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QUANTUM HAMILTONIAN AND DIPOLE MOMENT IDENTIFICATION IN PRESENCE OF LARGE CONTROL PERTURBATIONS

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Abstract. The problem of recovering the Hamiltonian and dipole moment is considered in a bilinear quantum control framework. The process uses as inputs some measurable quantities (observables) for each admissible control. If the implementation of the control is noisy the data available is only in the form of probability laws of the measured observable. Nevertheless it is proved that the inversion process still has unique solutions (up to phase factors). Both additive and multiplicative noises are considered. Numerical illustrations support the theoretical results.

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1. Introduction and motivation

Successful manipulation of quantum dynamics (see [5] and references therein for a recent review) leads to interesting perspectives among which is the possibility to identify the system through measurements of control-dependent observations. This technique, called quantum identification or quantum inversion, was documented both theoretically [1,4,16,23] and numerically [8,11,18]. However although the numerical implementations show interesting robustness of the identification process with respect to noise, there is less theoretical guidance to explain this fact. Two fundamental questions concerning the well-posedness of this problem arise: the existence and the uniqueness of the Hamiltonian, and/or the dipole moment, compatible with the given measurements. In this work we only study the uniqueness.

More specifically we start from the setting in [16] which treats the case without noise. After some technical preliminaries in Section 3 we address the noise-free case in Section 4 and relax many of the assumptions used in the previous work. Then in Section 5 we introduce the possibility that the control is subject at each time to unknown perturbations. We consider both additive and multiplicative noise. Since the actual control that acts on the system is unknown, only the probability laws of the observations are available. We explain which are the properties of the set of measurements required to determine uniquely (up to phase factors) the free Hamiltonian and dipole moment.

Then a numerical implementation is presented in Section 6. Some closing remarks are the object of Section 7.

Keywords and phrases. Quantum control, quantum identification.

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1.1. Notations

We introduce the following notations

- $\mathbb{L}_{M_1,M_2,\dots,M_m}$ is the Lie algebra spanned by the matrices $M_1, M_2, \dots, M_m$;
- for any matrix or vector X we denote by $\overline{X}$ its conjugate (the matrix whose entries are the complex conjugates of the entries of X) and by X^* its adjoint (the transpose conjugate);
- $\mathcal{H}_N$ is the set of all Hermitian matrices $\mathcal{H}_N = \{X \in \mathbb{C}^{N\times N} | X^* = X\}$;
- $\mathcal{S}_N$ is the unit sphere of $\mathbb{C}^N$: $\mathcal{S}_N = \{v \in \mathbb{C}^N | \|v\| = 1\}$;
- $\Psi(t, H, u(\cdot), \mu, \Psi_0)$ is the solution of the equation (2.1) below; to simplify the notation, when there is no ambiguity, we denote it $\Psi(t)$;
- $\lambda_k(X)$, $k = 1, \dots, N$ are the eigenvalues of $X \in \mathcal{H}_N$ taken in increasing order; we also introduce $\phi_k(X)$ $k = 1, \dots, N$ to be eigenvectors of X (forming an orthonormal basis of $\mathbb{C}^N$) corresponding to eigenvalues $\lambda_k(X)$; note that Span$\{\phi_k(X)\}$ may not be unique;
- $SU(N)$ is the special unitary group of degree N, which is the group of $N \times N$ unitary matrices with determinant 1;
- $\mathfrak{su}(N)$ is the Lie Algebra of skew-Hermitian matrices (the Lie algebra of $SU(N)$);

2. The model

We present the mathematical framework following closely the notations of the previous work [16].

Consider a controlled quantum system with time-dependent wave-function $\Psi(t)$ satisfying the Schrödinger equation:

$$\begin{cases} i\dot{\Psi}(t, H, u(\cdot), \mu, \Psi_0) = (H + u(t)\mu)\Psi(t, H, u(\cdot), \mu, \Psi_0) \\ \Psi(0, H, u(\cdot), \mu, \Psi_0) = \Psi_0, \end{cases} \tag{2.1}$$

where H is the internal ("free") Hamiltonian and μ the coupling operator between the control $u(t) \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+; \mathbb{R})$ and the system. We work in a finite dimensional framework, therefore $H, \mu \in \mathcal{H}_N$ for some $N \in \mathbb{N}^*$. The goal is to determine the matrix entries of H and μ from laboratory measurements of some observables depending on $\Psi(t)$. The control $u(t)$ can be changed in order to gather enough information on the system.

However, contrary to [16], we allow in this work some time independent perturbations to appear in the control $u(t)$. That is, when the control is implemented in practice the nominal control intensity required by the experimentalist, denoted $\epsilon(t)$, is perturbed by Y which means that $u = u(t, \epsilon(\cdot), Y)$; here Y is a discrete random variable with possible outcomes $y_1, y_2, \dots$. We assume that the law of the random variable Y is time independent. A first example is the additive perturbation $u(t) = \epsilon(t) + Y$. Such perturbation models have already been used in the quantum computing literature under the name of "fixed systematic errors", see section VI.A. equation (40) of [14] or "systematic control error", see [15]. In [19] the authors use a noise model called "low frequency noise" (see Sect. IV.C. of [12]): it is defined as the portion of the (control) amplitude noise that has a correlation time that is long (up to 10^3 times) compared to the timescale of the dynamics therefore it can be considered as constant in time. Additional noise models (additive or multiplicative) are presented in [24].

The perturbation Y is unknown and thus $\Psi(t)$ is a random variable, as are all measurements depending on $\Psi(t)$. Repeating the control experiment several times the experimentalist will only learn the law of the measurements. From now on we will denote by $\mathcal{L}_Y Z$ the law of the random variable Z (that is measurable with respect to the sigma-algebra generated by Y).

Two different settings are considered depending on which parameters are to be identified and the nature of the information available:

- Setting **(S1)**: The Hamiltonian H is known and the goal is to identify the dipole moment μ.
- Setting **(S2)**: Both the Hamiltonian H and the dipole moment μ are unknown.

The measurements are of the form $\langle O\Psi(T, H, u, \mu, \Psi_0), \Psi(T, H, u, \mu, \Psi_0)\rangle$ with $O \in \mathcal{H}_N$ a member of a list of possible measurements. Often, the experimentalist only measures one observable in a list (but can repeat the experiment many times). This means that for general $O_1, O_2 \in \mathcal{H}_N$ no information is available on the joint distribution of the values $\langle O_1\Psi(T,H,u,\mu,\Psi_0), \Psi(T,H,u,\mu,\Psi_0)\rangle$ and $\langle O_2\Psi(T,H,u,\mu,\Psi_0), \Psi(T,H,u,\mu,\Psi_0)\rangle$ of these two observables.

3. Some technical preliminaries

3.1. Complete sets of commuting observables

We recall in this section several facts about complete sets of commuting observables (hereafter abbreviated CSCO). We refer the reader to ([6], p. 146) for details.

First, recall that an observable is a self-adjoint operator on $\mathbb{C}^N$. Once a basis of $\mathbb{C}^N$ is chosen the observable can be represented as a matrix $O \in \mathcal{H}_N$.

A set of observables $\mathcal{O} = \{O_1, \ldots, O_K\}$ is called *set of commuting observables* (named SCO hereafter) if $[O_k, O_\ell] = 0$, $\forall k, \ell \in \{1, \ldots, K\}$.

When all observables in the SCO are multiples of the identity operator the SCO is said to be trivial; unless specified otherwise, we only work with non-trivial SCO.

All observables in the SCO $\mathcal{O}$ can be diagonalized simultaneously *i.e.*, there exists at least an orthonormal basis $\Phi = \{\phi_1, \ldots, \phi_N\}$ of $\mathbb{C}^N$ such that any $O \in \mathcal{O}$ is diagonal in the basis Φ. This means that in particular any ϕ_ℓ is an eigenvector of any observable $O \in \mathcal{O}$. In general the basis Φ is not unique because of possible degeneracies in the spectrum of the observables in $\mathcal{O}$. By definition a SCO is called a *complete set of commuting observables* (CSCO) if the orthonormal basis that diagonalizes the SCO is unique up to phase factors and permutations, *i.e.*, if $\{\varphi_1, \ldots, \varphi_N\}$ is another orthonormal basis rendering all $O \in \mathcal{O}$ diagonal then there exists a permutation σ of $\{1, \ldots, N\}$ and phases $\beta_1, \ldots, \beta_N \in \mathbb{R}$ such that $\varphi_k = \mathrm{e}^{i\beta_k}\phi_{\sigma(k)}$ for all $k = 1, \ldots, N$.

Examples:

(1) Let H be a Hamiltonian with all eigenvalues $\lambda_\ell(H)$ of multiplicity 1. Then $\mathcal{O} = \{H\}$ is a CSCO.

(2) Let $\{v_1, \ldots, v_N\}$ be an orthonormal basis of $\mathbb{C}^N$. Then defining P_k to be the projection on v_k (that is $P_k = v_k v_k^*$) the set $\mathcal{O} = \{P_k, 1 \le k \le N\}$ is a CSCO. In this case P_k are called populations of the states v_k.

(3) Consider $N = 3$ and $\mathcal{O} = \{O_d\}$ with:

$$O_d = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/2 \end{pmatrix}. \tag{3.1}$$

Because the eigenspace corresponding to the eigenvalue 1/2 is of dimension 2 $\mathcal{O}$ is not a CSCO. In this case both the canonical base of $\mathbb{C}^3$: $\{(1,0,0)^T, (0,1,0)^T, (0,0,1)^T\}$ and the orthonormal basis $\{(1,0,0)^T, (0,1/2,-\sqrt{3}/2)^T, (0,\sqrt{3}/2,1/2)^T\}$ render O_d diagonal.

