also limited to the *second*order statistics of the RV $\mathbf{c}_{\mathbf{k}}$, i.e. to a second-order joint moment which is their cross-correlation and (ii) as mentioned above, this information cannot be accessed when one only considers $\text{Tr}(\rho \hat{A})$ and \hat{A} is diagonal.

In contrast, our approach, based on RCPS themselves, yields much richer information because it allows one to access all the statistics of $\mathbf{p}_{\mathbf{k}}$, as detailed further in this paper. Besides, performing measurements in the computational basis for a d-dimensional RCPS (2) yields estimates for d RV $\mathbf{p}_{\mathbf{k}}$ defined by (7), with $0 \leq k \leq d-1$. Among these RV, up to (d-1) may be statistically independent because they sum to one, as shown by (4). For d > 2, one may therefore wonder whether this set of (d-1) > 1 quantities provides richer information than the single scalar value $Tr(\rho \hat{A})$ only considered in the usual approach. This topic will be investigated in future papers but, in Section III, we show that, even for d = 2, our approach to RCPS based on the probabilities $\mathbf{p}_{\mathbf{k}}$ is more powerful than the approach based on the associated density operator.

D. Exploiting higher-order statistics of RCPS

As outlined above, the statistics respectively accessible with the RV $\mathbf{p}_{\mathbf{k}}$ associated with an RCPS and with the approach based on its density operator ρ and $\text{Tr}(\rho A)$ yield a fundamental difference, which will be better appreciated by first considering the classical counterpart of this phenomenon. Statistical methods for processing classical random signals, images or other types of data are often limited to the use of two types of parameters. The first one is their *first-order statistics*, especially the first-order moment, or expectation, $E\{\mathbf{X}\}$ of an RV **X**. The second one is their *second-order statistics*, which especially include (i) the second-order moment $E\{\mathbf{X}\mathbf{Y}^*\}$ of RV \mathbf{X} and \mathbf{Y} , and (ii) the associated centered secondorder moment, i.e. covariance, $E\{\tilde{\mathbf{X}}\tilde{\mathbf{Y}}^*\}$ of \mathbf{X} and \mathbf{Y} , with the centered version of **X** defined as $\tilde{\mathbf{X}} = \mathbf{X} - E\{\mathbf{X}\}$ and the same for $\tilde{\mathbf{Y}}$. Second-order statistics also include the restriction of the above parameters to a single RV, i.e. when $\mathbf{X} = \mathbf{Y}$, which is connected with mean power and variance, as partly discussed above.

The above parameters were sufficient for developing powerful methods, such as Principal Component Analysis (PCA) [21, 22] or Adaptive Noise Cancellation (ANC) [23, 24]. ANC typically makes it possible to restore an unknown signal of interest from a measured signal that is a so-called "mixture", i.e. combination, of that useful signal and of noise, but ANC requires that another measurement provide the noise signal alone.

In contrast, more difficult classical signal processing problems need more advanced tools, closely related to so-called *higher-order statistics* or HOS (see e.g. the surveys in [19, 20] and more details in [16–18, 25]). "Higher" here means "higher than 2" and refers to the fact that these methods (also) exploit other parts of the information contained in the data than the above-defined firstorder and second-order parameters. In a basic form, this means exploiting *m*th-order moments with $m \geq 3$, these moments being defined as $E\{\mathbf{X}^m\}$ for one real RV **X** and $E\{\mathbf{X}^{m_1}\mathbf{Y}^{m_2}\}$ with $m_1 + m_2 = m$ for joint moments of two real RV \mathbf{X} and \mathbf{Y} (and so on for more than two RV). Here again, the corresponding *centered* moments are obtained by replacing \mathbf{X} and \mathbf{Y} by their centered versions $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$. HOS methods also use (i) higher-order cumulants, that may be expressed as specific combinations of moments having attractive properties, (ii) generalized moments $E\{q(\mathbf{X})\}$ and $E\{q(\mathbf{X})h(\mathbf{Y})\}$ where g and h are arbitrary nonlinear functions and (iii) other quantities, that exploit all the pdf $f_{\mathbf{X}}$ or joint pdf $f_{\mathbf{X},\mathbf{Y}}$ of RV, such as differential entropy or mutual information [16–20, 25]. Besides, all these parameters extend to more than two RV, as illustrated below for their quantum version (see (19)).

In particular, the above tools have been used for classical Independent Component Analysis (ICA) for so-called i.i.d. signals. ICA is a major class of methods for solving the Blind Source Separation (BSS) well-known signal processing problem, which consists of extracting a set of source signals from measured signals that all are "mixtures", i.e. combinations, of these source signals. ICA is a required extension of PCA and ANC because, for i.i.d. signals, the above-defined BSS problem cannot be solved with only second-order statistical methods, including PCA and ANC, but it can be solved by exploiting the additional information that is provided by HOS for non-Gaussian signals and that is used in ICA (see details e.g. in Chapter 7 of [16] or in Chapter 12 of [18]). This problem is also closely related to blind system or mixture identification [26–28], because BSS and hence ICA essentially require one to estimate the inverse of the function, i.e. "system", that mixes the source signals.

Having the above classical data processing background in mind, we now move to the quantum framework. Our approach based on the RV $\mathbf{p}_{\mathbf{k}}$ associated with an RCPS may then be expected to be able to solve QIP problems that cannot be handled by restricting oneself to (i) the density operator ρ associated with an RCPS and (ii) the corresponding mean of observable $\text{Tr}(\rho \hat{A})$. More precisely, to extend QIP capabilities, one may exploit the HOS of the RV $\mathbf{c}_{\mathbf{k}}$ through the statistics of the RV $\mathbf{p}_{\mathbf{k}}$ at orders higher than one whereas, as explained above, ρ and $\text{Tr}(\rho \hat{A})$ essentially access the first-order statistics of $\mathbf{p}_{\mathbf{k}}$ and anyway only the second-order statistics of $\mathbf{c}_{\mathbf{k}}$.

In a basic form, this means exploiting fourth-order parameters of any $\mathbf{c}_{\mathbf{k}}$ with $0 \leq k \leq d-1$, through the second-order moment, i.e. mean power, $E\{(\mathbf{p}_{\mathbf{k}})^2\}$ of $\mathbf{p}_{\mathbf{k}}$, or through is centered second-order moment, i.e. variance,

$$E\{(\mathbf{p}_{\mathbf{k}} - E\{\mathbf{p}_{\mathbf{k}}\})^{2}\} = E\{(\mathbf{p}_{\mathbf{k}})^{2}\} - (E\{\mathbf{p}_{\mathbf{k}}\})^{2}.$$
 (18)

Other statistical parameters of the RV $\mathbf{p}_{\mathbf{k}}$ may also be

considered by extending, to the quantum framework, the parameters that we summarized above for the classical framework. This first includes parameters for a single RV $\mathbf{p}_{\mathbf{k}}$, such as various higher-order moments $E\{(\mathbf{p}_{\mathbf{k}})^m\}$ or generalized moments $E\{g(\mathbf{p}_{\mathbf{k}})\}$. Importantly, this also includes parameters associated with *several* of these RV, such as their joint moments

$$E\{\prod_{k\in I} (\mathbf{p}_{\mathbf{k}})^{m_k}\}\tag{19}$$

where I is an arbitrary subset of the set of indices k with $0 \le k \le d-1$ and m_k are integers, that define the overall order of the considered moment [29].

