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yannick Deville, Alain Deville

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Yannick Deville [*]
Université de Toulouse, UPS, CNRS, CNES, OMP, IRAP (Institut de Recherche en Astrophysique et Planétologie), F-31400 Toulouse, France

Alain Deville [†]
Aix-Marseille Université, CNRS, IM2NP UMR 7334, F- 13397 Marseille, France

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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 require one to know, hence to very 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. In contrast, we propose "single-preparation BQPT methods" (SBQPT) , i.e., methods which can operate with only one instance of each considered input state. These two concepts are here illustrated with practical (S)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 and (ii) the considered quantum process is based on cylindrical-symmetry Heisenberg spin coupling. As a benchmark, we moreover introduce nonblind QPT methods dedicated to the considered Heisenberg process, we analyze their theoretical behavior (this requires the tools developed in this paper for random input states), and we numerically test their sensitivity to systematic and nonsystematic errors, which are most likely to occur in practice. This shows that, even for very low preparation errors (especially systematic ones), these nonblind QPT methods yield much lower performance than our SBQPT methods. Our blind and single-preparation QPT concepts may be extended, e.g., to a much wider class of processes and to SBQPT methods based on other quantum state properties, as outlined in this paper.

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I. INTRODUCTION

System identification and system inversion are two closely related problems. First, considering classical, i.e., nonquantum, 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 [1] is stated to be "nonblind" by the signal and image processing community [2] or "supervised" by the machine learning and data analysis community [3]. The more challenging version of that problem is the blind [2] 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 semiblind). 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 nonblind 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.

[*] yannick.deville@irap.omp.eu
[†] alain.deville@univ-amu.fr

The blind MIMO version of the above system inversion problem is almost the same as blind source separation (BSS) [4–6]: 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 [4–6], which may be seen as an extension of more conventional principal component analysis, or PCA [7]. (PCA alone cannot achieve BSS [6]). 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 [4–6].

We now consider quantum information processing (QIP) [8] and quantum machine learning [9–11], 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 nonblind system identification, especially (see [12]) introduced in 1997 in Ref. [13] and called "quantum process tomography" or QPT by the QIP community: See, e.g., Refs. [8,14–22]. 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 Ref. [23]. 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., Refs. [23,24]) or, more precisely, quantum-source independent component analysis (or QSICA, see, e.g., Ref. [25]) 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 Refs. [26,27] and then especially detailed in Ref. [28]. 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 Ref. [29].

In the present paper, our first contribution (see Sec. IV) concerns yet another type of unsupervised quantum machine learning methods [9], 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 Ref. [30] and we only outlined some resulting BQPT methods in that and some subsequent short conference papers (especially Ref. [31]), but only as spin-offs of corresponding BQSS methods. In contrast, 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: In contrast, 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 Secs. V D and VIII.

(2) This BQPT method therefore first performs measurements at the output of the system, i.e., quantum process, to be identified (see Sec. 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 Sec. 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., nonblind, 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 Sec. 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 Sec. VI . This performance is then compared to that of nonblind QPT methods also dedicated to Heisenberg coupling, that we introduce in Sec. VII, where we also provide an analysis of their theoretical properties. The applications of BQPT methods are presented in Sec. VIII, together with conclusions drawn from this investigation and an outline of its potential extensions.

II. CONSIDERED QUANTUM PROCESS AND STATE PROPERTIES

In standard QPT, if one focuses on the time evolution of the system of interest A, constrained by its couplings to its environment B, the bipartite system $\{A, B\}$ (supposed to be globally isolated at the chosen timescale) is assumed to be initially in a product mixed state $\rho \otimes \rho_B$, where ρ and ρ_B are density operators describing the initial states of A and B respectively. Then, at a later time t, A may be described with a density operator ρ'. In the general context of quantum information, the mapping $\rho \to \rho' = \mathcal{E}(\rho)$ is a so-called quantum operation. In the more specific QPT context, the global transform of $\{A, B\}$ is unitary, and when A is coupled to B, then $\mathcal{E}$, which is not a unitary transform, still happens to be a trace-preserving completely positive mapping (TPCP) [13,32]. This formalism is quite general, but is practically associated with a high complexity (cf., e.g., [16,33]). The particular case when $\mathcal{E}$ is itself a unitary transform is both simpler and important, as it corresponds to a limiting behavior in the presence of weak coupling and

because quantum logic gates, which play a major role in the development of quantum computers, have to implement at least nearly unitary mappings [14]. In this paper, we address such a class of unitary transforms $\mathcal{E}$, by considering a device composed of two distinguishable qubits [28] implemented as electron spins 1/2, that are internally coupled according to the cylindrical-symmetry Heisenberg model, which is, e.g., relevant for spintronics applications [34,35]. We stress that this type of coupling is only used as a concrete example to show how to fully implement the proposed general concepts in a relevant case, but that these concepts and resulting practical BQPT algorithms may then be extended, e.g., to other classes of quantum processes and associated applications, as discussed at the end of Sec. VIII.

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:

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

where

(1) $G = g\mu_e$, 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,

(2) 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, and

(3) 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 the first notation i in the exponentials is the imaginary unit, and with $0 \leqslant r_i \leqslant 1$ 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 $t \geqslant t_0$.

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 [24] 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 Ref. [24], 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,

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

(2) without using or knowing values of its input state $|\psi(t_0)\rangle$,

(3) 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 Ref. [36] 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 Sec. 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 [24,25]

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

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

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

with

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

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

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

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., Refs. [13,15,24,25]).