(4) Consider the truncated spin-less Hydrogen atom whose eigenstates can be labeled by a set of three indexes $\phi_{n,l,m}$ with $n = 1, 2, \ldots, N_t$, $l = 0, 1, \ldots, n-1$, $m = -l, -l+1, \ldots, l-1, l$. Here $N_t \in \mathbb{N}$ is a fixed truncation threshold. A CSCO is given by the operators H (Hamiltonian), L^2 (square of the angular momentum operator), L_z (the z component of the angular momentum operator) which act on the eigenstate $\phi_{n,l,m}$ as:

$$H\phi_{n,l,m} = \frac{C_H}{n^2}\phi_{n,l,m},\ L^2\phi_{n,l,m} = l(l+1)\hbar^2\phi_{n,l,m},\ L_z\phi_{n,l,m} = m\hbar\phi_{n,l,m}, \tag{3.2}$$

with C_H an universal constant and $\hbar$ the Plank constant. Here n is called principal quantum number, l the angular momentum quantum number and m the magnetic quantum number. Note that in this case $\{H, L^2\}$ is a SCO but not a CSCO.

Measuring simultaneously all observables in a CSCO is in principle possible as it is compatible with the Heisenberg uncertainty principle since all observables in a CSCO commute two by two; therefore the values of those observables may be simultaneously computed with infinite precision.

The following characterization of a CSCO will be used in the following sections:

Lemma 3.1. *Let $\mathcal{O} = \{O_1, \ldots, O_K\}$ be a SCO. Then $\mathcal{O}$ is a CSCO iff there exist $\gamma_1, \ldots, \gamma_K \in \mathbb{R}$ such that all eigenvalues of $\sum_{k=1}^K \gamma_k O_k$ have multiplicity one.*

Proof. We prove first the direct implication. Consider a basis $\Phi = \{\phi_1, \ldots, \phi_N\}$ of $\mathbb{C}^N$ that renders all O_k diagonal and denote $(O_k)_j$ the jth eigenvalue of O_k, that is $O_k\phi_j = (O_k)_j\phi_j$. Suppose now by contradiction that for any $\gamma = (\gamma_1, \ldots, \gamma_K) \in \mathbb{R}^K$ there exists $i(\gamma) \neq j(\gamma) \leq N$, such that $\sum_{k=1}^K \gamma_k (O_k)_{i(\gamma)} = \sum_{k=1}^K \gamma_k (O_k)_{j(\gamma)}$. Define the functions $g^{\ell_1,\ell_2} : \mathbb{R}^K \to \mathbb{R}$ by $g^{\ell_1,\ell_2}(\gamma_1, \ldots, \gamma_K) = \sum_{k=1}^K \gamma_k[(O_k)_{\ell_1} - (O_k)_{\ell_2}]$ and let $A^{\ell_1,\ell_2} = \{\gamma \in \mathbb{R}^K; g^{\ell_1,\ell_2}(\gamma) = 0\}$. We obtain that $\cup_{1\leq \ell_1<\ell_2\leq N} A^{\ell_1,\ell_2} = \mathbb{R}^K$. By the Baire's theorem at least a couple (ℓ_1^*, ℓ_2^*) exists such that $A^{\ell_1^*,\ell_2^*}$ has non empty interior. Therefore the analytic function $g^{\ell_1^*,\ell_2^*}$ is null on a non empty open set hence it is null everywhere.

But this means that $(O_k)_{\ell_1^*} = (O_k)_{\ell_2^*}$ for all $k = 1, \ldots, K$. Therefore for all $O_k \in \mathcal{O}$ the ℓ_1^*th eigenvalue is of multiplicity 2 (the ℓ_1^*th eigenvector and the ℓ_2^*th eigenvector are associated to the same eigenvalue) which contradicts the uniqueness of the basis that diagonalizes $\mathcal{O}$, and hence we obtain a contradiction with the definition of a CSCO.

The reverse implication is more straightforward. Any basis $\Phi = \{\phi_1, \ldots, \phi_N\}$ that renders all $O_k \in \mathcal{O}$ diagonal will also render $\sum_{k=1}^K \gamma_k O_k$ diagonal. But by hypothesis all eigenvalues of $\sum_{k=1}^K \gamma_k O_k$ are distinct and therefore the basis Φ is unique (up to permutation and phases) and hence $\mathcal{O}$ is a CSCO.

3.2. Background on controllability results

Let $L \in \mathbb{N}^*$ and $G_1, \ldots, G_L$ be L finite dimensional, connected, compact and simple Lie groups with the identity element Id. Let $A_\ell, B_\ell \in \mathfrak{g}_\ell$ for all $\ell = 1, \ldots, L$ where $\mathfrak{g}_\ell$ is the Lie algebra of G_ℓ.

Definition 3.2. Consider L bilinear systems on the Lie groups G_ℓ:

$$\begin{cases} \frac{\mathrm{d}X_\ell(t)}{\mathrm{d}t} = (A_\ell + u(t)B_\ell)X_\ell(t), \\ X_\ell(0) = Id. \end{cases} \tag{3.3}$$

The systems are called *simultaneously controllable (or ensemble controllable)* if there exists $T_{A_1,\ldots,A_L,B_1,\ldots,B_L} > 0$ such that for all $T \geq T_{A_1,\ldots,A_L,B_1,\ldots,B_L}$ and for all $V_\ell \in G_\ell$, $\ell = 1, \ldots, L$ arbitrary, there exists a control $u \in \mathrm{L}^1([0, T], \mathbb{R})$ with $X_\ell(T) = V_\ell$, $\forall \ell = 1, \ldots, L$.

Let $\mathcal{A} = A_1 \bigoplus \ldots \bigoplus A_L \in \bigoplus_{\ell=1}^L \mathfrak{g}_\ell$ and $\mathcal{B} = B_1 \bigoplus \ldots \bigoplus B_L \in \bigoplus_{\ell=1}^L \mathfrak{g}_\ell$. The following simultaneous controllability results are proved in ([21], Thms. 1 & 2 and [3], Lem. 3, p. 29).

Theorem 3.3. *The collection (3.3) of L bilinear systems is simultaneously controllable if and only if $\mathbb{L}_{\mathcal{A},\mathcal{B}} = \bigoplus_{\ell=1}^L \mathfrak{g}_\ell$ or equivalently $dim_{\mathbb{R}}\mathbb{L}_{\mathcal{A},\mathcal{B}} = \sum_{\ell=1}^L dim_{\mathbb{R}}\mathfrak{g}_\ell$.*

Lemma 3.4. *We suppose that $\mathbb{L}_{A_\ell,B_\ell} = \mathfrak{g}_\ell$, for all $\ell = 1, \ldots, L$. Then $\mathbb{L}_{\mathcal{A},\mathcal{B}} \neq \bigoplus_{\ell=1}^L \mathfrak{g}_\ell$ if and only if there exist $\ell, \ell' \in \{1, \ldots, L\}$, $\ell \neq \ell'$ and an isomorphism $f : \mathfrak{g}_\ell \to \mathfrak{g}_{\ell'}$ such that $f(A_\ell) = A_{\ell'}$ and $f(B_\ell) = B_{\ell'}$.*

Theorem 3.5. *Let G be a finite dimensional, connected, compact and simple Lie group and $\mathfrak{g}$ be its Lie algebra. Let $A, B \in \mathfrak{g}$ such that $\mathbb{L}_{A,B} = \mathfrak{g}$ and $\alpha_1, \ldots, \alpha_L \in \mathbb{R}$ be real constants, $\alpha_i \neq \alpha_j$ $\forall i \neq j$. Consider the collection of control systems on G:*

$$\begin{cases} \frac{\mathrm{d}X_\ell(t)}{\mathrm{d}t} = \{A + (u(t) + \alpha_\ell)B\}X_\ell(t), \\ X_\ell(0) = Id. \end{cases} \tag{3.4}$$

Then the collection of systems (3.4) is simultaneously controllable.

Remark 3.6. Although the Theorems 3.3 and 3.5 are formulated on a Lie group, this is enough to obtain controllability for the wave-function; recall that if $X(t, H, u(\cdot), \mu) : \mathbb{R} \times \mathcal{H}_N \times \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+; \mathbb{R}) \times \mathcal{H}_N \to SU(N)$ satisfies the following equation:

$$\begin{cases} i\dot{X}(t, H, u(\cdot), \mu) = (H + u(t)\mu)X(t, H, u(\cdot), \mu), \\ X(0, H, u(\cdot), \mu) = Id, \end{cases} \tag{3.5}$$

then $\Psi(t, H, u(\cdot), \mu, \Psi_0) = X(t, H, u(\cdot), \mu)\Psi_0$ is the solution of (2.1). Since $SU(N)$ is transitive on the sphere $\mathcal{S}_N$ (see [7], p. 88), if the control system is controllable on the Lie group $SU(N)$ then it will also be controllable in the wave-function formulation.