How the above statistical parameters are used depends on the considered QIP task. A large set of potential applications deal with the estimation of parameters of a quantum system (or of a quantum state), therefore with a close relationship with quantum process (or state) tomography and with Hamiltonian estimation. The resulting classes of QIP methods especially include the quantum extension of so-called moment matching methods used for classical data processing (see e.g. Section 4.3 of [16]). This consists of expressing the RV $\mathbf{p}_{\mathbf{k}}$, and then some of their moments, with respect to quantities including the unknown parameters (e.g. of the considered system) to be estimated. Each such moment thus yields an equation with respect to the unknown parameters. Estimates of these moments may be derived from measurements as explained above. One then uses these estimates instead of the actual moments in the above equations. Considering enough moments thus yields enough equations, from which the values of the unknown parameters are derived. These values are therefore those that match the estimated moments, hence the name of this approach.

Although we did not explicitly mention that quantum moment matching concept in our application-driven QIP papers, we already used it in several of them: see e.g. [1– 3], [4] (Section 1.7.2), [6]. These applications concerned the quantum version of BSS, i.e. BQSS, and of blind system and parameter identification, i.e. BQPT and BHPE. They were focused on a specific type of quantum process/system (which corresponds to the mixing function of classical BSS): we considered two gubits coupled according to the Heisenberg model. In addition, a new application of the above quantum moment matching procedure is detailed below in Section III. This new investigation has complementary features with respect to our abovementioned previous works. First, whereas we previously only considered the statistics of the probabilities $\mathbf{p}_{\mathbf{k}}$ associated with an RCPS, we here moreover compare the capabilities thus achieved with those of the appproach to RCPS based on ρ and $\text{Tr}(\rho \hat{A})$ that we defined in Section IIC. We thus explicitly prove that the approach based on the statistics of $\mathbf{p}_{\mathbf{k}}$ is more powerful. Besides, we only used first-order moments of $\mathbf{p}_{\mathbf{k}}$ in the previous works [1-3], [4] (Section 1.7.2), [6] (we also used other statistical parameters, but for quantities that are only indirectly related to \mathbf{p}_k : see [30]). In constrast, we here

also take advantage of the second-order moment of $\mathbf{p_k}$. Moreover, we here investigate the estimation of parameters of a quantum process, which is a task closely related to BQPT and BHPE, but we here consider a different class of processes. That class is much more general than the above-mentioned Heisenberg process in the sense that it addresses any energy-preserving process, represented by an arbitrary unitary matrix, although it is only considered for a single qubit for the sake of clarity. Finally, we not only propose blind estimation methods, but also non-blind ones.

Before we focus on that QIP task in Section III, the remainder of the present section is dedicated to the presentation of other general features of RCPS. We first stress that a very large number of moments (19), and therefore e.g. of moment-based equations in the above quantum moment matching procedure, may be defined from the same set of measurements. This is very attractive because it may drastically reduce the number of types of measurements required to estimate the parameters of interest, whereas this is currently a bottleneck as soon as the dimensionality of the considered system or state increases. The experimental complexity of performing various types of quantum measurements (e.g. spin components along various directions) will thus be, at least partly, replaced by additional processing of a reduced set of measurement results on a classical computer, which is much simpler. More precisely, various previously reported QIP methods use only a *single* quantity, namely the first-order moment (i.e. the mean), for each type of measurement, and they therefore require various types of measurements to obtain enough information about the considered phenomenon. In contrast, our approach based on RCPS can get enough information with a lower number of types of measurement, by exploiting various parameters of the quantities $\mathbf{p}_{\mathbf{k}}$, including their mean power and higher-order statistical parameters, derived on a classical computer from all measurement results obtained for each given type of measurement. We plan to investigate this topic in future papers for general configurations, but we already illustrate it with an example in Section III of the present paper.

E. Limitations of usual statistics of observables

We stress that, for a given physical quantity A and a given RCPS $|\psi\rangle$, the approach proposed in this paper exploits statistical parameters of (one or several) $RV \mathbf{p_k}$, not those of the (single) RV defined by the measured values of A (note also that the RV $\mathbf{p_k}$ may be continuous-valued or discrete-valued as discussed in Section IV, whereas the RV defined by A is generally discrete-valued). Our motivation is that this approach based on the statistical parameters of interest of $\mathbf{p_k}$ yields much more information than the usual approach based on A, as will now be shown. To this end, we hereafter first revisit the concept of the mean of a physical quantity, that we only partly addressed is Section II C, but now without resorting to the density operator of an RCPS. This then allows us to naturally proceed further, by combining the approach used here with some HOS concepts introduced in Section II D.

Let us first consider the mean, hence the first-order statistics, of A. Using an arbitrary orthonormal basis $\{|k\rangle\}$, the RCPS $|\psi\rangle$ is defined by (2), whereas A is represented by a possibly non-diagonal matrix whose elements are denoted as $a_{k\ell}$. The usual expression (12) of the mean of A for a deterministic-coefficient pure state is here first used for the state $|\psi(\alpha)\rangle$ associated with a single outcome α . This yields

$$E\{A\}_{|\psi(\alpha)\rangle} = \sum_{k} \sum_{\ell} c_k(\alpha)^* c_\ell(\alpha) a_{k\ell}.$$
 (20)

Then using the expectation of the latter quantity over all outcomes α yields the mean of A for the RCPS $|\psi\rangle$, which reads

$$E\{A\}_{|\psi\rangle} = \sum_{k} \sum_{\ell} E\{\mathbf{c}_{\mathbf{k}}^* \mathbf{c}_{\ell}\} a_{k\ell}.$$
 (21)

That mean of A therefore has two limitations. First, it is only related to (part of) the *second-order* statistics of the RV $\mathbf{c}_{\mathbf{k}}$, that include two aspects:

- 1. Moments that each involve a single RV. They correspond to the terms with $k = \ell$ in (21), namely to the probabilities $\mathbf{p}_{\mathbf{k}}$ defined by (7).
- 2. Joint moments of two RV, that correspond to the terms with $k \neq \ell$ in (21). When A is represented by a diagonal matrix, these terms disappear from (21).

When the dimension d of the state space is higher than 2, using only the mean of A yields an additional limitation: estimating that mean yields only a *single* equation with respect to estimates of (some: see above) statistics of all RV $\mathbf{c_k}^* \mathbf{c_\ell}$, including all $\mathbf{p_k}$, as shown by (21). In contrast, our approach based on the probabilities $\mathbf{p_k}$ of an RCPS themselves allows one to separately estimate (all) the statistics of *each* of these probabilities. In the specific case when d = 2, i.e. for a single qubit, this difference between the considered two approaches reduces, because only one independent probability $\mathbf{p_k}$ exists, as shown by (9), but several statistical parameters of that $\mathbf{p_k}$ can still be exploited, as explained above [31].