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 Ref. [37], these probabilities have the following properties:

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

where

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

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

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

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

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

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

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

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

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 BLIND QPT METHODS

We first consider the estimation of parameter v. This is achieved by exploiting (15). If we were developing a conventional, i.e., nonblind, 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 $|\psi(t)\rangle$ (such methods are presented in addition in Sec VII). 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., Ref. [13]); 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

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

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 Refs. [24,25] for BQSS methods intended for the Heisenberg coupling model, setting the constraint

$$0 < r_1 < \tfrac{1}{2} < r_2 < 1 \quad (29)$$

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

$$r_i = \left\{\tfrac{1}{2}\left[(1+p_{1zz}-p_{4zz}) + \epsilon_i\sqrt{(1+p_{1zz}-p_{4zz})^2-4p_{1zz}}\right]\right\}^{1/2} \quad i\in\{1,2\} \quad (30)$$

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 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 statistically independent and have the same statistics): Then, (28) straightforwardly yields

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

In some configurations, the sign of v is known [24,25], 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 BLIND QPT 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 nonblind 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} (this is illustrated by the methods presented in Sec VII). In contrast, 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 [38], 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 the considered spin component, for each of the two spins; 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 Sec. 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 Sec. 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 Sec. IV for our multiple-preparation BQPT method. However, these expressions involve $E\{r_1^2\}$ and $E\{r_2^2\}$ which, unlike in Sec. 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 Sec. 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

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

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

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

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

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 $E\{\sin\Delta_I\} \neq 0$. Equation (28) then yields

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

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

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

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 and (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 constrained to be statistically independent. Besides, r_1 and r_2 are here requested to have the same statistics. Finally, $(\phi_1 - \theta_1)$ and $(\phi_2 - \theta_2)$ are here required to have the same statistics, moreover with the constraints

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

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

which is, e.g., obtained with RVs $(\phi_i - \theta_i)$ whose probability density functions are even and nonzero on $[-\frac{\pi}{2}, \frac{\pi}{2}]$. In that case, (14), (20)–(22), and (27) yield [39] (with the same statistics for $i = 1$ and 2, due to the above constraints):

$$E\{p_{1zz}\} = \big(E\{r_i^2\}\big)^2, \tag{39}$$

$$E\{p_{1xx}\} - E\{p_{4xx}\} = E\{R_{14}\}w_1 - E\{I_{14}\}w_2, \tag{40}$$

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

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

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

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

$$E\{r_i^2\} = \sqrt{E\{p_{1zz}\}}. \tag{44}$$

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

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

Using (25), (44), and (45), Eqs. (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 Eq. (40), by taking into account that w_1 and w_2 are the cosine and sine of the same angle [see (23) and (24)]. However, the solutions of such an equation yield a problematic indeterminacy. This problem is avoided by creating *two* linearly independent Eq. (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. Equations (18) and (19) may then be inverted as

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

with

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

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

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

with

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

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.

Equations (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 Sec. V B yields an estimate $\widehat{v}$ 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 $\widehat{v}$ 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

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

Similarly, the procedure defined in Sec. V C 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

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

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

$$\frac{\widehat{J}_{xy}\tau_1}{\hbar} = \frac{J_{xy}\tau_1}{\hbar} + \Delta k_{xy}\pi, \tag{52}$$

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

with

$$\Delta k_{xy} = \widehat{k}_{xy} - k_{xy}, \tag{54}$$

$$\Delta k_z = \widehat{k}_z - k_z. \tag{55}$$

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) and (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 $e^{i\Delta k_{xy}2\pi} = 1$)

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

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 disappears 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 Refs. [8,16,17,19,20,22], QPT (and hence our blind extension) may especially be used as a major tool for characterizing the *actual* behavior of quantum gates, which are the building blocks of quantum computers. This characterization is typically performed in an "identification phase," taking place before the "computation phase" which uses these quantum processes and gates. Moreover, one may consider scenarios where these processes and gates are used in consistent 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 or 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 gates or processes 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 is equivalent to the first one presented in this section, except that, from the point of view of the computation phase, (i) it uses 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. A summary of this extended BQPT method is provided as a pseudoalgorithm in Algorithm 1.

VI. TEST RESULTS FOR BLIND QPT METHODS

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), and (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), Eqs. (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

Algorithm 1. Second single-preparation blind quantum process tomography method.

Input : Outcomes of measurements of spin components along Oz and Ox axes associated with output process states $|\psi(t)\rangle$, when using single-preparation unknown-value input process states $|\psi(t_0)\rangle$.

Output: An estimate of the quantum process matrix M involved in (7) (to be then used with the write-read time interval $(t-t_0)$ set to τ_3 in the computation phase: see text).

begin

`/* 1. Estimate parameter` v, `with write-read time interval` $(t-t_0)$ `set to` τ_1: `*/`

Derive estimates of $E\{p_{1zz}\}$, $E\{p_{2zz}\}$ and $E\{p_{4zz}\}$ from measurement outcomes;

Estimate $E\{r_1^2\}$ and $E\{r_2^2\}$ by using (34);

Derive estimate of v^2 from (31);

if *sign of* v *unknown* **then**

Derive estimates of $E\{p_{1zz}\}$, $E\{p_{2zz}\}$ and $E\{p_{4zz}\}$ from measurement outcomes;

`/* use state preparations with other statistics than above */`

Estimate $E\{r_1^2\}$ and $E\{r_2^2\}$ by using (34);

Derive sign of v from (36);

end

Derive estimate $\widehat{v}$ of v from its known or estimated sign and from estimate of v^2;

`/* 2. Estimate parameters` w_1 `and` w_2, `with write-read time interval` $(t-t_0)$ `set to` $\tau_2 = 2\tau_1$: `*/`

for *two sets of statistics of parameters of* $|\psi(t_0)\rangle$ **do**

Derive estimates of $E\{p_{1zz}\}$, $E\{p_{1xx}\}$ and $E\{p_{4xx}\}$ from measurement outcomes;

`/* use state preparations with other statistics than when estimating` v `*/`

Estimate $E\{R_{14}\}$ and $E\{I_{14}\}$ by using (41) and (42) with (25), (44) and (45);

end

Solve two equations (40) to get estimates $\widehat{w}_1$ and $\widehat{w}_2$ of w_1 and w_2; `/* one equation for each set of statistics of parameters of` $|\psi(t_0)\rangle$ `*/`