4. Inversion without noise

Theorem 4.1 (Setting **(S1)**). *Let H, μ_1, $\mu_2 \in \mathcal{H}_N$, H diagonal, $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$ and denote for $a = 1, 2$ and $\epsilon \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+, \mathbb{R})$: $\Psi_a(t, \epsilon) = \Psi(t, H, \epsilon(\cdot), \mu_a, \Psi_0^a)$. Let $\mathcal{O}$ be a (non-trivial) SCO. We suppose that $N \geq 3$ and:*

- **(A1):** $\mathbb{L}_{iH, i\mu_1} = \mathbb{L}_{iH, i\mu_2} = \mathfrak{su}(N)$.
- **(A2):** $tr(H) = tr(\mu_1) = tr(\mu_2) = 0$.
- *the eigenvalues of H are all of multiplicity one.*

Then there exists $T > 0$ such that if:

$$\langle O\Psi_1(T, \epsilon), \Psi_1(T, \epsilon)\rangle = \langle O\Psi_2(T, \epsilon), \Psi_2(T, \epsilon)\rangle \quad \forall \epsilon \in L^1([0, T]; \mathbb{R}), \quad \forall O \in \mathcal{O}, \tag{4.1}$$

then for some $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$:

$$(\mu_1)_{jk} = \mathrm{e}^{i(\alpha_j - \alpha_k)}(\mu_2)_{jk}, \ \forall j, k \leq N. \tag{4.2}$$

Remark 4.2.

(1) Assumption **(A1)** is required for the simultaneous controllability, see Theorem 3.3 and Lemma 3.4.
(2) The assumption **(A2)** can be made without loss of generality according to [16]. In fact, changing the Hamiltonian H and/ or dipole moment μ by adding a multiple of the identity operator Id, does not change the observations. In this case, the state $\Psi(t)$ is replaced by $\mathrm{e}^{i\varphi}\Psi(t)$ with the phase $\varphi \in \mathbb{R}$ depending on $tr(H)$, $tr(\mu)$ and on the control u.

Remark 4.3. The proof also shows that the values of any additional observable commuting with H are identical for both systems, in particular all populations are always identical.

Moreover, when μ_1 and μ_2 are matrices of dipole operators (*i.e.*, have the form of real potentials) truncated to dimension N, then μ_1 and μ_2 are real symmetric matrices; the Theorem implies $(\mu_1)_{jk} = \pm(\mu_2)_{jk}$ for all j, k. In general this is not enough to conclude that $\mu_1 = \mu_2$ as it can be seen from the counter-example 1 from ([16], p. 381) where $N = 3$, $\Psi_0^1 = \Psi_0^2 = (1, 0, 0)^T$:

$$H = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{pmatrix}, \quad \mu_1 = \begin{pmatrix} 0 & -\mu_\alpha & 0 \\ -\mu_\alpha & 0 & \mu_\beta \\ 0 & \mu_\beta & 0 \end{pmatrix}, \quad \mu_2 = \begin{pmatrix} 0 & \mu_\alpha & 0 \\ \mu_\alpha & 0 & \mu_\beta \\ 0 & \mu_\beta & 0 \end{pmatrix}, \ E_1, E_2, \mu_\alpha, \mu_\beta \in \mathbb{R} \text{ (arbitrary)}. \tag{4.3}$$

In this case all control fields give rise to identical populations for both systems. This under-determination can be mitigated under additional hypothesis as in Remark 4.8.

Remark 4.4. When eigenvalues of H are degenerate but $\mathcal{O}$ is a CSCO the Theorem 4.6 below should be used instead.

Proof. Consider the collection of two systems (H,μ_1) and (H,μ_2) seen as a control system on $SU(N)\bigoplus SU(N)$ with operators $iH\bigoplus iH$, $i\mu_1\bigoplus i\mu_2 \in \mathfrak{su}(N)\bigoplus\mathfrak{su}(N)$. This collection can either be controllable or not. Denote $\mathcal{R}_t = \{(\Psi_1(t,\epsilon),\Psi_2(t,\epsilon))|\epsilon\in L^1([0,t];\mathbb{R})\}$, $\mathcal{R}_\infty = \cup_{t\geq 0}\mathcal{R}_t$. It is known (see [13], Thm. 6.5 item (ii) p. 322) that there exists T such that $\mathcal{R}_T = \mathcal{R}_\infty$.

Since $\mathcal{O}$ is a non-trivial SCO it contains at least an observable, denoted O, that is not multiple of the identity. For this observable there exist $\Psi_x,\Psi_y\in\mathcal{S}_N$ such that $\langle O\Psi_x,\Psi_x\rangle \neq \langle O\Psi_y,\Psi_y\rangle$. But the condition (4.1) shows that no control ϵ exists that drives Ψ_0^1 to Ψ_x and Ψ_0^2 to Ψ_y; therefore the joint system $iH\bigoplus iH$, $i\mu_1\bigoplus i\mu_2$ is not controllable simultaneously. Then it exists an automorphism of $\mathfrak{su}(N)$ that sends iH to iH and $i\mu_1$ to $i\mu_2$. But the automorphisms of $\mathfrak{su}(N)$ are of the form $X\in\mathfrak{su}(N)\mapsto WXW^{-1}\in\mathfrak{su}(N)$ or $X\in\mathfrak{su}(N)\mapsto W\overline{X}W^{-1}\in\mathfrak{su}(N)$ for some $W\in SU(N)$. Recall that the matrix H is real (because it is diagonal and in $\mathcal{H}_N$). Consider first that one can find $W\in SU(N)$ such that $H = WHW^{-1}$ and $\mu_2 = W\mu_1W^{-1}$. The first identity shows that $[H,W]=0$ and therefore W is diagonal with the diagonal containing entries of the form $\mathrm{e}^{i\alpha_\ell}$, $\ell\leq N$; the conclusion follows from the second identity. Consider now that there exists $W\in SU(N)$ such that $iH = W\overline{iH}W^{-1}$; then $[H^2,W]=0$, thus W diagonal and therefore $H=-H$, impossible.

Remark 4.5. The result is stronger than the Theorem 1 in ([16], p. 380) which requires:

- A stronger condition on the spectrum of H (the non-degenerate transition condition); recall that the transitions of H are called non-degenerate if the eigenvalues $\lambda_k(H)$ of H satisfy $\lambda_i(H)-\lambda_j(H)\neq\lambda_a(H)-\lambda_b(H)$ for all $(a,b)\neq(i,j)$. Here we only ask that the eigenvalues have multiplicity one.
- That observables in $\mathcal{O}$ are the populations (thus in particular $\mathcal{O}$ is a CSCO). Here a single non-trivial observable is enough.
- That the equality (4.1) take place at all times $T\geq 0$. Here only one time (large enough) is required.

Theorem 4.6 (Setting **(S2)**)**.** *Let $\mu_1,\mu_2,H_1,\ H_2\in\mathcal{H}_N$, $\Psi_0^1,\Psi_0^2\in\mathcal{S}_N$ and denote for $a=1,2$ and $\epsilon\in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}_+,\mathbb{R})$: $\Psi_a(t,\epsilon)=\Psi(t,H_a,\epsilon(\cdot),\mu_a,\Psi_0^a)$. We suppose that $N\geq 3$ and the following assumptions hold true:*
(A1): $\mathbb{L}_{iH_1,i\mu_1} = \mathbb{L}_{iH_2,i\mu_2} = \mathfrak{su}(N)$;
(A2): $tr(H_1)=tr(H_2)=tr(\mu_1)=tr(\mu_2)=0$;
Let $\mathcal{O}=\{O_1,\ldots,O_K\}$ be a CSCO and $\Phi=\{\phi_1,\ldots,\phi_N\}$ an orthonormal basis that diagonalizes $\mathcal{O}$.
Then there exists $T>0$ such that if:

$$\langle O_k\Psi_1(T,\epsilon),\Psi_1(T,\epsilon)\rangle = \langle O_k\Psi_2(T,\epsilon),\Psi_2(T,\epsilon)\rangle \quad \forall\epsilon\in L^1([0,T];\mathbb{R}),\quad \forall k=1,\ldots,K, \tag{4.4}$$

then there exist $(\alpha_i)_{i=1}^N\in\mathbb{R}^N$ and $\theta\in\mathbb{R}$ such that for all $j,k\leq N$ either

$$\langle\mu_1\phi_j,\phi_k\rangle = \mathrm{e}^{i(\alpha_j-\alpha_k)}\langle\mu_2\phi_j,\phi_k\rangle,\ \langle H_1\phi_j,\phi_k\rangle = \mathrm{e}^{i(\alpha_j-\alpha_k)}\langle H_2\phi_j,\phi_k\rangle,\ \langle\Psi_0^1,\phi_j\rangle = \mathrm{e}^{i(\theta-\alpha_j)}\langle\Psi_0^2,\phi_j\rangle, \tag{4.5}$$

or

$$\langle\mu_1\phi_j,\phi_k\rangle = -\mathrm{e}^{i(\alpha_j-\alpha_k)}\overline{\langle\mu_2\phi_j,\phi_k\rangle},\quad \langle H_1\phi_j,\phi_k\rangle = -\mathrm{e}^{i(\alpha_j-\alpha_k)}\overline{\langle H_2\phi_j,\phi_k\rangle},\ \langle\Psi_0^1,\phi_j\rangle = \mathrm{e}^{i(\theta-\alpha_j)}\overline{\langle\Psi_0^2,\phi_j\rangle}. \tag{4.6}$$

