Quantum process tomography with unknown single-preparation input states

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Quantum Process Tomography (QPT) methods aim at identifying, i.e. estimating, a given quantum process. QPT is a major quantum information processing tool, since it especially allows one to characterize the actual behavior of quantum gates, which are the building blocks of quantum computers. However, usual QPT procedures are complicated, since they set several constraints on the quantum states used as inputs of the process to be characterized. In this paper, we extend QPT so as to avoid two such constraints. On the one hand, usual QPT methods requires one to know, hence to precisely control (i.e. prepare), the specific quantum states used as inputs of the considered quantum process, which is cumbersome. We therefore propose a Blind, or unsupervised, extension of QPT (i.e. BQPT), which means that this approach uses input quantum states whose values are unknown and arbitrary, except that they are requested to meet some general known properties (and this approach exploits the output states of the considered quantum process). On the other hand, usual QPT methods require one to be able to prepare many copies of the *same* (known) input state, which is constraining. On the contrary, we propose "single-preparation methods", i.e. methods which can operate with only one instance of each considered input state. These two new concepts are here illustrated with practical BQPT methods which are numerically validated, in the case when: i) random pure states are used as inputs and their required properties are especially related to the statistical independence of the random variables that define them, ii) the considered quantum process is based on cylindrical-symmetry Heisenberg spin coupling. These concepts may be extended to a much wider class of processes and to BQPT methods based on other input quantum state properties.

I. INTRODUCTION

System identification and system inversion are two closely related problems. First considering classical, i.e. non-quantum, signals and systems, the basic version of system identification concerns single-input single-output (SISO) systems. It consists of estimating the unknown parameter values of such a system (i.e. of the transform that it performs) belonging to a known class, by using known values of its input (source signal s) and output (signal x). This version [23] is stated to be "non-blind" by the signal and image processing community [1] or "supervised" by the machine learning and data analysis community [32]. The more challenging version of that problem is the blind [1] or unsupervised one, where the input values are unknown and uncontrolled, but it may be known that the input signal belongs to a given class (due to this partial knowledge, these methods are sometimes stated to be semi-blind). Both versions may then be extended to multiple-input multiple-output (MIMO) systems.

Besides, in various applications, what is needed is not the direct transform performed by the above system, but the inverse of that transform (assuming it is invertible).

For SISO non-blind and blind configurations, this is motivated by the fact that one eventually only accesses the ouput x of the above direct system, and one aims at deriving a signal y which ideally restores the original source signal s. To this end, one may first use the above-mentioned system identification methods in order to estimate the direct system, then derive its inverse and eventually transfer the output x of the direct system through the inverse system. Alternatively, one may develop methods for initially identifying the *inverse* system itself. Extended versions of this "(unknown) system inversion" task concern MIMO configurations, where a set of original source signals s_1 to s_M are to be respectively restored on the outputs y_1 to y_M of the inverse system.

The blind MIMO version of the above system inversion problem is almost the same as blind source separation (BSS) [7],[15],[21]: as in system inversion, BSS aims at canceling the contributions of all sources but one in each output signal of the separating system; however, in BSS, one often allows each output signal to be equal to a source signal only up to an acceptable residual transform. These transforms, called indeterminacies, cannot be avoided because only limited constraints are set on the source signals and on the direct system which combines (i.e., "mixes", in BSS terms) these signals. In particular, the first class of BSS methods that was developed and that is still of major importance is Independent Component Analysis, or ICA [7],[15],[21], which may be seen

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as an extension of more conventional Principal Component Analysis, or PCA [22] (PCA alone cannot achieve BSS [21]). ICA is a statistical approach, which essentially requires statistically independent random source signals. Thus, for the simplest class of mixtures, ICA is guaranteed to restore the source signals up to limited indeterminacies [7],[15],[21].

We now consider quantum information processing (QIP) [27] and quantum machine learning [3],[8],[29], i.e. processing of quantum data and/or processing with quantum means, and we still focus on system identification and inversion problems. Among these problems, the one which was first studied is the quantum version of non-blind system identification, especially [35] introduced in 1997 in [6] and called "quantum process tomography" or QPT by the QIP community: see e.g. [2], [4], [5], [25], [26], [27], [30], [31], [33], [34]. The quantum version of the above-mentioned classical source separation, called Quantum Source Separation, or QSS, and especially its blind version, or BQSS, were then introduced in 2007 in [9]. Two main classes of BQSS methods were developed since then. The first one may be seen as a quantum extension of the above-mentioned classical ICA methods, since it takes advantage of the statistical independence of the parameters that define random source quantum states (qubit states). It is called Quantum Independent Component Analysis (or QICA, see e.g. [9],[10]) or, more precisely, Quantum-Source Independent Component Analysis (or QSICA, see e.g. [13]) to insist on the quantum nature of the considered source data, whereas it uses classical processing means (after quantum/classical data conversion). The second main class of BQSS methods was introduced in 2013-2014 in [11],[12] and then especially detailed in [16]. It is based on the unentanglement of the considered source quantum states and it typically uses quantum processing means to restore these unknown states from their coupled version. Independently from the above quantum extensions of ICA, a quantum version of PCA was introduced in 2014 in [24].

In the present paper, our first contribution (see Section IV) concerns yet another type of unsupervised quantum machine learning methods [3], namely Blind Quantum Process Tomography, or BQPT. Here again, the term "blind", or "unsupervised", refers to the fact that we consider situations where the input values of the process to be identified are unknown, but they are requested to meet some (hereafter statistical) properties. We briefly introduced that BQPT concept in 2015 in [14] and we only outlined some resulting BQPT methods in that and some subsequent short conference papers, but only as spin-offs of corresponding BQSS methods. On the contrary, the present paper is the first one where we provide a detailed description of a method which combines the following features:

1. This method is primarily intended for BQPT, not for BQSS. To this end, it only uses classical processing means: on the contrary, using quantum processing means requires one to precisely characterize

them beforehand, which is a significant drawback here, since BQPT, as QPT, is especially developed as a tool for characterizing quantum gates, as discussed in Sections V D and VII.

2. This BQPT method therefore first performs measurements at the output of the system, i.e. quantum process, to be identified (see Section III), in order to convert quantum states into classical-form data before they are processed with classical means.

3. Moreover, for the Heisenberg coupling process considered below as an example (see Section II), we aim at minimizing the number of types of measurements performed to fully characterize that process.

As detailed further in this paper, usual, i.e. non-blind, QPT, as well as the above first form of BQPT, use sample frequencies of the above-mentioned measurement outcomes at the output of the process (i.e. normalized cumulative values associated with these outcomes), derived from many copies of each considered state value. To apply such methods, one should therefore be able to *prepare* many copies of the *same* input state, which is cumbersome. Our second contribution in this paper (see Section V) then consists of extensions of the above BQPT methods, which also allow one to use few copies or even one instance (i.e. preparation) of each quantum state. The numerical performance of this second type of methods is reported in Section VI, whereas its applications are presented in Section VII, together with conclusions drawn from this investigation.

II. CONSIDERED QUANTUM PROCESS AND STATE PROPERTIES

In QPT and BQPT problems, the system or process to be identified receives a quantum state $|\psi(t_0)\rangle$, e.g. associated with a set of qubits considered at time t_0. This system outputs a quantum state $|\psi(t)\rangle$ associated with the same set of qubits at a later time t. The behavior of the system is defined by an operator which may be rather general (e.g. an arbitrary unitary operator) or which may be restricted to a given class of operators corresponding to a specific type of physical devices (see e.g. [26]). In this paper, we address the second case and we consider a device composed of two distinguishable qubits [16] implemented as electron spins 1/2, that are coupled according to the cylindrical-symmetry Heisenberg model, which is e.g. relevant for spintronics applications. We stress that this type of coupling is only used as a concrete example, to show how to fully implement the proposed concepts in a relevant case, but that these concepts and resulting practical BQPT algorithms may then be transposed by the reader to other classes of quantum processes and associated applications.

The symmetry axis of the Heisenberg model is here denoted as Oz. The considered spins are supposed to be

placed in a magnetic field (also oriented along Oz and with a magnitude B) and thus coupled to it. Moreover, we assume an isotropic $\overline{\overline{g}}$ tensor, with principal value g. The time interval when these spins are considered is supposed to be short enough for their coupling with their environment to be negligible. In these conditions, the temporal evolution of the state of the device composed of these two spins is governed by the following Hamiltonian:

$$H = Gs_{1z}B + Gs_{2z}B - 2J_{xy}(s_{1x}s_{2x} + s_{1y}s_{2y})$$
$$-2J_z s_{1z}s_{2z} \tag{1}$$

where:

- $G = g\mu_e$, where μ_e is the Bohr magneton, i.e. $\mu_e = e\hbar/2m_e = 0.927 \times 10^{-23} JT^{-1}$ and $\hbar$ is the reduced Planck constant,

- s_{ix}, s_{iy}, s_{iz}, with $i \in \{1,2\}$, are the three components of the vector operator $\overrightarrow{s_i}$ associated with spin i in a cartesian frame,

- J_{xy} and J_z are the principal values of the exchange tensor.