`/* 3. Estimate matrix` M `of quantum process, for a write-read time interval` $(t-t_0)$ `equal to` $\tau_3 = 2\tau_2$: `*/`

Derive an estimate $\widehat{\Delta}_{Ed}$ of Δ_{Ed} by using $\widehat{v}$ in (47);

Derive scaled shifted estimate $\frac{\widehat{J}_{xy}(\tau_1)\tau_1}{\hbar}$ of J_{xy} by using (50) with an arbitrary integer $\widehat{k}_{xy}$, e.g. $\widehat{k}_{xy} = 0$;

Derive an estimate $\widehat{\Delta\Phi}_{1,0d}$ of $\Delta\Phi_{1,0d}$ by using $\widehat{w}_1$ and $\widehat{w}_2$ in (49);

Derive a scaled shifted estimate $\frac{\widehat{J}_z(\tau_2)\tau_2}{\hbar}$ of J_z by using (51), modified as described in text, with an arbitrary integer $\widehat{k}_z$, e.g. $\widehat{k}_z = 0$;

Derive estimate $\widehat{D}$ of D by inserting $\frac{\widehat{J}_{xy}(\tau_1)\tau_3}{\hbar}$ and $\frac{\widehat{J}_z(\tau_2)\tau_3}{\hbar}$ into (11)-(13);

Estimate M by using (9) and (10) with $\widehat{D}$;

end

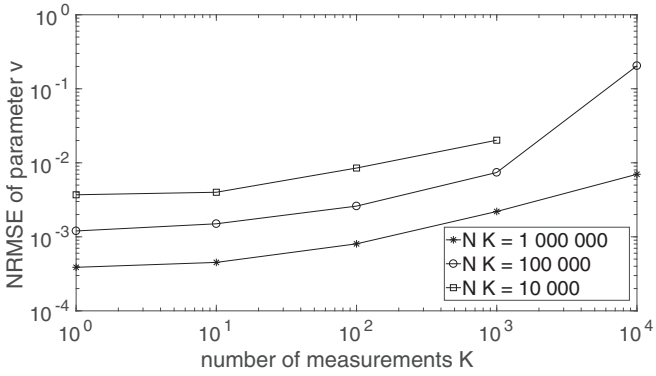

FIG. 1. Normalized root mean square error (NRMSE) of estimation of parameter v vs number K of preparations of each of the N used states.

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 Figs. 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 decrease 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

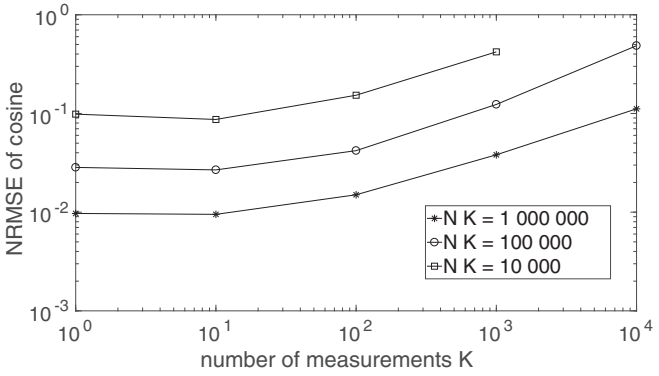

FIG. 2. NRMSE of estimation of parameter w_1 vs number K of preparations of each of the N used states.

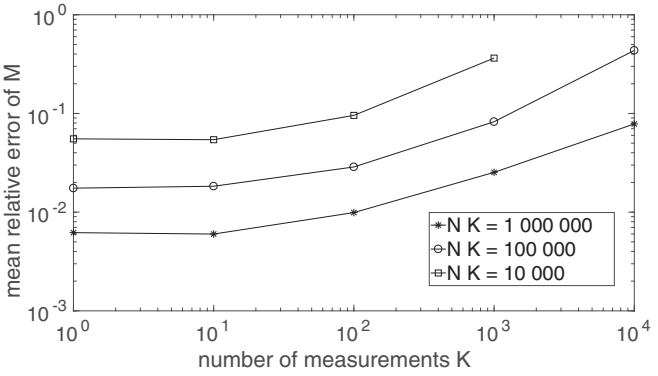

FIG. 4. Mean relative error of estimation of matrix M vs number K of preparations of each of the N used states.

1.75% for $N = 10^5$ or 0.62% for $N = 10^6$. In these tests, we used a simple protocol; 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, Figs. 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 an 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.

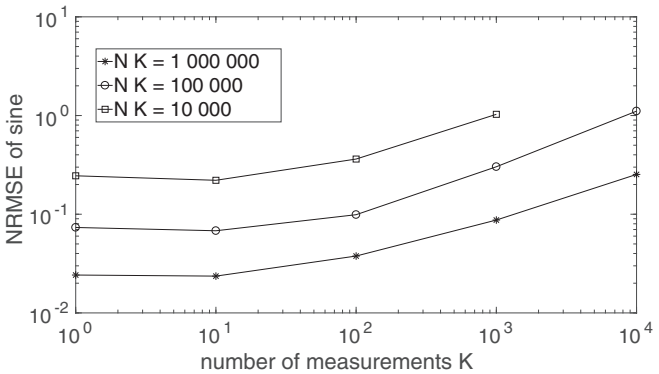

FIG. 3. NRMSE of estimation of parameter w_2 vs number K of preparations of each of the N used states.

VII. NONBLIND QPT METHODS

From the point of view of their principles, nonblind (i.e., traditional) QPT methods and blind QPT methods that were proposed in this paper mainly have a *qualitative* difference: As explained above, a major advantage of blind methods is that they can operate with unknown input states, moreover without requiring each such state to be repeatedly prepared for the single-preparation version that can be developed for blind methods. In contrast, when first *designing* a nonblind method, one must select the value of each of the states to be repeatedly (i.e., multiple-preparation approach; see comments in Sec. V A) provided to the input of the process to be characterized. Then, when actually *applying* such a method, different cases may be considered concerning each stage of the method that is assumed to use one input state value selected by the designer of this method:

(1) The case of "ideal preparation" would occur if one would be able to make all actually prepared input states equal to the "assumed state" selected when designing this QPT method. This case is ideal only from the point of view of the *values* of the input states, but the performance is then still limited by the fact that a *finite* number of copies of the assumed state is prepared, which limits estimation accuracy.