Remark 4.7. When $\mathcal{O}$ is not a CSCO, the same proof allows only to obtain that an isomorphism of Lie algebras exists that sends iH_1 to iH_2 and $i\mu_1$ to $i\mu_2$. In general it is not possible to obtain more than a general isomorphism as shown by the following counter-example:

$$H_1 = \begin{pmatrix}1 & 0 & 0\\ 0 & -1/2 & 0\\ 0 & 0 & -1/2\end{pmatrix}, W = \begin{pmatrix}1 & 0 & 0\\ 0 & 1/2 & \sqrt{3}/2\\ 0 & -\sqrt{3}/2 & 1/2\end{pmatrix},\quad \mu_1 = \begin{pmatrix}0 & 1 & 2\\ 1 & 0 & 0\\ 2 & 0 & 0\end{pmatrix}, \tag{4.7}$$

$$H_2 = WH_1W^{-1} = H_1, \mu_2 = W\mu_1 W^{-1} = \begin{pmatrix} 0 & \sqrt{3}+1/2 & 1-\sqrt{3}/2 \\ \sqrt{3}+1/2 & 0 & 0 \\ 1-\sqrt{3}/2 & 0 & 0 \end{pmatrix}, \Psi_0^2 = W\Psi_0^1, \mathcal{O} = \{O_d\}. \tag{4.8}$$

It is immediate to see that $\langle O_d\psi, \psi\rangle = 1/2 - 3/2|\langle \psi, (1,0,0)^T\rangle|^2$ and that $W(1,0,0)^T = (1,0,0)^T$. When the control ϵ on the first system realizes the transformation X the observable is $1/2 - 3/2|\langle X\Psi_0^1, (1,0,0)^T\rangle|^2$; at the same time the control realizes the transformation WXW^{-1} on the second system giving the observable $1/2 - 3/2|\langle WXW^{-1}W\Psi_0^1, (1,0,0)^T\rangle|^2$. But $\langle WXW^{-1}W\Psi_0^1, (1,0,0)^T\rangle = \langle X\Psi_0^1, W^{-1}(1,0,0)^T\rangle = \langle X\Psi_0^1, (1,0,0)^T\rangle$. Therefore it is not possible to distinguish between the couple (H_1, μ_1) and (H_2, μ_2) (at least for this initial data).

Remark 4.8. If, for physical reasons, we know the initial state of the system, then $\Psi_0^1 = \Psi_0^2$; when this initial state has non-zero components along every element of the basis, *i.e.* $\langle \Psi_0^1, \phi_k\rangle \neq 0$, for all $k \geq 1$ the equation (4.5) implies $e^{i\alpha_j} = e^{i\theta}$ for all $j = 1, \ldots, N$ which means $H_1 = H_2$ and $\mu_1 = \mu_2$. When some coefficients $\langle \Psi_0^1, \phi_k\rangle$ are zero, further symmetries may occur and one can have, for instance, $\mu_1 \neq \mu_2$: see counter-example 1 from ([16], p. 381) presented in Remark 4.3.

On the other hand, in this case, the conclusion (4.6) can be written more conveniently in the adapted basis $\{v_1 = e^{-i\alpha_1/2}\phi_1, \ldots, v_N = e^{-i\alpha_N/2}\phi_k\}$:

$$\langle \mu_1 v_j, v_k\rangle = -\overline{\langle \mu_2 v_j, v_k\rangle},\ \langle H_1 v_j, v_k\rangle = -\overline{\langle H_2 v_j, v_k\rangle},\ \Psi_0^1 = \Psi_0^2 = e^{i\theta/2}\sum_{\ell=1}^{N} \varsigma_\ell v_\ell,\ \varsigma_\ell \in \mathbb{R}. \tag{4.9}$$

Proof. Denote by T the time at which the couple of systems (H_1, μ_1), (H_2, μ_2), seen as a control system on $SU(N)\bigoplus SU(N)$ with operators $iH\bigoplus iH$, $i\mu_1\bigoplus i\mu_2 \in \mathfrak{su}(N)\bigoplus \mathfrak{su}(N)$ reaches all attainable states. Since a CSCO is a non-trivial SCO it follows as in the Theorem 4.1 that there exists an isomorphism of $f : \mathfrak{su}(N) \to \mathfrak{su}(N)$ such that $iH_2 = f(iH_1)$, $i\mu_2 = f(i\mu_1)$.

All isomorphisms of $\mathfrak{su}(N)$ are of the form $\mathfrak{X} \in \mathfrak{su}(N) \mapsto W\mathfrak{X}W^{-1} \in \mathfrak{su}(N)$ or $\mathfrak{X} \in \mathfrak{su}(N) \mapsto W\overline{\mathfrak{X}}W^{-1} \in \mathfrak{su}(N)$ for some $W \in SU(N)$. We only treat here the "exotic" case $f(\mathfrak{X}) = W\overline{\mathfrak{X}}W^{-1}$ as the second alternative is similar. Thus $H_2 = -W\overline{H_1}W^{-1}$ and $\mu_2 = -W\overline{\mu_1}W^{-1}$. With the notations in the equation (3.5) we write:

$$X(t, H_2, u(\cdot), \mu_2) = X(t, -W\overline{H_1}W^{-1}, u(\cdot), -W\overline{\mu_1}W^{-1}) = W\overline{X(t, H_1, u(\cdot), \mu_1)}W^{-1}. \tag{4.10}$$

As the first system is controllable then every state $X \in SU(N)$ can be reached by some control $u(\cdot)$ thus

$$\langle O_k X\Psi_0^1, X\Psi_0^1\rangle = \langle O_k W\overline{X}W^{-1}\Psi_0^2, W\overline{X}W^{-1}\Psi_0^2\rangle, \forall X \in SU(N), \forall k \leq K. \tag{4.11}$$

Note that (4.11) also holds for any linear combination of observables in $\mathcal{O}$. We invoke the Lemma 3.1 and obtain the existence of an observable O, diagonal in the basis Φ and with all eigenvalues distinct, such that

$$\langle OX\Psi_0^1, X\Psi_0^1\rangle = \langle OW\overline{X}W^{-1}\Psi_0^2, W\overline{X}W^{-1}\Psi_0^2\rangle, \forall X \in SU(N). \tag{4.12}$$

The vectors ϕ_k are eigenvectors of O and denote as $\lambda_k(O)$ the corresponding eigenvalues. In particular $O = \sum_{k=1}^N \lambda_k(O)\phi_k\phi_k^*$. We can suppose that $\lambda_1(O) < \lambda_2(O) < \ldots < \lambda_N(O)$ (otherwise re-index the vectors).

Let us write $\overline{W^{-1}\Psi_0^2} = x\Psi_0^1 + yv$ with $x, y \in \mathbb{C}$, $|x|^2 + |y|^2 = 1$, $v \in \mathcal{S}_N$, $v \perp \Psi_0^1$.

Suppose $y \neq 0$; then there exists $X \in SU(N)$ such that $X\Psi_0^1 = \phi_N$ and $Xv \in \mathrm{Span}\{\overline{W^{-1}\phi_N}, \phi_N\}^\perp$. Then $\langle OX\Psi_0^1, X\Psi_0^1\rangle = \lambda_N(O) = \langle OW\overline{X}W^{-1}\Psi_0^2, W\overline{X}W^{-1}\Psi_0^2\rangle$. Since $\lambda_N(O)$ is the maximum possible value for O and all eigenspaces of O are of dimension 1 it follows that $W\overline{X}W^{-1}\Psi_0^2 \in \mathrm{Span}\{\phi_N\}$ hence $X\overline{W^{-1}\Psi_0^2} \in \mathrm{Span}\{\overline{W^{-1}\phi_N}\}$. Then:

$$1 = |\langle X\overline{W^{-1}\Psi_0^2}, \overline{W^{-1}\phi_N}\rangle| = |\langle X(x\Psi_0^1 + yv), \overline{W^{-1}\phi_N}\rangle| = |\langle x\phi_N, \overline{W^{-1}\phi_N}\rangle| = |x||\langle \phi_N, \overline{W^{-1}\phi_N}\rangle|. \tag{4.13}$$

It follows $y = 0$, $|x| = 1$; therefore $\overline{W^{-1}\Psi_0^2} \in \text{Span}\{\Psi_0^1\}$ which means that there exists $\theta \in \mathbb{R}$ such that $\Psi_0^2 = \mathrm{e}^{i\theta} W \overline{\Psi_0^1}$; after trivial simplifications the equality (4.12) can be written

$$\langle OX\Psi_0^1, X\Psi_0^1\rangle = \langle OW\overline{X\Psi_0^1}, W\overline{X\Psi_0^1}\rangle, \forall X \in SU(N). \tag{4.14}$$

But $X \in SU(N)$ means that $X\Psi_0^1$ can be chosen arbitrary in $\mathcal{S}_N$; we have therefore:

$$\forall w \in \mathcal{S}_N: \ \langle Ow, w\rangle = \langle OW\overline{w}, W\overline{w}\rangle = \langle W^*OW\overline{w}, \overline{w}\rangle = \langle \overline{W^*OW}w, w\rangle. \tag{4.15}$$

But this implies $O = \overline{W^*OW}$ and thus:

$$\sum_{k=1}^N \lambda_k(O)\phi_k\phi_k^* = O = \overline{W^*OW} = \overline{W^*\left(\sum_{k=1}^N \lambda_k(O)\phi_k\phi_k^*\right)W} = \sum_{k=1}^N \lambda_k(O)(\overline{W}^*\overline{\phi_k})(\overline{W}^*\overline{\phi_k})^*. \tag{4.16}$$

Since all eigenvalues of O are non-degenerate the representation $O = \sum_{k=1}^N \lambda_k(O)\phi_k\phi_k^*$ is unique up to phases. Therefore there exist $\alpha_k \in \mathbb{R}$ such that $\overline{W}^*\overline{\phi_k} = \mathrm{e}^{-i\alpha_k}\phi_k$ or, equivalently, $W^*\phi_k = \mathrm{e}^{i\alpha_k}\overline{\phi_k}$.