One may then try to access richer information by considering the mean $E\{g(A)\}_{|\psi\rangle}$ of a function g of A, as the quantum counterpart of the generalized moments $E\{g(\mathbf{X})\}$ of classical RV, and similarly to the quantum generalized moments $E\{g(\mathbf{p_k})\}$, both defined in Section II D. Here, g is an arbitrary function, and this e.g. includes the specific case when

$$g(x) = \left(x - E\{A\}_{|\psi\rangle}\right)^2 \tag{22}$$

for which $E\{g(A)\}_{|\psi\rangle}$ is the variance of A for the RCPS $|\psi\rangle$ (this is coherent with the corresponding expression

of the variance for a usual, i.e. deterministic-coefficient, pure state: see e.g. p. 295 of [14]). However, even for arbitrary functions g, that approach based on $E\{g(A)\}_{|\psi\rangle}$ has limited capabilities, as will now be shown. Using an arbitrary orthonormal basis $\{|k\rangle\}$, the expression of the matrix that represents g(A) may be derived from the considered physical quantity A and function g: see e.g. [32]. Its elements are hereafter denoted as $g_{k\ell}$ and their expressions are not needed here: using the same approach as in (20)-(21) yields

$$E\{g(A)\}_{|\psi\rangle} = \sum_{k} \sum_{\ell} E\{\mathbf{c}_{\mathbf{k}}^* \mathbf{c}_{\ell}\}g_{k\ell}$$
(23)

again with the connection (7) with the probabilities $\mathbf{p}_{\mathbf{k}}$ for the terms of (23) with $k = \ell$. The main conclusion and limitation that may be derived from (23) is that this quantity too only depends on the *second-order* statistics of the coefficients $\mathbf{c}_{\mathbf{k}}$: introducing the function g yields a nonlinearity in the expressions of the matrix elements $g_{k\ell}$ [32], not in the statistics of the coefficients $\mathbf{c}_{\mathbf{k}}$ [33], [34].

F. Other connection of RCPS with density operators

Another connection between RCPS and the usual framework of deterministic-coefficient pure states is now introduced as follows. Starting from an RCPS $|\psi\rangle$, we consider each associated deterministic-coefficient pure state $|\psi(\alpha)\rangle$. We use its density operator in the usual sense of quantum mechanics: it is defined by adapting (14) and (15) to $|\psi(\alpha)\rangle$ instead of $|\psi\rangle$. This yields

$$\tilde{\rho}_{k\ell}(\alpha) = c_k(\alpha)c_\ell(\alpha)^* \tag{24}$$

where we denote as $\tilde{\rho}(\alpha)$ the density matrix and density operator of $|\psi(\alpha)\rangle$. We moreover introduce the original *random* operator and the associated random matrix, both denoted as $\tilde{\rho}$, as follows: it is the operator/matrix which depends on the outcome α and whose realization associated with any outcome α is $\tilde{\rho}(\alpha)$. The elements of the matrix $\tilde{\rho}$ then read

$$\tilde{\boldsymbol{\rho}}_{k\ell} = \mathbf{c}_{\mathbf{k}} \mathbf{c}_{\boldsymbol{\ell}}^*. \tag{25}$$

This random operator $\tilde{\rho}$ thus consists of an ensemble of usual density operators $\tilde{\rho}(\alpha)$. It should be distinguished from the single, deterministic, density operator ρ defined by (16), that we previously associated with an RCPS. Yet, they are closely connected, since ρ is the expectation of $\tilde{\rho}$, as shown by (16) and (25). Besides, (25) shows that the diagonal elements of $\tilde{\rho}$ are nothing but the quantities $\mathbf{p}_{\mathbf{k}}$ that we previously introduced in (7). This operator $\tilde{\rho}$ therefore also contains the wealth of all the statistics of the random probabilities $\mathbf{p}_{\mathbf{k}}$ upon which we focus in this paper, plus its off-diagonal elements to be further investigated. The random operator $\tilde{\rho}$ associated with the above-mentioned ensemble of $\tilde{\rho}(\alpha)$ is thus much richer than its plain expectation consisting of the density operator ρ of (16).

Besides, it is thus not surprising that we succeeded in associating *several* RCPS (in the sense of (16)) with a given density operator in our very recent investigation [8]: knowing the mean operator ρ is not sufficient for imposing all the statistics of the coefficients $\mathbf{c_k}$ of an RCPS nor those of its random operator $\tilde{\rho}$ (similarly, knowing the mean of a classical RV is not sufficient for imposing all the statistics of that RV).

If one would like to use all $\tilde{\rho}$, one would then have to define how to access related properties in practice, typically by means of measurements, as we did above for $\mathbf{p}_{\mathbf{k}}$, i.e. for the diagonal of $\tilde{\rho}$. The non-diagonal elements of $\tilde{\rho}$ will be analyzed in our future papers, whereas we keep on focusing on $\mathbf{p}_{\mathbf{k}}$ hereafter.

III. AN APPLICATION TO QUANTUM PARAMETER ESTIMATION

A. Considered quantum system and task

A well-known QIP task is Quantum Process Tomography (QPT), especially [35] introduced in 1997 in [9]. QPT is the quantum version of classical non-blind system identification (see e.g. [12, 36-44]) and is also closely connected with non-blind quantum channel estimation and phase estimation [2]. It e.g. applies to a quantum system that here does not interact with its environment, whose input is here an RCPS $|\psi_{in}\rangle$ equal to the initial state of the system, and whose output is then an RCPS $|\psi_{out}\rangle$ equal to the final state of the system. The process/transform applied by the system to its input is unknown and is to be identified, i.e. estimated. It is represented by a unitary matrix M: multiplying the vector of coefficients of the input ket $|\psi_{in}
angle$ by that matrix yields the vector of coefficients of the output ket $|\psi_{out}\rangle$ (see (27) below for an example).

For a given initial-to-final time interval, the expression of the above matrix M is defined by the Hamiltonian of the quantum system, which may be known to belong to a given class, whereas the values of the parameters of that model are unknown and are to be estimated. A related task is therefore (non-blind) Hamiltonian Parameter Estimation (HPE) [45–47]. Such parameter estimation problems are also addressed, but often referred to as Hamiltonian identification, e.g. in [43, 48, 49] and partly [50].

Standard QPT and HPE methods are non-blind in the sense that they estimate the considered quantities by knowing the input values of the process, in addition to measurement results associated with its output. We extended these approaches to their blind version, which is more powerful because it does not require one to know each value of the applied input but only some of their statistical properties: see e.g. our previous works in [5, 6, 51] for blind QPT (BQPT) and [2] for blind HPE (BHPE). As stated above, these previous investigations of blind methods were focused on a specific class of two-qubit processes and associated Hamiltonian, based on cylindricalsymmetry Heisenberg coupling. In contrast, we here consider a very generic class of processes: we address any unitary process, yet focusing on single-qubit processes. Single-qubit processes are considered both for the sake of clarity and to show that our approach to RCPS based on probability statistics yields better performance than the approach to RCPS based on the density operator and $Tr(\rho \hat{A})$ even for a single qubit, i.e. when the wealth of our approach does not result from the availability of *several* independent probabilities $\mathbf{p}_{\mathbf{k}}$ (see Section II C).

