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Classical-processing and quantum-processing signal separation methods for qubit uncoupling

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Abstract The Blind Source Separation problem consists in estimating a set of unknown source signals from their measured combinations. It was only investigated in a non-quantum framework up to now. We propose its first quantum extensions. We thus introduce the Quantum Source Separation field, investigating both its blind and non-blind configurations. More precisely, we show how to retrieve individual quantum bits (qubits) only from the global state resulting from their undesired coupling. We consider cylindrical-symmetry Heisenberg coupling, which e.g. occurs when two electron spins interact through exchange. We first propose several qubit uncoupling methods which typically measure repeatedly the coupled quantum states resulting from individual qubits preparations, and which then statistically process the classical data provided by these measurements. Numerical tests prove the effectiveness of these methods. We then derive a combination of quantum gates for performing qubit uncoupling, thus avoiding repeated qubit preparations and irreversible measurements.

Keywords blind source separation (BSS) · cylindrical-symmetry Heisenberg coupling · quantum bit (qubit) · quantum circuit · quantum source separation · spin uncoupling ·

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1 Introduction

Various areas within the information processing field developed very rapidly during the last decades. This includes the generic Blind Source (or Signal) Separation (BSS) problem, which consists in estimating a set of unknown source signals from a set of observed (i.e. measured) signals which are so-called mixtures[1], i.e. combinations, of these source signals [10], [12], [13], [24], [25]. BSS methods thus apply to a wide range of signal denoising and component extraction problems (see e.g. Chapter 16 of [13] for an overview). This especially concerns communications, e.g. when a set of radio-frequency reception antennas provide linear combinations (which are a simple class of "mixtures") of several emitted signals and one aims at retrieving each emitted signal only from their received combinations (see e.g. a typical application in [16] and the survey presented in Chapter 17 of [13]). Similarly, this applies to the generic acoustic configuration based on a set of microphones, which perform recordings in a room where several people are simultaneously talking (this is known as the "cocktail party" effect). Each microphone then records a superposition of filtered speech signals, and BSS methods aim at extracting each original speech signal from all available microphone recordings (see e.g. [28] and Chapter 19 of [13]). Applications of BSS approaches have also been reported in many other fields,

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[1] The word "mixture" and related terms are used in the BSS sense in all this paper: we are not considering "statistical mixtures" in the Quantum Physics sense, as detailed in Appendix A.

especially in the biomedical domain (see e.g. [32] and Chapter 18 of [13]).

Another growing area is Quantum Information Processing (QIP), which is closely related to Quantum Physics (QP) [6], [9], [30], [35]. QIP uses abstract representations of systems whose behavior is requested to obey the laws of QP. This already yielded new and powerful information processing methods, to be contrasted with "classical", i.e. non-quantum, methods such as the existing above-mentioned BSS approaches. Their effective implementation then requires one to develop practical quantum systems, which is only an emerging topic today [30].

To our knowledge, no connection has been made between the classical BSS and QIP/QP areas in any journal before this paper. One may expect, however, that undesired "coupling" between individual "signals" (i.e. quantum states) will also have to be considered in the QIP/QP area. Such a coupling e.g. occurs when two electron spins interact through exchange. In this paper, we consider two spins with cylindrical-symmetry Heisenberg coupling and we investigate how each individual spin state may be retrieved from the global state resulting from that coupling. We thus introduce quantum extensions of the "fully classical" BSS field (i.e. BSS for initially classical signals and with classical processing means). As a consequence of Bohr's correspondence principle, any classical phenomenon can be viewed as the limit of some quantum phenomenon. An extension of BSS from the classical to the quantum domain is therefore legitimate, even if it is not a direct consequence of the development of experimental methods and/or theoretical advances in the QIP field. Our approach for introducing quantum BSS is also relevant because, to a large extent, classical BSS belongs to the more general Statistical Signal Processing (SSP) field: since QIP and QP are essentially based on a *probabilistic* view of physical phenomena, trying to bridge the gap between SSP/BSS and QIP/QP is a priori a reasonable attempt.

The proposed extensions of the (B)SS field to the quantum domain may yield two types of separation methods and two types of applications because, **whereas both the initial data (source signals) and their mixtures resulting from undesired coupling have a quantum nature, these mixtures may be *processed* either by classical means (after measurements) or by quantum means.** In this paper, we investigate both types of processing which allow to retrieve quantum source information:

– we first propose methods using measurements (of quantum observables). In that context, a major feature of the (B)SS problem is that, *whatever the details of the measurement process, these measurements necessarily lead to classical data*, and hence to *classical processing* (i.e. processing of classical data). Therefore, without having to wait for the development of practical quantum circuits, this classical-processing version of our approach already applies to possible experiments requiring methods for retrieving information about individual quantum states from measurements performed after undesired coupling between these states, e.g. when dealing with quantum phenomena involving electron or nuclear spins 1/2.

– We then more briefly examine a method where the processed data are still in quantum form (i.e. no measurements are performed before processing). Our method for *quantum processing* was clearly suggested by the already existing experimental and theoretical results in the field of quantum computing. The general principles used in that field, rooted in the ideas mainly introduced by Feynman [20], [21], Benioff [4], Deutsch [14] and Bennett [5], and respecting the postulates of quantum mechanics, have been successfully tested experimentally. This is especially true for the unitary time evolution of the quantum gates, e.g. tested using high resolution liquid state pulsed NMR.

In this context, a potential application of our quantum extensions of (B)SS concerns the core of future quantum computers, where both the data to be processed and the processing means will have a quantum nature. When developing our quantum-processing method, we keep the usual approach of quantum computing, thoroughly presented in the reference book [30], which e.g. states that "a quantum computer is built from a quantum circuit containing wires and elementary quantum gates to carry around and manipulate the quantum information" (p. 17).

In our quantum-processing method, once the quantum source information has been retrieved, it has of course to be used. It may e.g. be decided that quantum measurements should be made (reading). This last step is outside the subject of source separation, a point of view similar to that adopted in quantum computing, as can be e.g. again seen in [30]. Its authors: 1) state that "a final element used in quantum circuits, almost implicitly sometimes, is measurement" (p. 185), 2) consider that both the very first stage for *preparing* the input quantum states and the final stage for *reading* the final quantum data are not part of the core quantum circuit structure, so that these stages are most often omitted from the representations of these circuits, as is done

e.g. for the quantum circuit implementing Deutsch's algorithm (p. 33) or for the circuit devoted to the quantum Fourier transform (p. 219).

As explicitely stated in [30], (p. 324): "Traditional quantum computation requires the system be prepared in a pure state". Keeping the case of NMR quantum gates, since a high number of nuclear spins are involved in NMR experiments, the so-called pseudo-pure states rather than pure states are then used. However, experiments with *electron spins* using a single (or a small number of) spin(s) are under development [27], [34], [39]. The present paper, when briefly considering physical rather than formal quantum bits (qubits), implicitly refers to experiments of the latter kind, involving a few quantum particles, which are not restricted to electron *spins*, but are far more general. One may think both of the Devoret group using the *charge* of electron in single-electron devices [19], [31], or using carbon nanotubes for the implementation of *quantum wires* [36] and of several groups working with *molecules* in the optical range [29].

The necessity of considering a pair of simple signals with undesired coupling in this introductory paper presently limits this application to quantum computing, excluding e.g. the correction of the consequences of a possible undesired coupling betwen the *outputs* of two-input quantum gates.

One should once for all note that, whereas we are here concerned with configurations where one aims at extracting information about quantum states after *undesired* coupling (following Heisenberg's model), on the contrary a two-qubit gate using liquid NMR *takes advantage* [37] of the scalar coupling [1].

The remainder of this article contains parts of different natures, i.e. mainly dealing with SSP/BSS or QIP/QP. It is organized as follows. In Section 2, we remind the reader of a major QIP concept used throughout this paper, i.e. the qubit (for a more detailed presentation of QIP, see [30]). Section 2 also describes the temporal evolution of a qubit, which is of utmost importance for the quantum data analyzed in this paper. Based on this general qubit concept, we then move in Section 3 to the specific quantum data model considered in this paper, which consists of two qubits coupled according to the cylindrical-symmetry Heisenberg model. We first define the resulting system quantum state itself, and then determine the expressions of the classical data derived from these coupled qubits by means of measurements. These classical data are the "mixed observations" (in the BSS sense) which may then be processed by classical BSS methods. The "mixing model" thus obtained turns out to be nonlinear and different

from those previously studied in the classical BSS literature (for a survey of nonlinear BSS, see e.g. [13], [25]). Therefore, in Section 4 we propose various classical signal separation methods for processing such mixed observations, considering "ideal", non-blind and blind configurations. The performance of the three types of methods thus introduced is assessed by means of numerical tests in Section 5. Then, as a quantum-processing alternative to the above classical-processing methods, in Section 6 we propose a quantum circuit structure for directly processing the coupled qubits, so as to restore their original uncoupled values. Conclusions are drawn from this investigation in Section 7, and more specific topics are detailed in the appendices. In particular, Appendix B details some aspects of the relationship between the Quantum Source Separation (QSS) field that we introduce in this paper and some other fields within the QIP domain, in addition to their relationships described above.

2 Definition of a single qubit

The fundamental concept used in abstract QIP is the quantum bit, or qubit. While a (classical) bit can only take two values, usually denoted 1 and 0, a qubit may be in any state $|\psi>$ expressed as

$$|\psi> = \alpha|+> + \beta|-> \tag{1}$$

in the basis defined by the two orthonormal vectors that we denote $|+>$ and $|->$ hereafter[2], where α and β are two complex-valued coefficients constrained to meet the condition

$$|\alpha|^2 + |\beta|^2 = 1 \tag{2}$$

which expresses that the state $|\psi>$ is normalized. From a QP point of view, this abstract mathematical model especially concerns electron or nuclear spins 1/2, which are quantum (i.e. non-classical) objects. The component of such a spin along a given arbitrary axis Oz defines a two-dimensional linear operator s_z. The two eigenvalues of this operator are equal to $+\frac{1}{2}$ and $-\frac{1}{2}$ in normalized units, and the corresponding eigenvectors are therefore denoted $|+>$ and $|->$. The value obtained when measuring this spin component can only be $+\frac{1}{2}$ or $-\frac{1}{2}$. Moreover, let us assume this spin is in the state $|\psi>$ defined by (1) when performing such a

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[2] These vectors $|+>$ and $|->$ are often respectively denoted $|0>$ and $|1>$ (see e.g. [30]). We here use the notations $|+>$ and $|->$, and the resulting notations for the basis $\mathcal{B}_+ = \{|++>, |+->, |-+>, |-->\}$ introduced in Section 3, in order to avoid confusion with the vectors of the other basis that we also have to consider specifically in this paper, i.e. $\mathcal{B}_1 = \{|1,1>, |1,0>, |0,0>, |1,-1>\}$ (see Appendix C).

measurement. Then, the probability that the measured value is equal to $+\frac{1}{2}$ (respectively $-\frac{1}{2}$) is equal to $|\alpha|^2$ (respectively $|\beta|^2$), i.e. to the squared modulus of the coefficient in (1) of the associated eigenvector $|+>$ (respectively $|->$).

The above discussion concerns the state of the considered spin at a given time. In addition, this state evolves with time. The spin is here supposed to be placed in a magnetic field and thus coupled to it. The time interval when it is considered is assumed to be short enough for the coupling between the spin and its environment to be negligible. In these conditions, the spin has a Hamiltonian. Therefore, if the spin state $|\psi(t_0)>$ at time t_0 is defined by (1), it then evolves according to Schrödinger's equation and its value at any time t is

$$|\psi(t)> = \alpha e^{-i\omega_p(t-t_0)}|+> +\beta e^{-i\omega_m(t-t_0)}|-> \qquad (3)$$

where $i = (-1)^{\frac{1}{2}}$ and the real (angular) frequencies ω_p and ω_m depend on the considered physical setup.