(2) Moreover, the input state values prepared in practice are not equal to the assumed state, due to unavoidable state preparation errors (see, e.g., Refs. [14,15,17,20,40,41]). The first type of such errors is systematic preparation errors, i.e., bias. It corresponds to the situation when all the states which are actually prepared are equal to one another but different from the assumed state.

(3) The second type of errors is nonsystematic preparation errors. It corresponds to the situation when all (or at least some

of) the states which are actually prepared are different from one another and hence different from the assumed state. When the mean value of all these prepared states is equal to the assumed state, these nonsystematic preparation errors involve only spread but no bias.

Considering this practical procedure for applying nonblind QPT methods, one may disregard their above-mentioned qualitative difference with respect to blind QPT methods and anyway aim at *quantitatively* comparing the practical performance reported in Sec. VI for blind methods to the performance of some nonblind methods, depending on the nature and magnitude of the preparation errors. Providing such a numerical comparison is one of our contributions reported in this section. This analysis is again based on the estimation accuracy achieved by the considered methods concerning the matrix M that defines the studied quantum process, depending on the considered "resources" in terms of the total number of input state preparations used in each stage of these methods.

The question is then which nonblind QPT method should be used in this benchmark. A natural approach would consist of using the most standard QPT method, defined in Refs. [8,13]. However, the resulting performance comparison may be considered not to be fair because standard QPT requires a very large number of state preparations (see, e.g., Refs. [16,33]), which is the price to pay for allowing it to apply to a wide class of quantum processes, thus without requiring (nor using, if any) detailed prior knowledge about the considered process. In contrast, beyond the general blind and single-preparation QPT concepts introduced in this paper, the practical BQPT methods that we reported are dedicated to a situation when prior knowledge is available: We focused on the class of Heisenberg processes defined in Sec. II. Therefore, a more relevant comparison is performed by testing a nonblind QPT method dedicated to such processes, preferably with processing stages that are (nonblind but) similar to those used in our blind method, e.g., in terms of the types of spin components that are measured. To our knowledge, no such methods have been reported in the literature (except "indirectly" and for their first part only; see comments about our previous paper in Ref. [42]). Therefore, as an additional contribution in this section, we hereafter introduce a new nonblind method (with some variants) intended for such processes.

As explained above, when *designing* this method, it is assumed that all prepared states provided to the input of the process are equal to one another and to the "assumed state" selected by the designer, thus leading to a multiple-preparation QPT method, as usual in the QPT literature. However, the situation when all prepared input states are different is also of interest, because this situation is also faced in practice (for nonsystematic errors), as stated above. This situation should therefore also be theoretically *analyzed*, before numerically testing it, in order to predict the expected behavior of this QPT method in this situation. This cannot be done in a traditional QPT framework, because that framework only applies to multiple-preparation (i.e., multiple-copy) QPT, whereas nonsystematic errors yield a single instance of each actually used input state. But the latter situation exactly belongs to the original single-preparation QPT framework that we introduced in this paper. A third contribution in this section therefore consists of also using that framework to analyze the studied nonblind QPT method by taking preparation errors, including nonsystematic ones, into account.

A. Design of nonblind QPT methods

1. General structure and considered configuration

The studied nonblind QPT method (and its variants) keeps the same general structure as its blind counterpart of Sec. V:

(1) It first uses spin component measurements along the Oz axis and the associated data model (14)–(19), in order to estimate the mixing parameter v.

(2) It then uses spin component measurements along the Ox axis (but not along the Oz axis, here) and the associated data model (20)–(27), in order to estimate the mixing parameters w_1 and w_2.

(3) It eventually uses the above estimates of v, w_1, and w_2, with exactly the same approach as in Sec. V D, to derive an estimate of the matrix M.

The difference between this approach and the above blind one lies in the method used to estimate v, w_1, and w_2, which is here different because the assumed knowledge about the input states $|\psi(t_0)\rangle$ is different. For each stage of the studied nonblind method, the parameters of the *assumed* input state $|\psi(t_0)\rangle$, that are defined in (3), are hereafter denoted as r_{ia}, θ_{ia}, and ϕ_{ia}, with $i \in \{1, 2\}$. The corresponding value of Δ_I, defined by (17), is denoted as Δ_{Ia}.

2. Estimating the parameter of Oz measurements

In the studied nonblind QPT method, we estimate v by starting from (14)–(16) with r_i and Δ_I respectively replaced by r_{ia} and Δ_{Ia}. The estimate $\widehat{v}$ of v may be obtained by using only (15) (i.e., neither (14) nor (16), unlike in our blind method [43]), which here yields

$$\widehat{p}_{2zz} = r_{1a}^2\left(1-r_{2a}^2\right)\left(1-\widehat{v}^2\right) + \left(1-r_{1a}^2\right)r_{2a}^2\widehat{v}^2 - 2r_{1a}r_{2a}\sqrt{1-r_{1a}^2}\sqrt{1-r_{2a}^2}\sqrt{1-\widehat{v}^2}\widehat{v}\sin\Delta_{Ia} \quad (61)$$

where $\widehat{p}_{2zz}$ is an estimate of probability p_{2zz}, computed as explained in Sec. VII B.

