Orthogonality relations in quantum tomography

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Abstract

Quantum estimation of the operators of a system is investigated by analyzing its Liouville space of operators. In this way it is possible to easily derive some general characterizations for the sets of observables (i.e., the possible *quorums*) that are measured for the quantum estimation. In particular we analyze the reconstruction of operators of spin systems. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

Two fundamental restrictions limit the possibility of devising a state reconstruction method. On one hand, the quantum complementarity principle does not allow to recover the quantum state from measurements on a single system, unless we have some prior information on it. On the other hand, the no cloning theorem ensures that it is not possible to make exact copies of a quantum system, without having prior knowledge of its state. Hence, the only possibility for devising a state reconstruction procedure is to provide a measuring strategy that employs numerous identical (although unknown) copies of the system, so that different measurements may be performed on each of the copies.

The problem of state estimation resorts essentially to estimating arbitrary operators of a quantum system by using the result of measurements of a set of observables. If this set of observables is sufficient to give full knowledge of the system state, then it is defined as a quorum [1]. Notice that, in general, a system may allow various, different quorums. Quantum tomography was born [2] as a state reconstruction technique in the optical domain, and has recently been extended [3] to a vast class of systems. By extension, we now denote as "Quantum Tomography" all unbiased quantum state reconstruction procedures, i.e., those procedures which are affected only by statistical errors that can be made arbitrarily small by increasing the number of measurements. Tomography makes use of the results of the quorum measurements in order to reconstruct the expectation value of arbitrary operators (even not observables) acting on the system Hilbert space $\mathcal{H}$.

The purpose of this Letter is to present in a formally familiar manner (employing the Dirac notation also on operator space) a constructive method to derive tomographic formulas for quantum systems, at least for finite dimensional Hilbert spaces. This is achieved by giving conditions to build quorums and to check whether a given set of operators is a quorum. In this way, we obtain an extension of the recently proposed group tomography [3], where similar conditions were

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derived for systems with an underlying group structure.

In Section 2 we give the definitions and the conditions to identify a quorum of operators by analyzing the space of operators of a system as a linear vector space. We derive a constructive algorithmic procedure to obtain tomographic formulas in the case of finite quorums. In Section 3 we give some examples of applications of the presented method in the domain of spin systems, where various different quorums are available [3,4].

2. General estimation

Consider the set of system operators, i.e., the Liouville space $\mathcal{L}(\mathcal{H})$. If we initially restrict ourselves to Hilbert–Schmidt operators in $\mathcal{L}(\mathcal{H})$, then this set is itself a Hilbert space of operators, with the scalar product

$$\langle \hat{A} | \hat{B} \rangle \overset{\text{def}}{=} \text{Tr}\big[\hat{A}^\dagger \hat{B}\big]. \tag{1}$$

It is then possible to employ all the properties of linear vector algebra, and to use the Dirac notation, by using the following definitions for bra and ket vectors:

$$\hat{O} \to |\hat{O}\rangle,$$
$$\text{Tr}[\bullet \hat{O}^\dagger] \to \langle \hat{O} | \bullet. \tag{2}$$

In this vision, quantum tomography consists of expressing the operator $\hat{A}$ we want to evaluate as an expansion on the observables of the quorum as

$$|\hat{A}\rangle = \int_{\mathcal{X}} dx \, |\hat{C}(x)\rangle \langle \hat{B}(x)|\hat{A}\rangle, \tag{3}$$

where $|\hat{A}\rangle$ is a generic operator in $\mathcal{L}(\mathcal{H})$, $|\hat{C}(x)\rangle$ (with $x \in \mathcal{X}$) is the set of quorum observables ($C(x)$ is a generally complex function of a selfadjoint operator, hence it is observable in this sense), and the set $\langle \hat{B}(x)|$ is the dual of the quorum. In ordinary notation, Eq. (2) is the tomography identity, i.e.,

$$\hat{A} = \int_{\mathcal{X}} dx \, \text{Tr}\big[\hat{B}(x)^\dagger \hat{A}\big] \hat{C}(x). \tag{4}$$