The conclusion follows from the relationships $H_2 = -W\overline{H_1}W^*$, $\mu_2 = -W\overline{\mu_1}W^*$ and $\Psi_0^2 = \mathrm{e}^{i\theta}W\overline{\Psi_0^1}$.

5. Inversion in presence of noise

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a discrete probability space, $\mathcal{V} = \{y_\ell \in \mathbb{R}^d | \ell \in \mathcal{I} \subset \mathbb{N}\}$ a set of values in $\mathbb{R}^d$ (possibly infinite) and let $Y : \Omega \to \mathcal{V}$ be a random variable. We can suppose that for all $y_\ell \in \mathcal{V}$, $\mathbb{P}(Y = y_\ell) > 0$ (otherwise we eliminate all y_ℓ such that $\mathbb{P}(Y = y_\ell) = 0$). Moreover after re-indexing $\mathcal{I}$ we can suppose that $\mathcal{I} = \mathbb{N}^*$ or $\mathcal{I} = \{1, \ldots, L_0\}$ for some $L_0 \in \mathbb{N}^*$. Denote $\xi_k = \mathbb{P}(Y = y_k)$, $\forall k \in \mathcal{I}$.

We can suppose that $(\xi_\ell)_{\ell\geq 1}$ is a decreasing sequence (re-indexing if necessary).

5.1. Technical preliminaries: a correspondence lemma

Let $J_a : \mathbb{C}^{N\times N} \to \mathbb{R}$, $a = 1, 2$ and $h : \mathbb{R}^{d+1} \to \mathbb{R}$ be real analytic functions with J_a bounded.

Lemma 5.1. *Let $A_a, B_a \in \mathfrak{su}(N)$, $T > 0$, $\epsilon \in \mathrm{L}^1([0,T], \mathbb{R})$ and denote by $X_a(t, y_\ell, \epsilon)$ the solution of*

$$\begin{cases} \frac{\mathrm{d}X_a(t,y_\ell,\epsilon)}{\mathrm{d}t} = (A_a + h(\epsilon(t), y_\ell)B_a)X_a(t, y_\ell, \epsilon) \\ X_a(0, y_\ell, \epsilon) = Id, \end{cases} \tag{5.1}$$

for $a = 1, 2$ and any $\ell \in \mathcal{I}$. Suppose that the following equality in law holds

$$\mathcal{L}_Y(J_1(X_1(T, Y, \epsilon))) = \mathcal{L}_Y(J_2(X_2(T, Y, \epsilon))) \quad \forall \epsilon \in \mathrm{L}^1([0,T], \mathbb{R}). \tag{5.2}$$

Then for any $\ell \in \mathcal{I}$, there exists $n_0(\ell, \xi_1, \ldots, \xi_n, \ldots)$ and $\kappa(\ell) \in \mathcal{I}$, $\kappa(\ell) \leq n_0(\ell, \xi_1, \ldots, \xi_n, \ldots)$ such that

$$J_1(X_1(T, y_\ell, \epsilon)) = J_2(X_2(T, y_{\kappa(\ell)}, \epsilon)) \quad \forall \epsilon \in \mathrm{L}^1([0,T], \mathbb{R}). \tag{5.3}$$

Proof. Let $\ell \in \mathcal{I}$. The proof is divided in several steps.

Step 1:
Fix a control ϵ. We introduce the notation:

$$v_a^k = J_a(X_a(T, y_k, \epsilon)), \qquad a = 1, 2 \quad \text{and} \quad k \in \mathcal{I}.$$

According to the assumption (5.2) we know that $J_1(X_1(T,Y,\epsilon))$ and $J_2(X_2(T,Y,\epsilon))$ follow the same law. Thus $\mathbb{P}(J_1(X_1(T,Y,\epsilon)) = v_1^\ell) = \mathbb{P}(J_2(X_2(T,Y,\epsilon)) = v_1^\ell)$. Then

$$\sum_{k'\in\mathcal{I}/v_2^{k'}=v_1^\ell} \xi_{k'} = \sum_{k\in\mathcal{I}/v_1^k=v_1^\ell} \xi_k \geq \xi_\ell > 0. \tag{5.4}$$

Therefore $\{k' \in \mathcal{I}/v_2^{k'} = v_1^\ell\} \neq \emptyset$. In addition, there exists a $n_0(\ell) \in \mathcal{I}$ such that $\sum_{k>n_0(\ell),k\in\mathcal{I}} \xi_k < \xi_\ell$ and $\sum_{k>n_0(\ell)-1,k\in\mathcal{I}} \xi_k \geq \xi_\ell$ (by convention a sum over an empty set of indexes is zero). So we have $\{k' \in \mathcal{I}/k' \leq n_0(\ell), v_2^{k'} = v_1^\ell\} \neq \emptyset$. The index $n_0(\ell)$ depends only on the law of Y and the index ℓ.

Letting ϵ vary in $L^1([0,T];\mathbb{R})$ we obtain a function $\kappa_1 : L^1([0,T];\mathbb{R}) \to \{k \in \mathcal{I}, k \leq n_0(\ell)\}$ such that

$$J_1(X_1(T,y_\ell,\epsilon)) = J_2(X_2(T,y_{\kappa_1(\epsilon)},\epsilon)). \tag{5.5}$$

Note: when the index $\kappa_1(\epsilon)$ with the property (5.5) is not unique, any compatible value in the set $\{k \in \mathcal{I}, k \leq n_0(\ell)\}$ can be chosen.

Step 2:
Let $n \in \mathbb{N}^*$. We consider the space $\mathcal{P}_n$ of piecewise constant controls $\mathcal{P}_n = \{f : [0,T] \to \mathbb{R}| \quad f = \alpha_1 \mathbf{1}_{[0,\frac{T}{n}]} + \alpha_2 \mathbf{1}_{]\frac{T}{n},\frac{2T}{n}]} + \ldots + \alpha_n \mathbf{1}_{]\frac{(n-1)}{n}T,T]}, \quad \alpha_1,\ldots,\alpha_n \in \mathbb{R}\}$. Denote $\alpha = (\alpha_1,\ldots,\alpha_n)$. Therefore for any $k \in \mathcal{I}$, we can define the functions g_k from $\mathbb{R}^n$ to $\mathbb{R}$ by

$$g_k(\alpha) = J_2(X_2(T,y_k,\epsilon_\alpha)) - J_1(X_1(T,y_\ell,\epsilon_\alpha)),$$

with $\epsilon_\alpha = \alpha_1 \mathbf{1}_{[0,\frac{T}{n}]} + \alpha_2 \mathbf{1}_{]\frac{T}{n},\frac{2T}{n}]} + \ldots + \alpha_n \mathbf{1}_{]\frac{(n-1)}{n}T,T]}$. We know that

$$X_a(T,y_k,\epsilon_\alpha) = \mathrm{e}^{(A_a+h(\alpha_n,y_k)B_a)\frac{T}{n}} \mathrm{e}^{(A_a+h(\alpha_{n-1},y_k)B_a)\frac{T}{n}} \ldots \mathrm{e}^{(A_a+h(\alpha_1,y_k)B_a)\frac{T}{n}} \quad a = 1,2. \tag{5.6}$$

Therefore the functions X_a are analytic in α (recall that the function h is analytic in α), and since J_a are analytic, the functions g_k are analytic. We denote $A_k = \{\alpha \in \mathbb{R}^n / g_k(\alpha) = 0\}$. Each A_k is closed because g_k is continuous. In Step 1, it is proved that

$$\exists \kappa^{\mathcal{P}} : \mathbb{R}^n \to \{k \in \mathcal{I}, k \leq n_0(\ell)\} \quad \text{such} \quad \text{that} \quad \forall \alpha \in \mathbb{R}^n \quad g_{\kappa^{\mathcal{P}}(\alpha)}(\alpha) = 0. \tag{5.7}$$

So $\bigcup_{k\in\mathcal{I},k\leq n_0(\ell)} A_k = \mathbb{R}^n$. By the Baire's theorem, it exists a k such that A_k has an interior point. This means that g_k is analytic and identically zero on a not empty open set. Therefore, $g_k \equiv 0$. So $\forall n$, $\exists \kappa_2(n) \in \{k \in \mathcal{I}, k \leq n_0(\ell)\}$ such that $g_{\kappa_2(n)}(\epsilon) = 0$, for any control $\epsilon \in \mathcal{P}_n$.

Step 3:
Take $q \in \mathbb{N}$ and denote $B_q = \{k \in \mathcal{I}, k \leq n_0(\ell)\}/g_k(\epsilon) = 0, \quad \forall \epsilon \in \mathcal{P}_{2^q}\}$. In Step 2 it is proved that for any $q \in \mathbb{N}$ the set B_q is not empty. Obviously $(B_q)_{q\in\mathbb{N}}$ is a decreasing sequence and B_q becomes constant from a certain term, thus $B_\infty = \bigcap_{q\geq 0} B_q \neq \emptyset$. This means that there exists $\kappa(\ell) \in \{k \in \mathcal{I}, k \leq n_0(\ell)\}$ such that $g_{\kappa(\ell)}(\epsilon) = 0$, $\forall \epsilon \in \mathcal{P}_{2^q}$ for all q. Yet, $\bigcup_{q=0}^\infty \mathcal{P}_{2^q}$ is dense in $L^1([0,T];\mathbb{R})$. So we have $g_{\kappa(\ell)}(\epsilon) = 0$, for any control ϵ in $L^1([0,T];\mathbb{R})$.

5.2. Main results

We set $d = 1$.