We first use a single assumed input state value which is such that $\sin\Delta_{Ia} = 0$ (this may especially be achieved with $\theta_{ia} = 0$ and $\phi_{ia} = 0$). The resulting version of (61) yields

$$\widehat{v}^2 = \frac{\widehat{p}_{2zz} - r_{1a}^2\left(1-r_{2a}^2\right)}{r_{2a}^2 - r_{1a}^2}. \quad (62)$$

As in our blind approach, additional processing is then required to derive $\widehat{v}$ if its sign is not known. To this end, we use another single assumed state, but now with θ_{ia} and ϕ_{ia} such that $\sin\Delta_{Ia} \neq 0$. Extracting $\widehat{v}$ from (61) then yields

$$\widehat{v} = \frac{r_{1a}^2\left(1-r_{2a}^2\right) + \left(r_{2a}^2 - r_{1a}^2\right)\widehat{v}^2 - \widehat{p}_{2zz}}{2r_{1a}r_{2a}\sqrt{1-r_{1a}^2}\sqrt{1-r_{2a}^2}\sqrt{1-\widehat{v}^2}\sin\Delta_{Ia}}. \quad (63)$$

Taking the sign of this equation results in

$$\mathrm{sgn}(\widehat{v}) = \mathrm{sgn}\big(r_{1a}^2(1-r_{2a}^2) + (r_{2a}^2 - r_{1a}^2)\widehat{v}^2 - \widehat{p}_{2zz}\big) \times \mathrm{sgn}(\sin\Delta_{Ia}) \tag{64}$$

All quantities in the right-hand term of (64) are known [using (62)], which makes it possible to derive $\mathrm{sgn}(\widehat{v})$ from that equation, and then $\widehat{v}$, by combining its sign with $|\widehat{v}|$ derived from (62).

It should be noted that Eqs. (62) and (64), which define the first part of this nonblind QPT method, are the counterparts of Eqs. (31) and (36) derived above for our blind method [42,44].

3. *Estimating the parameters of Ox measurements*

We here estimate w_1 and w_2 by starting from (20)–(27), with r_i, θ_i, and ϕ_i respectively replaced by r_{ia}, θ_{ia}, and ϕ_{ia}. The values of R_{14} and I_{14} in (21) and (22) are thus known, and only (20) is used to estimate w_1 and w_2 (therefore without using measurements of spin components along the Oz axis in addition, unlike in our blind method). More precisely, we here again create *two* linearly independent Eq. (20), each of them with probability estimates $\widehat{p}_{1xx}$ and $\widehat{p}_{4xx}$ derived from a set of prepared input states which are ideally equal to the same assumed value. We then solve these two equations with respect to the estimates of w_1 and w_2.

B. Analysis of nonblind QPT methods

The above-mentioned probability estimates $\widehat{p}_{2zz}$, $\widehat{p}_{1xx}$, and $\widehat{p}_{4xx}$ are here again typically equal to the sample frequencies of the corresponding measurement outcomes over the considered K actually prepared input states involved in each stage of the studied nonblind QPT method. This approach is expected to yield the following performance, depending on the considered case in terms of preparation errors, among the three cases defined at the beginning of Sec. VII, and considering measurements along the Oz axis as an example.

In the case when all K input states are prepared without errors, when K increases, $\widehat{p}_{2zz}$ tends to get closer to the actual value p_{2zz} associated with the single prepared state value. Moreover, this p_{2zz} is consistent with the values r_{ia} and Δ_{Ia} that were inserted into (62) and (64). When K increases, the solution $\widehat{v}$ of these equations therefore tends to (with statistical fluctuations from one estimation of v to another, due to the fluctuations of measurement results) get closer to the actual value v, asymptotically with $\widehat{v} \to v$ when $K \to +\infty$.

In the case of systematic preparation errors only, the same input state value is used in all K preparations so that, here again, when K increases, $\widehat{p}_{2zz}$ tends to get closer to the value p_{2zz} associated with this single input state value [defined by (15)] and $\widehat{p}_{2zz} \to p_{2zz}$ when $K \to +\infty$. However, unlike in the above "ideal preparation" case, this value p_{2zz} and the values r_{ia} and Δ_{Ia} that were inserted into (62) and (64) are here *not* consistent, because they respectively correspond to the actually prepared and assumed input states, which are here different. Therefore, the estimate $\widehat{v}$ derived from the inconsistent values of (62) and (64) remains biased with respect to v even when $K \to +\infty$.

Things get more complex when finally considering the case of spread errors (with or without bias). On the one hand, the method introduced in Sec. VII A was *designed* by considering a single repeatedly prepared input state in each stage, as traditional nonblind QPT methods, hence involving a single probability value p_{2zz} in each of Eqs. (62) and (64) that are used to derive $\widehat{v}$. But on the other hand, the K actually prepared input states are here all different. One may try and consider each of the K probability values p_{2zz}, defined by (15), that are associated with all these states, but anyway (i) each of these p_{2zz} cannot be estimated separately in practice because only a single instance of the corresponding state is available, and (ii) Eqs. (62) and (64) used to derive $\widehat{v}$ do not each involve such a set of K probability values p_{2zz}. The traditional multipreparation nonblind QPT framework therefore does not allow one to *analyze* the situation considered here.

But we can now solve this problem by taking into account the single-preparation framework that we introduced in this paper. To this end, we consider all K *random* input states and the associated *random* probabilities p_{2zz}. As in our single-preparation blind method, we then consider the expectation of (15), but here with r_i and Δ_I respectively replaced by r_{ia} and Δ_{Ia}, which correspond to the single assumed state considered here. This yields

$$E\{p_{2zz}\} \approx r_{1a}^2(1-r_{2a}^2)(1-v^2) + (1-r_{1a}^2)r_{2a}^2v^2 - 2r_{1a}r_{2a}\sqrt{1-r_{1a}^2}\sqrt{1-r_{2a}^2}\sqrt{1-v^2}v\sin\Delta_{Ia} \tag{65}$$