Among the above parameters, the value of g may be experimentally determined, and B can be measured. The values of J_{xy} and J_z are here assumed to be unknown.

We here suppose that each spin i, with $i \in \{1,2\}$, is prepared, i.e. initialized, at a given time t_0, in the pure state

$$|\psi_i(t_0)\rangle = \alpha_i|+\rangle + \beta_i|-\rangle \tag{2}$$

where $|+\rangle$ and $|-\rangle$ are eigenkets of s_{iz}, for the eigenvalues $1/2$ and $-1/2$ respectively. We will further use the polar representation of the qubit parameters α_i and β_i, which reads

$$\alpha_i = r_i e^{i\theta_i} \quad \beta_i = q_i e^{i\phi_i} \quad i \in \{1,2\} \tag{3}$$

where i is the imaginary unit, and with $0 \le r_i \le 1$ and

$$q_i = \sqrt{1 - r_i^2} \quad i \in \{1,2\} \tag{4}$$

because each spin state $|\psi_i(t_0)\rangle$ has unit norm. Moreover, for each couple of phase parameters θ_i and ϕ_i, only their difference has a physical meaning. After they have been prepared, these spins are coupled according to the above-defined model for $t \ge t_0$.

Hereafter, we consider the state of the overall system composed of these two distinguishable spins. At time t_0, this state is equal to the tensor product of the states of both spins defined in (2). It therefore reads

$$|\psi(t_0)\rangle = |\psi_1(t_0)\rangle \otimes |\psi_2(t_0)\rangle \tag{5}$$
$$= \alpha_1\alpha_2|++\rangle + \alpha_1\beta_2|+-\rangle$$
$$+ \beta_1\alpha_2|-+\rangle + \beta_1\beta_2|--\rangle \tag{6}$$

in the four-dimensional basis $\mathcal{B}_+ = \{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$.

The state of this two-spin system then evolves with time. Its value $|\psi(t)\rangle$ at any subsequent time t may be derived from its above-defined Hamiltonian. It is defined [10] by

$$C_+(t) = MC_+(t_0) \tag{7}$$

where $C_+(t_0)$ and $C_+(t)$ are the column vectors of components of $|\psi(t_0)\rangle$ and $|\psi(t)\rangle$, respectively, in basis $\mathcal{B}_+$. For instance, as shown by (6),

$$C_+(t_0) = [\alpha_1\alpha_2, \alpha_1\beta_2, \beta_1\alpha_2, \beta_1\beta_2]^T \tag{8}$$

where ^{T} stands for transpose. Moreover, the matrix M of (7), which defines the transform applied to $|\psi(t_0)\rangle$, reads

$$M = QDQ^{-1} = QDQ \tag{9}$$

with

$$Q = Q^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{10}$$

and D equal to

$$\begin{bmatrix} e^{-i\omega_{1,1}(t-t_0)} & 0 & 0 & 0 \\ 0 & e^{-i\omega_{1,0}(t-t_0)} & 0 & 0 \\ 0 & 0 & e^{-i\omega_{0,0}(t-t_0)} & 0 \\ 0 & 0 & 0 & e^{-i\omega_{1,-1}(t-t_0)} \end{bmatrix}. \tag{11}$$

The four real (angular) frequencies $\omega_{1,1}$ to $\omega_{1,-1}$ in (11) depend on the physical setup. In [10], it was shown that they read

$$\omega_{1,1} = \frac{1}{\hbar}\left[GB - \frac{J_z}{2}\right], \quad \omega_{1,0} = \frac{1}{\hbar}\left[-J_{xy} + \frac{J_z}{2}\right], \tag{12}$$

$$\omega_{0,0} = \frac{1}{\hbar}\left[J_{xy} + \frac{J_z}{2}\right], \quad \omega_{1,-1} = \frac{1}{\hbar}\left[-GB - \frac{J_z}{2}\right]. \tag{13}$$

Since the values of the parameters J_{xy} and J_z of the Hamiltonian of (1) are presently unknown, the values of the parameters $\omega_{1,1}$ to $\omega_{1,-1}$ of the quantum process involved in (7) are also unknown.

In this paper, we address the (B)QPT problem, i.e. we aim at estimating the matrix M involved in (7), which defines the considered quantum process. Moreover, we estimate it in a blind, i.e. unsupervised, way, that is:

- by using values of the output state $|\psi(t)\rangle$ of this process,

- without using nor knowing values of its input state $|\psi(t_0)\rangle$,

- but by knowing and exploiting some properties of these states $|\psi(t_0)\rangle$. In this paper, these requested properties are as follows. The states $|\psi(t_0)\rangle$ are

required to be unentangled (as shown by (5)). Besides, the proposed BQPT methods are statistical approaches and the six parameters r_i, θ_i and ϕ_i, with $i \in \{1,2\}$, defined in (3) are constrained to have properties that are similar to those requested in the above-mentioned QSICA methods: (i) these parameters are random valued, so that we here consider random pure quantum states $|\psi_i(t_0)\rangle$ (see [17] for more details) and (ii) some combinations of the random variables (RVs) r_i, θ_i and ϕ_i are statistically independent and have a few known statistical features, as detailed further in this paper.

As explained in Section I, the considered BQPT task is performed by using only classical-form processing means. To this end, the available quantum-form data, namely the output states $|\psi(t)\rangle$, are first converted into classical-form data, by means of measurements, as described hereafter.

III. MEASUREMENTS FOR PROCESS OUTPUTS

The first type of proposed BQPT approaches uses a set of copies of each output state $|\psi(t)\rangle$. For each copy, it measures the components of the considered two spins along the above-defined Oz direction. The result of each such measurement has four possible values, that is $(+\frac{1}{2}, +\frac{1}{2})$, $(+\frac{1}{2}, -\frac{1}{2})$, $(-\frac{1}{2}, +\frac{1}{2})$ or $(-\frac{1}{2}, -\frac{1}{2})$ in normalized units (see Appendix A 1). Their probabilities are respectively denoted as p_{1zz} to p_{4zz} hereafter. Using the polar representation (3), these probabilities read [10],[13]

$$p_{1zz} = r_1^2 r_2^2 \tag{14}$$

$$p_{2zz} = r_1^2(1-r_2^2)(1-v^2) + (1-r_1^2)r_2^2 v^2$$
$$- 2r_1 r_2 \sqrt{1-r_1^2}\sqrt{1-r_2^2}\sqrt{1-v^2}\, v \sin \Delta_I \tag{15}$$

$$p_{4zz} = (1-r_1^2)(1-r_2^2) \tag{16}$$

with

$$\Delta_I = (\phi_2 - \theta_2) - (\phi_1 - \theta_1) \tag{17}$$

$$\Delta_E = -\frac{J_{xy}(t-t_0)}{\hbar} \tag{18}$$

$$v = \text{sgn}(\cos \Delta_E) \sin \Delta_E. \tag{19}$$

Probability p_{3zz} is not considered hereafter because the sum of p_{1zz} to p_{4zz} is equal to 1.

In practice, for each value of state $|\psi(t)\rangle$, estimates of probabilities p_{1zz} to p_{4zz} are derived, typically as the sample frequencies of the associated measurement outcomes obtained for all copies of $|\psi(t)\rangle$ (see e.g. [4],[6],[10],[13]).

Similarly, these BQPT approaches use another set of copies of each output state $|\psi(t)\rangle$, by measuring the two spin components along an axis Ox which is orthogonal to Oz. These measurements yield the same four possible outcomes as above, but with different probabilities, which

are denoted as p_{1xx} to p_{4xx} hereafter. As shown in [18], these probabilities have the following properties

$$p_{1xx} - p_{4xx} = R_{14}w_1 - I_{14}w_2 \tag{20}$$

where

$$R_{14} = r_1^2 r_2 \sqrt{1-r_2^2}\cos(\phi_2 - \theta_2)$$
$$+ r_2^2 r_1 \sqrt{1-r_1^2}\cos(\phi_1 - \theta_1)$$
$$+ (1-r_1^2)r_2\sqrt{1-r_2^2}\cos(\phi_2 - \theta_2 - \Delta\Phi_{1,-1})$$
$$+ (1-r_2^2)r_1\sqrt{1-r_1^2}\cos(\phi_1 - \theta_1 - \Delta\Phi_{1,-1}) \tag{21}$$

$$I_{14} = -r_1^2 r_2 \sqrt{1-r_2^2}\sin(\phi_2 - \theta_2)$$
$$- r_2^2 r_1 \sqrt{1-r_1^2}\sin(\phi_1 - \theta_1)$$
$$+ (1-r_1^2)r_2\sqrt{1-r_2^2}\sin(\phi_2 - \theta_2 - \Delta\Phi_{1,-1})$$
$$+ (1-r_2^2)r_1\sqrt{1-r_1^2}\sin(\phi_1 - \theta_1 - \Delta\Phi_{1,-1}) \tag{22}$$

$$w_1 = \cos \Delta\Phi_{1,0} \tag{23}$$

$$w_2 = \sin \Delta\Phi_{1,0} \tag{24}$$

$$\Delta\Phi_{1,-1} = -\frac{2GB(t-t_0)}{\hbar} \tag{25}$$

$$\Delta\Phi_{1,0} = \frac{(t-t_0)}{\hbar}\left(-J_{xy} + J_z - GB\right). \tag{26}$$