Theorem 5.2. *Consider the same setting and assumptions as in the Theorem 4.6 with the exception of the relation (4.4). Then there exists $T > 0$ such that if:*

$$\mathcal{L}_Y \langle O_k \Psi_1(T,\epsilon+Y), \Psi_1(T,\epsilon+Y)\rangle = \mathcal{L}_Y \langle O_k \Psi_2(T,\epsilon+Y), \Psi_2(T,\epsilon+Y)\rangle \quad \forall \epsilon \in L^1([0,T];\mathbb{R}), \quad \forall k = 1,\ldots,K, \tag{5.8}$$

then either the conclusion (4.5) or the conclusion (4.6) of the Theorem 4.6 holds (see also Rem. 4.8).

Remark 5.3. When $\mathcal{O}$ is not a CSCO, the same proof allows only to obtain that an isomorphism of Lie algebras exists that sends iH_1 to iH_2 and $i\mu_1$ to $i\mu_2$.

Remark 5.4. Relation (5.8) does not imply that for any $\gamma_k \in \mathbb{R}$:

$$\forall \epsilon \in L^1([0,T];\mathbb{R}) :$$
$$\mathcal{L}_Y \left\langle \left(\sum_{k=1}^{K} \gamma_k O_k\right) \Psi_1(T,\epsilon+Y), \Psi_1(T,\epsilon+Y) \right\rangle = \mathcal{L}_Y \left\langle \left(\sum_{k=1}^{K} \gamma_k O_k\right) \Psi_2(T,\epsilon+Y), \Psi_2(T,\epsilon+Y) \right\rangle, \quad (5.9)$$

because the probability laws are not additive. This is in contrast with the situation in the Theorem 4.6 (see Eqs. (4.11) and (4.12)). But the relation remains true for any operator of the form $aO_k + bId$, $a, b \in \mathbb{R}$.

Proof. Choose $m_0 \in \mathbb{N}$ such that $m_0\xi_1 > 1$. Then there exists some $\eta > 0$ small enough with $\sum_{m=0}^{m_0}(\xi_1 - m\eta) > 1$ and $\xi_1 - m_0\eta > \eta$. As $\sum_{k\in\mathcal{I}} \xi_k = 1$, there exists $n_0' \in \mathcal{I}$ such that $\sum_{k\in\mathcal{I}, k>n_0'} \xi_k < \eta$ (by convention a sum over an empty set of indexes is zero). According to Definition 3.2, for all $\ell, \ell' \in \{1,\ldots,n_0'\}$, if the collection of 2 systems (3.3) for $A_1 = -iH_1 + y_\ell(-i\mu_1) \in \mathfrak{su}(N)$, $B_1 = -i\mu_1 \in \mathfrak{su}(N)$ and $A_2 = -iH_2 + y_{\ell'}(-i\mu_2) \in \mathfrak{su}(N)$, $B_2 = -i\mu_2 \in \mathfrak{su}(N)$ is simultaneously controllable, then there exists $T_{H_1,H_2,\mu_1,\mu_2,y_\ell,y_{\ell'}} > 0$ such that the collection is simultaneously controllable at all times $T \geq T_{H_1,H_2,\mu_1,\mu_2,y_\ell,y_{\ell'}}$. If the collection is not controllable, we take $T_{H_1,H_2,\mu_1,\mu_2,y_\ell,y_{\ell'}}$ to be the time required to control one system (to any target). According to Theorem 3.5, we know that the collection of n_0' systems (3.4) with $A = -iH_2$, $B = -i\mu_2$ and $(\alpha_1,\ldots,\alpha_{n_0'}) = (y_1,\ldots,y_{n_0'})$ is simultaneously controllable therefore there exists $T_{H_2,\mu_2,y_1,\ldots,y_{n_0'}}$ such that the collection is simultaneously controllable at any time $T \geq T_{H_2,\mu_2,y_1,\ldots,y_{n_0'}}$. Let $T = max_{1\leq \ell,\ell' \leq n_0'}(T_{H_2,\mu_2,y_1,\ldots,y_{n_0'}}, T_{H_1,H_2,\mu_1,\mu_2,y_\ell,y_{\ell'}})$. Suppose that the observations follow the same law at time T. Recall that $\Psi_a(T,\epsilon+y_\ell) = X_a(T,\epsilon+y_\ell)\Psi_0^a$ with $X_a(t,\epsilon+y_\ell)$ solutions of (5.1) where $A_a = -iH_a$, $B_a = -i\mu_a$, for $a = 1,2$ respectively and $h(\epsilon(t), y_\ell) = \epsilon(t) + y_\ell$.

The second part of Remark 5.4 implies that we can suppose, without loss of generality, that any $\tilde{O} \in \mathcal{O}$ has the smallest eigenvalue equal to 0 and the largest one equal to 1. Fix now $\tilde{O} \in \mathcal{O}$. We apply the Lemma 5.1 to $X \mapsto \langle \tilde{O}X\Psi_0^a, X\Psi_0^a\rangle$, $a = 1,2$ which are obviously analytic with respect to X. Then for all $\ell \in \mathcal{I}$, $\exists\kappa(\ell)$ such that

$$\langle \tilde{O}\Psi_1(T,\epsilon+y_\ell), \Psi_1(T,\epsilon+y_\ell)\rangle = \langle \tilde{O}\Psi_2(T,\epsilon+y_{\kappa(\ell)}), \Psi_2(T,\epsilon+y_{\kappa(\ell)})\rangle. \quad (5.10)$$

Recall equation (5.4) in Lemma 5.1 (we use the same notations):

$$\sum_{k\in\mathcal{I}/v_1^k=v_1^\ell} \xi_k = \sum_{k'\in\mathcal{I}/v_2^{k'}=v_1^\ell} \xi_{k'},$$

for any control $\epsilon(t) \in \mathrm{L}^1([0,T],\mathbb{R})$. Now let us take $\ell = 1$. In Lemma 5.1 we proved that $\kappa(1) \leq n_0(1)$ with $\sum_{k>n_0(1)-1} \xi_k \geq \xi_1 > \xi_1 - m_0\eta > \eta > \sum_{k>n_0'} \xi_k$. Thus $n_0' \geq n_0(1) \geq \kappa(1)$. By simultaneous controllability, there exists a control ϵ such that $\langle \tilde{O}\Psi_2(T,\epsilon+y_{\kappa(1)}), \Psi_2(T,\epsilon+y_{\kappa(1)})\rangle = 1$ and $\langle \tilde{O}\Psi_2(T,\epsilon+y_j), \Psi_2(T,\epsilon+y_j)\rangle = 0$ for all $j \leq n_0'$ and $j \neq \kappa(1)$. In addition, Lemma 5.1 proves that for any control ϵ, $v_1^1 = v_2^{\kappa(1)} = 1$. So for this ϵ,

$$\xi_1 \leq \sum_{k\in\mathcal{I}/v_1^k=v_2^{\kappa(1)}} \xi_k = \sum_{k'\in\mathcal{I}/v_2^{k'}=v_2^{\kappa(1)}} \xi_{k'} \leq \xi_{\kappa(1)} + \sum_{k>n_0'} \xi_k \leq \xi_{\kappa(1)} + \eta. \quad (5.11)$$

We deduce that $\xi_{\kappa(1)} \geq \xi_1 - \eta$. With the same reasoning and by recurrence we demonstrate that $\xi_{\kappa^m(1)} \geq \xi_1 - m\eta$ for any $m \in \{1,\ldots,m_0\}$ thanks to the relationship $\sum_{k>n_0(\kappa^m(1))-1} \xi_k \geq \xi_{\kappa^m(1)} \geq \xi_1 - m\eta \geq \xi_1 - m_0\eta > \eta > \sum_{k>n_0'} \xi_k$. If $1, \kappa(1), \ldots, \kappa^{m_0}(1)$ are all distinct, then $1 = \sum_{k\in\mathcal{I}} \xi_k \geq \sum_{m=0}^{m_0} \xi_{\kappa^m(1)} > 1$, which leads to a contradiction. So at least two among the $1, \kappa(1), \ldots, \kappa^{m_0}(1)$ are equal.

On the other hand equation (5.10) implies that the collection of the two systems

$$\begin{cases} \frac{\mathrm{d}X_1(t,\epsilon)}{\mathrm{d}t} = [-i(H_1 + y_{\kappa^m(1)}\mu_1) + \epsilon(t)(-i\mu_1)]X_1(t,\epsilon) \\ X_1(0,\epsilon) = Id \end{cases} \quad (5.12)$$

and

$$\begin{cases} \frac{\mathrm{d}X_2(t,\epsilon)}{\mathrm{d}t} = [-i(H_2 + y_{\kappa^{m+1}(1)}\mu_2) + \epsilon(t)(-i\mu_2)]X_2(t,\epsilon) \\ X_2(0,\epsilon) = Id \end{cases} \tag{5.13}$$