A model representing all single-qubit unitary processes is obtained by expressing the above matrix M as follows (see [12] p. 176):

$$M = e^{iv_1} \begin{bmatrix} e^{i(-v_2/2 - v_4/2)} \cos\left(\frac{v_3}{2}\right) & -e^{i(-v_2/2 + v_4/2)} \sin\left(\frac{v_3}{2}\right) \\ e^{i(v_2/2 - v_4/2)} \sin\left(\frac{v_3}{2}\right) & e^{i(v_2/2 + v_4/2)} \cos\left(\frac{v_3}{2}\right) \\ \end{array}$$
(26)

The problem addressed below is the estimation of all or at least part of the parameters v_1 to v_4 . To this end, we propose both non-blind and blind estimation methods.

Since the output state of the considered process and hence the matrix M are defined only up to a phase factor, one may anticipate that v_1 cannot be estimated (and that this is not an issue). This is confirmed by the operation of the methods proposed below.

B. Considered states and measurements

The random-coefficient state $|\psi_{in}\rangle$ applied to the input of the considered process is defined by the right-hand term of (5). The resulting output state $|\psi_{out}\rangle$ of that process is defined by the right-hand term of (2) with d =2. Its coefficients $\mathbf{c_k}$ here form the vector

$$\begin{bmatrix} \mathbf{c_0} \\ \mathbf{c_1} \end{bmatrix} = M \begin{bmatrix} \mathbf{r} \\ \sqrt{1 - \mathbf{r}^2} e^{i\phi} \end{bmatrix}.$$
 (27)

Measurements are then performed for copies of each realization of the state $|\psi_{out}\rangle$ that corresponds to an outcome α . In a practical QIP setup, only some types of measurements are allowed. To perform a fair comparison of the two processing methods respectively based on the probabilities $\mathbf{p}_{\mathbf{k}}$ and on the density operator ρ , both methods should be considered for the same type(s) of measurements. We hereafter analyze the case when only measurements in the computational basis are allowed [52]. From a physical point of view, this e.g. corresponds to implementing the considered qubit as a spin 1/2 and measuring its s_z spin component (the basis vectors $|0\rangle$ and $|1\rangle$ in (5) might then be denoted as $|+\rangle$ and $|-\rangle$). These measurements have two possible results, whose probabilities are defined by (7). Using (26)and (27), this may be shown to yield

$$\mathbf{p_0} = \cos(v_3)\mathbf{r}^2 + \frac{1 - \cos(v_3)}{2}$$

$$-\cos(v_4 + \boldsymbol{\phi})\sin(v_3)\mathbf{r}\sqrt{1 - \mathbf{r}^2} \qquad (28)$$

$$\mathbf{p_1} = 1 - \mathbf{p_0}.\tag{29}$$

C. Approach based on the mean value $Tr(\rho \hat{A})$

We first investigate an approach based on the principles presented in Section II C. In the considered basis, the measured physical quantity, as defined in Section III B, is represented by the matrix

$$\hat{A} = \begin{bmatrix} \frac{1}{2} & 0\\ 0 & -\frac{1}{2} \end{bmatrix}.$$
(30)

Therefore

$$Tr(\rho \hat{A}) = \frac{1}{2}(\rho_{00} - \rho_{11}).$$
(31)

. Using (17) and (29), this yields

$$\operatorname{Tr}(\rho \hat{A}) = E\{\mathbf{p}_0\} - \frac{1}{2}.$$
(32)

As an example, for all quantum parameter estimation methods investigated in this paper, we moreover set the same following constraints on the statistics of the input state $|\psi_{in}\rangle$ (but not on its individual values). **r** and ϕ are statistically independent RV. **r** has a uniform distribution over the interval $[r_1, r_2]$ and ϕ has a uniform distribution over the interval $[-B_{\phi}, B_{\phi}]$, where r_1, r_2 and B_{ϕ} are free parameters. In these conditions, (28) yields

$$E\{\mathbf{p_0}\} = \cos(v_3)E\{\mathbf{r}^2\} + \frac{1 - \cos(v_3)}{2}$$
(33)
$$-\cos(v_4)\sin(v_3)E\{\cos(\phi)\}E\{\mathbf{r}\sqrt{1 - \mathbf{r}^2}\}.$$

Eq. (32) and (33) lead to the following conclusions. First, $\operatorname{Tr}(\rho \hat{A})$ dos not depend on v_1 , as expected from Section III A. Besides, $Tr(\rho \hat{A})$ turns out not to depend on v_2 , due to the considered type of measurements (and this is also true for \mathbf{p}_0 itself, not only for its expectation, as shown by (28)). Therefore, the approach considered here cannot estimate v_1 and v_2 . Finally, by deriving an estimate of the mean value $Tr(\rho A)$ from measurements, (32) and (33) only provide a *single* equation with *two* unknowns, namely v_3 and v_4 (the required statistics of **r** and ϕ are known, as explained in Section III D). This single equation is therefore not sufficient for deriving the values of these two unknowns, so that this approach fails to solve the considered problem. In contrast, we will now show that our approach to RCPS based on probability statistics succeeds in estimating v_3 and v_4 from the same type of measurement results as in the method considered here, by further exploiting these classical-form data.

D. Approach based on the statistics of the random probability p_0

We here propose an approach that is based on the principles introduced in Section II D and that therefore exploits statistical parameters of the RV \mathbf{p}_0 . As shown by (28), this RV and hence its statistical parameters only depend on v_3 and v_4 , not on v_1 and v_2 . Therefore, we here only aim at estimating v_3 and v_4 (see the above comment about the possible use of other types of measurements to estimate v_2). To this end, we consider two statistical parameters of \mathbf{p}_0 , in order to define two (independent) equations with unknowns v_3 and v_4 . Focusing on the simplest parameters, we first again consider the first-order moment (33) of \mathbf{p}_0 . In addition, we here use its second-order moment, that is, $E\{(\mathbf{p}_0)^2\}$ [53]. Due to (7), with respect to the random coefficient \mathbf{c}_0 of the considered quantum state, the statistical parameters used here are thus $E\{|\mathbf{c}_0|^2\}$ and $E\{|\mathbf{c}_0|^4\}$, i.e. second-order and fourth-order statistics of the RV \mathbf{c}_0 .