3 Coupling/mixing models for two qubits

3.1 Quantum point of view: spin coupling model

Future QIP systems will simultaneously handle several qubits, which will e.g. be physically implemented as sets of spins. One may expect that undesired coupling between these spins will appear in quantum physical setups, in the same way as current classical signal processing systems involve undesired signal coupling. We here consider a system composed of two such distinguishable spins. These spins are assumed to be coupled according to the version of the Heisenberg model which has a cylindrical-symmetry axis, denoted Oz (this includes the isotropic Heisenberg model as a specific case). These 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. Here again, 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 system composed of these two spins is governed by the following Hamiltonian

$$H = Gs_{1z}B + Gs_{2z}B - 2J_{xy}(s_{1x}s_{2x} + s_{1y}s_{2y})$$
$$-2J_z s_{1z}s_{2z} \qquad (4)$$

where:

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

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

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

We then assume that these two spins, called spin 1 and spin 2 hereafter, are respectively initialized with states

$$|\psi_1(t_0)> = \alpha_1|+> +\beta_1|-> \qquad (5)$$

and

$$|\psi_2(t_0)> = \alpha_2|+> +\beta_2|-> \qquad (6)$$

at a given time t_0. The $|+>$ vectors in (5) and (6) are different: they are respectively associated with spin 1 and spin 2. These spins are then coupled according to the above-defined model for $t \geq t_0$.

Hereafter, we consider the state $|\psi(t)>$ 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 (5)-(6). It may therefore be expressed as

$$|\psi(t_0)> = |\psi_1(t_0)> \otimes |\psi_2(t_0)> \qquad (7)$$
$$= \alpha_1\alpha_2|++> +\alpha_1\beta_2|+->$$
$$+\beta_1\alpha_2|-+> +\beta_1\beta_2|--> \qquad (8)$$

in the four-dimensional basis $\mathcal{B}_+ = \{|++>, |+->, |-+>, |-->\}$ which corresponds to the operators s_{1z} and s_{2z} respectively associated with the components of the two spins along the symmetry axis Oz.

The state of this two-spin system then evolves with time. Its value at any subsequent time t may be derived from its above-defined Hamiltonian. We show in Appendix C that it reads

$$|\psi(t)> = \sum_{j=1}^{4} c_j(t-t_0)|b_j> \qquad (9)$$

where $|b_j>$ are the basis vectors composing the four-dimensional basis $\mathcal{B}_+$ and the expressions of the corresponding amplitudes $c_j(t-t_0)$ are detailed in (68).

We here started from a concrete (i.e. physical) setup, thus considering a QP point of view. This led us to the state expression in (9). From here on, we move to an abstract QIP point of view, and we aim at restoring the state of each qubit at time t_0 only from the state of the qubit pair at time $t > t_0$ as described by (9).

3.2 Statistical signal processing point of view: new mixing model for classical-processing separation methods

The first approach proposed in this paper consists in converting the above overall quantum state into clas-

sical data by performing measurements, and then processing the latter data with classical means. We here derive the model of these classical data, while the associated processing methods will then be described in Section 4.

This approach is based on a "repeated write/read" (RWR) procedure, which consists in performing K times the same "write/read" step. In each occurence k of this step, a user W first writes (i.e. prepares) both qubits at time $t_w(k)$, respectively with the states defined in (5)-(6), and then, at time $t_r(k)$, a user R reads the state of the system composed of the two coupled qubits. This state is defined by (9), with $(t - t_0)$ replaced by $T(k) = t_r(k) - t_w(k)$, which yields the coefficients $c_j(T(k))$. Reading the system's state means that user R measures the couple of values associated with s_{1z} and s_{2z}. This couple is then equal (in normalized units) to one of the four possible values $(+\frac{1}{2}, +\frac{1}{2})$, $(+\frac{1}{2}, -\frac{1}{2})$, $(-\frac{1}{2}, +\frac{1}{2})$ and $(-\frac{1}{2}, -\frac{1}{2})$, respectively with probabilities[3] p_1, p_2, p_3 and p_4 equal to the squared moduli of the coefficients $c_j(T(k))$ associated with the states composing $\mathcal{B}_+$ in the modified version of (9), i.e.

$$|c_j(T(k))|^2 = p_j \qquad \forall\, j \in \{1 \dots 4\}. \tag{10}$$

Using the expressions of the coefficients c_j provided in (68), Eq. (10) reads

$$\left| \alpha_1 \alpha_2 e^{-i\omega_{1,1} T(k)} \right|^2 = p_1 \tag{11}$$

$$\frac{1}{4} \left| (\alpha_1 \beta_2 + \beta_1 \alpha_2) e^{-i\omega_{1,0} T(k)} \right.$$
$$\left. + (\alpha_1 \beta_2 - \beta_1 \alpha_2) e^{-i\omega_{0,0} T(k)} \right|^2 = p_2 \tag{12}$$

$$\frac{1}{4} \left| (\alpha_1 \beta_2 + \beta_1 \alpha_2) e^{-i\omega_{1,0} T(k)} \right.$$
$$\left. - (\alpha_1 \beta_2 - \beta_1 \alpha_2) e^{-i\omega_{0,0} T(k)} \right|^2 = p_3 \tag{13}$$

$$\left| \beta_1 \beta_2 e^{-i\omega_{1,-1} T(k)} \right|^2 = p_4. \tag{14}$$

Eq. (11) and (14) do not depend on their phase factors, i.e. they reduce to

$$|\alpha_1 \alpha_2|^2 = p_1 \tag{15}$$
$$|\beta_1 \beta_2|^2 = p_4. \tag{16}$$

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[3] We provided a preliminary description related to this mixing model in our conference papers [17],[18]. As compared to these papers, we here modify the respective indices of the probabilities associated with the four possible measured values. This modification is made in order for these indices to be directly related to the order of the corresponding vectors in the above-defined basis $\mathcal{B}_+$. Similarly, as compared to our conference papers, we here reorder the vectors in basis $\mathcal{B}_1$, which is defined in Appendix C. This aims at simplifying the description of the quantum-processing approach which is introduced in Section 6, which was not considered at all in our conference papers.

In order to use our statistical signal processing (SSP) approach, (12)-(13) should involve the same parameter values in all occurences k of the write/read step. The write-read time interval $T(k)$ should therefore be the same for all occurences. It is denoted T hereafter.

Estimates of p_1 to p_4 may then be straightforwardly obtained as the relative frequencies of occurence of the four values $(+\frac{1}{2}, +\frac{1}{2})$ to $(-\frac{1}{2}, -\frac{1}{2})$ respectively, in the measurements of our RWR procedure[4]. Unfortunately, as a consequence of the exchange coupling, these estimated probabilities do not directly yield the parameters α_i and β_i that user R aims at determining, i.e. the considered two qubits are "mixed" (in the source separation sense) in these measured data defined by (12), (13), (15) and (16). This therefore defines a new problem similar to fully classical Source (or Signal) Separation (SS). The new nonlinear SS configuration thus obtained involves the following three items at this *preliminary* stage: (i) the observed data consist of the measured probabilities p_1 to p_4, (ii) the "source signals" to be extracted from them are the parameters α_i and β_i and (iii) the unknown coefficients of the considered set of nonlinear "mixing" (in SS terms) equations are the frequencies $\omega_{i,j}$. These three items deserve the following comments.

Let us first note that the equations in the complete mixture model, i.e. (12), (13), (15), (16), are partly redundant: we always have

$$p_1 + p_2 + p_3 + p_4 = 1 \tag{17}$$

because the initial states defined by (5)-(6), are normalized, so that the state $|\psi(t_w(k)) >$ defined by (7) is normalized, and this state then evolves according to Schrödinger's equation, which keeps norm unchanged. We therefore only consider p_1, p_2 and p_4 as the observed data hereafter, and (12), (15), (16) as the mixing equations[5]. Using standard SS notations, the "observation vector" (composed of the measured parameters) is therefore $x = [x_1, x_2, x_3]^T$ with $x_1 = p_1, x_2 = p_2$ and $x_3 = p_4$, and where ^{T} stands for transpose.

To derive the final expressions of the mixing model and the definition of sources, we then express each complex-valued qubit parameter in polar form, i.e.

$$\alpha_1 = r_1 e^{i\theta_1} \quad \beta_1 = q_1 e^{i\phi_1} \quad \alpha_2 = r_2 e^{i\theta_2} \quad \beta_2 = q_2 e^{i\phi_2}. \tag{18}$$

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[4] Instead of this sequential RWR procedure (or combined with it), one may use a parallel system where several couples of qubits, all with the same Hamiltonian and initial state, are read, and frequencies of occurence are computed over them (too). This increases system speed, but also complexity.

[5] Since we have to remove one of the initial four mixing equations, we choose to remove the one associated with p_3 because it has the most complicated expression (together with the equation for p_2).

Eq. (15) and (16) are then easily shown to be equivalent to

$$r_1^2 r_2^2 = p_1 \tag{19}$$
$$q_1^2 q_2^2 = p_4. \tag{20}$$

Longer calculations using phase factorizations show that (12) may be expressed as

$$(r_1 q_2 \cos \Delta_E)^2 + (q_1 r_2 \sin \Delta_E)^2$$
$$-2 r_1 r_2 q_1 q_2 \cos \Delta_E \sin \Delta_E \sin \Delta_I = p_2 \tag{21}$$

where

$$\Delta_I = (\phi_2 - \phi_1) - (\theta_2 - \theta_1) \tag{22}$$

and

$$\Delta_E = \frac{(\omega_{1,0} - \omega_{0,0})T}{2}. \tag{23}$$

Eq. (65) and (66) then yield

$$\Delta_E = -\frac{J_{xy}T}{\hbar}. \tag{24}$$

Moreover, each initial qubit state meets the normalization condition (2), so that

$$q_i = \sqrt{1 - r_i^2} \quad i = 1, 2. \tag{25}$$

Therefore, among all four modulus parameters in the right-hand expressions in (18), one may consider only the two parameters r_i as independent variables, i.e. "sources", while the parameters q_i are then derived from these r_i by means of (25). The mixing equation (20) may then be rewritten as

$$(1 - r_1^2)(1 - r_2^2) = p_4. \tag{26}$$

Similarly, the four phase parameters in the right-hand expressions in (18) only yield a single "source", i.e. the parameter Δ_I defined in (22), since only this combination of the phase parameters is involved in the mixing equations (19), (21), (26) and may therefore be retrieved from the observed data. To avoid ambiguities, one may therefore fix three of the phase parameters θ_1, ϕ_1, θ_2, and ϕ_2 (e.g. to 0) and only use the fourth parameter to store information. Using standard SS notations, the "source vector" (composed of the parameters that we aim at retrieving) is therefore $s = [s_1, s_2, s_3]^T$ with $s_1 = r_1, s_2 = r_2$ and $s_3 = \Delta_I$.