Notice that the extension of the theory to non-normalizable vectors in the operator Hilbert space is immediate: one only has to require the existence of the trace

of Eq. (4). If, for example, $\hat{A}$ is a trace-class operator, then we do not need to require $\hat{B}(x)$ to be of Hilbert–Schmidt class, since it is sufficient to require $\hat{B}(x)$ bounded. Through Eq. (3), the tomographic reconstruction procedure is immediately obtained. In fact, by measuring the observables $|\hat{C}(x)\rangle$ of the quorum, we can [1] express the mean value of any operator $\langle \hat{A} \rangle$ in terms of the eigenvalues of $|\hat{C}(x)\rangle$ as

$$\langle \hat{A} \rangle = \int_{\mathcal{X}} dx \sum_m p(m,x) \lambda_m^{(x)} \, \text{Tr}\big[\hat{B}^\dagger(x)\hat{A}\big], \tag{5}$$

where $p(m,x)$ is the probability of obtaining the eigenvalue $\lambda_m^{(x)}$ when measuring the quorum observable $\hat{C}(x)$. In particular, the reconstruction of the density matrix on a given orthonormal basis $|n\rangle \in \mathcal{H}$ corresponds to employing Eq. (5) with the generalized projector $\hat{A} = |n\rangle\langle n'|$.

Since we want Eq. (3) to be valid for a generic operator $|\hat{A}\rangle$ in $\mathcal{L}(\mathcal{H})$ (or also in a subspace of $\mathcal{L}(\mathcal{H})$), then we must require that the $|\hat{C}(x)\rangle$ constitute a spanning set for the operator (sub)space, with the set of $\langle \hat{B}(x)|$ acting as its dual. A spanning set is a generalized basis for a vector space: it is a complete set of vectors but it is not, in general, composed of linearly independent (or normalized) vectors. Define dual $\langle \hat{B}(x)|$ of the set $|\hat{C}(x)\rangle$ as the set constructed so to have

$$\langle \hat{B}(x)|\hat{C}(x')\rangle = \text{Tr}\big[\hat{B}^\dagger(x)\hat{C}(x')\big] = \delta(x,x'),$$
$$\forall x, x' \in \mathcal{X}, \tag{6}$$

where $\delta(x,x')$ is a reproducing kernel for $\langle \hat{B}(x)|$, i.e.,

$$\int_{\mathcal{X}} dx \, \delta(x,x') \langle \hat{B}(x)| = \langle \hat{B}(x')|. \tag{7}$$

Since $|\hat{C}(x)\rangle$ is a complete set, $\delta(x,x')$ is a reproducing kernel also for this set, i.e.,

$$\int_{\mathcal{X}} dx \, \delta(x,x') |\hat{C}(x)\rangle = |\hat{C}(x')\rangle. \tag{8}$$

From linear vector algebra we obtain the following four equivalent definitions of spanning set:

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[1] Eq. (5) is obtained by taking the expectation value of both members of Eq. (3) and by calculating the expectation value trace using the eigenvectors of the quorum observables $|\hat{C}(x)\rangle$.

A set of vectors $|\hat{C}(x)\rangle$ (with dual $\langle\hat{B}(x)|$) is a spanning set $\Leftrightarrow$

(i)

$\forall|\hat{A}\rangle \in \mathcal{L}(\mathcal{H})$,

$$|\hat{A}\rangle = \int_{\mathcal{X}} dx\,|\hat{C}(x)\rangle\langle\hat{B}(x)|\hat{A}\rangle,$$

i.e., the tomographic identity, namely Eq. (3).

(ii) $|\hat{C}_n\rangle$ is complete, i.e., (no nonzero element is orthogonal to $|\hat{C}(x)\rangle$ $\forall x$):

$$\langle\hat{A}|\hat{C}(x)\rangle = \langle\hat{B}(x)|\hat{A}\rangle = 0,$$
$$\forall x \in \mathcal{X} \Rightarrow |\hat{A}\rangle = 0. \qquad (9)$$

(iii) The following operatorial identity resolution applies,

$$\int_{\mathcal{X}} dx\,|\hat{C}(x)\rangle\langle\hat{B}(x)| = \hat{\hat{1}}, \qquad (10)$$

where $\hat{\hat{1}}$ is the identity super-operator, namely the operator acting on operators such that $\hat{\hat{1}}[\hat{A}] = \hat{A}$ $\forall\hat{A} \in \mathcal{L}(\mathcal{H})$.