The value of $\Delta\Phi_{1,-1}$ in (25) is known, since it can be derived from the above-defined known quantities. Moreover

$$p_{1xx} + p_{4xx} = \frac{1}{2} + r_1 r_2 \sqrt{1-r_1^2}\sqrt{1-r_2^2}\left[\cos \Delta_I\right.$$
$$\left. + \cos\left((\phi_1 - \theta_1) + (\phi_2 - \theta_2) - \Delta\Phi_{1,-1}\right)\right]. \tag{27}$$

The BQPT methods proposed in this paper therefore consist of two major steps. The first step aims at estimating the unknown values of the parameters v, w_1 and w_2 of the mappings from the parameters r_i, θ_i and ϕ_i of the initial qubit states $|\psi(t_0)\rangle$ to the probabilities of measurement outcomes, namely p_{jzz} and p_{jxx}, with $j = 1$ to 4, or their combinations. The second step then uses the estimated values of v, w_1 and w_2 to derive an estimate of matrix D of (9) and hence of the complete matrix M of (9), which defines the considered process. We now proceed to the description of these methods.

IV. MULTIPLE-PREPARATION BQPT METHODS

We first consider the estimation of parameter v. This is achieved by exploiting (15). If we were developing a

conventional, i.e. non-blind, QPT method, we would use one or several instances of Eq. (15), and each of these instances would involve (i) known values of the input parameters r_i, θ_i, ϕ_i and hence Δ_I of $|\psi(t_0)\rangle$ and (ii) an estimate of the set of output probabilities p_{jzz}, derived from a set of copies of $|\psi(t)\rangle$. This approach is constraining because it requires one to *precisely* prepare each state *value* $|\psi_i(t_0)\rangle$ (for state preparation and associated errors, see e.g. [6]), otherwise the errors in r_i and Δ_I yield errors in the estimated value of v.

The above drawback is avoided by our BQPT methods. Following the above-defined terminology, these methods are blind in the sense that they estimate v by using only a set of estimated values of output probabilities p_{jzz}, without knowing the values of the input parameters r_i, θ_i, ϕ_i and hence Δ_I, but requesting them to have some known properties. More precisely, we here consider statistical methods, which operate with a set of random states $|\psi_i(t_0)\rangle$ and which thus only set constraints on some of the *statistical parameters* of (combinations of) r_i, θ_i, ϕ_i, not on their *individual values* for each state $|\psi_i(t_0)\rangle$. In particular, the versions of these BQPT methods considered in this paper use only the first-order mean statistics of the available quantities p_{jzz}, i.e. their expectations $E\{p_{jzz}\}$. When assuming r_1, r_2 and Δ_I to be statistically independent RVs, (15) yields

$$
\begin{aligned}
E\{p_{2zz}\} = {} & E\{r_1^2\}(1 - E\{r_2^2\})(1 - v^2) \\
& + (1 - E\{r_1^2\})E\{r_2^2\}v^2 \\
& - 2E\{r_1\sqrt{1 - r_1^2}\}E\{r_2\sqrt{1 - r_2^2}\}\sqrt{1 - v^2}v \\
& \times E\{\sin \Delta_I\}.
\end{aligned}
\tag{28}
$$

In this equation, $E\{p_{2zz}\}$ is known: in practice, it is estimated as the sample mean of the estimates of all values of p_{2zz}, themselves typically estimated with sample frequencies, as explained above. Besides, as detailed e.g. in [10],[13] for BQSS methods intended for the Heisenberg coupling model, setting the constraint

$$
0 < r_1 < \frac{1}{2} < r_2 < 1
\tag{29}
$$

allows one to derive r_1 and r_2 from (14) and (16) without any ambiguity, for each unknown state $|\psi(t_0)\rangle$. This yields

$$
\begin{aligned}
r_i = \Bigg[\frac{1}{2} \Big[& (1 + p_{1zz} - p_{4zz}) \\
& + \epsilon_i\sqrt{(1 + p_{1zz} - p_{4zz})^2 - 4p_{1zz}} \Big] \Bigg]^{1/2} \quad i \in \{1, 2\}
\end{aligned}
\tag{30}
$$

with $\epsilon_1 = -1$ and $\epsilon_2 = 1$. Taking the sample mean of any function of r_i defined by (30) then yields estimates of all statistics of r_i involved in (28). Finally, we only set the following constraint on one statistical parameter of the used values of θ_i and ϕ_i, again without having to know their individual values. We request the states $|\psi(t_0)\rangle$ to be prepared with a procedure which is such that the

value of $E\{\sin \Delta_I\}$ is known. With these constraints on input state statistics, the only unknown in (28) is v. By solving this type of equations, this BQPT method then yields the desired estimate of v. In particular, a simple case consists of using $E\{\sin \Delta_I\} = 0$ (which may e.g. be achieved by preparing the two spins with states such that $(\phi_1 - \theta_1)$ and $(\phi_2 - \theta_2)$ are statisticially independent and have the same statistics): then, (28) straightforwardly yields

$$
v^2 = \frac{E\{p_{2zz}\} - E\{r_1^2\}(1 - E\{r_2^2\})}{E\{r_2^2\} - E\{r_1^2\}}.
\tag{31}
$$

In some configurations the sign of v is known [10],[13], so that the value of v may be derived from (31). Otherwise, it may be derived from another instance of (28), using data that yield another value of $E\{\sin \Delta_I\}$: details about how to solve this sign indeterminacy and how to also estimate parameters w_1 and w_2 are provided below for an improved version of our methods. Indeed, the above version of BQPT is attractive because it does not require each value of $|\psi(t_0)\rangle$ to be known, but it still yields a limitation: it requires one to be able to prepare the *same* value $|\psi(t_0)\rangle$ a large number of times, to derive an associated frequency-based estimate of each set of probabilities p_{jzz}. This still requires some control of the input states of the process, that we would like to avoid, in order to simplify the practical operation of BQPT methods and to make them "blinder". We hereafter show how to avoid this preparation of many copies of each state $|\psi(t_0)\rangle$.

V. SINGLE-PREPARATION BQPT METHODS

A. Single-preparation QIP

As a second contribution in this paper, we now extend (B)QPT methods so that they can operate with a few copies or even a single instance of each considered input state $|\psi(t_0)\rangle$. For non-blind methods as defined above, this does not seem to be possible, because they need many copies of each state $|\psi(t_0)\rangle$ and associated outcomes of measurements performed for each state $|\psi(t)\rangle$, in order to derive a frequency-based estimate of each set of probabilities p_{jzz}. On the contrary, our blind versions of QPT can be extended so as to reach this goal, because they only need one to estimate *expectations* of these (now random) probabilities p_{jzz}, i.e. $E\{p_{jzz}\}$, not each of their individual values p_{jzz} for each state $|\psi(t_0)\rangle$. In the short conference paper [19], we very recently introduced a general QIP framework (i.e., not restricted to BQPT) for estimating expectations $E\{p_j\}$ of probabilities p_j of outcomes of general types of quantum measurements. Its principle is summarized hereafter, whereas its detailed description and properties are provided in Appendix A.

For each expectation $E\{p_j\}$ of a random probability p_j to be estimated, as discussed above, in practice the expectation operator $E\{.\}$ is replaced by a sample mean,

i.e. by a *sum* (of values, moreover normalized). Similarly, each probability p_j is replaced by a sample frequency, i.e. by a *sum* (of 1 and 0, depending whether the considered event occurs or not for each trial defined by a preparation of the initial quantum states (2) and by an associated measurement of a couple of spin components; this summation is here again followed by a normalization, by the total number of trials). $E\{p_j\}$ is therefore estimated by a (normalized) "sum of sums", which may then be reinterpreted as a single global sum, and what primarily matters is the total number of preparations of initial quantum states (2) involved in that global sum, whereas the number of preparations for each state value (2) may be decreased, down to 1, as confirmed by simulations in Section VI (which also justifies why even better performance is obtained when decreasing the number of preparations per state for a given total number of preparations, i.e. while increasing accordingly the considered number of different states). The corresponding BQPT methods are therefore called single-preparation BQPT methods. It should be clear that they can be freely used with either one instance or several (e.g. many) copies per state, i.e. the above terminology means that these methods *allow* one to use a single instance of each state. On the contrary, our so-called multiple-preparation BQPT methods *force* one to use many state copies to achieve good performance.