is not ensemble controllable for all $m \in \{0, \dots, m_0 - 1\}$. Applying Theorem 3.3 and Lemma 3.4 to $G = SU(N)$, $A_1 = -i(H_1 + y_{\kappa^m(1)}\mu_1)$, $A_2 = -i(H_2 + y_{\kappa^{m+1}(1)}\mu_2)$, $B_1 = -i\mu_1$ and $B_2 = -i\mu_2$ there exist f_m automorphisms of $\mathfrak{su}(N)$ such that $f_m(-i(H_1 + y_{\kappa^m(1)}\mu_1)) = -i(H_2 + y_{\kappa^{m+1}(1)}\mu_2)$ and $f_m(-i\mu_1) = -i\mu_2$. By linearity of f_1 and f_m, we obtain $(f_m^{-1} \circ f_1)(-iH_1) = -iH_1 + [(y_{\kappa(1)} - y_1) - (y_{\kappa^{m+1}(1)} - y_{\kappa^m(1)})](-i\mu_1)$ and $(f_m^{-1} \circ f_1)(-i\mu_1) = -i\mu_1$. Denote $f = f_m^{-1} \circ f_1$ and $\beta = (y_{\kappa(1)} - y_1) - (y_{\kappa^{m+1}(1)} - y_{\kappa^m(1)})$, then we have $-iH_1 = f(-iH_1) + i\beta\mu_1 = f(f(-iH_1) + i\beta\mu_1) + i\beta\mu_1 = f^2(-iH_1) + 2i\beta\mu_1$ and by recurrence $-iH_1 = f^p(-iH_1) + ip\beta\mu_2$ for all $p \in \mathbb{N}$. All automorphisms of $\mathfrak{su}(N)$ belong to a compact set hence the set $\{f^p(-iH_1) \in \mathfrak{su}(N), p \geq 0\}$ is bounded for all m. Therefore the sequence $(ip\beta\mu_2)_{p\geq 0}$ is bounded which implies $\beta\mu_2 = 0$. According to assumption (**A1**), $\mu_2 \neq 0$. Thus $\beta = 0$. Denote $C = y_{\kappa(1)} - y_1$, then $y_{\kappa^{m+1}(1)} = y_{\kappa^m(1)} + C \ \forall m \in \{0, \dots, m_0 - 1\}$. As $1, \kappa(1), \dots, \kappa^{m_0}(1)$ are not all different, $C = 0$.

Since $\tilde{O} \in \mathcal{O}$ was arbitrary we proved so far that the systems without noise $(H_1 + y_1\mu_1, \mu_1)$ and $(H_2 + y_1\mu_2, \mu_2)$ give the same observations for the CSCO $\mathcal{O}$; the conclusion follows from the Theorem 4.6.

Remark 5.5. Here and in all similar results, the time T should be understood as 'if the time is large enough': the proof can be trivially adapted to treat the situation when the equality in law holds at some other final time T^* provided that T^* is larger than the time T given by the theorem.

A similar reasoning allows to prove for the setting **(S1)** the following:

Corollary 5.6. *Consider the same setting and assumptions as in Theorem 4.1 with the exception of the relation (4.1). Then there exists $T > 0$ such that if:*

$$\mathcal{L}_Y \langle O\Psi_1(T, \epsilon + Y), \Psi_1(T, \epsilon + Y)\rangle = \mathcal{L}_Y \langle O\Psi_2(T, \epsilon + Y), \Psi_2(T, \epsilon + Y)\rangle \quad \forall \epsilon \in L^1([0,T];\mathbb{R}), \quad \forall O \in \mathcal{O}, \tag{5.14}$$

then the conclusion (4.2) of the Theorem 4.1 holds.

5.3. The multiplicative perturbation case

In this section we consider the multiplicative perturbation, which means the control is in the form of $u = Y \cdot \epsilon$. We suppose moreover that this perturbation is positive: $\mathcal{V} \subset \mathbb{R}^+$.

Corollary 5.7. *Consider the same setting and assumptions as in the Theorem 4.6 with the exception of the relation (4.4). Then there exists $T > 0$ such that if:*

$$\mathcal{L}_Y \langle O_k\Psi_1(T, \epsilon Y), \Psi_1(T, \epsilon Y)\rangle = \mathcal{L}_Y \langle O_k\Psi_2(T, \epsilon Y), \Psi_2(T, \epsilon Y)\rangle \quad \forall \epsilon \in L^1([0,T];\mathbb{R}), \quad \forall k = 1, \dots, K, \tag{5.15}$$

then either the conclusion (4.5) or the conclusion (4.6) of the Theorem 4.6 holds (see also Rem. 4.8).

Proof. The proof is similar with the exception that the simultaneous controllability result to be used is Corollary 5, page 25 in [3].

Remark 5.8. When $\mathcal{V}$ also contains negative values, a similar result can be stated. The only difference is that one obtains:

$$\langle \mu_1\phi_j, \phi_k\rangle = \pm \mathrm{e}^{i(\alpha_j - \alpha_k)}\langle \mu_2\phi_j, \phi_k\rangle, \ \langle H_1\phi_j, \phi_k\rangle = \pm \mathrm{e}^{i(\alpha_j - \alpha_k)}\langle H_2\phi_j, \phi_k\rangle, \ \langle \Psi_0^1, \phi_j\rangle = \pm \mathrm{e}^{i(\theta - \alpha_j)}\langle \Psi_0^2, \phi_j\rangle, \tag{5.16}$$

and a similar relation for the conjugate case. Furthermore, the polynomial situation $\mathcal{V} \subset \mathbb{R}^d$ with $d > 1$, $u(t) = \sum_{a=0}^d Y_a\epsilon^a(t)$ can be studied. But although this case is also tractable with the controllability result in [20], the conclusion is very cumbersome to formulate and we leave it as an exercise for the reader.

TABLE 1. Law of Y for the numerical example in Section 6. Here $L_0 = 10$; the second row presents the values y_ℓ, $\ell \leq L_0$ which have been chosen randomly (uniformly) in $[0, 0.1 * \frac{\|H\|_{l^\infty}}{\|\mu\|_{l^\infty}} = 0.0012]$. The third row displays the probabilities ξ_ℓ, $\ell \leq L_0$ which have been chosen at random, uniformly in $[0,1]$, the sum rescaled to 1 and then ordered such that $(\xi_\ell)_{\ell \geq 1}$ is a decreasing sequence.

ℓ	1	2	3	4	5	6	7	8	9	10
y_ℓ	0.000400	0.000066	0.001025	0.000224	0.000816	0.000679	0.000740	0.000975	0.000211	0.000156
ξ_ℓ	0.181810	0.163630	0.145450	0.127270	0.109090	0.090900	0.072720	0.054540	0.036360	0.018180

6. Numerical application

Numerical tests are presented for the setting of the Theorem 5.2. We consider the 4-level system ($N = 4$) in [8] and want to recover the Hamiltonian matrix H_{real} and the dipole moment matrix μ_{real}:

$$H_{\text{real}} = \begin{pmatrix} 0.0833 & -0.0038 & -0.0087 & 0.0041 \\ -0.0038 & 0.0647 & 0.0083 & 0.0038 \\ -0.0087 & 0.0083 & 0.0036 & -0.0076 \\ 0.0041 & 0.0038 & -0.0076 & 0.0357 \end{pmatrix}, \quad \mu_{\text{real}} = \begin{pmatrix} 0 & 5 & -1 & 0 \\ 5 & 0 & 6 & -1.5 \\ -1 & 6 & 0 & 7 \\ 0 & -1.5 & 7 & 0 \end{pmatrix}.$$

Note that:

$$H_{\text{real}} = \mathrm{e}^{\mathcal{P}_{\text{real}}} D \mathrm{e}^{-\mathcal{P}_{\text{real}}}, \quad D = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.0365 & 0 & 0 \\ 0 & 0 & 0.0651 & 0 \\ 0 & 0 & 0 & 0.0857 \end{pmatrix}, \; \mathcal{P}_{\text{real}} = \begin{pmatrix} 0 & 1 & -1 & 1 \\ -1 & 0 & 1 & 1 \\ 1 & -1 & 0 & -1 \\ -1 & -1 & 1 & 0 \end{pmatrix}.$$

In practice the eigenvalues of the free Hamiltonian are measured by spectrometry and hence known with high precision, see also the discussion in ([16], p. 379 and Rem. 7, p. 384). Accordingly, we suppose that the eigenvalues of H_{real} are known *i.e.*, the matrix D is known. So identifying H_{real} is equivalent to identifying the anti-Hermitian rotation matrix $\mathcal{P}_{\text{real}}$.

The law of the perturbation Y is given in Table 1. We consider a finite set of test control fields of the form:

$$\epsilon(t) = \exp\left(-40(t - T/2)^2/T^2\right) \sum_{i<j,i,j=1}^{N} A_{i,j} \sin[(\lambda_j(H_{\text{real}}) - \lambda_i(H_{\text{real}}))t + \theta_{i,j}]. \tag{6.1}$$

Here $\lambda_i(H_{\text{real}})$ are eigenvalues of H_{real}, $i \leq N$ and $A_{i,j}$, $\theta_{i,j}$ are parameters to be chosen later. The total simulation time is $T = 3200$ which means about 10 periods of the smallest transition frequency $\lambda_4(H_{\text{real}}) - \lambda_3(H_{\text{real}})$.

Let $\{e_k; k \leq N\}$ be the canonical basis of $\mathbb{C}^N$ and $\mathcal{O} = \{e_k e_k^*, k \leq N\}$ (populations).