(iv)

$$\int_{\mathcal{X}} dx\,\langle\hat{A}|\hat{C}(x)\rangle\langle\hat{B}(x)|\hat{A}\rangle = \|\hat{A}\|^2 \overset{\text{def}}{=} \mathrm{Tr}[\hat{A}^\dagger\hat{A}],$$

$$\forall|\hat{A}\rangle \in \mathcal{L}(\mathcal{H}).$$

In the usual notation, these equivalent definitions write as [5]:

(i)

$$\hat{A} = \int_{\mathcal{X}} dx\,\mathrm{Tr}[\hat{B}^\dagger(x)\hat{A}]\hat{C}(x).$$

(ii)

$$\mathrm{Tr}[\hat{B}^\dagger(x)\hat{A}] = \mathrm{Tr}[\hat{A}^\dagger\hat{C}(x)] = 0,$$
$$\forall x \in \mathcal{X} \Rightarrow \hat{A} = 0.$$

(iii)

$$\int_{\mathcal{X}} dx\,\langle i|\hat{C}(x)|j\rangle\langle k|\hat{B}^\dagger(x)|l\rangle = \delta_{il}\delta_{jk},$$

where $\{|n\rangle\}$ is a basis for the system Hilbert space $\mathcal{H}$.

(iv)

$$\int_{\mathcal{X}} dx\,\mathrm{Tr}[\hat{A}^\dagger\hat{C}(x)]\,\mathrm{Tr}[\hat{B}^\dagger(x)\hat{A}] = \mathrm{Tr}[\hat{A}^\dagger\hat{A}],$$

$$\forall\hat{A} \in \mathcal{L}(\mathcal{H}).$$

In order to obtain the dual set $\langle\hat{B}(x)|$ starting from a given set $|\hat{C}(x)\rangle$, one in general has to solve the operatorial equation (6) that defines the quorum. For finite quorums, this resorts to a matrix inversion. An alternative procedure is now proposed. It derives from the Gram–Schmidt orthogonalization method [6], which allows to derive a basis starting from a complete set of vectors. Namely, one obtains a basis $|y_k\rangle$, given the complete set $|C_k\rangle$ (assume for simplicity that all $|C_k\rangle$ are non-zero and that in $\{|C_k\rangle\}$ there are no couples of proportional vectors), recursively defined as

$$\begin{cases} |y_0\rangle \doteq \frac{1}{N_0}|C_0\rangle \\ |y_k\rangle \doteq \frac{1}{N_k}\left(|C_k\rangle - \sum_{j=0}^{k-1}|y_j\rangle\langle y_j|C_k\rangle\right), \end{cases} \qquad (11)$$

where $N_0 \doteq \||C_0\rangle\|$ and

$$N_k \doteq \left\||C_k\rangle - \sum_{j=0}^{k-1}|y_j\rangle\langle y_j|C_k\rangle\right\|.$$

Notice that in the recursion (11) one must take care of eliminating all the vectors $|C_k\rangle$ which are a linear combination of the $|y_j\rangle$ with $j < k$.

Write the identity resolution for the basis obtained with procedure (11), i.e.,

$$\hat{1} = \sum_{k=0}^{\infty}|y_k\rangle\langle y_k|$$

$$\equiv \frac{|C_0\rangle}{N_0}\langle y_0|$$

$$+ \sum_{k=1}^{\infty}\frac{1}{N_k}\left(|C_k\rangle - \sum_{j=0}^{k-1}|y_j\rangle\langle y_j|C_k\rangle\right)\langle y_k|. \qquad (12)$$

By using repeatedly Eq. (11) (expressing $|y_j\rangle$ of Eq. (12) in terms of the $|C_n\rangle$s) and by reorganizing the terms in the sums, we can find the dual set $\langle B_n|$ as

$$\langle B_0| = \frac{\langle y_0|}{N_0} - \frac{\langle y_0|C_1\rangle\langle y_1|}{N_0 N_1}$$

$$+ \left(-\frac{\langle y_0|C_2\rangle}{N_0 N_2} + \frac{\langle y_0|C_1\rangle\langle y_1|C_2\rangle}{N_0 N_1 N_2}\right)\langle y_2| + \cdots,$$

$$\langle B_1| = \frac{\langle y_1|}{N_1} - \frac{\langle y_1|C_2\rangle\langle y_2|}{N_1 N_2}$$
$$+ \left(-\frac{\langle y_1|C_3\rangle}{N_1 N_3} + \frac{\langle y_1|C_2\rangle\langle y_2|C_3\rangle}{N_1 N_2 N_3} \right)\langle y_3| + \cdots,$$
$$\vdots \tag{13}$$

Eq. (12) guarantees that it is possible to write

$$\hat{1} = \sum_n |C_n\rangle\langle B_n|, \tag{14}$$

which is just definition (iii) (i.e., Eq. (10)) of spanning set.