B. Estimating the parameter of Oz measurements

We here aim at using the single-preparation approach of Section V A to estimate the parameter v involved in the probabilities p_{jzz}. We hereafter again take advantage of (28), and especially of its version (31), derived in Section IV for our multiple-preparation BQPT method. However, these expressions involve $E\{r_1^2\}$ and $E\{r_2^2\}$ which, unlike in Section IV, cannot here be estimated by using the expectation of the square of (30) because this involves expectations of *nonlinear combinations* of the above probabilities p_{1zz} to p_{4zz}, whereas we here aim at developing a *single-preparation* algorithm, for which Section V A only defined how to estimate the expectations of p_{1zz} to p_{4zz} themselves. We here solve this problem by using a modified approach, where we first take the expectation of (14) and (16), again for statistically independent RVs r_1 and r_2. This yields

$$E\{p_{1zz}\} = E\{r_1^2\}E\{r_2^2\} \tag{32}$$

$$E\{p_{4zz}\} = (1 - E\{r_1^2\})(1 - E\{r_2^2\}). \tag{33}$$

These equations involve only the unknown of interest, $E\{r_1^2\}$ and $E\{r_2^2\}$. Again setting the constraint (29), they yield the unique solution

$$E\{r_i^2\} = \frac{1}{2}\left[(1 + E\{p_{1zz}\} - E\{p_{4zz}\})\right.$$
$$\left. + \epsilon_i \sqrt{(1 + E\{p_{1zz}\} - E\{p_{4zz}\})^2 - 4E\{p_{1zz}\}}\right]$$
$$i \in \{1, 2\} \tag{34}$$

again with $\epsilon_1 = -1$ and $\epsilon_2 = 1$. If the sign of v is known, the value of v may thus be derived from (31), therefore using data such that $E\{\sin \Delta_I\} = 0$. Otherwise, (31) is first used to estimate v^2, which yields $|v|$, and the sign of v is then derived from another set of spin state preparations, now considering the case when $E\{\sin \Delta_I\} \neq 0$. Eq. (28) then yields

$$v = \frac{E\{r_1^2\}(1 - E\{r_2^2\}) + (E\{r_2^2\} - E\{r_1^2\})v^2 - E\{p_{2zz}\}}{2E\{r_1\sqrt{1-r_1^2}\}E\{r_2\sqrt{1-r_2^2}\}\sqrt{1 - v^2}E\{\sin \Delta_I\}}. \tag{35}$$

Taking the sign of this equation, where a factor is guaranteed to be positive, results in

$$\text{sgn}(v) = \text{sgn}\left(E\{r_1^2\}(1 - E\{r_2^2\}) + (E\{r_2^2\} - E\{r_1^2\})v^2\right.$$
$$\left. - E\{p_{2zz}\}\right)\text{sgn}(E\{\sin \Delta_I\}). \tag{36}$$

For this second set of spin state preparations, (i) we do not request the *value* of $E\{\sin \Delta_I\}$ but only its *sign* to be known, (ii) the values of $E\{r_1^2\}$, $E\{r_2^2\}$ and $E\{p_{2zz}\}$ may again be estimated as explained above. Also using the above estimate of v^2, Eq. (36) then allows one to estimate the sign of v.

C. Estimating the parameters of Ox measurements

We then show how to estimate the parameters w_1 and w_2 of (20), using measurements of spin components along the Ox axis, in addition to the Oz axis, and the corresponding expectations $E\{p_{jxx}\}$ and $E\{p_{jzz}\}$. Here again, we only constrain the statistical parameters of the RVs r_i and $(\phi_i - \theta_i)$, not their individual deterministic values, in order to be able to solve (20) with respect to w_1 and w_2. More precisely, the RVs r_1, r_2, $(\phi_1 - \theta_1)$ and $(\phi_2 - \theta_2)$ are here statistically independent. Besides, r_1 and r_2 have the same statistics. Finally, $(\phi_1 - \theta_1)$ and $(\phi_2 - \theta_2)$ have the same statistics, moreover with

$$E\{\sin(\phi_i - \theta_i)\} = 0 \qquad i \in \{1, 2\} \tag{37}$$
$$E\{\cos(\phi_i - \theta_i)\} > 0 \qquad i \in \{1, 2\}, \tag{38}$$

which is e.g. obtained with RVs $(\phi_i - \theta_i)$ whose probability density functions are even and non-zero on $[-\frac{\pi}{2}, \frac{\pi}{2}]$. In that case, (14), (20)-(22) and (27) yield [37] (with the same statistics for $i = 1$ and 2):

$$E\{p_{1zz}\} = (E\{r_i^2\})^2 \tag{39}$$
$$E\{p_{1xx}\} - E\{p_{4xx}\} = E\{R_{14}\}w_1 - E\{I_{14}\}w_2 \tag{40}$$

$$E\{R_{14}\} = E\{r_i\sqrt{1-r_i^2}\}E\{\cos(\phi_i - \theta_i)\}$$
$$\times 2\left[E\{r_i^2\}(1 - \cos \Delta\Phi_{1,-1}) + \cos \Delta\Phi_{1,-1}\right] \tag{41}$$

$$E\{I_{14}\} = -E\{r_i\sqrt{1-r_i^2}\}E\{\cos(\phi_i - \theta_i)\}$$
$$\times 2(1 - E\{r_i^2\})\sin \Delta\Phi_{1,-1} \tag{42}$$

$$E\{p_{1xx}\} + E\{p_{4xx}\} = \left[E\{r_i\sqrt{1-r_i^2}\}E\{\cos(\phi_i - \theta_i)\} \right]^2$$
$$\times (1 + \cos\Delta\Phi_{1,-1}) + \frac{1}{2}. \qquad (43)$$

Once $E\{p_{1zz}\}$, $E\{p_{1xx}\}$ and $E\{p_{4xx}\}$ have been estimated as explained above, Eq. (39), with $E\{r_i^2\} \geq 0$ due to $r_i \geq 0$, yields

$$E\{r_i^2\} = \sqrt{E\{p_{1zz}\}}. \qquad (44)$$

Moreover, $r_i \geq 0$, (38) and (43) yield

$$E\{r_i\sqrt{1-r_i^2}\}E\{\cos(\phi_i - \theta_i)\} = \left[\frac{E\{p_{1xx}\} + E\{p_{4xx}\} - \frac{1}{2}}{1 + \cos\Delta\Phi_{1,-1}} \right]^{\frac{1}{2}} \qquad (45)$$

Using (25), (44) and (45), Eq. (41) and (42) then yield estimates of $E\{R_{14}\}$ and $E\{I_{14}\}$. The only unknowns of (40) are then w_1 and w_2. One could try and solve a single equation (40), by taking into account that w_1 and w_2 are the cosine and sine of the same angle (see (23)-(24)). However, the solutions of such an equation yield a problematic indeterminacy. This problem is avoided by creating *two* linearly independent equations (40), by using two sets of statistics for r_1, r_2, $(\phi_1 - \theta_1)$ and $(\phi_2 - \theta_2)$. Solving these two equations yields w_1 and w_2.

D. Estimating the quantum process

We finally show how the estimates of the parameters v, w_1 and w_2 obtained above may be used to estimate the matrix D of (11) and hence the complete matrix M of (9), which defines the considered process in the standard basis.

In a first method, we only consider a single value of the time interval $(t - t_0)$ involved in (11), that we hereafter denote as τ_1. Eq. (18)-(19) may then be inverted as

$$\frac{J_{xy}\tau_1}{\hbar} = -\Delta_{Ed} + k_{xy}\pi \qquad (46)$$

with

$$\Delta_{Ed} = \arcsin(v) \qquad (47)$$

where Δ_{Ed} is one determination associated with the actual value Δ_E, i.e. Δ_{Ed} is equal to Δ_E up to the additive constant $-k_{xy}\pi$, where k_{xy} is an integer. Similarly, (23)-(24) and (26) may be inverted as

$$\frac{J_z\tau_1}{\hbar} = \Delta\Phi_{1,0d} + 2k_z\pi + \frac{J_{xy}\tau_1}{\hbar} + \frac{GB\tau_1}{\hbar} \qquad (48)$$

with

$$\Delta\Phi_{1,0d} = \text{sgn}(w_2)\arccos(w_1) \qquad (49)$$

where $\Delta\Phi_{1,0d}$ is one determination associated with the actual value $\Delta\Phi_{1,0}$, i.e. $\Delta\Phi_{1,0d}$ is equal to $\Delta\Phi_{1,0}$ up to the additive constant $2k_z\pi$, where k_z is an integer.