The only mixing parameters involved in the mixing equations (19), (21), (26) are functions of Δ_E, which is defined in (23). These mixing parameters only concern (21), which can be transformed as follows, in order to express it with respect to a *single* mixing parameter. As a first step, let us consider the intermediate variable u defined as

$$u = \sin \Delta_E. \tag{27}$$

We then have

$$\cos \Delta_E = \epsilon \sqrt{1 - u^2} \tag{28}$$

with

$$\epsilon = \mathrm{sgn}(\cos \Delta_E). \tag{29}$$

Also using (25), Eq. (21) may then be rewritten as

$$r_1^2(1 - r_2^2)(1 - u^2) + (1 - r_1^2)r_2^2 u^2$$
$$-2 r_1 r_2 \sqrt{1 - r_1^2}\sqrt{1 - r_2^2}\sqrt{1 - u^2}\epsilon u \sin \Delta_I = p_2. \tag{30}$$

Moreover, the two parameters ϵ and u may eventually be merged into a single mixing parameter v defined as

$$v = \epsilon u. \tag{31}$$

Indeed, we thus have

$$v^2 = u^2 \tag{32}$$

so that (30) may be rewritten as

$$r_1^2(1 - r_2^2)(1 - v^2) + (1 - r_1^2)r_2^2 v^2$$
$$-2 r_1 r_2 \sqrt{1 - r_1^2}\sqrt{1 - r_2^2}\sqrt{1 - v^2}v \sin \Delta_I = p_2. \tag{33}$$

This yields the final form of our new "mixing model", in SS terms. This model is composed of (19), (26), (33), and was derived above from the "polar complex-valued cylindrical-symmetry Heisenberg spin coupling model", in QP terms. This mixing model may be expressed in compact form as

$$x = F(s), \tag{34}$$

where the nonlinear mixing function F has three components F_1 to F_3, with $x_i = F_i(s)$, $\forall i \in \{1 \ldots 3\}$. These components F_i are respectively defined by (19), (33) and (26). The only mixing parameter involved in this mixing model is v.

We now have two models for the data that we are considering in this paper, i.e. a quantum model (9) and a classical one, composed of (19), (26), (33). While more specific comments about conditions for applying these models are provided in Appendix D, we here move to the resulting qubit uncoupling methods, by first considering the approaches based on the classical form of these data.

4 Classical-processing methods for qubit separation

4.1 Invertibility of SS mixing model

The next step of this investigation consists in determining whether and how the above-defined classical source signals, i.e. the qubit parameters r_1, r_2 and Δ_I, may be retrieved by user R only from

- the observations, i.e. the measured estimates of p_1, p_2 and p_4,
- and the mixing parameter v, which will be obtained as explained below.

The first issue is therefore the invertibility of the mixing model (34): given an observation vector x and the mixing parameter v, we must derive the number and expressions of the source vectors s which are such that $x = F(s)$. The mixing equations (19) and (26) only involve the two sources $s_1 = r_1$ and $s_2 = r_2$. They are easily solved, thus showing that both sources r_i are defined by

$$r_i = \sqrt{\frac{1}{2}\left[(1 + p_1 - p_4) + \epsilon\sqrt{(1 + p_1 - p_4)^2 - 4p_1}\right]} \quad (35)$$

with $\epsilon = 1$ for one of these sources and $\epsilon = -1$ for the other one. This permutation ambiguity, which is usual in fully classical SS, results in two solutions for the couple (r_1, r_2). We here solve it by requesting the qubit initialization to always be performed with

$$0 < r_1 < \frac{1}{2} < r_2 < 1 \quad (36)$$

which guarantees that only the solution with $r_1 < r_2$ is relevant.

Eq. (33) then directly yields a single solution for $\sin \Delta_I$, provided the factor of $\sin \Delta_I$ in (33) is non-zero, i.e. provided r_1, r_2 and v^2 are different from 0 and 1. This yields a single solution for source $s_3 = \Delta_I$, provided the qubit phases are initialized so as to meet

$$-\frac{\pi}{2} \leq \Delta_I \leq \frac{\pi}{2}. \quad (37)$$

This solution reads

$$\Delta_I = \arcsin\left[\frac{r_1^2(1 - r_2^2)(1 - v^2) + (1 - r_1^2)r_2^2 v^2 - p_2}{2r_1 r_2\sqrt{1 - r_1^2}\sqrt{1 - r_2^2}\sqrt{1 - v^2}v}\right]. \quad (38)$$

The above description completely solves the problem if user R does not aim at retrieving information stored in the phase parameters of the qubits defined in (18): r_1 and r_2 are derived from (35), and the other modulus parameters in (18) are then obtained from (25). This especially concerns the case when these qubits are constrained to be initialized by user W so that all four phases in (18) are zero; all the information stored by user W in the qubits is thus retrieved by user R. On the contrary, if user R also aims at deriving the phase qubit parameter Δ_I from (38), he needs the value of the mixing parameter v. The last issue to be addressed in this procedure is then: how does user R get this value of v ? In a given configuration, v is fixed. This yields three possible cases and associated classes of SS methods. The general features of these cases are described hereafter in Section 4.2, while corresponding specific SS methods are then proposed in Sections 4.3 and 4.4.

4.2 How to get the value of mixing parameter v

The three possible ways to obtain the value of the mixing parameter v may be defined as follows.

4.2.1 Ideal case

The preferred situation is faced when user R knows the exact value of v, typically because he knows the values of the frequencies $\omega_{i,j}$ of the considered system, as shown by (31), (29), (27) and (23). This situation therefore requires very detailed knowledge of the physical properties of this system (exchange integrals), which is usually hard to obtain by means of theoretical or experimental physical analysis of the system.

To avoid this constraint, we hereafter consider the situation when v is not known a priori. The approach that we propose then consists in using data (i.e. observations and/or source values, as detailed below) to estimate v. This approach, only based on signal values, as opposed to the above-mentioned theoretical or experimental determination of physical quantities, yields the two possible scenarios described hereafter.

4.2.2 Non-blind approach for estimating v

Our first data-driven solution makes it possible to determine v easily, but requests the system to be first operated with at least one *known* vector of source values r_1, r_2 and Δ_I: also measuring the probability p_2 for this or these source vectors allows one to derive v from (33), using the methods detailed in Section 4.3.

This general approach for estimating v is called a "non-blind" approach, since it requires one to know some source values, in addition to the observations x.

4.2.3 Blind approach for estimating v

On the contrary, blind SS (BSS) methods only use the observations x to first estimate the mixing parameter v and to then retrieve unknown source values by using the inversion equations (35) and (38). They are therefore more attractive (but more complex) than the above non-blind solution, since they do not require any known source values. Various blind methods may be developed for the mixing model introduced in this paper, by resorting to different SSP tools. These SSP methods are based on a common approach, which consists in using (at least) one sequence of different values for the couple of qubits, where these values are unknown as stated above, but some of their statistical properties are assumed to be known. We propose simple BSS methods based on this approach in Section 4.4 and we comment about possible extensions in Section 7.

4.3 Non-blind methods for estimating mixing parameter v

As stated above, the non-blind methods for estimating the mixing parameter v essentially consist in deriving v from (at least) one known source vector $[r_1, r_2, \Delta_I]^T$ and from the associated measured value(s) of the probability p_2, using (33). This general approach yields several methods, depending whether some (limited) prior knowledge about the system is available or not, and depending on which known source vector(s) is used. Three such methods are detailed hereafter.

4.3.1 A method using a simple source vector

An attractive method based on the above principle consists in using a source vector $[r_1, r_2, \Delta_I]^T$ such that

$$\sin \Delta_I = 0 \tag{39}$$

e.g. with $\Delta_I = 0$, since the solution of (33) is then much simpler: (33) is then a linear equation with respect to v^2. However, this equation thus only yields v^2, so that one should then define some means to obtain the sign of v, in order to eventually derive the value of v itself.

In some cases, this sign ambiguity on v due to (33) may be solved thanks to limited physical knowledge about the system. More precisely, Δ_E is defined by (24). Let us therefore consider the case when the user-defined parameter T can be set to a value which is low enough to guarantee that

$$-\frac{\pi}{2} \leq \Delta_E \leq \frac{\pi}{2}. \tag{40}$$

Eq. (29) then yields

$$\epsilon = 1 \tag{41}$$

so that (31) and (27) result in

$$v = \sin \Delta_E. \tag{42}$$

The parameter v then has the same sign as Δ_E, due to (40). In other words, to obtain the requested sign of v in this case, the only physical knowledge required about the considered system is not the exact value of Δ_E, but only its sign. Eq. (24) shows that this eventually amounts to requesting the sign of J_{xy} to be known. This is not constraining since, for a given physical system, this sign of J_{xy} can be determined.

As stated above, this approach applies if T can be set to a value which is low enough to guarantee that Condition (40) is met. The question is then: may such values of T be reached in actual systems ? This topic is therefore addressed in Appendix E, where we investigate the magnitude of Δ_E. The physical analysis presented in that appendix has the following consequences for the data processing methods considered in this paper:

- since there exist physical situations where $|\Delta_E|$ is significantly lower than 1, Condition (40) can be met, so that the processing method proposed in this Section 4.3.1 is indeed of interest. This case when $\sin \Delta_I = 0$ and the sign of v is known therefore yields a simple method, which is used in the tests reported further in this paper.
- However, there also exist physical situations where $|\Delta_E|$ is significantly higher than 1. We should therefore also develop processing methods applicable to the case when the sign of v is not known. We describe such methods hereafter.

4.3.2 A method using a simple couple of source vectors

As explained above, we here consider the case when the sign of v is not known. The method described in Section 4.3.1 is then not sufficient to derive the value of v, but can still be used as the first stage of the extended approach proposed here. That first stage provides v^2. Once this value has been obtained, we then again use (33) in the second stage of our extended method, but now with another source vector, denoted $[\tilde{r}_1, \tilde{r}_2, \tilde{\Delta}_I]^T$, which is selected so that $\sin \tilde{\Delta}_I \neq 0$ and which yields a probability $\tilde{p}_2$. We consider the case when $\tilde{r}_1, \tilde{r}_2$ and v^2 are different from 0 and 1, as explained above. For this second source vector, (33) therefore yields

$$v = \frac{\tilde{r}_1^2(1 - \tilde{r}_2^2)(1 - v^2) + (1 - \tilde{r}_1^2)\tilde{r}_2^2 v^2 - \tilde{p}_2}{2\tilde{r}_1 \tilde{r}_2 \sqrt{1 - \tilde{r}_1^2}\sqrt{1 - \tilde{r}_2^2}\sqrt{1 - v^2}\sin \tilde{\Delta}_I}. \tag{43}$$

This equation makes it possible to derive v, since all the parameters in its right-hand term (including v^2) are known at this stage.

4.3.3 A method using a general couple of source vectors

In the above two methods, we used at least a source vector such that $\sin \Delta_I = 0$, because of the simplicity of the corresponding solutions of (33). Using this type of source vector is not mandatory however, as shown in the third method that we will now present, which also does not require the sign of v to be known. In this method, we use two source vectors $[r_1, r_2, \Delta_I]^T$ and $[\tilde{r}_1, \tilde{r}_2, \tilde{\Delta}_I]^T$, which are selected so that $\sin \Delta_I \neq 0$ and $\sin \tilde{\Delta}_I \neq 0$, and which respectively yield probabilities p_2 and $\tilde{p}_2$. We again consider the case when $r_1, r_2, \tilde{r}_1, \tilde{r}_2$ and v^2 are different from 0 and 1. Eq. (33) applied to both source vectors yields

$$\frac{r_1^2(1 - r_2^2)(1 - v^2) + (1 - r_1^2)r_2^2 v^2 - p_2}{2r_1 r_2 \sqrt{1 - r_1^2}\sqrt{1 - r_2^2}\sin \Delta_I}$$
$$= \sqrt{1 - v^2}\, v$$

$$= \frac{\tilde{r}_1^2(1 - \tilde{r}_2^2)(1 - v^2) + (1 - \tilde{r}_1^2)\tilde{r}_2^2 v^2 - \tilde{p}_2}{2\tilde{r}_1 \tilde{r}_2 \sqrt{1 - \tilde{r}_1^2}\sqrt{1 - \tilde{r}_2^2}\sin\tilde{\Delta}_I}. \qquad (44)$$

The first and last terms in (44) yield a linear equation with respect to v^2, from which one derives v^2. The value of v itself may then be obtained as in our second method, i.e. by using (43).