Summarizing, we described a method for deriving tomographic formulas for arbitrary systems. One must start from a set of operators $\hat{C}_n$ he or she would like to use as a quorum, and verify that such a set is complete, i.e., that no nonzero element of $\mathcal{L}(\mathcal{H})$ is orthogonal to all $\hat{C}_n$:

$$\langle \hat{A}|\hat{C}_n\rangle = \text{Tr}[\hat{A}^\dagger \hat{C}_n] = 0, \quad \forall n \Rightarrow |\hat{A}\rangle = 0. \tag{15}$$

If the set is finite, then one can employ the orthogonalization procedure outlined previously to derive the dual set. If the set is infinite discrete or continuous, then one can only resort to finding appropriate solutions for Eq. (6). Once the dual is known, the tomographic identity (3) can be written explicitly. The reconstruction procedure, in terms of the probabilities of measurements of quorum observables, follows straightforwardly and yields Eq. (5), which allows to obtain arbitrary operator expectation values in terms of quorum outcome probabilities. Of course, one may think of similar procedures based on different orthogonalization algorithms.

Since no hypotheses were made on the structure of the system Hilbert space, the theory presented in this section is valid for any quantum system. In the following section we will give some example applications.

3. Example of application: spin tomography

Here we show an application of the theory presented in the previous section by rederiving the spin tomography [3,4], where various different quorums may be employed.

The simplest possible example is a spin $s = \frac{1}{2}$ system. In this case we expect that the Pauli matrix and the identity constitute a quorum (since any 2×2 matrix can be written on such a basis). Take the

quorum $\mathcal{Q} \stackrel{\text{def}}{=} \{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z, \hat{1}\}$: it is immediate to verify that it is complete. Since the quorum operators are orthogonal, i.e., $\hat{\sigma}_\alpha \bullet \hat{\sigma}_{\alpha'} = \hat{1}\delta_{\alpha\alpha'}$ ($\alpha, \alpha' = x, y, z$), using the Gram–Schmidt procedure it is immediate to obtain the dual set as $\mathcal{C} = \{\frac{1}{2}\hat{\sigma}_x, \frac{1}{2}\hat{\sigma}_y, \frac{1}{2}\hat{\sigma}_z, \frac{1}{2}\hat{1}\}$. Expansion (3) of a matrix $\hat{A}$ is, thus

$$|\hat{A}\rangle = \frac{1}{2}\left[\sum_{\alpha=x,y,z} |\hat{\sigma}_\alpha\rangle\langle\hat{\sigma}_\alpha^\dagger|\hat{A}\rangle + |\hat{1}\rangle\langle\hat{1}|\hat{A}\rangle \right], \tag{16}$$

which immediately yields the reconstruction procedure

$$\langle\hat{A}\rangle = \sum_{m=-1/2}^{1/2} \sum_{\alpha=x,y,z} p(m, \vec{n}_\alpha) m \, \text{Tr}[\hat{A}\hat{\sigma}_\alpha]$$
$$+ \frac{1}{2}\text{Tr}[\hat{A}], \tag{17}$$

where $p(m, \vec{n}_\alpha)$ is the probability to obtain the eigenvalue $m = \pm\frac{1}{2}$ while measuring $\vec{S} \bullet \vec{n}_\alpha$. This equation allows the reconstruction of the expectation value of any spin $s = \frac{1}{2}$ operator $\hat{A}$ from the measurement of the spin in the x, y, z directions.