Eq. (46)-(49) define the expressions of the scaled *actual* principal values J_{xy} and J_z with respect to the *actual* values of v, w_1 and w_2. The latter values are unknown but, in practice, the procedure defined in Section VB yields an estimate $\hat{v}$ of the value of v (for the considered value τ_1). From this, one may derive an estimate $\widehat{\Delta}_{Ed}$ of Δ_{Ed} by using $\hat{v}$ in (47). One would then like to derive an estimate $\widehat{J}_{xy}$ of J_{xy} from (46). But one does not know the actual value k_{xy} involved in (46) in the fully blind case considered here, i.e. when no prior information is available about the value of J_{xy} (as opposed to the case when one at least knows in which range of values J_{xy} is situated, which defines the minimum and maximum possible values of k_{xy}). In this blind method, one can then only select an arbitrary integer $\widehat{k}_{xy}$ and derive the corresponding scaled "shifted estimate" of J_{xy} by using

$$\frac{\widehat{J}_{xy}\tau_1}{\hbar} = -\widehat{\Delta}_{Ed} + \widehat{k}_{xy}\pi. \qquad (50)$$

Similarly, the procedure defined in Section VC yields estimates $\widehat{w}_1$ and $\widehat{w}_2$ of the values of w_1 and w_2 (for the considered value τ_1). From this, one first derives an estimate $\widehat{\Delta\Phi}_{1,0d}$ of $\Delta\Phi_{1,0d}$ by using $\widehat{w}_1$ and $\widehat{w}_2$ in (49). Then, based on (48), one derives a scaled shifted estimate $\widehat{J}_z$ of J_z by using

$$\frac{\widehat{J}_z\tau_1}{\hbar} = \widehat{\Delta\Phi}_{1,0d} + 2\widehat{k}_z\pi + \frac{\widehat{J}_{xy}\tau_1}{\hbar} + \frac{GB\tau_1}{\hbar} \qquad (51)$$

where $\widehat{k}_z$ is an arbitrarily selected integer. When neglecting estimation errors for v, w_1 and w_2, and hence for Δ_{Ed} and $\Delta\Phi_{1,0d}$, and when taking the difference between (46) and (50), then between (48) and (51), one gets

$$\frac{\widehat{J}_{xy}\tau_1}{\hbar} = \frac{J_{xy}\tau_1}{\hbar} + \Delta k_{xy}\pi \qquad (52)$$

$$\frac{\widehat{J}_z\tau_1}{\hbar} = \frac{J_z\tau_1}{\hbar} + 2\Delta k_z\pi + \Delta k_{xy}\pi \qquad (53)$$

with

$$\Delta k_{xy} = \widehat{k}_{xy} - k_{xy} \qquad (54)$$

$$\Delta k_z = \widehat{k}_z - k_z. \qquad (55)$$

The shifted estimates $\frac{\widehat{J}_{xy}\tau_1}{\hbar}$ and $\frac{\widehat{J}_z\tau_1}{\hbar}$ provided by this method are therefore equal to the quantities of interest, that is $\frac{J_{xy}\tau_1}{\hbar}$ and $\frac{J_z\tau_1}{\hbar}$, only up to (the above neglected estimation errors and) additive constants which are integer multiples of π. These constants are the "undeterminacies" of this method in the classical BSS sense, i.e. the undesired remaining differences between the above estimated and actual quantities, from the point of view of the quantities $\frac{J_{xy}\tau_1}{\hbar}$ and $\frac{J_z\tau_1}{\hbar}$. They then yield the following indeterminacies from the point of view of the matrix M of the considered quantum process, which is eventually to be estimated. Using the above estimates $\frac{\widehat{J}_{xy}\tau_1}{\hbar}$ and $\frac{\widehat{J}_z\tau_1}{\hbar}$, one derives the associated estimate of the matrix M (i)

by inserting these estimates, which may be expressed as (52)-(53), into (11)-(13), which yields the corresponding estimate $\widehat{D}$ of D, and (ii) finally by using (9) and (10) to derive the associated estimate of M. These calculations especially yield (taking into account that $e^{i\Delta k_z 2\pi} = 1$ and $e^{\Delta k_{xy} 2\pi} = 1$)

$$\widehat{D} = e^{i(\Delta k_z \pi - \Delta k_{xy}\frac{\pi}{2})} D. \tag{56}$$

The estimate $\widehat{D}$ provided by this first method is therefore equal to the actual matrix D up to the phase factor $e^{i(\Delta k_z \pi - \Delta k_{xy}\frac{\pi}{2})}$. More specifically, this factor is equal to 1 and thus diseappears for part of the possible values of the integers Δk_z and Δk_{xy}, e.g. when Δk_z is a multiple of 2 and Δk_{xy} is a multiple of 4. This yields the same phenomenon for M. The general phase factor $e^{i(\Delta k_z \pi - \Delta k_{xy}\frac{\pi}{2})}$ cannot be avoided with this method if no additional information is available. It is the only and quite weak indeterminacy of this BQPT method from the point of view of D and M. Moreover, we hereafter introduce an extended version of that method, which completely removes this indeterminacy by taking the typical applications of (B)QPT methods into account.

As discussed e.g. in [5], [25], [27], [30], [31], [34], QPT (and hence our blind extension) may especially be used as a tool for characterizing quantum gates, which are the building blocks of quantum computers. This characterization is typically performed before using the considered gates for quantum computation, thus leading to a two-phase approach, composed of an "identification phase" and then of a "computation phase", for these quantum processes/gates. Moreover, one may consider scenarios where these processes/gates are used in coherent but somewhat different conditions during the identification and computation phases. We hereafter propose such an approach for extending the above BQPT method so as to remove its indeterminacy. We do not claim that the Heisenberg coupling model considered in this paper could be used as a suitable process/gate for quantum computers: it is just used as an example hereafter, to illustrate a possible procedure for removing BQPT indeterminacies, thus then allowing the reader to extend this procedure to other processes/gates that could be of interest in other configurations.

The approach that we propose uses three values of the time interval $(t - t_0)$ involved in (11), that we hereafter denote as τ_1, τ_2 and τ_3. The first step of the identification phase uses the time interval τ_1, essentially to obtain an estimate of J_{xy} associated with this value τ_1, that we hereafter denote as $\widehat{J}_{xy}(\tau_1)$ for the sake of clarity. More precisely, this first step of the identification phase derives the shifted estimate $\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar}$ in the same way as in the above first BQPT method, i.e. using (50), with $\widehat{J}_{xy}$ here replaced by $\widehat{J}_{xy}(\tau_1)$. Therefore, when neglecting estimation errors, this again yields (52), but with our modified

notations, that is

$$\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar} = \frac{J_{xy}\tau_1}{\hbar} + \Delta k_{xy}\pi. \tag{57}$$

The second step of the identification phase then uses the time interval τ_2, with $\tau_2 = 2\tau_1$ (τ_2 may instead be set to any other even multiple of τ_1, but we keep the values of τ_1, τ_2 and τ_3 as close as possible to one another, in order to minimize the differences in the conditions of operation in the two steps of the identification phase and in the computation phase). This second step of the identification phase essentially aims at obtaining an estimate of J_z associated with the value τ_2, that we therefore hereafter denote as $\widehat{J}_z(\tau_2)$. More precisely, this second step derives the shifted estimate $\frac{\widehat{J}_z(\tau_2)\tau_2}{\hbar}$ in the same way as $\frac{\widehat{J}_z\tau_1}{\hbar}$ in the above first BQPT method, except that this step is here performed with τ_2, so that it uses (51) with τ_1 replaced by τ_2, moreover taking into account that the term $\frac{\widehat{J}_{xy}\tau_2}{\hbar}$ of this modified version of (51) is here obtained as being equal to the value $\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar}$ of this second BQPT method multiplied by 2. When neglecting estimation errors, taking the difference between the modified versions of (48) and (51), and using (57), Eq. (53) is thus replaced by

$$\frac{\widehat{J}_z(\tau_2)\tau_2}{\hbar} = \frac{J_z\tau_2}{\hbar} + 2\Delta k_z\pi + 2\Delta k_{xy}\pi. \tag{58}$$

The computation phase then involves the same type of quantum process (9)-(11), but with a time interval $(t - t_0)$, between input state preparation at time t_0 and output state use at time t, which is set to τ_3, with $\tau_3 = 2\tau_2$ (again, τ_3 may instead be set to any other even multiple of τ_2, but we keep the values of τ_1, τ_2 and τ_3 as close as possible to one another). This computation phase should then be analyzed as follows. During that phase, the considered actual process is defined by (9)-(13), but with $(t - t_0)$ replaced by τ_3. From the point of view of that computation phase, the estimate of that actual process is obtained by replacing $\frac{J_{xy}(t-t_0)}{\hbar}$ and $\frac{J_z(t-t_0)}{\hbar}$ by $\frac{\widehat{J}_{xy}(\tau_1)\tau_3}{\hbar}$ and $\frac{\widehat{J}_z(\tau_2)\tau_3}{\hbar}$ in (9)-(13), the latter estimates being derived as explained above by our extended BQPT method (up to the factors τ_3/τ_1 and τ_3/τ_2). These estimates have the properties defined by (57) and (58). Since $\tau_3/\tau_1 = 4$ and $\tau_3/\tau_2 = 2$, this yields

$$\frac{\widehat{J}_{xy}(\tau_1)\tau_3}{\hbar} = \frac{J_{xy}\tau_3}{\hbar} + 4\Delta k_{xy}\pi \tag{59}$$

$$\frac{\widehat{J}_z(\tau_2)\tau_3}{\hbar} = \frac{J_z\tau_3}{\hbar} + 4\Delta k_z\pi + 4\Delta k_{xy}\pi. \tag{60}$$