which is the counterpart of (61), but where we use "$\approx$" instead of "$=$" to refer to the fact that the expectation $E\{p_{2zz}\}$ associated with *actual* input states and the *assumed* values r_{ia} and Δ_{Ia} were inserted in (65) independently, "inconsistently" as defined above (with a possibly large discrepancy). The counterparts of (62) and (64) are then derived in the same way as (65). Then replacing $E\{p_{2zz}\}$ and v by their estimates in these equations yields an associated practical procedure for estimating v. The estimate of $E\{p_{2zz}\}$ used here is defined by the framework that we introduced in Sec. V A and Appendix A 2. The required probability estimate is thus equal to the sample frequency of the corresponding measurement outcome over the considered K actually prepared input states. This means that the practical algorithm thus obtained is exactly the same as the one that we derived above for the nonblind QPT method of Sec. VII A. The advantage is that this now allows us to analyze the expected behavior of the method of Sec. VII A for random preparations due to spread errors, with the tools of the single-preparation framework that we introduced in this paper. To this end, we consider (65) [the same approach then applies to the counterpart of (62) and (64) that involves $E\{p_{2zz}\}$]. In practice, the term $E\{p_{2zz}\}$ of (65) is replaced by its above-defined estimate, which has statistical fluctuations as compared with the theoretical value $E\{p_{2zz}\}$, so that the estimate of v derived from (65) (or its subsequent versions) also has statistical fluctuations. Moreover, when $K \to +\infty$, this estimate of $E\{p_{2zz}\}$ has a limit, which is $E\{p_{2zz}\}$ itself (see Appendix A 2). This entails that, if that value $E\{p_{2zz}\}$ is equal to the value p_{2zz} that corresponds to the considered assumed state, i.e., if the actually prepared states have spread but no asymptotic bias, then, when $K \to +\infty$, all quantities in (65) become consistent and hence $\widehat{v} \to v$.

The expected behavior of the studied nonblind method is therefore different for preparations with bias and preparations with spread but no bias. Numerical tests are used hereafter to confirm this theoretical analysis.

C. Test results for nonblind QPT methods

We tested our nonblind method of Sec. VII A in the same conditions as the single-preparation blind one, except for the input states. We hereafter define their assumed and actual values. For each stage of our nonblind method and each of the six input parameters r_i, θ_i, and ϕ_i, with $i \in \{1, 2\}$, the single assumed value r_{ia}, θ_{ia}, or ϕ_{ia} is here set to the middle of the range over which it was previously randomly drawn when testing our blind method (see Appendix B). We first performed tests with only systematic errors, i.e., biased actually prepared input states. θ_1 and θ_2 were fixed to 0 in all these tests. Besides, denoting u and u_a as the actual and assumed values of an arbitrary parameter among r_i and ϕ_i, that actual value was set to

$$u = u_a \pm f_b R_u \tag{66}$$

where R_u is the width of the range associated with parameter u, that is 0.5, 0.5, 2π, and 2π respectively for parameters r_1, r_2, ϕ_1, and ϕ_2 in all stages of this nonblind method. f_b (called the bias factor) then defines the magnitude of the bias considered for u in terms of a fraction of the above range. The considered fraction f_b is the same for all parameters u and all stages of the method, which allows us to tune a *single* parameter to investigate the sensitivity of our nonblind method to systematic errors. The sign "±" in (66) stands for "−", "+", "−", "+" respectively for parameters r_1, r_2, ϕ_1, and ϕ_2. Different signs are required for ϕ_1 and ϕ_2 because otherwise, with the specific protocol (66) here used for controlling the parameter biases, the resulting parameter of interest (17) for Oz measurements would remain unbiased whatever the value of the parameter f_b of that protocol.

We then performed tests with nonsystematic errors, i.e., spread actually prepared state, without bias. θ_1 and θ_2 were fixed to 0 in all these tests. Besides, again for any parameter u among r_i and ϕ_i, each actually prepared value of u was randomly, uniformly, drawn over the interval $[u_{\min}, u_{\max}]$ with

$$u_{\min} = u_a - f_s R_u \tag{67}$$

$$u_{\max} = u_a + f_s R_u \tag{68}$$

where f_s (called the spread factor) defines the magnitude of the spread considered for u in terms of the fraction of the above-defined range R_u. That single parameter f_s is used to investigate the sensitivity of our nonblind method to the spread of prepared states.

Figure 5 shows the results obtained for our blind method (operated with $K = 1$ and N varied, where N and K were defined in Sec. VI) and for our nonblind method (operated with $N = 1$ and K varied), receiving input states with systematic errors. The specific case $f_b = 0$ corresponds to no bias, i.e., "ideal preparation." We here again analyze the mean relative error for the matrix M, depending on the total number NK of preparations per stage. As expected for our blind method and for our nonblind method with "ideal preparation" (see Sec. VII B), performance continuously improves when NK increases. Moreover, the price to pay for the advantages of our blind method as compared with this ideal version of our nonblind method is only a limited performance degradation. When considering systematic errors that occur in practice, the performance of our nonblind method is altered in a way which is qualitatively consistent with our analysis of Sec. VII B (i.e., the error on M stops to decrease when NK exceeds a certain value) and which quantitatively yields a major limitation for that method: Even for a bias as low as 0.1% of the parameter ranges, our nonblind method yields much lower performance than the blind one in the range of values of NK for which the blind method yields particularly attractive performance (this blind method, e.g., yields an error significantly lower than 1% for $NK = 10^6$). Besides, for a low bias of 1%, the error of the nonblind method remains saturated to a high value whatever NK in the considered range. Therefore, although that nonblind method was designed specifically for the considered class of quantum processes, it is highly sensitive to systematic errors and our blind method is hence a much more attractive alternative.

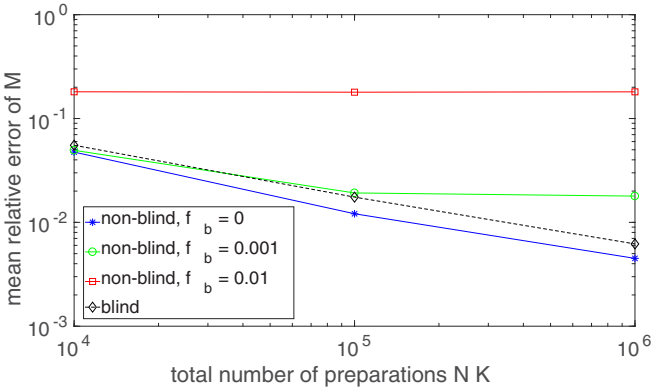

FIG. 5. Mean relative error of estimation of matrix M vs total number NK of preparations. Dashed black line: blind method. Solid color line: nonblind method receiving input states with systematic errors defined by f_b.