For an arbitrary spin s, a possible quorum is given by the spin component in all directions, i.e., the observable $\vec{S} \bullet \vec{n}$ ($\vec{S}$ being the spin operator and $\vec{n}$ a vector on the unit sphere). In order to find the dual $\langle\hat{B}|$, consider the exponential of the quorum, i.e., $\hat{D}(\psi, \vec{n}) = \exp(i\psi\vec{S}\bullet\vec{n})$, which satisfies definition (iii) (i.e., Eq. (10)) of spanning set. In fact, $\hat{D}(\psi, \vec{n})$ constitutes a unitary irreducible representation of the group $SU(2)$. The orthogonality relation between the matrix elements of the group representation $D(g)$ of dimension d writes as [7]

$$\int_R dg \, D_{jr}(g) D_{tk}^\dagger(g) = \frac{V}{d}\delta_{jk}\delta_{tr}, \tag{18}$$

where dg is the group Haar invariant measure, and $V = \int_R dg$. For $SU(2)$, with the $2s + 1$ dimension unitary irreducible representation $\hat{D}(\psi, \vec{n})$, Haar's invariant measure is $\sin^2\frac{\psi}{2}\sin\vartheta\,d\vartheta\,d\varphi\,d\psi$, and $V = 4\pi^2$. Thus, the orthogonality relations in this case are given by

$$\frac{2s+1}{4\pi^2}\int_\Omega d\vec{n}\int_0^{2\pi} d\psi \sin^2\frac{\psi}{2}\langle j|e^{i\psi\vec{n}\bullet\vec{S}}|r\rangle$$
$$\times \langle t|e^{-i\psi\vec{n}\bullet\vec{S}}|k\rangle = \delta_{jk}\delta_{tr}, \tag{19}$$
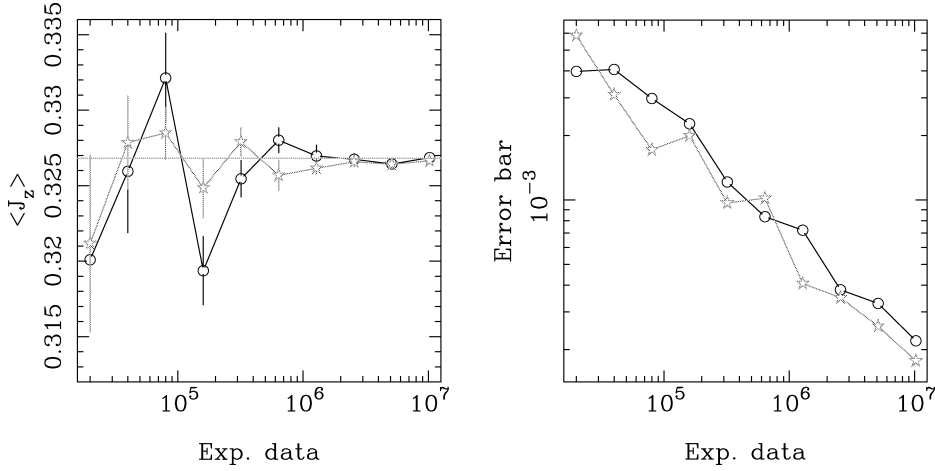
Fig. 1. Monte Carlo comparison between continuous and discrete tomography for a spin $s = 1/2$ system. Continuous tomography uses $\hat{D}(\psi, \vec{n})$ as quorum, while discrete tomography uses the quorum $\mathcal{Q} \stackrel{\text{def}}{=} \{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z, \hat{1}\}$. Left: convergence of the mean value of $\langle s_z \rangle$ for a coherent $\alpha = 2$ spin state for increasing number of experimental data (the theoretical value is given by the horizontal line). The circles ∘ refer to continuous, the stars ⋆ to discrete tomography. Right: plot of the statistical error bars of the graphs on the left *vs* experimental data. The error bars are obtained by dividing the experimental data into 20 statistical blocks. Notice that the two tomographic procedures are essentially equivalent.

which is the the spanning set definition (iii) for the set of operators $|\hat{D}\rangle = \hat{D}$, with dual $\langle \hat{D}^\dagger | \bullet = \text{Tr}[\hat{D}^\dagger \bullet]$.

Then, it is possible to write the spin tomography identity as

$$\hat{A} = \frac{2s + 1}{4\pi^2} \int_\Omega d\vec{n} \int_0^{2\pi} d\psi \sin^2 \frac{\psi}{2}$$
$$\times \text{Tr}[\hat{A}\hat{D}^\dagger(\psi, \vec{n})]\hat{D}(\psi, \vec{n}), \qquad (20)$$

from which the following reconstruction procedure is derived:

$$\langle \hat{A} \rangle = \frac{2s + 1}{4\pi^2} \sum_{m=-s}^{s} \int_\Omega d\vec{n}\, p(m, \vec{n}) \int_0^{2\pi} d\psi\, \sin^2 \frac{\psi}{2}$$
$$\times \text{Tr}[\hat{A}\, e^{-i\psi(\vec{S}\bullet\vec{n}-m)}], \qquad (21)$$

where $p(m, \vec{n})$ is the probability of obtaining m as the measurement result of $\vec{S} \bullet \vec{n}$. This equation allows the reconstruction of arbitrary spin s expectation values $\langle \hat{A} \rangle$, from spin measurements in all directions $\vec{n}$.