Considering the same conditions as in Section III C, the expression of $E\{(\mathbf{p_0})^2\}$ with respect to v_3 and v_4 is derived from (28). Then substituting v_4 thanks to (33) yields

$$E\{(\mathbf{p_0})^2\} = a_2 \cos^2(v_3) + a_1 \cos(v_3) + a_0 \tag{34}$$

with

$$a_{2} = \frac{1}{4} + \frac{1}{2} \left(E\{\mathbf{r}^{2}\} - E\{\mathbf{r}^{4}\} \right) \left(E\{\cos(2\phi)\} - 3 \right) + 2b_{1} \left(E\{\mathbf{r}^{2}\} - \frac{1}{2} \right) + b_{2} \left(E\{\mathbf{r}^{2}\} - \frac{1}{2} \right)^{2}$$
(35)

$$a_{1} = (1 - 2E\{\mathbf{p_{0}}\}) \left(b_{1} + b_{2} \left(E\{\mathbf{r}^{2}\} - \frac{1}{2}\right)\right)$$
(36)

$$a_{0} = E\{\mathbf{p}_{0}\} - \frac{1}{4} + b_{2} \left(E\{\mathbf{p}_{0}\} - \frac{1}{2}\right)^{2} + \frac{1}{2} \left(1 - E\{\cos(2\phi)\}\right) \left(E\{\mathbf{r}^{2}\} - E\{\mathbf{r}^{4}\}\right)$$
(37)

where

$$b_1 = \frac{1}{2} - \frac{E\{\mathbf{r}^3\sqrt{1-\mathbf{r}^2}\}}{E\{\mathbf{r}\sqrt{1-\mathbf{r}^2}\}}$$
(38)

$$b_{2} = \frac{E\{\cos(2\phi)\} \left(E\{\mathbf{r}^{2}\} - E\{\mathbf{r}^{4}\}\right)}{\left[E\{\cos(\phi)\}E\{\mathbf{r}\sqrt{1-\mathbf{r}^{2}}\}\right]^{2}}.$$
 (39)

To estimate v_3 from (34), the required statistical parameters of \mathbf{r} and ϕ should be known. This yields two estimation methods. In the most conventional, i.e. nonblind, method, one performs measurements for (copies of) realizations of the input state $|\psi_{in}\rangle$ of the considered process and then derives sample statistics for the required statistical parameters. Instead, we hereafter focus on a blind, hence more challenging, method, i.e. without performing any measurements at the input of the considered process but only using some statistical properties imposed on that input [54]. More precisely, since we here again use the statistical distributions of \mathbf{r} and ϕ defined in Section III C, the statistical parameters of \mathbf{r} and ϕ used in (35)-(39) may be shown to read

$$E\{\mathbf{r}^2\} = \frac{1}{3}(r_1^2 + r_1r_2 + r_2^2) \tag{40}$$

$$E\{\mathbf{r}^{4}\} = \frac{1}{5}(r_{1}^{4} + r_{1}^{3}r_{2} + r_{1}^{2}r_{2}^{2} + r_{1}r_{2}^{3} + r_{2}^{4})$$
(41)

$$E\{\mathbf{r}\sqrt{1-\mathbf{r}^2}\} = \frac{-1}{3(r_2-r_1)} \left(\left(1-r_2^2\right)^{3/2} - \left(1-r_1^2\right)^{3/2} \right)$$
(42)

$$E\{\mathbf{r}^{3}\sqrt{1-\mathbf{r}^{2}}\} = \frac{1}{r_{2}-r_{1}} \left[-\frac{1}{3} \left(\left(1-r_{2}^{2}\right)^{3/2} - \left(1-r_{1}^{2}\right)^{3/2} \right) + \frac{1}{5} \left(\left(1-r_{2}^{2}\right)^{5/2} - \left(1-r_{1}^{2}\right)^{5/2} \right) \right]$$
(43)

$$E\{\cos(\phi)\} = \frac{\sin(B_{\phi})}{B_{\phi}} \tag{44}$$

$$E\{\cos(2\phi)\} = \frac{\sin(2B_{\phi})}{2B_{\phi}}.$$
(45)

Therefore, when r_1 , r_2 and B_{ϕ} are fixed to known values and estimates of $E\{\mathbf{p}_0\}$ and $E\{(\mathbf{p}_0)^2\}$ are derived from measurements, (34) yields a second-order polynomial equation with respect to $\cos(v_3)$.

The corresponding solutions for $v_3 \in [-\pi, \pi]$ read

$$v_{3} = \epsilon_{2} \arccos\left(\frac{-a_{1} + \epsilon_{1}\sqrt{a_{1}^{2} - 4a_{2}\left(a_{0} - E\{(\mathbf{p_{0}})^{2}\}\right)}}{2a_{2}}\right)$$
(46)

with $\epsilon_1 = \pm 1$ and $\epsilon_2 = \pm 1$. The value of $v_4 \in [-\pi, \pi]$ is then derived from (33), which yields

$$v_{4} = \epsilon_{3} \arccos\left(\frac{-E\{\mathbf{p}_{0}\} + \cos(v_{3})E\{\mathbf{r}^{2}\} + \frac{1-\cos(v_{3})}{2}}{\sin(v_{3})E\{\cos(\phi)\}E\{\mathbf{r}\sqrt{1-\mathbf{r}^{2}}\}}\right)$$
(47)

with $\epsilon_3 = \pm 1$.

First disregarding the choice of ϵ_1 , ϵ_2 and ϵ_3 , the main result thus obtained is that (46) and (47) show that our approach succeeds in estimating v_3 and v_4 . We again stress that this is achieved by using $E\{(\mathbf{p_0})^2\}$, i.e. the statistics of $\mathbf{p_0}$ beyond the first order and hence the statistics of $\mathbf{c_0}$ beyond the second order. In constrast, by only using second-order statistics of $\mathbf{c_0}$, the approach based on the density operator and the associated mean of measurements $\text{Tr}(\rho \hat{A})$ fails to estimate v_3 and v_4 , as shown in Section III C.

In the basic version of the method proposed here, estimates of v_3 and v_4 are obtained up to some so-called indeterminacies, corresponding to the fact that this method does not define whether each of the parameters ϵ_1 , ϵ_2 and ϵ_3 should be set to 1 or -1. Various types of indeterminacies also exist in classical BSS and blind system/mixture identification, due to the limited information available in *blind* methods. Part of these indeterminacies can e.g. be avoided by requesting some additional prior knowledge, that would here e.g. correspond to knowing to which intervals the unknown values of v_3 and v_4 belong. Indeterminacies also appeared in the basic version of our previous BQPT [6] and BHPE methods [2]. We succeeded in removing them in refined versions of our methods, where we used additional occurrences of the same type of measurements, but with different statistics for the input quantum states. One might also investigate the use of such measurements in order to remove the indeterminacies on v_3 and v_4 here, if one would like to solve this problem completely, i.e. beyond the above illustration of the general capabilities of higher-order statistics of $\mathbf{c_0}$.