Comparing these expressions with (52) and (53) shows that this second BQPT method it equivalent to the first one presented in this section, except that, from the point of view of the computation phase, (i) it use the time interval τ_3 and (ii) Δk_{xy} and Δk_z are respectively replaced by $4\Delta k_{xy}$ and $2\Delta k_z$. The analysis provided above for

the first method therefore also applies here when taking the above modifications into account. In particular, (56) also applies here, but its phase factor $e^{i(\Delta k_z \pi - \Delta k_{xy}\frac{\pi}{2})}$ here becomes $e^{i(2\Delta k_z \pi - 2\Delta k_{xy}\pi)}$ and is therefore always equal to one. In other words, this extended BQPT method is equivalent to forcing Δk_{xy} and Δk_z to be respectively equal to multiples of 4 and 2 from the point of view of the computation phase, which suppresses the indeterminacy that the first method has in that phase.

The above discussion first means that any value of Δk_{xy} and hence $\widehat{k}_{xy}$ may be used during the identification phase of our extended BQPT method. From a practical point of view, the simplest implementation of this method therefore consists of selecting $\widehat{k}_{xy} = 0$ in the modified version of (50), i.e. it consists of setting the estimate $\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar}$ to $-\widehat{\Delta}_{Ed}$. This estimate is then multiplied by $\tau_3/\tau_1 = 4$ when considering it from the point of view of the computation phase. Similarly, during the identification phase one sets the estimate $\frac{\widehat{J}_z(\tau_2)\tau_2}{\hbar}$ by using (51), with τ_1 replaced by τ_2 and with $\widehat{k}_z$ preferably set to 0 (and with $\frac{\widehat{J}_{xy}\tau_2}{\hbar}$ obtained by multiplying the above estimate $\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar}$ by $\tau_2/\tau_1 = 2$). This estimate $\frac{\widehat{J}_z(\tau_2)\tau_2}{\hbar}$ is then multiplied by $\tau_3/\tau_2 = 2$ when considering it from the point of view of the computation phase.

VI. TEST RESULTS

The physical implementation of qubits is an emerging topic which is beyond the scope of this paper. We therefore assessed the performance of the extended BQPT method proposed above by means of numerical tests performed 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 input states $|\psi(t_0)\rangle$. Each such state is obtained by randomly drawing its six parameters r_i, θ_i and ϕ_i, with $i \in \{1, 2\}$, and then using (3), (4), (6) (the state (6) is defined by the above six parameters, but only the four parameters r_i and $\phi_i - \theta_i$ have a physical meaning). We then process the states $|\psi(t_0)\rangle$ according to (7), with given values of the parameters of the matrix M which defines the quantum process to be identified. This yields the states $|\psi(t)\rangle$. More precisely, we eventually use simulated measurements of spin components associated with these states $|\psi(t)\rangle$. For measurements along the Oz axis, this means that we use the model (14)-(16) with a given value of the mixing parameter v, corresponding to the above values of the parameters of the matrix M. For each of the N states $|\psi(t_0)\rangle$, corresponding to parameter values (r_1, r_2, Δ_I), Eq. (14)-(16) thus yield the corresponding set of probability values $(p_{1zz}, p_{2zz}, p_{4zz})$, which are used as follows. We use K prepared copies of the considered state $|\psi(t_0)\rangle$ to simulate K random-valued two-qubit spin component measurements along the Oz axis, drawn with the above probabilities $(p_{1zz}, p_{2zz}, p_{4zz})$. We then derive

the sample frequencies of the results of these K measurements, which are estimates of p_{1zz}, p_{2zz} and p_{4zz} for the considered state $|\psi(t_0)\rangle$ (see (A6)). Then computing the averages of these K-preparation estimates over all N source vectors $|\psi(t_0)\rangle$ yields (NK)-preparation estimates of probability expectations $E\{p_{jzz}\}$ (see (A9)). Spin component measurements for the Ox axis are handled similarly, thus yielding estimates of probability expectations $E\{p_{jxx}\}$. Both types of estimates of probability expectations are then used by our extended BQPT method, as explained in the previous sections, to derive the estimates $\frac{\widehat{J}_{xy}\tau_1}{\hbar}$ and $\frac{\widehat{J}_z\tau_2}{\hbar}$, from which we then derive the estimates of D and eventually M corresponding to the computation phase that uses the time interval τ_3.

In these tests, the above parameters N and K were varied as described further in this section, whereas the numerical values of the other parameters were fixed as explained in Appendix B, so that we used the same values for the parameters v, w_1 and w_2 and for the matrix M in all tests. 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 states $|\psi(t_0)\rangle$, in order to assess the statistical performance of the considered BQPT method over 100 estimations of the same set of parameter values. The performance criteria used to this end are defined as follows. Separately for each of the scalar parameters v, w_1 and w_2, we computed the Normalized Root Mean Square Error (NRMSE) of that parameter over all 100 estimations, defined as the ratio of its RMSE to its actual value. For the *matrix* M, we first derived a *scalar* relative error for each test, defined as the ratio of the Frobenius norm of the "error matrix" $(\widehat{M} - M)$, where $\widehat{M}$ is the estimate of M provided by our BQPT method, to the Frobenius norm of the actual matrix M (the Frobenius norm of a matrix A with entries a_{ij} is defined as $\sqrt{\sum_i \sum_j a_{ij}^2}$). We then computed the average of this relative error over all 100 estimations.

The values of these four performance criteria are shown in Fig. 1 to 4, where each plot corresponds to a fixed value of the product NK, i.e. of the complexity of the BQPT method in terms of the total number of state preparations. Each plot shows the variations of the considered performance criterion vs. K, hence with N varied accordingly, to keep the considered fixed value of NK. This first shows that the proposed BQPT method is able to operate with a number K of preparations per state $|\psi(t_0)\rangle$ decreased down to one, as expected. Moreover, for a fixed value of NK, the errors improve when K decreases, which is expected to be due to the fact that the number N of *different* used states thus increases, allowing the estimation method to better explore the statistics of the considered random process. Thus using $K = 1$, the mean relative error for the matrix M defining the considered quantum process (see Fig. 4) can e.g. here be made equal to 5.53 % for $N = 10^4$ or 1.75 % for $N = 10^5$ or 0.62 % for $N = 10^6$. In these tests, we used a simple pro-

tocol, i.e. we considered the same values of K and N in the six series of state preparations used for estimating all parameters (v, w_1 and w_2), so that the total number of preparations is equal to $6NK$. Different values of K and N might be used in these six series of state preparations, in order to optimize the total number of preparations used to achieve a given error for M. In particular, when estimating the *sign* of v, the result is a binary decision, not a continuous value which should be accurately estimated, so that this sign could be obtained without errors with a significantly lower number of state preparations, thus making the total number of state preparations closer to $5NK$. Besides, Fig. 1 to 3 show that, when using the same values of K and N, the parameter v is estimated much more accurately than w_1 and w_2. This is reasonable, because the measurements along the Oz axis, which are used to estimate v, yield a simpler model and hence a simpler estimation procedure than the measurements along the Ox (and Oz) axis, which are used to estimate w_1 and w_2. When aiming at optimizing the use of state preparations, one may therefore think of reducing the number of state preparations for estimating v as compared with those used for estimating w_1 and w_2, in order to balance the estimation accuracies for these parameters. However, it is not guaranteed that the estimation accuracy for M will thus be significantly improved: in Fig. 1 to 4, the estimation accuracy for M has in intermediate value between the accuracies achieved for the parameters v, w_1 and w_2 upon which M depends, i.e. the accuracy of M is not limited by those of its "worst parameters", namely w_1 and w_2, but takes advantage of its best parameter v. Based on all above results and considerations, a typical performance level to be eventually kept in mind for the matrix M which defines the considered quantum process is a mean relative error of around 1 % for around 500,000 state preparations.
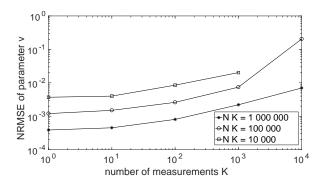

FIG. 1. Normalized Root Mean Square Error (NRMSE) of estimation of parameter v vs. number K of preparations of each of the N used states.
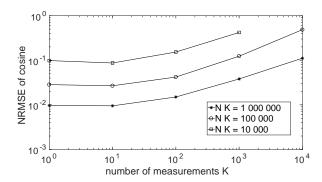

FIG. 2. NRMSE of estimation of parameter w_1 vs. number K of preparations of each of the N used states.
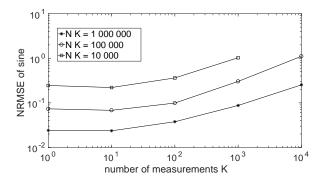

FIG. 3. NRMSE of estimation of parameter w_2 vs. number K of preparations of each of the N used states.