4.4 Blind methods for estimating mixing parameter v

Following the general approach that we defined in Section 4.2.3, we here introduce simple methods for blindly estimating the mixing parameter v. For each of the three sources, these methods use (at least) one realization of a sequence of random variables, indexed by n. These sequences are denoted in short $r_1(n)$, $r_2(n)$ and $\Delta_I(n)$, respectively for each of the three sources. The random source signals composed of these sequences are assumed to be such that, for each source, the corresponding random variables are identically distributed throughout the sequence. Moreover, these source signals are assumed to be mutually statistically independent. The BSS methods that we introduce below therefore belong to Independent Component Analysis (ICA), which is one of the current major classes of BSS methods [13], [24].

Our BSS methods operate as follows. We consider the expectation (i.e. the statistical average) of (33), denoted $E\{.\}$. This yields

$$E\{r_1^2(n)\}(1 - E\{r_2^2(n)\})(1 - v^2)$$
$$+ (1 - E\{r_1^2(n)\})E\{r_2^2(n)\}v^2$$
$$- \Big[2E\{r_1(n)\sqrt{1 - r_1^2(n)}\}E\{r_2(n)\sqrt{1 - r_2^2(n)}\}\times$$
$$\sqrt{1 - v^2}\,v E\{\sin\Delta_I(n)\}\Big] = E\{p_2(n)\} \qquad (45)$$

where averaging is performed in practice over the considered sequence of source vectors. The modulus parameters $r_i(n)$ for each couple of qubits in the sequence(s) may again be estimated from (35). They are then used to estimate the expectations involving $r_i(n)$ which appear in (45). $E\{p_2(n)\}$ is also estimated from this sequence(s). By constraining the sequence(s) of qubit values to be such that its statistical parameter $E\{\sin\Delta_I(n)\}$ has a known value, the only unknown in (45) is v. Eq. (45) therefore makes it possible to estimate v in various ways. More precisely, (45) has the same nature as (33) from the point of view of the unknown v, i.e. the only difference between these equations concerns the parameter values which are known or estimated. Various methods for the blind case may therefore be developed, by solving (45) according to the same approaches as described in Section 4.3 for solving (33) in the non-blind case.

It should be kept in mind that each occurence of (33) corresponding to a single source vector in the non-blind case is here replaced by (45) corresponding to a *sequence* of source vectors (which have the same statistics). Therefore, among all the methods described in Section 4.3, the one introduced in Section 4.3.1 is here especially attractive (when the ambiguity on the sign of v may be solved as explained above), because it only requires a *single* sequence of source vectors. These vectors should be such that $E\{\sin\Delta_I(n)\} = 0$, as the averaged version of Condition (39) which is set in the corresponding non-blind method. The case when $E\{\sin\Delta_I(n)\} = 0$ and the sign of v is known therefore yields a simpler method, which is used in the tests reported below.

The methods described in Sections 4.3.2 and 4.3.3 may also be extended to the blind case by taking their average, but they then require *two* sequences of source vectors, with different statistics from one sequence to the other, which is more constraining.

5 Numerical results with classical-processing methods

The three cases that we introduced in Section 4.2 resulted in the above-defined three types of methods for qubit uncoupling. These methods use classical processing means, since they operate on data available in non-quantum form, essentially obtained by applying our RWR procedure to quantum states. Our approach for determining the performance of these SS methods uses two stages, i.e:

– a mixing stage, which creates a set of observation vectors x corresponding to known source vectors s, mixed according to the considered Heisenberg model with a given v,
– a separating stage, which possibly first estimates v. It then processes the above observation vectors and thus derives estimates $\hat{s}$ of the actual sources s from which these observation vectors x were computed. Comparing the actual and estimated sources then makes it possible to check that the proposed methods succeed in separating these sources, and to determine the accuracy of this separation, i.e. the magnitude of the deviation of the estimated sources $\hat{s}$ with respect to the actual sources[6] s.

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[6] This performance assessment procedure can only be used when *developing* and testing the considered SS methods, with actual source values s which are *known* (but which are not used in the SS methods themselves, except possibly to estimate v non-blindly). On the contrary, in the actual setup which is to be eventually used, the actual sources are *unknown*, and one precisely aims at estimating them ! They cannot therefore be compared to their estimated values.
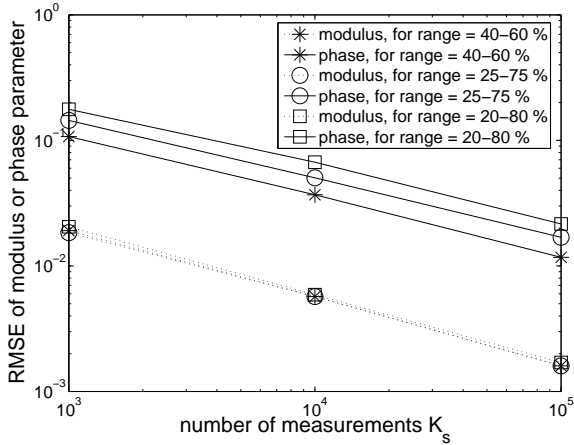
Fig. 1 Performance when restoring sources with value of mixing parameter v of first tested SS method (i.e. exact value of v). Performance is measured by RMSE of source modulus or phase parameters. It is plotted vs number of measurements K_s used when restoring sources. Each plot corresponds to a specific range for the random source parameters.

A natural approach for implementing the above mixing stage would consist in developing a real quantum system composed of two qubits, interacting through Heisenberg coupling. However, this involves quite sophisticated physical devices as stated above, so that the development of such a system would require a complete investigation, which is out of the scope of this article. Instead, we here use another approach, which consists in developing a realistic software simulation of this system, described in Appendix F.

As a reference, we initially test the first of our three types of SS methods, that we described in Section 4.2.1: in the separating stage, we restore the three source values from (35) and (38), with the exact value of v which was previously used in the mixing stage to create the estimated probabilities $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ with our RWR procedure. This corresponds to the above-defined "ideal case" concerning the value of v used in the separating stage. However, this configuration is not ideal concerning the measured probabilities $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$, whose accuracy depends on the number of measurements K_s used in our RWR procedure in the separating stage.

Fig. 1 shows how the separation accuracy of this SS approach depends on K_s. This accuracy is computed for r_1 and r_2 on the one hand ("modulus" in Fig. 1) and for Δ_I on the other hand ("phase" in Fig. 1). It is measured by the Root-Mean-Square Error (RMSE) achieved for the considered source component(s), measured over a set of $L = 100$ initializations of the couple of qubits. These RMSE are defined in Appendix G. The qubit parameter values are here randomly selected within a sub-range of their 0%-100% allowed range de-

fined by (36) and (37). Three cases are considered for this sub-range i.e. 40%-60%, then 25%-75% and 20%-80% of the allowed range. The parameter v is set to 0.5 in these tests. Fig. 1 shows that the logarithm of the RMSE of each source component linearly decreases with respect to the logarithm of K_s. This decrease may be explained as follows. When the number of measurements K_s tends to infinity, the measured values $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ converge towards the associated asymptotic values, i.e. p_1, p_2, p_4 respectively. Therefore, when estimating the sources with $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ in (35) and (38), and using the exact value of v, these estimated sources converge towards the source values which were actually used to create the observations $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$. The RMSE between the actual and estimated source therefore converges to zero. Moreover, Fig. 1 shows that setting K_s to a few thousand measurements is enough to achieve good separation accuracy.

We then modify the above test procedure as follows, in order to evaluate the version of our non-blind SS methods which is based on $\Delta_I = 0$ and which was described in Section 4.3.1 (we here assume that the sign of v is known). In the separating stage, we first derive an estimate $\hat{v}$ of v, using our above-defined approach based on (33). To this end, we apply our RWR procedure to a known qubit initialization, with a number of measurements K_m (for estimating p_2 when used in (33)) which may be different from K_s (involved in subsequent estimation of p_1, p_2, p_4, when they are used in (35) and (38) to perform separation). In this initial characterization of the mixing phenomenon in the system, one may allow a K_m value much higher than the K_s value in the final use of $\hat{v}$ for separation. To evaluate separation accuracy, we then still restore the three source values from (35) and (38), but now using $\hat{v}$.

Fig. 2 shows the performance thus achieved for several K_m values and for source parameters selected in the 20%-80% sub-range. Only the phase source Δ_I is considered because, as stated above, the estimates of r_1 and r_2 do not depend on the considered estimate of v and are therefore the same for all three types of SS methods. Fig. 2 shows that RMSE again decreases when K_s is increased. However, when K_s becomes very high, RMSE now converges towards a value which is lower when a higher value of K_m is used. This phenomenon occurs because, unlike with our first tested SS method, even if $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ are close to their associated asymptotic values in the separating stage, when estimating Δ_I with (38) the accuracy is limited by the approximate value $\hat{v}$ used in (38). Anyway, Fig. 2 shows that, by using a high enough K_m (the required value depends on K_s), this second SS method succeeds in achieving the same accuracy as the first, i.e. "ideal", one.
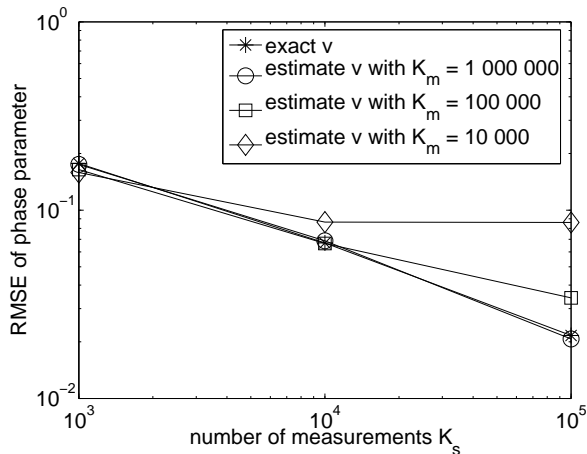
Fig. 2 Performance when restoring sources with value of $\hat{v}$ of first tested SS method (i.e. exact value of v) or second tested SS method (i.e. non-blind estimate of v). Performance is measured by RMSE of source phase parameter. It is plotted vs number of measurements K_s used when restoring sources. Each plot for the second SS method corresponds to a specific number of measurements K_m used when estimating v.

Fig. 3 Performance when restoring sources with value of $\hat{v}$ of first tested SS method (i.e. exact value of v) or third tested SS method (i.e. blind estimate of v derived from 100 qubit initializations). Performance is measured by RMSE of source phase parameter. It is plotted vs number of measurements K_s used when restoring sources. Each plot for the third SS method corresponds to a specific number of measurements K_m used when estimating v.

Our third tested SS method then uses the same procedure as the second one, except that $\hat{v}$ is here derived blindly from a set of qubit initializations which are such that $E\{\sin \Delta_I(n)\} = 0$ (the sign of v is again assumed to be known). This corresponds to the simplest version of the type of methods described in Section 4.4. Fig. 3 shows the performance obtained for 100 such initializations. These results are qualitatively similar to those for our second method, but the moderate number of qubit initializations used for deriving $\hat{v}$ here limits the accuracy of this estimated parameter and therefore the RMSE of the method. This limitation disappears when increasing this number of initializations: Fig. 4 shows that, for 1000 initializations, this method achieves almost the same accuracy as the "ideal" one in all the considered range.