E. Test results

To validate the blind method of Section IIID and to evaluate its accuracy, we performed numerical tests with data derived from a software simulation of the considered configuration. Each elementary test consists of the following stages. We first create a set of N realizations of the random-coefficient pure input state $|\psi_{in}\rangle$ defined by the right-hand term of (5). Each of these N realizations is obtained by randomly drawing the parameters \mathbf{r} and ϕ and then using (5). We then transfer each such realization of $|\psi_{in}\rangle$ through the quantum process to be identified. This corresponds to using (27) with a given value of the matrix M defined by (26) and hence with given values of the parameters v_1 to v_4 . This yields N realizations of the set of coefficients $\mathbf{c}_{\mathbf{k}}$ of the state $|\psi_{out}\rangle$. Besides, we eventually use simulated measurements associated with these states, as defined in Section III B. For each of the N realizations of the set of coefficients $\mathbf{c}_{\mathbf{k}}$, Eq. (7) yields the corresponding realization of the probability \mathbf{p}_0 , which is used as follows. We use K prepared copies of the considered realization of the state $|\psi_{in}\rangle$ to simulate K random-valued measurements, drawn with the above value of the probability \mathbf{p}_0 . We then derive the sample frequency, over these K measurements, of the measurement result associated with the ket $|0\rangle$. This sample frequency is an estimate of the considered realization of \mathbf{p}_0 . Then computing the average of these K-preparation estimates, over all N realizations of the states $|\psi_{in}
angle$ and hence $|\psi_{out}\rangle$, yields an (NK)-preparation estimate of the probability expectation $E\{\mathbf{p}_0\}$. Similarly, the mean of the squares of the estimates of all N realizations of $\mathbf{p_0}$ yields an estimate of $E\{(\mathbf{p}_0)^2\}$. Both expectation estimates are then used by our quantum parameter estimation method defined in Section IIID, to derive estimates of v_3 and v_4 .

As an example, the parameters of the matrix M of (26) to be identified were set to the same values in all tests, namely $v_1 = \pi/10$, $v_2 = 2v_1$, $v_3 = 3v_1$ and $v_4 = 4v_1$. Besides, the RV **r** and ϕ that define the input state of the considered process (see (27)) were uniformly drawn, respectively over the intervals [0, 1] and $[-\pi/4, \pi/4]$. The above parameters N and K were varied as described further in this section. For each considered set of conditions defined by the values of N and K, we performed 100 above-defined elementary tests, with different sets of realizations of the state $|\psi_{in}\rangle$, in order to assess the statistical performance of the considered estimation method over 100 estimations of the same set $\{v_3, v_4\}$ of parameter values.

The considered performance criteria are defined as follows. Separately for each of the parameters v_3 and v_4 , we computed the Normalized Root Mean Square Error (NRMSE) of that parameter over all 100 obtained estimates, defined as the ratio of its RMSE to its actual (positive) value. The values of these two performance criteria are shown in Fig. 1, where each plot corresponds to one of the parameters v_3 and v_4 and to a fixed value of N. Each plot shows the variations of the considered performance criterion vs. K. We here use the values of ϵ_1, ϵ_2 , and ϵ_3 that yield the lowest NRMSE, based on the considerations provided in Section III D.

Fig. 1 first shows that the estimation error decreases when K or N increase, as expected. More precisely, each plot for a fixed N shows that the NRMSE tends to an asymptotic value when is K sufficiently increased. This occurs because the (fixed number N of) realizations of \mathbf{p}_0 are thus accurately estimated. To further decrease that asymptotic value of NRSME, one should then increase the number of (estimated) values of \mathbf{p}_0 over which averaging is performed, i.e. the value of N, as confirmed by Fig. 1. This figure moreover shows that the proposed method can achieve quite low NRMSE values, e.g. around 2×10^{-3} in the considered range of values of N and K.

IV. COMPARING DISCRETE RCPS WITH MIXED STATES

The RV $\mathbf{c_k}$, and hence the RV $\mathbf{p_k}$ derived from (7), may be continuous-valued or discrete-valued. For instance, in the QIP problem analyzed in Section III, the considered $\mathbf{c_k}$ and $\mathbf{p_k}$ are those of the output state $|\psi_{out}\rangle$ of the process, and the nature (continuous/discrete) of their statistics results from the nature of the statistics used for preparing the random input state $|\psi_{in}\rangle$, i.e. for drawing its parameters **r** and ϕ , as shown by (28).

Considering probabilistic phenomena in general, socalled discrete (i.e. discrete-valued) RV are especially obtained if the considered probability space Ω contains a finite number L of outcomes α . This then allows us to obtain a discrete RCPS especially by considering a situation with L "possible cases", i.e. L outcomes α , each with a probability of occurrence $P(\alpha)$. Selecting such an outcome α completely defines the corresponding values of the coefficients $c_k(\alpha)$ of the associated pure state $|\psi(\alpha)\rangle$, i.e. the value of α defines that deterministic-coefficient state $|\psi(\alpha)\rangle$, that thus has a probability $P(\alpha)$. The RV $\mathbf{c}_{\mathbf{k}}$, and hence the RV $\mathbf{p}_{\mathbf{k}}$ derived from (7), are thus discrete.

At first sight, the above discrete set of deterministiccoefficient pure states $|\psi(\alpha)\rangle$ and associated probabilities $P(\alpha)$ are reminiscent of how von Neumann introduces mixed states in Chapter IV of [14], before he moves to their description in terms of a density operator (pp. 295-296). However, the complete definition of how RCPS



FIG. 1. Estimation of parameters no. 3 and 4 of the matrix in (26), that is, v_3 and v_4 : Normalized Root Mean Square Error (NRMSE) of estimation vs. number K of measurements for (copies of) each of the N used states.

and mixed states are handled moreover contains the following major difference, which is the reason why they yield different properties for QIP tasks. When addressing mixed states, von Neumann considers all deterministiccoefficient pure states $|\psi(\alpha)\rangle$ as a whole and he only computes averages of physical quantities over all these states $|\psi(\alpha)\rangle$ (therefore involving the probabilities $P(\alpha)$), which corresponds to only considering the quantity $Tr(\rho \hat{A})$. The corresponding practical procedure is based on observable measurements, using what we here call "unsegmented data", i.e. computing a single observable average over all available data. In contrast, as explained in Section IIB, our multiple-preparation practical approach is based on segmented data. This means that we require the data to be created so that, separately for each outcome α , one accesses all measurement results for the single state $|\psi(\alpha)\rangle$. For a given α , this then makes possible to estimate all probabilities $p_k(\alpha)$ with $0 \leq k \leq d-1$. Then considering the complete set of data differently, separately for any index k with $0 \le k \le d-1$, we thus get the set of (estimated) values $p_k(\alpha)$ for all outcomes α . For any k, this defines the whole statistical distribution of the RV $\mathbf{p}_{\mathbf{k}}$. This distribution may then be exploited, thus providing QIP capabilities that cannot be achieved when only considering $Tr(\rho A)$ for a mixed state.

To summarize, richer information and hence better QIP capabilities are obtained with our randomprobability-based RCPS framework than with mixed states and $\text{Tr}(\rho \hat{A})$, but at the expense of adding a constraint, that is, using the above-defined segmented data of our multiple-preparation approach: this remains compatible with the results that von Neumann obtained in a *different* configuration than ours (unsegmented data) and with the idea that "there is no such thing as a free lunch", which is reasonable.