VII. DISCUSSION AND CONCLUSION

Non-blind or blind QPT may be defined as the identification, i.e. estimation, of a given quantum process or gate. As discussed in Section V D, this allows one to characterize the *actual* behavior of such a gate, so that (B)QPT is a major quantum information processing tool. The usual, i.e. non-blind, version of QPT requires one to know, hence to precisely control (i.e. prepare), the specific quantum states used as inputs of the quantum gate to be characterized. The blind version of this tool, i.e. BQPT, which is the first contribution proposed in this paper, then provides an attractive extension of QPT, since it allows one to use input quantum states whose values are unknown and arbitrary, except that they are requested to meet some general known properties.

Such blind approaches especially have two potential applications. The most natural one is when the input states of the considered process indeed cannot be known. Such methods could then be of interest for characterizing quantum gates while they are operating and when only their results (output states) are available to the user who is to characterize them (provided some output states $|\psi(t)\rangle$ are available to perform BQPT, with adequate values of the above-defined preparation-to-measurement time interval ($t - t_0$)). This on-line characterization may
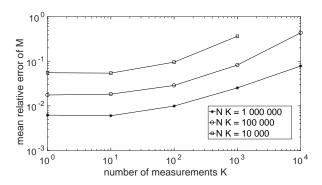
FIG. 4. Mean relative error of estimation of matrix M vs. number K of preparations of each of the N used states.

be useful e.g. if the transform performed by a quantum gate slowly evolves over time (e.g. due to aging) and must be monitored, by characterizing it from time to time. Besides, BQPT may be of even higher interest in more standard configurations, when the process input states may be prepared and known: BQPT then avoids the complexity of *accurately preparing the specific states* which are required by usual QPT methods, because BQPT can use *any* input states (which have the requested general properties).

The second constraint of usual QPT methods is that they require one to be able to prepare many copies of the *same* (known) input state, which is cumbersome. As a second contribution in this paper, we proposed methods which avoid this constraint, since they allow one to use one instance or several copies of each considered input state (and they provide even better performance when decreasing the number of preparations per state to one and increasing the number of different states accordingly, for a fixed total number of preparations, i.e. fixed complexity). Briefly, this quite attractive property is obtained because the proposed methods do not use the estimated probabilities separately associated which each considered random state, but only the expectations of these random probabilities.

It should also be noted that the solution provided by each of the proposed BQPT methods is defined by a unique set of closed-form expressions. This avoids the issues of estimation methods that are based on the numerical optimization of cost functions and that yield false solutions when they get trapped into local minima of these cost functions. Morever, the proposed BQPT methods only require a limited number of types of measurements (only spin component measurements along the Ox and Oz axes in the case considered here), which simplifies their practical use. This results from the fact that these methods only perform the types of measurements which are needed to get enough information about the required unknown parameter values. This should be contrasted with methods which use a larger set of types of measurements to first completely restore quantum states.

The main global result of this paper is therefore the joint concept of Single-preparation Blind QPT (SBQPT). It was here illustrated and numerically validated for a specific type of quantum process, based on cylindrical-symmetry Heisenberg coupling, for the sake of clarity. However, it may be applied to a much wider class of processes and to methods based on other statistical parameters of quantum measurement outcomes or other quantum state properties. Such extensions will be reported in future papers.

Appendix A: From multiple-preparation to single-preparation quantum information processing (QIP)

In this appendix, we first summarize the concepts and notations that are used in conventional, i.e. multiple-preparation, QIP (see Section A 1) and that we need to then introduce our non-conventional, single-preparation, approach to QIP (see Section A 2) for an arbitrary number of qubits.

1. Multiple-preparation QIP

Throughout this paper, qubits are physically implemented as spins $1/2$. If such a qubit, with index i, is described with a pure and "deterministic" quantum state, as defined in [17], it is represented by a normalized vector of a two-dimensional space $\mathcal{E}_i$, expressed as

$$|\psi_i\rangle = \alpha_i|+\rangle_i + \beta_i|-\rangle_i \qquad (A1)$$

where α_i and β_i are two fixed complex-valued coefficients constrained to meet the normalization condition for $|\psi_i\rangle$. The index i in the above notations $|+\rangle_i$ and $|-\rangle_i$ is most often omitted in the literature, but we keep it here, to clarify the notations that we hereafter introduce for *a set of* qubits.

Let us now consider an arbitrary number Q of distinguishable [16] qubits, with indices $i \in \{1,\dots,Q\}$. If the state $|\psi\rangle$ of this set of qubits is pure and deterministic, it belongs to the space $\mathcal{E}$ defined as the tensor product (denoted as $\otimes$) of the above spaces $\mathcal{E}_i$. The standard basis of $\mathcal{E}$ consists of the 2^Q vectors $|+\rangle_1 \otimes |+\rangle_2 \otimes \dots \otimes |+\rangle_{Q-1} \otimes |+\rangle_Q$ to $|-\rangle_1 \otimes |-\rangle_2 \otimes \dots \otimes |-\rangle_{Q-1} \otimes |-\rangle_Q$ that we hereafter respectively denote as $|j\rangle$, with $j \in \{1,\dots,2^Q\}$. The state of this set of qubits then reads

$$|\psi\rangle = \sum_{j=1}^{2^Q} c_j|j\rangle \qquad (A2)$$

where the complex-valued coefficients c_j are again fixed and arbitrary, except that they meet the normalization condition

$$\sum_{j=1}^{2^Q} |c_j|^2 = 1. \qquad (A3)$$

The result obtained for one measurement of the spin component s_{zi} of $\overrightarrow{s_i}$ along the quantization axis, for a single qubit i which is in state (A1) (see e.g. [10] for details), has a random nature and is $+\frac{1}{2}$ or $-\frac{1}{2}$ in normalized units. The probabilities of obtaining these two values are respectively equal to $|\alpha_i|^2$ and $|\beta_i|^2$, that is, to the squared moduli of the coefficients in (A1) which correspond to the vectors $|+\rangle_i$ and $|-\rangle_i$ that are respectively associated with the allowed values $+\frac{1}{2}$ and $-\frac{1}{2}$.

When simultaneously performing such a measurement for each of the qubits i of an overall set of Q qubits, the obtained result is a vector of Q values. The 2^Q possible values of this vector are $[+\frac{1}{2}, +\frac{1}{2}, \ldots, +\frac{1}{2}, +\frac{1}{2}]$, $[+\frac{1}{2}, +\frac{1}{2}, \ldots, +\frac{1}{2}, -\frac{1}{2}]$, and so on, these values being respectively associated with the above-defined 2^Q basis vectors $|j\rangle$ and hereafter indexed by j. Thus, the experiment consisting of this Q-qubit measurement yields a random result, and each elementary event [28] A_j is defined as: the result of the experiment is equal to the j-th Q-entry vector in the above series of possible values $[+\frac{1}{2}, +\frac{1}{2}, \ldots, +\frac{1}{2}, +\frac{1}{2}]$ and so on. Moreover, the probabilities of these events are defined according to the principle presented above for one qubit, that is

$$P(A_j) = |c_j|^2 \qquad \forall\, j \in \{1, \ldots, 2^Q\}. \qquad \text{(A4)}$$

The simplest procedure, applied in practice to estimate the above probabilities for a given Q-qubit state, uses a large number (typically from a few thousand up to one hundred thousand [10], [16]) of copies of that state, so that we hereafter call this approach "multiple-preparation QIP" (we previously called it "batch QIP" in [19]). These copies may be obtained in parallel from an ensemble of systems or successively for the same system ("repeated write/read", or RWR, procedure [9], [10], [13]). The above type of measurement is performed for each of these copies and one counts the number of occurrences of each of the possible results $[+\frac{1}{2}, +\frac{1}{2}, \ldots, +\frac{1}{2}, +\frac{1}{2}]$ and so on. The associated sample relative frequencies are then used as estimates of the probabilities $P(A_j)$.

2. Single-preparation QIP

The above description was provided for an arbitrarily selected deterministic pure quantum state $|\psi\rangle$. When developing our first class of BQSS methods [9], [10], [13], we had to extend that framework to *random* pure quantum states. We especially detailed that concept in [17]. Briefly, the coefficients α_i and β_i in (A1) and c_j in (A2) then become complex-valued random variables (RVs). Hence, the probabilities in (A4) also become RVs !