All above tests therefore prove the relevance of our three SS methods operating with classical processing means.

6 A quantum-processing method for qubit separation

Anticipating on the development of future practical full-quantum circuits, we now aim at proposing a quantum circuit structure for performing qubit uncoupling, as a quantum-processing alternative to the above classical-processing methods. We therefore still operate with the available quantum system state $|\psi(t) >$ defined by (9). This state is here considered as the result obtained

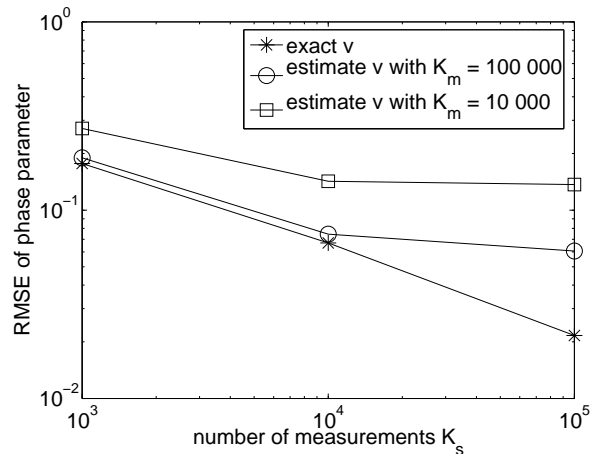when applying an operator $\overset{o}{M}$ to the initial state $|\psi(t_0) >$, i.e.

$$|\psi(t) > = \overset{o}{M}|\psi(t_0) > . \tag{46}$$

This Mixing operator $\overset{o}{M}$, in SS terms, corresponds to the temporal evolution of the system from time t_0 to time t, which is a reversible operation ([38], process (2)). We then aim at deriving a corresponding separating or Unmixing operator $\overset{o}{U}$, and an associated quantum circuit, which receives the available state $|\psi(t) >$ as its input, and which restores the quantum state $|\psi(t_0) >$
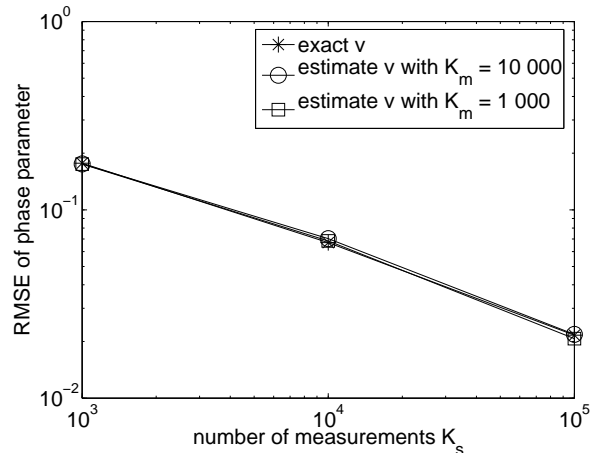

Fig. 4 Same as Fig. 3, but estimating v with 1000 qubit initializations in third SS method.

as its output[7]. This desired operator $\overset{o}{U}$ is therefore the inverse of the mixing operator, i.e

$$\overset{o}{U} = \overset{o}{M}{}^{-1}. \tag{47}$$

Our quantum-processing SS method is thus a reversible process, unlike our classical-processing methods, which include irreversible measurements ([38], process (1)). The mixing operation in (46) may also be expressed with respect to the column vector $C_+(t)$ composed of the complex magnitudes of the Components of $|\psi(t) >$ in basis $\mathcal{B}_+$ and to the vector $C_+(t_0)$ for $|\psi(t_0) >$. This reads

$$C_+(t) = M C_+(t_0) \tag{48}$$

where M is the mixing matrix in basis $\mathcal{B}_+$. For the considered Heisenberg mixing model, the entries of $C_+(t)$ are all $c_j(t - t_0)$ contained in (9) and defined in (68). As shown in Appendix H, this yields

$$C_+(t) = Q D Q^{-1} C_+(t_0) \tag{49}$$

with Q and D defined in (75) and (76). Eq. (48), (49) and (75) then show that, for two spins 1/2 and cylindrical-symmetry Heisenberg mixing

$$M = Q D Q^{-1} = Q D Q. \tag{50}$$

Our separating system then restores $C_+(t_0)$ from $C_+(t)$ by inverting (48), i.e.

$$C_+(t_0) = U C_+(t) \tag{51}$$

where U is the separating matrix in basis $\mathcal{B}_+$ defined as

$$U = M^{-1} = Q D^{-1} Q^{-1} = Q D^* Q \tag{52}$$

where $*$ stands for complex conjugate (Eq. (50) and (52) correspond to the eigendecompositions of M and U, respectively). The overall mixing and separating configuration thus obtained is shown in Fig. 5[8]. The quantum circuit that we propose as an implementation of the separating stage therefore consists of the cascade of three simpler sub-circuits. We now detail the internal structures that we propose for these sub-circuits, using the notations defined in [30], where their $|0 >$ and $|1 >$ states respectively correspond to our $|+ >$ and $|- >$.

Fig. 5 Quantum mixing and separating configuration.

Fig. 6 Implementation of operator Q.

A possible implementation of the two Q operators of Fig. 5 is shown in Fig. 6. It uses two controlled-NOT gates (CNOTs) and a controlled-Hadamard gate[9]. The latter gate may be further decomposed, using the approach defined in pp. 180-181 of [30]. This e.g. yields the circuit shown in Fig. 7, which uses CNOTs, and standard rotation and S (phase) operators.

Eventually, a possible decomposition of the overall phase-based block D^* into simpler phase-based circuits is provided in Fig. 8, where the open circle notation indicates conditioning on the qubit being set to zero, as in [30] p. 184. Various cases may be defined for this block D^* depending whether its phase parameters, and therefore the values of the frequencies $\omega_{i,j}$ of the considered system, are known or not. As in our above SS methods operating with classical means, the *ideal case* is when these frequencies are known, but this is quite constraining and may be avoided by deriving these frequencies from (quantum) signal values. Besides, the estimation of the phase parameters of D (and hence of D^*) is nothing but the "phase estimation" problem [30] for the overall matrix M, i.e. the determination of the eigenvalues of M, identical to those of D. This prob-

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[7] A given quantum circuit restores a single state $|\psi(t_0) >$ only from a *single* preparation of the state $|\psi(t) >$, as opposed to the *repeated* write/reads required in the RWR procedure used for our classical-processing SS methods.

[8] The horizontal lines connecting the blocks of this diagram are crossed by short diagonal segments (i.e. "/") in order to make it clear that each connection is a "bus", involving a *set* of qubits (i.e. two qubits here). This corresponds to the usual convention, e.g. mentioned in [30] p. 223.
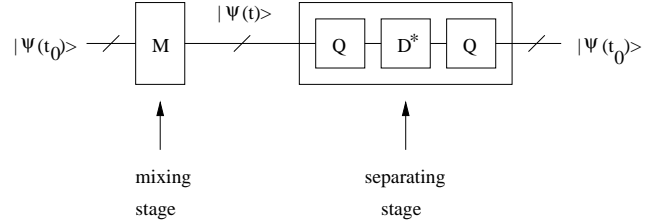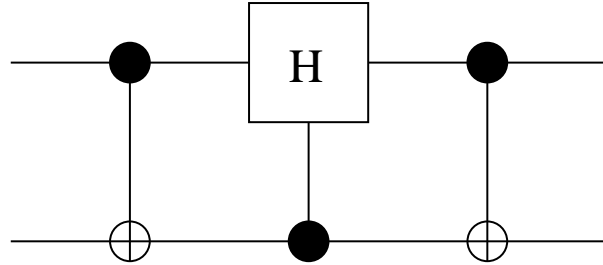
[9] The top and bottom inputs/outputs in Fig. 6 and 8 respectively correspond to qubits no. 1 and 2.
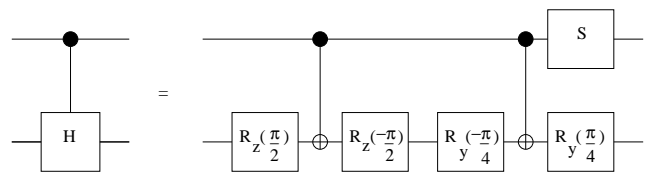

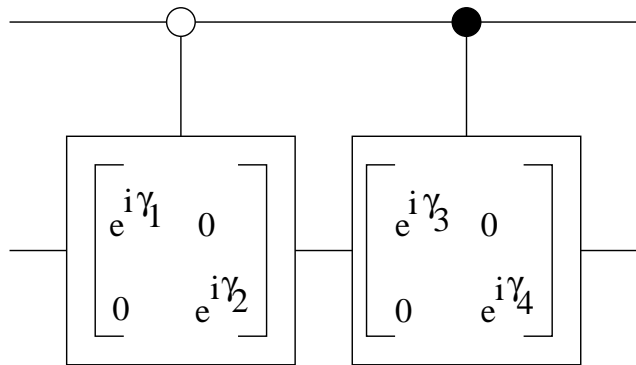**Fig. 7** An implementation of controlled-H operator used in Fig. 6.

Fig. 8 Implementation of operator D^*, with $\gamma_1 = \omega_{1,1}(t - t_0)$, $\gamma_2 = \omega_{1,0}(t-t_0)$, $\gamma_3 = \omega_{0,0}(t-t_0)$ and $\gamma_4 = \omega_{1,-1}(t-t_0)$.

lem may therefore be solved by using the procedure described in Chapter 5 of [30]. Moreover, the eigenvectors of M are known, as shown in Appendix C and in the expression of Q in (75). Using them as an input of the phase estimation procedure, and therefore considering a *non-blind approach* for estimating the mixing parameters, is attractive for this procedure, as explained in [30]. This procedure may however be used with other inputs than the eigenvectors of M, which may open the way to *blind approaches* for mixture estimation, but at the expense of introducing randomness into the algorithm [30]. Such blind approaches are a possible topic for future research.

7 Conclusions and future work

In this paper, we introduced the Quantum Source (or Signal) Separation (QSS) field. This term means that the data to be separated are initially available in quantum form, i.e. we investigate the uncoupling of qubits. This gives rise to two alternative approaches, i.e:

1. these qubits may first be converted into classical data by means of repeated measurements, then allowing one to process the latter data with classical (i.e. non-quantum) statistical processing methods. New SS methods must be developed for the considered QSS problem involving Heisenberg coupling, because this configuration turns out to yield a nonlinear SS model which has not yet been studied in the literature.
2. The other approach consists in directly processing the qubits by means of quantum circuits, which yields a full-quantum solution to the QSS problem.

We investigated both approaches in this paper and we thus proposed various types of QSS methods. Our methods based on classical processing may be implemented with currently available technological means,

i.e. software implementations of SS algorithms. These solutions are of interest in various current experiments involving quantum phenomena, as stated above. On the contrary, the practical application of our approach based on quantum processing will require actual quantum circuits, which are only starting to be developed today, as explained above. This future quantum-processing solution will have the advantage of avoiding the repeated qubit preparations and irreversible measurements required in our classical-processing methods. It is of potential interest for future quantum computers.

The source separation problem treated in this paper may moreover be seen as an *operation of disentanglement after an undesired entanglement,* which is a quantum problem without any classical version.