In other words, von Neumann defines mixed states by explicitly assuming: "if we do not even know what state is actually present – for example, when several states [...] with the respective probabilities [...] constitute the description", where the "several states" and "respective probabilities" he mentions are $|\psi(\alpha)\rangle$ and $P(\alpha)$ with our notations. In practice, these mixed states are handled by repeatedly drawing a pure state at random, measuring a given quantity, and finally averaging all measurement results, as explained above. In our multiple-preparation approach to RCPS, each pure state $|\psi(\alpha)\rangle$ is also randomly drawn but, once it has been selected, many copies of it are created (as discussed in Section IIB) and considered apart from all the data associated with any other deterministic-coefficient pure state that is subsequently also randomly drawn. This allows us to perform averaging for measurements corresponding to only the copies of that single state $|\psi(\alpha)\rangle$. This multiple-preparation approach thus requires many copies of each pure state $|\psi(\alpha)\rangle$ to accurately estimate the statistical distributions of all RV $\mathbf{p}_{\mathbf{k}}$, with $0 \leq k \leq d-1$.

In contrast, we also recently developed singlepreparation QIP methods, intended for BQPT, BHPE, BQSS and related tasks, as well as intrusion detection in quantum channels: see details in [2, 6, 11, 55]. This single-preparation approach is different from the multiple-preparation one but does not contradict it, as will now be shown. As suggested by its name, our singlepreparation approach can operate with few or even with only one preparation of each drawn pure state $|\psi(\alpha)\rangle$. This is acceptable because, for any index k, we did not use this approach to estimate the individual probabilities $p_k(\alpha)$ for all outcomes α , but only the expectation $E\{\mathbf{p}_{\mathbf{k}}\}$, i.e. the first-order moment of the RV $\mathbf{p}_{\mathbf{k}}$, using our procedure that we described in [2, 6, 11, 55]. When we developed that single-preparation approach, we did not comment about whether it could be extended to second-order and higher-order statistics of $\mathbf{p}_{\mathbf{k}}$, but we expected that it would be difficult, and possibly infeasible for some of those statistical parameters, because some linearity properties that we used for $E\{\mathbf{p}_k\}$ would not hold for other parameters. We can now extend that comment by taking into account, as follows, the considerations about von Neumann's mixed states that we provided above. We explained that our multiple-preparation approach to RCPS yields higher capabilities than the use of mixed states, because it segments the measured data and it is thus able to estimate some parameters (namely the probabilities $p_k(\alpha)$), for each segment. But when the length of each segment, i.e. the number of copies of each state $|\psi(\alpha)\rangle$, decreases down to one, not only the probabilities $p_k(\alpha)$ cannot be individually estimated, but the concept of segment itself vanishes: we are left we an overall set of states $|\psi(\alpha)\rangle$, with one copy of each such state, and the only averages we can compute are over this complete data set. This corresponds to the higher level of the two-level procedure that we defined above, after (9), for this multiple-preparation approach, whereas the lower level here disappears. But, if only computing an overall average for the complete set of data, we thus get back to von Neumann's approach based on mixed states. Therefore, unless we will disclose another trick for handling the single-preparation configuration differently for RCPS [56], at this stage it seems that it will face the same limitation as the approach based on mixed states.

Two RCPS-based approaches with complementary features are thus currently available. The first one is the multiple-preparation approach, which has the abovedefined advantages, that result from the use of the second-order and higher-order statistics of the probabilities $\mathbf{p}_{\mathbf{k}}$ and the drawback of requiring multiple and segmented preparations. The second one is the singlepreparation approach, which yields simpler operation or is even required in some applications (e.g. statistical intrusion detection), as detailed e.g. in [2, 6, 11, 55], but which currently applies only to QIP problems that can be solved by only using the expectation, i.e. first-order statistics, of $\mathbf{p}_{\mathbf{k}}$.

V. OTHER RELATED WORKS

The above-defined topics of this investigation also compare as follows with previous works from the literature. The first topic is the concept of RCPS themselves and hence its relationships with "random quantum states" in a broad sense. Of course, usual concepts of quantum mechanics already involve randomness, because a measurement performed for a deterministic-coefficient pure state usually yields a random result. In the present section we do not address that basic type of randomness (which corresponds to the lower level of our multiple-preparation procedure of Section IIB), but the types of randomness that may be defined in addition to that basic type and to von Neuman's concepts related to mixed states that we presented in Section IV (for our RCPS, the additional type of randomness corresponds to the higher level of our multiple-preparation procedure of Section IIB). This yields the following three aspects.

First, not yet focusing on RCPS, some papers from the literature contain limited statements about "random quantum states" in a broad sense. In particular, [57] especially deals with quantum thermal states and considers that "a random state [...] can be used to represent the outcome of a measurement process, or to describe the statistics of an ensemble" but does not use the concept of RCPS as defined in the present paper (for the quantum framework, [57] only mentions "random phases").

Second, [58] mainly considers a random quantum pure state as a whole, i.e. as a vector, without explicitly providing its mathematical expression in a given basis: that paper is not very detailed. It briefly mentions "the components of the state vector, in some fixed basis" but does not refer to random variables for these components. Moreover, it is restricted to specific probability distributions for the above quantities, namely to the case when "pure states are distributed uniformly over the unit sphere" and possibly in addition e.g. "subjected to the restriction that all the components of the state vector in the given basis be real." In contrast, in the present paper, we allow arbitrary probability distributions for the ket coefficients. This is very important, because it is required for being able to address a wide range of QIP problems, especially blind (i.e. unsupervised) processing problems, where some probability distributions may be unknown.

Finally, quite a few papers, published more recently than our first papers (that include [1]), have closer relationships with our work: although they do not use the term RCPS, they use that concept or closely related ones, i.e. a ket whose coefficients are random variables, or at least related to random variables. More precisely, in [59] the ket coefficients are defined as "functions of complex-valued random variables $\boldsymbol{\xi}$ " where $\boldsymbol{\xi}$ is a vector, whereas in [60] these coefficients themselves "are chosen at random from some given probability distribution". Moreover, both [59] and [60] then only focus on quite specific probability distributions: see the symmetries and constraints on even and odd functions imposed in [59], together with the three specific probability densities defined in its Table I, e.g. leading to states that are uniformly distributed over the unit sphere; instead [60] "consider[s] the [ket coefficients] as iid (real, complex or quaternion-real) Gaussian variables with zero mean" (which, by the way, cannot be an accurate model of actual behavior: the modulus of a ket coefficient is upper bounded by one, so that this coefficient cannot have an unbounded Gaussian density). In contrast, as stated above, we allow arbitrary probability distributions for the ket coefficients.