The problem tackled in this section is the estimation of some statistical parameters of these RVs (A4), namely their expectations. The natural (global) procedure that may be used to this end, and that we used in the specific context of BQSS [9], [10], [13], consists of the following

two levels. The lower level only concerns one deterministic state (A2) and the associated probabilities (A4) which are estimated from a large number of copies of the considered state, using the multiple-preparation QIP framework of Section A 1. This is repeated for different states (A2) and then, at the higher level, the sample mean over all these states is separately computed for each probability $P(A_j)$ (with samples supposedly drawn from the same statistical distribution). We here aim at proceeding further: at the above-defined lower level, we aim at using *a small number* of copies of the considered state, or ultimately *a single* instance of that state, thus developing what we call "single-preparation QIP" (we called it "stochastic QIP" in [19]). At first sight, it might seem that this is not possible, because the lower level would thus not provide accurate estimates, that one could then confidently gather at the higher level. However, we claim and show below that this approach can be used if one only aims at estimating some statistical parameters of the considered quantum states.

We now first build the proposed approach by starting from the frequentist view of probabilities (see e.g. [28]) at the above-defined two levels of the considered procedure, that is:

- At the higher level, where one combines the contributions associated with N states of the set of Q qubits. These states are indexed by $n \in \{1, \ldots, N\}$ and denoted as $|\psi(n)\rangle$.

- At the lower level, which concerns one deterministic state $|\psi(n)\rangle$ and the associated probabilities $P(A_j, n)$ defined by (A4) but with coefficients $c_j(n)$ which depend on state $|\psi(n)\rangle$.

At the lower level, each probability $P(A_j, n)$ is defined as

$$P(A_j, n) = \lim_{K \to +\infty} \frac{\mathcal{N}(A_j, n, K)}{K} \qquad \text{(A5)}$$

provided this limit exists. $\mathcal{N}(A_j, n, K)$ is the number of occurrences of event A_j for the state $|\psi(n)\rangle$ when performing measurements for a set of K copies of that state $|\psi(n)\rangle$. In practice, one uses only a *finite* number K of copies of state $|\psi(n)\rangle$ and therefore only accesses the following approximation of the above probability:

$$P'(A_j, n, K) = \frac{\mathcal{N}(A_j, n, K)}{K}. \qquad \text{(A6)}$$

The higher level of the considered procedure then addresses the statistical mean associated with samples, indexed by n, of a given quantity, which is here theoretically $P(A_j, n)$. In the frequentist approach, this statistical mean is defined (if the limit exists) as

$$E\{P(A_j)\} = \lim_{N \to +\infty} \frac{\sum_{n=1}^{N} P(A_j, n)}{N}. \qquad \text{(A7)}$$

At the higher level too, in practice one uses only a *finite* number N of states $|\psi(n)\rangle$, which first yields the following

approximation if only performing an approximation at the higher level of the procedure:

$$E'\{P(A_j)\} = \frac{\sum_{n=1}^N P(A_j, n)}{N}. \qquad (A8)$$

The latter expression may then be modified by replacing its term $P(A_j, n)$ by its approximation (A6). This yields

$$E''\{P(A_j)\} = \frac{\sum_{n=1}^N \mathcal{N}(A_j, n, K)}{NK}. \qquad (A9)$$

$\sum_{n=1}^N \mathcal{N}(A_j, n, K)$ is nothing but the number, hereafter denoted as $\mathcal{N}(A_j, L)$, of occurrences of event A_j for the complete considered set of $L = NK$ measurements. Therefore, $E''\{P(A_j)\}$ is the relative frequency of occurrence of that event over these L measurements, or "'trials", using standard probabilistic terms [28]. This quantity (A9) may therefore also be expressed as

$$E''\{P(A_j)\} = \frac{\mathcal{N}(A_j, L)}{L} \qquad (A10)$$

$$= \frac{\sum_{\ell=1}^L \mathbb{1}(A_j, \ell)}{L} \qquad (A11)$$

where $\mathbb{1}(A_j, \ell)$ is the value of the indicator function of event A_j for trial ℓ, which takes the value 1 if A_j occurs during that trial, and 0 otherwise. When using (A11), one now considers the $L = NK$ trials as organized as a single series, with trials indexed by ℓ. One thus fuses the above-defined two levels of the procedure into a single one, thus disregarding the fact that, in this series, each block of K consecutive trials uses the same state $|\psi(n)\rangle$. One may therefore wonder whether the number K of used copies of each state $|\psi(n)\rangle$ may be freely decreased, and even set to one, while possibly keeping the same total number L of trials. A formal proof of the relevance of that approach, using Kolmogorov's view of probabilities, is provided in [19]. Moreover, [19] thus proves that the proposed estimator (A11) of $E\{P(A_j)\}$ is attractive because, for states independently randomly drawn with the same distribution and with one instance of each state, this estimator is asymptotically efficient, that is, when the number L of trials tends to infinity: (i) the mean of this estimator tends to the actual value $E\{P(A_j)\}$, i.e. this estimator is asymptotically unbiased (it is even unbiased for a *finite* number of trials), and (ii) the variance of this estimator tends to 0.

Appendix B: Test conditions

All tests reported in Section VI were performed in the following conditions. The six parameters r_i, θ_i and ϕ_i, with $i \in \{1, 2\}$, of each initial state $|\psi(t_0)\rangle$ were randomly drawn with a uniform distribution, over an interval which depends on the step of the considered BQPT method, in order to meet the constraints on the statistics of these parameters that are imposed by that BQPT method. The parameters q_1 and q_2 were then derived from (4). More precisely, as a first step, to estimate the absolute value of v as explained in the first part of Section V B, the qubit parameter values r_1 and r_2 were selected within the 20%-80% sub-range of their 0%-100% allowed range defined by (29), that is, $[0.1, 0.4[$ for r_1 and $[0.6, 0.9[$ for r_2, as in [13]. Besides, ϕ_1 and ϕ_2 were drawn over $[0, 2\pi[$ whereas θ_1 and θ_2 were fixed to 0 (as stated above, the parameters which have a physical meaning are $\phi_i - \theta_i$). These data are thus such that $E\{\sin \Delta_I\} = 0$, as required by this step of the considered BQPT method. Then, as a second step, to estimate the sign of v as explained in the second part of Section V B, the same conditions as in the above first step were used for r_i, θ_i and ϕ_i, with $i \in \{1, 2\}$, except that ϕ_1 was fixed to 0 and ϕ_2 was drawn over $[0, \pi[$. These data are thus such that $E\{\sin \Delta_I\}$ is non-zero and has a known sign (here, it is positive), as required by this step of the considered BQPT method. The above two steps were performed with $\tau_1 = 0.51$ ns [36]. Finally, to estimate w_1 and w_2, the method of Section V C uses measurements along the Oz and Ox axes, with $\tau_2 = 2\tau_1$. For each of the parameters r_i, θ_i and ϕ_i, with $i \in \{1, 2\}$, we used the same statistics for measurements along the Oz and Ox axes. For the first equation (40), r_1 and r_2 were drawn over $[0.1, 0.4[$ and ϕ_1 and ϕ_2 were drawn over $[-\pi/2, \pi/2[$, whereas θ_1 and θ_2 were fixed to 0. For the second equation (40), r_1 and r_2 were drawn over $[0.6, 0.9[$, whereas ϕ_1, ϕ_2, θ_1, and θ_2 were selected in the same way as for the first equation (40). All above conditions concern the identification phase. Then, in the computation phase, we used $\tau_3 = 2\tau_2$, as explained in Section V D.

Besides, the value of matrix M was set as follows. Conventional Electron Spin Resonance generally operates at X or Q bands (around 10 and 35 GHz respectively). For electron spins with $g = 2$, at 35 GHz, the resonance field is near 1.25 T. In the simulations, we used the values $g = 2$ and $B = 1$ T. Concerning the exchange coupling, we chose $J_z/k_B = 1$ K and $J_{xy}/k_B = 0.3$ K (see Appendix E of [10] and [20]).

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Erratum: replace two terms $E\{r_i\}E\{q_i\}$ in (33) of [9] by $E\{r_iq_i\}$, since q_i depends on r_i.

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[35] See also [27] p. 398 for the other earliest references.

[36] As a typical example, we aim at setting τ_1 to τ_3 around 1 ns. However, choosing $\tau_2 = 1$ ns exactly, and hence $\tau_1 = 0.5$ ns, yields a specific case: in the step of the proposed BQPT method when τ_2 is used (i.e., when estimating w_1 and w_2), the value of v is thus very close to 1, which is its maximum possible value, as shown by (19). To avoid being in such a specific case, we slightly shifted τ_1, and hence τ_2 and τ_3, by setting $\tau_1 = 0.51$ ns.

[37] In this part of our method, we do not use (30) and we therefore do not set the constraint (29).