Our first steps into this new QSS field suggest many potential developments, which will be presented in future papers. One of the most immediate extensions will consist in developing more powerful classical statistical blind qubit separation methods than the basic ones that we introduced in this paper by considering moment-based approaches. Especially, applying the maximum likelihood (ML) concept to QSS is an attractive approach, thanks to the statistical properties of ML methods.

A Mixtures in Quantum Physics and Source Separation

The term "mixture" (or "mixing") has distinct meanings in the Quantum Physics and Source Separation fields. In Quantum Physics, "a mixture" is an abbreviation for "a statistical mixture". A statistical mixture, described by a density operator $\rho(t)$, has to be opposed to a "pure state", described (in the Schrödinger representation) by a ket or state vector $|\psi(t)>$. It should be stressed that any linear combination of kets is itself a ket (principle of superposition of Quantum Mechanics) and therefore describes a pure state, *and not a mixture.* In the Source Separation field, an example of source mixing is obtained when, instead of receiving separately each source (or signal), a user receives data (experimental signals) which are each some linear superposition of the different sources. While in that situation the mixing is linear, on the contrary in the present paper, we are faced with a nonlinear mixing. It should be clear that, in this paper, the qubits are always considered in pure states, the words "mixture" and "mixing" being therefore systematically used with their meaning in the SS context. Pure states have also been considered in various QIP investigations reported in the literature (see e.g. [6], [7], [22], [26], [30]).

B Relationship between QSS and some other QIP fields

When taking up a comparison between our present Quantum Source Separation (QSS) methods and existing QIP tools, a first intuitive feeling may be that such a comparison is made

difficult by the wealth of the existing methods and literature devoted to QIP. On close scrutiny, it should first be noticed that our aim is not determining the quantum state (of the qubit pair) *after* the action of undesired coupling between the qubits. Our aim is the restoration of the quantum state (of each qubit) *before* this action, a much more specific and difficult task. It is possible to establish a link between our problem and the general theory of systems, using the following procedure: the coupling between the two qubits is described as a "system", possessing two 1-qubit inputs and two 1-qubit outputs. The states of the qubits before coupling (source signals) are seen as signals placed at each input of this system. The states resulting from their coupling (signals after "mixing" within the SS terminology, or observations) are seen as states appearing at the outputs of that system. Within this framework, our problem is not limited to (quantum) signals, but focused on (quantum) systems. Due to space limitations, a discussion of this question in the general context of classical and quantum systems will be presented elsewhere. We instead first move into a narrower context, the one which allowed the first experimental realization of quantum gates and is presently the most developed in the QIP field, namely that of (liquid state pulsed) NMR. Use of a specific experimental context allows a practical illustration of some points which have just been only suggested.

People familiar with NMR know that spin echo techniques are routinely used in NMR spectroscopy and are now also used in ESR spectroscopy. If the magnetic moments have been *initially oriented in a common well-chosen direction*, by a first well-chosen electromagnetic pulse, the spin-spin couplings then rapidly destroy this magnetic order. It is often said that the well-chosen second pulse produces a refocusing of the spins, which allows the birth of an echo [2], [37], and it is sometimes added that the pulse sequence allows the suppression of the effect of the spin-spin coupling. The spin-echo technique is generally used to measure the so-called spin-spin relaxation time T_2, a measure of the strength of the spin-spin coupling. Saying that refocusing allows the suppression of the undesired spin-spin coupling therefore seems improper. It seems better to say that refocusing takes advantage of the existence of this coupling to get information on its strength. It should then be clear that the spin-echo (or refocusing) technique has its own interest, but that its aim is quite distinct from that of our QSS methods, as it is not able to recover the state of the nuclear spins once spin-spin coupling has perturbed the quantum state of these nuclear spins, first prepared *in a rather general* quantum pure state.

Comparison of our QSS methods with possibly existing tools in the QIP field, either made within the general framework of the theory of (classical or quantum) systems, or within the quite distinct field of NMR used in the QIP context, leads to an examination of quantum tomography [30], then **carefully distinguishing between *state* tomography (QST) and *process* tomography (QPT).**

State tomography should be immediately discarded. The reason is that, if used in our context, it would at best help recovering what we called the signal present at the *output* of our system, i.e. the quantum state resulting from the undesired coupling (QST may not access the unknown source signals).

Quantum process tomography, on the contrary, in the present context helps recovering the signals present on the inputs of the system, i.e. the initial quantum state of each qubit (i.e. their states before the action of the undesired coupling). *The question is then: what is the interest of QPT compared to our QSS methods?* Before examining the answer, we insist that **focusing on state tomography and ignoring process tomography would be the signature, in the tomography field, of a confusion between a problem involving signals and one involving systems.**

A quantum system has the same number of inputs and of outputs, whereas e.g. in conventional digital electronics, a gate with two inputs and only one output does exist. The dimensions of the input and output state spaces of a quantum system are thus the same. This dimension is $d = 2^n$ if the system operates with n qubits. If one adopts the point of view of (Standard) QPT [30] (and we will simply write QPT instead of SQPT) for identifying the coupling between the two spins 1/2 studied in this paper, one should first introduce both the state space $\mathcal{E}_{1,2} = \mathcal{E}_1 \otimes \mathcal{E}_2$ of the pair of spins, with dimension $d = 2^2$, and a basis of orthonormal vectors $| \Phi_i >$. The Heisenberg coupling is then seen as a possible process (to be identified), and understood as a (part of a) "system", which then possesses *one* (two-qubit) input and *one* (two-qubit) output. If at $t = 0$ the state of the spin pair is described by a state vector $| \Psi_0 >$, and by the corresponding projector $| \Psi_0 >< \Psi_0 |$ (or more generally by a density matrix ρ_0), and if the state of the pair at time t in the presence of the Heisenberg coupling is $| \Psi(t) >$, QPT considers that the input of the system receives the projector $| \Psi_0 >< \Psi_0 |$ (or more generally the density matrix ρ_0) and that its output is the projector $| \Psi(t) > < \Psi(t) |$ (or more generally $\rho(t)$). QPT moreover introduces a new vector space with dimension $d^2 = 16$ and a basis composed of the d^2 "vectors" $| \Phi_i >< \Phi_j |$ (with $i = 1...d$, $j = 1...d$). Then QPT uses d^2 projectors $| \Pi_j >< \Pi_j |$ successively placed at the input of the system, and determines the corresponding states at its output, a priori assuming that for a given j, the corresponding output state is a statistical mixture described by a density operator ρ'_{Oj} (O: output), with:

$$\rho'_{Oj} = \sum_{k,l} (\rho'_{Oj})_{kl} \, | \Phi_k >< \Phi_l | . \tag{53}$$

ρ'_{Oj} being Hermitian, with trace 1, $(d^2 - 1)$ independent real parameters are necessary for describing the most general ρ'_{Oj}. The whole operation for the d^2 projectors leads to the determination of $d^2(d^2 - 1)$ i.e. $d^4 - d^2 = 240$ real quantities, the aim being the identification of the process (presently the Heisenberg coupling). The complexity of this QPT approach, as compared to our QSS method, has two reasons:

1. **one is linked to the input state:** our SS method uses a system where the input state is a product of a quantum state for each qubit, whereas QPT considers that the input state may be any state vector in $\mathcal{E}_{1,2}$, which means that entangled states are then implicitly allowed, while we do know that they should be excluded in the considered case. Moreover any statistical mixture at the input used in QPT is allowed, while we presently exclude them, and while if we assume them in the future, only statistical mixtures of the form $\rho_{01} \otimes \rho_{02}$ (0 for time $t = 0$, 1 for qubit 1, 2 for qubit 2) *will be allowed,* since we will aim at separately recovering each initial qubit state in our QSS framework.

2. **The other reason is linked to the process**, understood as a system. In the QPT approach, the process may be either internal to the qubit pair (which is true for the Heisenberg coupling) or external to that pair (e.g. a coupling of the pair to a thermal bath, or spin-lattice coupling) and no assumption is made about the process (see e.g. reference to T_2 or to T_1 in [11]), insofar as it conserves the trace of the density operator, i.e. the output is a density operator ρ'. On the contrary, in our QSS problem,

the process is known to be internal to the qubit pair, and is quite specific (thus depending on a single parameter in our method based on measurements).

Then, in the QPT approach, and considering again a given $| \Pi_j >< \Pi_j |$, and the corresponding ρ'_{Oj} (output), if one measures both s_{z1} and s_{z2}, this gives $(d-1)$ relations, and, in order to get (d^2-1) relations, one needs a total of $(d+1)$ pairs of successive measurements (e.g. (s_{z1}, s_{z2}), (s_{x_1}, s_{x_2}), (s_{y_1}, s_{y_2}) etc). This means that for the whole operation using the d^2 projectors, $d^2.2(d+1)$ i.e. 160 measurements (taking place after the corresponding preparations) are needed, a rather gigantic task. The reason is that QPT, while truly a quite general method, is much more complex than required in the present Source Separation problem since, through its very construction, it ignores what is presently known about both the state of the spins and their coupling.

If two spins 1 were considered instead of spins 1/2, and keeping initial pure states, the complexity of the problem would of course increase, but our discussion indicates that, keeping the other assumptions, the complexity of the QPT approach would even increase far more (the numbers of real parameters and of measurements then increase roughly as d^4 and d^3 respectively).

C Temporal evolution of the overall state of two coupled spins

The initial state of the overall system composed of the considered two spins is defined by (8). This state may also be expressed in the four-dimensional basis composed of the eigenvectors of the cylindrical-symmetry Heisenberg Hamiltonian. We here denote this basis $\mathcal{B}_1 = \{|1,1>,|1,0>,|0,0>,|1,-1>\}$. The expression of this basis with respect to $\mathcal{B}_+$ may be derived from QP calculations. Briefly, these calculations are based on the system's Hamiltonian defined by (4) and on the QP operators $s^+ = s_x + is_y$ and $s^- = s_x - is_y$. Calculations show that the eigenvectors of the matrix representing the Hamiltonian H in the $\mathcal{B}_+$ basis are

$$|1,1> = |++>\tag{54}$$

$$|1,0> = \frac{|+->+|-+>}{\sqrt{2}}\tag{55}$$

$$|0,0> = \frac{|+->-|-+>}{\sqrt{2}}\tag{56}$$

$$|1,-1> = |-->.\tag{57}$$

i.e the eigenkets common to S^2, S_z, s_1^2 and s_2^2 (with $\overrightarrow{S} = \overrightarrow{s_1} + \overrightarrow{s_2}$). This result reflects the fact that the cylindrical-symmetry Heisenberg coupling between two spins *one-half* accidentally commutes with S^2 and S_z (and of course with s_1^2 and s_2^2). In spherical symmetry ($J_{xy} = J_z$), this commutation property is true for any spin, a consequence of the equality $2\overrightarrow{s_1}\overrightarrow{s_2} = S^2 - s_1^2 - s_2^2$.