Similarly, Fig. 6 shows the results obtained for our blind and nonblind methods (both operated with $K = 1$ and N varied), receiving input states with nonsystematic errors. The specific case $f_s = 0$ corresponds to no spread, i.e., "ideal preparation." When considering nonsystematic errors that occur in practice, the performance of our nonblind method is altered in a way which is qualitatively consistent with our analysis of Sec. VII B (i.e., the error on M decreases when NK increases and it would disappear only when $NK \to +\infty$), but which quantitatively yields a significant limitation for that method: Even for a spread as low as 5% of the parameter ranges, our nonblind method yields much lower performance than the blind one in the range of values of NK for which the blind method yields particularly attractive performance (e.g., as stated above, an error significantly lower than 1% for $NK = 10^6$). Therefore, the sensitivity of that specifically designed nonblind method to spread errors it also significant (although it is much lower than its sensitivity to systematic errors), which confirms that our blind method is a much more attractive alternative.

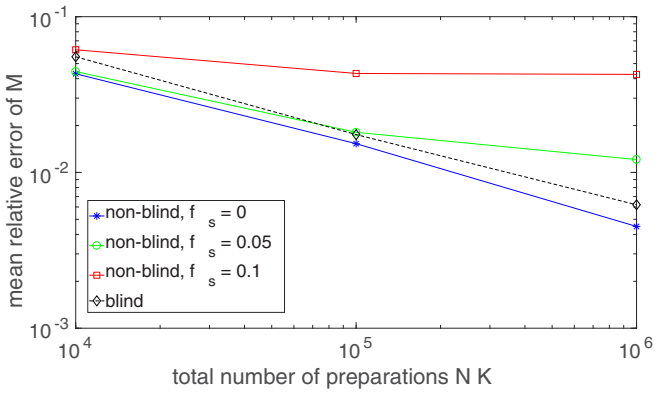

FIG. 6. Mean relative error of estimation of matrix M vs total number NK of preparations. Dashed black line: blind method. Solid color line: nonblind method receiving input states with nonsystematic errors defined by f_s.

VIII. DISCUSSION, PROSPECTS, AND CONCLUSION

As explained in the introduction, in a classical context, solutions to the system identification problem are well known, which was a reason for hoping that it should be possible to build up corresponding solutions in a quantum context. Such a hope reflects the existing consensus upon the idea that any experimental fact possessing a classical explanation may be interpreted as some limit of a quantum behavior. It is true that the correspondence principle was historically used as a heuristic tool for the building of quantum mechanics. But, e.g., in the field of information theory (IT) there exists no general recipe allowing one to build up a quantum IT from the existing classical IT. And when trying to move conceptually from a quantum to a classical description, it is not possible to subsume the difference through making $\hbar \longrightarrow 0$ in the quantum approach, and, e.g., the spin has no classical analog. The main reason for this difficulty of establishing a bridge between the two approaches is the existence of conceptual rather than quantitative differences between classical and quantum theories. Chapter 15 of Ref. [45] is devoted to a convincing discussion, by Ballentine, of the question of the classical limit. In the domain of quantum tomography (QT), a subfield of IT, one has to keep in mind both these reservations and the idea that the development of QT is a complex activity aiming at building a quantum version of system identification. And the present paper, together with [30,31], suggests that, in QT, any definition opposing a situation where the *states* are known and one in which the *process* is known should henceforth be restricted to *nonblind* QPT and quantum state tomography (QST) respectively. In contrast, the present paper deals with the *blind* version of quantum *process* identification, i.e., when not only that process but also its input state are unknown. More precisely, the features of nonblind and blind QPT may be contrasted as follows. The usual, i.e., nonblind, version of QPT requires one to know, hence to very precisely control (i.e., prepare), the specific quantum states used as inputs of the quantum process to be characterized (this is illustrated in Sec. VII, for the original nonblind QPT methods that we introduce in this paper). 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 (see Sec. V D) 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 online characterization may 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 with 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. Moreover, 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.

We therefore presented two main types of contributions in this paper. On the one hand, we introduced the general joint concept of single-preparation blind QPT (SBQPT). On the other hand, we showed in detail how to apply that concept to a specific type of quantum process, based on cylindrical-symmetry Heisenberg coupling, we numerically validated the performance thus achieved and we compared it to the performance of relevant, original, nonblind QPT methods (similarly,

various papers from the literature dealing with nonblind QPT are focused on other specific processes or class of processes; see, e.g., Refs. [18,20,46]). Beyond these two aspects, this investigation opens the way to various extensions of SBQPT, which will be reported in future papers and which may here be outlined as follows. First, still considering two qubits isolated from their environment, the specific (Heisenberg) coupling between them which was considered above may be replaced by another phenomenon, thus leading to another specific type of unitary process. At least for some of these processes, we anticipate that it will be rather easy to transpose to such processes the SBQPT procedure that we detailed above for one type of process. Besides, some other extensions will most likely require more in-depth investigations. This includes applying the proposed general concepts to processes with more than two input qubits [47], to arbitrary unitary processes and more generally to possibly nonunitary (but trace-preserving and completely positive) processes that take into account interactions of the qubits with their environment. Moreover, the extensions listed so far are focused on the considered process itself, but one may also focus on the *input values* of these processes. In the above investigation, we considered input pure states, described by the kets $|\psi(t_0)\rangle$, but we used an already extended framework by considering *random-valued* ket coefficients, unlike in standard *deterministic* pure states. In contrast, in the standard QPT framework described in Refs. [8,13], the process inputs are defined in terms of statistical mixtures represented by density operators. We started to discuss the connections between these two approaches in Ref. [36] (for other types of BQPT and BQSS methods), and this topic could be further investigated. Finally, one may consider extending SBQPT methods to other statistical parameters of quantum measurement outcomes or to other quantum state properties.