We choose $N_\epsilon = 36$ controls $\epsilon_1(t), \ldots, \epsilon_{N_\epsilon}(t)$ drawing θ_{ij} uniformly in $[0, 2\pi]$ and A_{ij} uniformly in $[0, 0.0012]$ and we define the functional to be minimized:

$$\mathcal{J}(\mathcal{P}, \mu) = \sum_{i=1}^{N_\epsilon} \sum_{j=1}^{N} d_{\mathcal{W}_1}(\mathcal{L}_Y(|\langle \Psi(T, \mathrm{e}^{\mathcal{P}} D \mathrm{e}^{-\mathcal{P}}, \epsilon_i + Y, \mu, \Psi_1^0), e_j \rangle|^2, \mathcal{L}_Y(|\langle \Psi(T, H_{\text{real}}, \epsilon_i + Y, \mu_{\text{real}}, \Psi_{\text{real}}^0), e_j \rangle|^2). \tag{6.2}$$

Here we use the 1-Wasserstein distance (see pp. 34–35 in [22]) $d_{\mathcal{W}_1}$ between two laws $L_Y Z_1$ and $L_Y Z_2$ defined as $d_{\mathcal{W}_1}(L_Y Z_1, L_Y Z_2) = \int_0^1 |F_{Z_1}^{-1}(x) - F_{Z_2}^{-1}(x)| \mathrm{d}x$ with F_{Z_1}(respectively F_{Z_2}) the cumulative distribution function of Z_1(respectively Z_2)(see pp. 73–75 in [22] for details). We start with 10% relative error on μ and $\mathcal{P}$ and we use

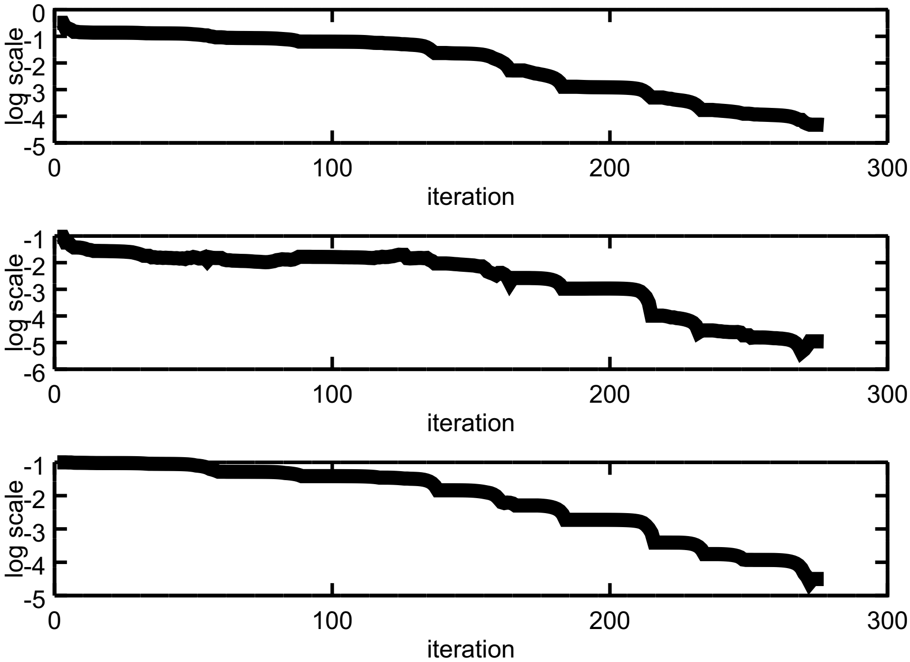

FIGURE 1. The (base 10) logarithm of $\mathcal{J}$ (upper plot), the (base 10) logarithm of the relative error on $\mathcal{P}$ (middle plot) and the (base 10) logarithm of the relative error on μ (lower plot) as a function of the iteration index.

a classical unconstrained nonlinear optimization algorithm to minimize $\mathcal{J}(\mathcal{P},\mu)$ (we used the Gnu Octave [9,10] procedure "fminunc"). After 277 iterations, we find:

$$\mathcal{P}_{277} = \begin{pmatrix} 0 & 0.999 & -0.999 & 1.002 \\ -0.999 & 0 & 1 & 0.999 \\ 0.999 & -1 & 0 & -1.002 \\ -1.002 & -0.999 & 1.002 & 0 \end{pmatrix}, \quad \mu_{277} = \begin{pmatrix} 0 & 4.999 & -0.998 & -0.003 \\ 4.999 & 0 & 6 & -1.5 \\ -0.998 & 6 & 0 & 7 \\ -0.003 & -1.5 & 7 & 0 \end{pmatrix}.$$

This corresponds to 0.003% relative error on μ and 0.001% relative error on $\mathcal{P}$. We note that the histograms for $(\mathcal{P}_{\text{real}},\mu_{\text{real}})$ and $(\mathcal{P}_{277},\mu_{277})$ are nearly the same. See Figures 1 and 2 for details.

7. PERSPECTIVES AND CONCLUDING REMARKS

Among the limitations of the present work is the requirement to consider only time-independent perturbations; it would be interesting to consider time-dependent perturbations and more elaborate noise models (beyond polynomial) and, of course, perturbations that can take values in an uncountable set (in the same spirit as in [2, 17]). Extension to infinite dimensional quantum systems can also be interesting; in all these cases one technical limitation is the absence of simultaneous controllability results analogue to Theorems 3.3 and 3.5, still missing in general even for finite dimensional models as soon as the dimension is larger than 4.

A distinct extension, which seems attainable with the tools presented here, is to consider a framework that involves density matrices instead of wave-functions.

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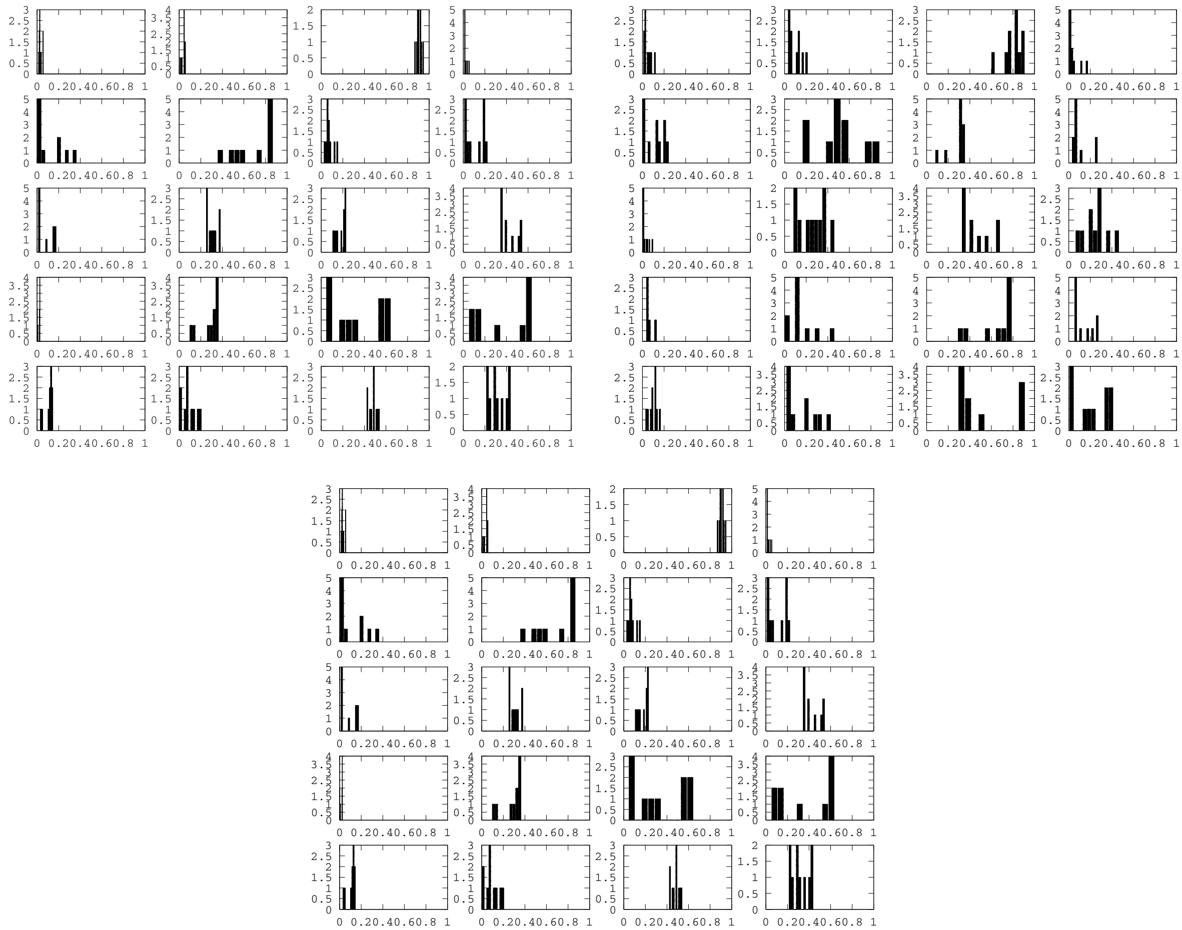

FIGURE 2. The optimization algorithm iterates starting from the initial guess $(\mathcal{P}_0, \mu_0)$ and constructs a sequence of estimations $(\mathcal{P}_k, \mu_k)$. We plot the histograms of the laws $\mathcal{L}_Y(|\langle \Psi(T, \mathrm{e}^{\mathcal{P}_k} D \mathrm{e}^{-\mathcal{P}_k}, \epsilon_i + Y, \mu_k, \Psi_1^0), e_j \rangle|^2$ for various choices of k, $i = 1, \ldots, 5$ and $j = 1, 2, 3, 4$. In the top picture are the histograms of the observations $(\mathcal{P}_{\text{real}}, \mu_{\text{real}})$, in the bottom left picture are the histograms for the initial guess $(\mathcal{P}_0, \mu_0)$ $(k = 0)$ and in the bottom right image the histograms for the final iteration $(\mathcal{P}_{277}, \mu_{277})$ $(k = 277)$. The optimization works well as there is an obvious match between the top and the bottom right histograms.

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