Eq. (54)-(57) may then be straightforwardly inverted, so as to obtain the expression of $\mathcal{B}_+$ with respect to $\mathcal{B}_1$, which reads

$$|++> = |1,1>\tag{58}$$

$$|+-> = \frac{|1,0>+|0,0>}{\sqrt{2}}\tag{59}$$

$$|-+> = \frac{|1,0>-|0,0>}{\sqrt{2}}\tag{60}$$

$$|--> = |1,-1>.\tag{61}$$

Inserting the latter expressions in (8) yields

$$|\psi(t_0)> = \alpha_1\alpha_2|1,1> + \frac{\alpha_1\beta_2+\beta_1\alpha_2}{\sqrt{2}}|1,0>$$
$$+\frac{\alpha_1\beta_2-\beta_1\alpha_2}{\sqrt{2}}|0,0> +\beta_1\beta_2|1,-1>.\tag{62}$$

The temporal evolution of this state then corresponds to phase rotations for each eigenvector, as in (3). In basis $\mathcal{B}_1$, the state at any time t then reads

$$|\psi(t)> = \alpha_1\alpha_2 e^{-i\omega_{1,1}(t-t_0)}|1,1>$$
$$+\frac{\alpha_1\beta_2+\beta_1\alpha_2}{\sqrt{2}}e^{-i\omega_{1,0}(t-t_0)}|1,0>$$
$$+\frac{\alpha_1\beta_2-\beta_1\alpha_2}{\sqrt{2}}e^{-i\omega_{0,0}(t-t_0)}|0,0>$$
$$+\beta_1\beta_2 e^{-i\omega_{1,-1}(t-t_0)}|1,-1>\tag{63}$$

where $\omega_{i,j}$ is the real frequency associated with the phase rotation for each eigenvector $|i,j>$. QP calculations show that these frequencies are equal to

$$\omega_{1,1} = \frac{1}{\hbar}\left[GB - \frac{J_z}{2}\right]\tag{64}$$

$$\omega_{1,0} = \frac{1}{\hbar}\left[-J_{xy} + \frac{J_z}{2}\right]\tag{65}$$

$$\omega_{0,0} = \frac{1}{\hbar}\left[J_{xy} + \frac{J_z}{2}\right]\tag{66}$$

$$\omega_{1,-1} = \frac{1}{\hbar}\left[-GB - \frac{J_z}{2}\right].\tag{67}$$

Using the expression of $\mathcal{B}_1$ with respect to $\mathcal{B}_+$ then yields the expression of the system state at any time t in basis $\mathcal{B}_+$

$$|\psi(t)> = \alpha_1\alpha_2 e^{-i\omega_{1,1}(t-t_0)}|++>$$
$$+\frac{1}{2}\left[(\alpha_1\beta_2+\beta_1\alpha_2)e^{-i\omega_{1,0}(t-t_0)}\right.$$
$$\left.+(\alpha_1\beta_2-\beta_1\alpha_2)e^{-i\omega_{0,0}(t-t_0)}\right]|+->$$
$$+\frac{1}{2}\left[(\alpha_1\beta_2+\beta_1\alpha_2)e^{-i\omega_{1,0}(t-t_0)}\right.$$
$$\left.-(\alpha_1\beta_2-\beta_1\alpha_2)e^{-i\omega_{0,0}(t-t_0)}\right]|-+>$$
$$+\beta_1\beta_2 e^{-i\omega_{1,-1}(t-t_0)}|-->.\tag{68}$$

D Applicability of considered data models

The quantum and SSP forms of the model defined in Section 3 are respectively used in the two types of signal separation methods that we propose in this paper, i.e.

– in our quantum-processing method, where we consider the evolution of the system in a time interval ranging from t_0 to t,
– in our classical-processing methods, where we use our RWR procedure and we therefore consider the evolution of the system in a series of time intervals, each ranging from $t_w(k)$ to $t_r(k)$.

This model and the resulting separation methods apply only if the system's Hamiltonian, and therefore the magnetic field $\overrightarrow{B}$, is the same throughout the above-defined time intervals and in all the considered system. For instance, in our RWR procedure, this requires users W (writer) and R (reader) to share the same constant magnetic field $\overrightarrow{B}$ throughout all time intervals $[t_w(k), t_r(k)]$.

Two major cases when $\overrightarrow{B}$ meets the above condition are defined hereafter. The first situation concerns quantum computers: such systems may be designed so that the writing and reading devices are close one to the other and thus placed in a magnetic field which is non-zero, spatially homogeneous and constant over the considered time period. The second situation is when there is no magnetic field. This may concern quantum computers, but also other potential applications, such as communication with quantum signals. In the latter application, using a zero field is attractive because, on the contrary, creating a spatially homogeneous, constant, *non-zero* field from the emitter to the receiver through the channel is often tricky. While the approach that we propose in this investigation may apply to future quantum computers, it is therefore also open to quantum communication applications. We do not claim however that it will be needed in the latter applications, i.e. that quantum communication always yields such coupling issues as those analyzed in this paper. Indeed, the most usual approach for quantum communication uses photons, and photons do not lead to coupling, except in nonlinear media.

The choice of the quantization axis used for measurements then deserves the following comments, depending whether a magnetic field exists or not in the considered configuration. If the magnetic field is non-zero, its direction defines a natural choice for the quantization axis. On the contrary, if the magnetic field is zero, its direction may not be used any more as the quantization axis. This is not a problem however, because any direction may be used for quantization: the only constraint is that the writing and reading devices must use the *same* direction. In particular, if coupling is indeed non-isotropic, i.e. if $J_{xy} \neq J_z$, a natural quantization axis is the symmetry axis of this coupling.

E Magnitude of Δ_E in real systems

Facing the difficult task of doing numerical estimations in a broad variety of possible physical situations, we first restrict this variety by excluding metals, then trying to identify the main phenomena and to get orders of magnitude for Δ_E, for electron and nuclear moments successively. In that spirit, we set $J_{xy} = J_z = J$. Eq. (24) then reads

$$\Delta_E = -\frac{JT}{\hbar}.$$

The choice of the value of T, the time interval between writing and reading, should be a compromise between opposite constraints. T must be long enough to allow the transfer from the writing device to the reading device. On the contrary, since during this time interval the coupled spins are assumed to be isolated from their environment, T must be significantly shorter than T_1, the so-called spin-lattice relaxation time, and we will take $T \leq T_1/10$. Therefore, both J and T values are linked to the physical properties of the spins, J directly and T because the choice of its value cannot ignore them. At the present time, experimental manipulations of magnetic moments widely use resonant methods (ESR, NMR), where the moments are submitted to a (quasi-)static magnetic field, and to an oscillating field at right angles to the static field. This oscillating field uses continuous waves or a pulsed mode, and its frequency fixes the value of the static field needed to get resonance.

We first pay attention to *electron magnetic moments,* in solid insulators. Ions of the 3d or 4f transition series replacing cations in non-magnetic (i.e diamagnetic) ionic insulators

(e.g. the II-VI oxides SrO and ZnO, or sulfides SrS and ZnS) often have an *electron* magnetic moment. When the 3d or 4f shell is half-filled, e.g. Mn^{2+} with the ground configuration $3d^5$, or Eu^{2+} $(4f^7)$, this magnetic moment has no orbital component. It is possible to replace for instance a part of the Sr^{2+} ions in SrS by Eu^{2+}, then obtaining the compound $Eu_x Sr_{1-x} S$. Europium sulfide EuS (total substitution) is a Heisenberg ferromagnetic insulator presently used in the context of spintronics, with a Curie temperature $T_C = 16.5$ K. Since we have adopted the view that the coupling between the qubits is undesired, we have preferred EuS to EuO, a Heisenberg ferromagnet with $T_C = 69$ K, both values being far smaller than the T_C value of the metal iron, 1043 K. The high value of T_C in these ferromagnetic insulators cannot be the result of a magnetic coupling. It is due to the exchange coupling between neighboring spins, a result of the Coulomb electrostatic force, together with the Pauli exclusion principle, in the presence of a significant overlap of electron wave functions [23]. Within the mean field approximation and assuming exchange between nearest neighbors (n.n) only, T_C is related to J through:

$$J = \frac{3k_B T_C}{2zS(S+1)}$$

where z is the number of n.n of a given spin S. This relation expresses that the thermal energy $k_B T_C$ at T_C has a value comparable to $zJS(S+1)$, which can then be interpreted as the mean exchange energy per spin (each spin has z n.n, and the exchange Hamiltonian between two n.n spins is $-2J\overrightarrow{S_1}\overrightarrow{S_2}$). This expression yields $J/k_B = 0.13$ K for EuS $(S = 7/2, z = 12)$. In fact, experience shows that the exchange between next nearest neighbors (n.n.n) is not negligible against that between n.n, and yields respectively $J_1/k_B = 0.22$ K for n.n and $J_2/k_B = -0.10$ K (antiferromagnetic coupling) for n.n.n [8]. The same J value between n.n spins 1/2 instead of spins 7/2, all others things being kept unchanged, would lead to a far smaller T_C value, $S(S+1)$ being then equal to 3/4 instead of 63/4.

In EuS, each moment is coupled to 12 n.n moments. Using for instance $Eu_x Sr_{1-x} S$ with e.g. $x = 10^{-4}$ (diluted sample), would suppress exchange, but the spins would not be strictly independent, because of the existence of the dipolar coupling, caused by the magnetic field created by each moment. At a distance r from a moment $\overrightarrow{\mu}$, the magnitude of this dipolar field is roughly equal to $(\mu_0/4\pi). \parallel \overrightarrow{\mu} \parallel /r^3$ (SI units), which is about 0.014 Tesla for a free electron spin and $r = 4$ Å. If x is in the $0.01-0.1$ range, the probability of existence of pairs of n.n is significant and higher than that of clusters or more numerous spins, and the dipolar energy between these pairs $(r = 4$ Å) is significantly weaker than the exchange energy. At the same time, having this high enough concentration of spins may be interesting for sensitivity reasons.

MnO and MnS are antiferromagnets, with a Néel temperature of 116 and 160 K respectively. In antiferromagnetic oxides or sulfides, the exchange coupling between n.n magnetic ions (direct exchange) is often weaker than that between magnetic ions separated by a diamagnetic ion, a coupling called superexchange, where the electrons of that diamagnetic ion (O^{2-} in MnO) make a link between the two moments [23]. The superexchange Hamiltonian is still of the form $-2J\overrightarrow{s_1}\overrightarrow{s_2}$, but with $J < 0$.

If we accept $J/k_B = +0.1$ K, $T_1 = 10^{-7}$ s and $T = 10^{-8}$ s, then $\Delta_E = -131$. In fact, at 300 K electron spins generally have a shorter T_1. For instance, in the diamagnetic II-VI oxides or sulfides already cited, if a small part of the cations have been replaced each by a magnetic ion, the quantized

vibrations of the ions (phonons) often play the role of the lattice (thermal bath) for the electron moment [2]. When the magnetic moment has no orbital part, its spin is only *weakly* coupled to the phonons. But even in this favorable case, T_1 at 300 K is rather short. For instance, for Mn^{2+} in ZnS, while $T_1 = 0.9$ s at 1.3 K [15], $T_1 = 4\times 10^{-9}$ s at 300 K [33]. As a consequence, if it is necessary to have a longer time T, for instance $T = 10^{-6}$ s, and then to have at least $T_1 = 10^{-5}$ s, use of electron spins could impose working below room temperature. With such T values and electron spins, $\mid \Delta_E \mid$ will probably be significantly greater than 1.