Let us then focus on the only above-mentioned papers from the literature that are connected with RCPS, namely [59, 60] and, to a much lower extent, [58]. Those papers completely differ from the present one concerning its other topics, beyond the RCPS concept. First, the core feature analyzed in this paper consists of the second-order and especially higher-order moments of the random ket coefficients and associated random probabilities, including their practical estimation. Instead, [59] only mentions a very limited set of moments (see the three moments in Table I), whereas [58, 60] do not mention them at all. Second, apart from quantum theory, the present paper aims at exploiting the above moments for performing various QIP tasks, e.g. related to QPT and quantum parameter estimation. In contrast, [59] has other goals (quantum numerical simulation) and only mentions (quite a few) moments as a by-product.

Finally, we stress that some papers from the quantum literature mention concepts related to higher-order moments, but in quite different frameworks than ours. In particular, in [61] Mielnik considers non-standard frameworks as announced in his title: "Generalized quantum mechanics". He especially imagines what could be done in "hypothetical theories" where one would "assume that the class of observables F is not the set of the quadratic forms like in orthodox theory but the set F_{2n} of all the continuous 2n-th order forms". He thus develops "higher order schemes" and comments about "higher order multipole moments". This is quite different from our approach, that has the following features. We stick to orthodox measurements for each deterministic pure state considered in the lower level of our procedure, so that each outcome probability is equal to (the modulus of) a "quadratic function of a ket coefficient". This relates to Mielnik's statement: "one might define the orthodox quantum mechanics as a theory of such a *c*-number wave for which only the quadratic forms are the observables". But, unlike Mielnik, we perform our complete set of orthodox measurements for our new type of states, namely RCPS, i.e. we organize these measurements according to the higher level of our procedure. Our complete approach is thus compatible with the orthodox theory, but yields a new feature: it allows us to introduce the higher-order moments associated with the (random) ket coefficients of the considered new type of states. Besides, Mielnik explains that "Since the quadratic character of the observables is conditioned by the linearity of the evolution processes the most obvious [situation where the orthodox quantum theory would not apply] consists in hypothetical evolution processes in which the quantum mechanical wave function would undergo a non-linear change". This leads him to "non-linear versions of quantum mechanics in which a non-linear wave equation would play the role of the Schrödinger equation". In contrast, our approach is fully compatible with Schrödinger's picture of quantum mechanics and our "higher-order effects" come from the advanced use of the statistics of random ket coefficients. allowed by the existence of RCPS themselves.

VI. CONCLUSION

As explained in Section IIC, when considering mixed states, von Neumann claimed that one only needs to use the density operator ρ and the mean of observable $Tr(\rho A)$. In the present paper, we provide a detailed theoretical analysis of another type of states, that we repeatedly used in our application-driven papers since 2007. We call these states "random-coefficient pure states" or RCPS, since their coefficients c_k in a given basis are random variables (we compared RCPS with mixed states in Section IV). With these RCPS too, one can associate a density operator. However, restricting the use of RCPS to that operator ρ and moreover possibly to a mean of observable $Tr(\rho A)$ would result in only considering the second-order statistics of the random variables $\mathbf{c}_{\mathbf{k}}$ and therefore in ignoring a large part of the information available from RCPS. Instead, we proposed to exploit the higher-order (i.e. higher than 2) statistics of $\mathbf{c}_{\mathbf{k}}$, through the second-order and higher-order statistics of the associated random probabilities $\mathbf{p}_{\mathbf{k}} = |\mathbf{c}_{\mathbf{k}}|^2$. We showed that this allows one to access much richer information and to solve quantum information processing (QIP) problems that cannot be handled with the mean value $Tr(\rho A)$ only. We illustrated that phenomenon for one concrete QIP problem, related to the well-known quantum process tomography task. Many other potential applications of RCPS exist. Some of them were suggested above and we plan to investigate such applications in future work.

So, having in mind Feynman's general statement that "There's plenty of room at the bottom" e.g. for computing, we may summarize our main claim in this paper as follows: to exploit the wealth of the information available from random-coefficient pure states, there is plenty of room at the higher orders (of the statistics of the random coefficients $\mathbf{c_k}$ of these quantum states).

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- [30] Our previous investigations related to BQSS, BQPT and BHPE involve a quantum process. The above-mentioned papers [1–3], [4] (Section 1.7.2), [6] directly use statistical parameters of the probabilities $\mathbf{p}_{\mathbf{k}}$ of measurements performed at the output of that process. In contrast, other investigations, dealing with BQSS, first use the individual values of these classical-form data $\mathbf{p}_{\mathbf{k}}$ as the input of a classical processing system, called the separating system. The outputs of that system aim at restoring modulus parameters and combinations of phase parameters of coefficients of several single-qubit quantum states. These parameters thus have some relationships with the quantities $\mathbf{r}_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ in (10). These BQSS methods are based on

various statistical parameters of the outputs of the separating system: their generalized moments are used in Section 1.7.3 of [4] and their cumulants in [62], whereas their whole pdf are exploited through their mutual information (see Section 1.5 of [4]), with a connection with the maximum likelihood approach (see Section 1.6 of [4]). All these approaches thus have an indirect link with the higher-order statistics of the $\mathbf{r}_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ parameters, and hence with those of $\mathbf{p}_{\mathbf{k}}$.

- [31] Although the mean of an observable is here intentionally analyzed without resorting to the content of Section II C, these two parts of this paper are clearly connected, because (21) is nothing but the quantity $\text{Tr}(\rho \hat{A})$ defined in Section II C for an RCPS, and the discussion provided after (21) therefore has connections with the comments we made in Section II C, mainly about the density operator ρ of an RCPS and partly about the resulting $\text{Tr}(\rho \hat{A})$.
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- [34] The mean of a function of an observable was not explicitly addressed in Section II C and was therefore independently detailed in the present section. However, its connection with Section II C may be shown as follows. G = g(A) is nothing but another observable, with an associated operator \hat{G} . Eq. (23) defines the mean $E\{G\}_{|\psi\rangle}$ of that new observable, that could also be expressed as $\operatorname{Tr}(\rho \hat{G})$ and that therefore has the limitations that we defined for $E\{A\}_{|\psi\rangle} = \operatorname{Tr}(\rho \hat{A})$ in Section II C and at the beginning of the present section, when considering an *arbitrary* observable A.
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- [54] Classical Blind Source Separation (BSS) methods are sometimes stated to be "semi-blind", rather than "blind", because they require some prior knowledge about the source signals to be separated, e.g. these signals may be requested to be statistically independent. That term "semi-blind" is especially used for methods that are more constraining concerning that prior knowledge, e.g. methods that constrain some source moments to be known or to belong to known intervals in addition to requesting source independence. From that point of view, the basic version of the quantum estimation method pro-

posed hereafter might be stated to be "semi-blind" because, in addition to requesting \mathbf{r} and ϕ to be statistically independent, it uses additional constraints on the marginal statistics of \mathbf{r} and ϕ , as detailed in Section III C (in fact, the proposed quantum estimation method does not require one to know all the statistical distributions of \mathbf{r} and ϕ but only the resulting parameters defined in (40)-(45)). Anyway, it remains that this proposed quantum estimation method does not require the *individual* values of the input to be known, which is the main feature of blind and associated methods.

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