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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 Sec. A 1) and that we need, in order to then introduce our nonconventional, single-preparation, approach to QIP (see Sec. 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 Ref. [36], it is represented by a normalized vector of a two-dimensional space $\mathcal{E}_i$, expressed as

$$|\psi_i\rangle = \alpha_i|+\rangle_i + \beta_i|-\rangle_i \tag{A1}$$

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 [28] qubits, with indices $i \in \{1, \ldots, Q\}$. 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 $|+\rangle_1 \otimes |+\rangle_2 \otimes \cdots \otimes |+\rangle_{Q-1} \otimes |+\rangle_Q$ to $|-\rangle_1 \otimes |-\rangle_2 \otimes \cdots \otimes |-\rangle_{Q-1} \otimes |-\rangle_Q$ that we hereafter respectively denote as $|j\rangle$, with $j \in \{1, \ldots, 2^Q\}$. The state of this set of qubits then reads

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

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

$$\sum_{j=1}^{2^Q} |c_j|^2 = 1. \tag{A3}$$

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., Ref. [24] 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 [48] A_j is defined as follows: The result of the experiment is equal to the jth 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

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

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 [24,28]) of copies of that state, so that we hereafter call this approach "multiple-preparation QIP" (we previously called it "batch QIP" in Ref. [38]). These copies may be obtained in parallel from an ensemble of systems or successively for the same system ("repeated write-read," or RWR, procedure [23–25]). 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 [23–25], we had to extend that framework to *random* pure quantum states. We especially detailed that concept in Ref. [36]. 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 [23–25], 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 Sec. 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 Ref. [38]). 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., Ref. [48]) at the above-defined two levels of the considered procedure:

(1) 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 $|\psi(n)\rangle$.

(2) 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

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

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:

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

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

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

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:

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

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

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

$\sum_{n=1}^{N} \mathcal{N}(A_j, n, K)$ 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 [48]. This quantity (A9) may therefore also be expressed as

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

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

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 Ref. [38]. Moreover, Ref. [38] 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 Sec. 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 Sec. V B, the qubit parameter values r_1 and r_2 were selected within the 20–80% subrange 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 Ref. [25]. 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 Sec. 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 nonzero 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 [49]. Finally, to estimate w_1 and w_2, the method of Sec. 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 Eq. (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 Eq. (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 Eq. (40). All above conditions concern the identification phase. Then, in the computation phase, we used $\tau_3 = 2\tau_2$, as explained in Sec. 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 Ref. [24] and Ref. [50]) .

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[42] The first part of our nonblind QPT method of Sec. VII A is also connected as follows to our paper [24]. In Ref. [24], the target task is nonblind and blind quantum source separation (QSS), only considering spin component measurements. But this QSS task itself requires one to estimate the parameter v related to Heisenberg coupling. The main nonblind method proposed to this end in Ref. [24] is nothing but the variant defined in Ref. [44] for the part of the nonblind QPT method dedicated to v that we independently derived in Sec. VII A 2 from the associated blind QPT method. Reference [24] also contains a modified method for estimating v that could therefore also be used here. It would be helpful if one would like to avoid using input states such that $\sin\Delta_{Ia}=0$. In contrast, Ref. [24] does not consider measurements of spin components along the Ox axis. The part of our nonblind QPT method dedicated to such measurements (which are needed to estimate w_1 and w_2 and hence the complete process) is therefore studied in the present paper, in Sec. VII A 3.
[43] A variant of the nonblind QPT method introduced in Sec. VII A may be obtained by replacing, in (15), r_1 and r_2 by $\widehat{r}_1$ and $\widehat{r}_2$, essentially derived in the same way as in our blind multiple-preparation method, i.e., by solving with respect to estimates of r_1 and r_2 the version of (14) and (16) which involves estimates of p_{1zz} and p_{4zz}; see (30). However, this variant entails estimation errors for r_1 and r_2 and is therefore likely to yield lower performance than the method presented in Sec. VII A that uses r_{1a} and r_{2a}, except especially in the case when the following conditions are met: (i) these estimation errors for r_1 and r_2 are low, i.e., the number K of prepared states is high (but this is not the case of main interest due to its complexity) and (ii) the method of Sec. VII A entails significant errors by using r_{1a} and r_{2a}, because the actually prepared state value(s) have large errors.
[44] Another variant of the nonblind QPT method introduced in Sec. VII A is obtained by using (63), with $\widehat{v}^2$ defined by (62), to *directly* derive $\widehat{v}$ [instead of using (64)], thanks to the fact that, in the nonblind case, the value of $\sin\Delta_{Ia}$ is known. This variant may seem to be more natural than the version described in Sec. VII A. But the two nonblind QPT methods which consist of the variant defined here and of the main version described in Sec. VII A deserve the following comments. Let us consider the single-preparation blind counterparts, based on (35) instead of (63), of these two nonblind QPT methods, namely method (a) which is the blind counterpart of the nonblind variant that we here introduced by directly deriving $\widehat{v}$ from (63) and method (b) which is the blind counterpart of the nonblind version of Sec. VII A; i.e., method (b) is the method of Sec. V. Method (a) is much less attractive than method (b), first because, to derive v directly from (35), method (a) requires the *value* of $E\{\sin\Delta_I\}$ to be known, instead of just its *sign* in the blind version of Sec. V, and requesting the user to know this value makes the method less blind. Similarly, method (a) requires the values of $E\{r_i\sqrt{1-r_i^2}\}$ in (35) to be known. Therefore, for blind methods, we selected the version of Sec. V and then, for nonblind methods, to obtain a version which is as similar as possible to the blind approach proposed in Sec. V, we focus on the version of Sec. VII A in the remainder of this paper.
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