We now come to *nuclear* spins. While exchange between electron spins can be quite strong, on the contrary, when two identical nuclei each carry a spin, their Coulomb repulsion does not give rise to any exchange coupling between the two *nuclear* spins, because the nuclear wave functions do not overlap, their spatial extension being far smaller than the internuclear distance (we have discarded the peculiar exception of solid ^3He, a quantum solid) [3]. On the contrary, the dipolar coupling still exists. For instance, the nucleus of each hydrogen atom (proton) creates a field roughly equal to 2×10^{-5} Tesla at a distance $r = 4$ Å. In NMR experiments with liquids, the Brownian motion of molecules averages the effects of the dipolar fields *on the spectra*. This average happens to be zero, and then the NMR lines are not broadened (nor shifted) by the dipolar coupling [1]. It is time to say that in resonance experiments with electron spins (ESR) in insulators with a high spin concentration, the lines are often quite narrower than expected in the presence of the dipolar coupling, because the then strong exchange coupling reduces its effect (exchange narrowing) [1],[2]. It should be clear that the observation of *conventional* NMR in diamagnetic solid insulators is generally difficult, because of the presence of dipolar broadening of the NMR spectra, as there is then neither motional nor exchange narrowing [1]. Quite elaborate methods have developed, which enable one to average out the effects of the dipolar couplings in the NMR spectra in these solids. When the electrical cloud around the nucleus does not have spherical symmetry, so-called quadrupolar effects can both complicate the NMR spectra and induce relaxation phenomena. But these effects vanish for spins 1/2 [1], and we may ignore them, since in the context of qubits we are restricted to spins 1/2.

In diamagnetic insulators, there still exists a spin-spin coupling called *pseudo-exchange*, or *scalar coupling* [1], with a short range (contrary to the dipolar coupling with its r^{-3} dependence) and of the form $-2J\overrightarrow{I_1}\overrightarrow{I_2}$ between two nuclear spins $\overrightarrow{I_1}$ and $\overrightarrow{I_2}$. It exists when an electron wave function is not zero on both nuclei. The first nuclear moment then somewhat polarizes the electron cloud, which then acts on the second nuclear moment. It is usual to write the numerical value J/h, in Hz, rather than that of J. With neighboring nuclei in molecules, it is often in the range 10^3 $Hz - 1$ Hz.

Nuclear spins are generally very weakly coupled to the lattice. We exclude the presence of paramagnetic impurities, which have several strong effects on the nuclear spins, and which for instance drastically shorten their T_1 (oxygen, for instance, is paramagnetic, and its presence in solutions shortens T_1, unless precautions are taken). In diamagnetic insulating solids, at 300 K, a T_1 value greater than 10^{-2} s is frequent (e.g. in ^{127}I in KI, $T_1 = 0.04$ s, and in $NaCl$ $T_1(Na) = T_1(Cl) \simeq 10$ s [1]). In liquids without paramagnetic impurities and in the absence of quadrupolar relaxation, spin-lattice relaxation is generally provided by the dipolar coupling in the presence of the static field, together with the Brownian motion of the molecules which is then the thermal bath. At

room temperature, T_1 is generally greater than 10^{-2} s. For instance, in water at 20 °C, for the proton, $T_1 = 3.6$ s [1].

We assume to have conditions such that the effects of the dipolar coupling are negligible against the scalar coupling. If $J/h = 10^3$ Hz and $T = 10^{-7}$ s, then $\Delta_E \simeq 6\times 10^{-4}$. In the present situation, it is possible, at room temperature, to use quite longer T durations, for instance $T = 10^{-4}$ s, and with the same J value $\mid \Delta_E \mid \simeq 0.6$.

As a conclusion:

- with electron spins, one should rather expect that $\mid \Delta_E \mid >$ 1 and possibly $\mid \Delta_E \mid \gg 1$. In order to avoid extremely short T durations, one should have to work at low temperature in order to increase T_1, unless it is possible to find spins 1/2 with a long T_1 at 300 K (free radicals present in so-called natural melanin, for instance, have been reported to have $T_1 = 10^{-4}$ s at 300 K).
- When considering nuclear spins, the short range spin-spin scalar coupling is far weaker than the exchange coupling previously found between neighboring electron spins, and taking $T = 10^{-7}$ s or 10^{-6} s, for instance, at 300 K, is not prohibited by the existence of a shorter spin-lattice relaxation time, and consequently $\mid \Delta_E \mid < 1$ and even $\mid \Delta_E \mid \ll 1$ seem likely.

F Software simulation of two coupled qubits

This appendix concerns a realistic software simulation of a quantum system composed of two qubits, interacting according to the cyclindrical-symmetry Heisenberg model. We developed this software package in order to validate the operation of the three classical-processing SS methods tested in Section 5. The core of this software consists of a simulator of our above-mentioned RWR procedure. To perform one run of this procedure, we first initialize the two qubits defined by (18). More precisely, we only choose the values of their three free parameters which appear in our final mixing model, i.e. r_1, r_2 and Δ_I, which define the considered source vector[10]. We also select the value of the mixing parameter v. This value corresponds to the considered spin coupling model and to the selected write-read interval, since (27), (29) and (31) show that

$$v = \mathrm{sgn}(\cos \Delta_E) \sin \Delta_E \tag{69}$$

with Δ_E defined by (24).

As stated above, we then aim at simulating the operation of a real two-qubit system in these conditions. So, before we proceed to the description of this simulator, let us make it clear how the operation of the real system itself would be defined. One could consider two aspects of this operation:

1. The *theoretical* (or asymptotic) behavior of this real system is represented by (19), (26), (33) which define with which probabilities p_1, p_2, p_4 one obtains each of the corresponding three possible measurement outcomes for one

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[10] If one would want to completely define all parameters in (18), this could be achieved as follows (but it must be clear that this is not used in our software simulation of the system, which only requires us to explicitly use r_1, r_2 and Δ_I !): starting from the above parameters r_1, r_2 and Δ_I, the other modulus parameters of the initial qubits state are then derived from (25), while the phase parameters in (18) are e.g. set to $\theta_1 = \Delta_I$, $\phi_1 = \theta_2 = \phi_2 = 0$, as explained in Section 3.2.

step of our RWR procedure, i.e. for one measurement performed with our two-qubit system.

As stated above, this system has a fourth possible measurement outcome, but the corresponding probability p_3 is completely fixed by the above three probabilities p_1, p_2, p_4, since all four probabilities sum to one.

2. The *practical* behavior of this system is obtained by applying our RWR procedure, i.e. by performing K times our write/read step and counting how many times each of the above three possible measurement outcomes occurs over these K trials. This yields three frequencies of (outcome) occurences, which are respectively estimates of p_1, p_2, p_4 and are therefore denoted $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$.

If one could perform an infinite number of measurements (i.e. $K \to \infty$), the measured values $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ would converge towards the associated asymptotic values, which are respectively equal to p_1, p_2, p_4. On the contrary, in practice, due to the finite number K of measurements, the measured values $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ are different from p_1, p_2, p_4. In other words, the observation vectors actually provided to our classical-processing SS methods then do not exactly follow the assumed mixing model defined by (19), (26), (33). This corresponds to so-called "noisy mixtures" in a fully classical SS context and this degrades the accuracy of SS. The magnitude of this degradation increases if the gap between the measured values $\hat{p}_1$, $\hat{p}_2$, $\hat{p}_4$ and the associated theoretical values p_1, p_2, p_4 increases. Therefore, this degradation tends to increase if K decreases.

From a mathematical point of view, the above *theoretical* behavior of the real system may be modelled as a discrete random variable, which has four possible values, with corresponding probabilities p_1 to p_4. We may use any set of four values as the possible values of this random variable, since these values have no importance in the model that we aim at developing: as explained below, they are only used to estimate the corresponding probabilities p_1 to p_4 (or even p_1, p_2, p_4), which are used in our approach. For instance, if the result $(+\frac{1}{2}, +\frac{1}{2})$ is obtained when measuring s_{1z} and s_{2z} in the considered physical system, what is needed to perform our separation process is the value of the probability p_1 of that result, but not the explicit result of that measurement.

The above *practical* behavior of the real system may therefore be modelled using a software program based on a pseudorandom generator defined as follows. The theoretical distribution of the data created by this generator is a discrete random variable, which has four arbitrarily selected possible values, with corresponding probabilities p_1 to p_4, where the values of p_1, p_2, p_4 are computed by using (19), (26), (33) and the selected values of r_1, r_2, Δ_I, v. In practice, K trials are performed with this generator. Its four possible outcomes are thus respectively obtained with frequencies of occurence that we derive from the data actually provided by the generator, and which are denoted $\hat{p}_1$ to $\hat{p}_4$. The software program that we thus defined is the simulator of the practical operation of the real system that we used to perform the SS tests described in Section 5.

G Performance criteria

Each elementary test performed with the software defined in Appendix F uses a single initialization of the coupled qubits, i.e. a single value of the source vector $s = [s_1, s_2, s_3]^T$ with $s_1 = r_1, s_2 = r_2$ and $s_3 = \Delta_I$. Such a test yields an estimate of the above source vector. The estimated source components

are denoted $\hat{r}_1, \hat{r}_2$ and $\hat{\Delta}_I$ hereafter. More generally speaking, we here consider a series of L such tests. Each test with index ℓ is performed with a source vector defined by $r_1(\ell), r_2(\ell)$ and $\Delta_I(\ell)$. The estimated values obtained for these three components are denoted $\hat{r}_1(\ell), \hat{r}_2(\ell)$ and $\hat{\Delta}_I(\ell)$.

The separation accuracy may be measured by the associated Mean Square Error (MSE) between these initial and estimated source vectors, or by the corresponding Root Mean Square Error (RMSE). We compute these parameters separately for: (i) r_1 and r_2 on the one hand, and (ii) Δ_I on the other hand. The motivations for considering separately these two sets of components are as follows:

– they are of different natures.
– The ranges in which they are varied have different widths. Therefore, it would be misleading to add their respective MSE with the same scale factor.
– Anyway, we need to compute the MSE (or RMSE) for these two sets of components separately: the MSE for the modulus components r_1 and r_2 is the same for all three classical-processing SS methods tested in Section 5. It is therefore only computed once. On the contrary, component Δ_I yields different MSE for each SS method. The MSE restricted to Δ_I should therefore be computed separately for each method.

The explicit expressions of the two above-defined MSE and corresponding RMSE are

$$MSE(r_1, r_2) = \frac{1}{2L} \sum_{\ell=1}^{L} \Big[(\hat{r}_1(\ell) - r_1(\ell))^2$$

$$+ (\hat{r}_2(\ell) - r_2(\ell))^2 \Big] \qquad (70)$$

$$RMSE(r_1, r_2) = \sqrt{MSE(r_1, r_2)} \qquad (71)$$

$$MSE(\Delta_I) = \frac{1}{L} \sum_{\ell=1}^{L} (\hat{\Delta}_I(\ell) - \Delta_I(\ell))^2 \qquad (72)$$

$$RMSE(\Delta_I) = \sqrt{MSE(\Delta_I)} \qquad (73)$$

with $\hat{\Delta}_I(\ell)$ and $\Delta_I(\ell)$ in radians.

H Matrix form of spin coupling model

The analysis that we presented in Section 3 may also be expressed in matrix form. To this end, we denote as $C_+(t)$ the column vector composed of the complex magnitudes of the Components of $|\psi(t)>$ in basis $\mathcal{B}_+$, i.e. composed of all coefficients $c_j(t - t_0)$ contained in (9) and defined in (68). Similarly, we represent the system state at time t_0 (defined in (7)) by the column vector $C_+(t_0)$. The analysis that we presented in Section 3 showed that the expression of $|\psi(t)>$ is derived from that of $|\psi(t_0)>$ by means of a 3-step procedure, i.e. basis-to-basis transform, phase rotations in eigenbasis and inverse basis-to-basis transform. This 3-step procedure may then be straightforwardly rewritten so as to express $C_+(t)$ with respect to $C_+(t_0)$, using a succession of 3 matrix products respectively corresponding to the above 3 steps. This yields explicitly

$$C_+(t) = QDQ^{-1}C_+(t_0) \qquad (74)$$

with

$$Q = Q^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad (75)$$

and D equal to

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

(76)

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