Numerical simulations show that the two preceding quorums are (for spin $s = \frac{1}{2}$) equivalent, namely the same number of experimental measurement data yield the same results and the same statistical error bars, apart from statistical fluctuations. In Fig. 1

a Monte Carlo comparison of the two spin reconstruction strategies based on the two different quorums is given. Both reconstructions are applied to a coherent spin state, defined as $|\alpha\rangle \stackrel{\text{def}}{=} \exp(\alpha S_+ - \alpha^* S_-)|-s\rangle$, where S_+, S_- are the spin lowering and raising operators and $|-s\rangle$ is the eigenvector of S_z relative to the minimum eigenvalue.

Weigert has shown [4] that another spin s quorum can be obtained by taking $N_s \stackrel{\text{def}}{=} (2s + 1)^2$ arbitrary[2] directions $\vec{n}_k$ and measuring the observables $\hat{Q}_k \stackrel{\text{def}}{=} |\vec{n}_k\rangle\langle\vec{n}_k|$, which are the projectors for the eigenspace relative to the maximum eigenvalue s of the observables $\vec{S} \bullet \vec{n}_k$. We define a dual $\langle\hat{Q}_k|$ for the $|\hat{Q}_k\rangle$ by requiring

$$\langle \hat{Q}_k | \hat{Q}_{k'} \rangle = \delta_{kk'}, \qquad (22)$$

i.e., Eq. (11) of [4], which is just the dual set definition (6). Condition (22) together with the completeness of the chosen quorum, guarantee that $|\hat{Q}_k\rangle$ (with dual $\langle\hat{Q}_k|$) is a spanning set for $\mathcal{L}(\mathcal{H})$, thus allowing

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[2] Actually the choice of the directions is not completely arbitrary, but "almost" [4] any choice yields a complete set of operators in $\mathcal{L}(\mathcal{H})$.

the tomographic identity

$$|\hat{A}) = \sum_{k=1}^{N_s} |\hat{Q}_k)(\hat{Q}_k|\hat{A}), \qquad (23)$$

i.e., (using the notation of [4])

$$\hat{A} = \sum_{k=1}^{N_s} \mathrm{Tr}[\hat{A}\hat{Q}^k]\hat{Q}_k, \qquad (24)$$

where $\hat{Q}^k$ is the dual operator of $\hat{Q}_k$. The explicit form of the dual set $\hat{Q}^k$ can be derived by a matrix inversion starting from Eq. (22) or by the Gram–Schmidt based procedure method given above. The reconstruction procedure is, in this case,

$$\langle \hat{A} \rangle = s \sum_{k=1}^{N_s} p(s, \vec{n}_k) \, \mathrm{Tr}[\hat{A}\hat{Q}^k], \qquad (25)$$

where $p(s, \vec{n}_k)$ is the probability of obtaining the maximum eigenvalue s, when measuring $\vec{S} \cdot \vec{n}_k$. This allows the reconstruction of arbitrary spin operators $\hat{A}$ from measurements of the spin along N_s fixed directions.

4. Conclusions

Recent group tomography [3] gives a general framework that allows to derive all the state reconstruction procedures that employ quorums which exhibit a group symmetry. Here we extended these results to generic state reconstruction procedures. In fact, we have seen how it is possible to give a characterization of tomographic formulas in terms of linear vector algebra on the vectors of the Liouville space of the system.

A constructive method to derive new tomographic formulas has been proposed starting from the Gram–Schmidt orthogonalization procedure. At least in principle, it allows to calculate the quorum dual for the quantum systems that allow a discrete quorum. We have given some examples of the method in the spin domain, by re-obtaining all the known spin tomographies using linear vector algebra arguments. For the sake of illustrating the method, we limited our analysis to the description of spin systems, but all known tomographies can be analyzed in this framework [5]. Moreover, one may expect to employ the presented procedures to uncover new tomographies for quantum systems for which state reconstruction procedures are not presently known.

Acknowledgements

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