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HAMILTONIAN IDENTIFICATION IN PRESENCE OF LARGE PERTURBATIONS

Ying FU^1 and Gabriel TURINICI²

Abstract. The inversion problem of recovering the Hamiltonian and dipole moment is considered in a quantum control framework. The inversion process uses as inputs some measurable quantities (observables) for each admissible control; however the implementation of the control is noisy (the perturbations are additive constants in a countable set of values) and therefore the data available is only in the form of the law of the measured observable. Nevertheless it is proved that the inversion process still has unique solutions (up to some phase factors). Numerical illustrations support the theoretical results.

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1. INTRODUCTION AND MOTIVATION

Successful manipulation of quantum dynamics (for a recent review see [6] and references therein) leads to interesting prospects among which is the possibility to identify the system through measurements of controldependent observations. This technique, called quantum identification or quantum inversion, was documented both theoretically [2,5,13,23] and numerically [7,9,15]. 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. In this context we propose a result that addresses this question. More specifically we start from the setting in [13] and introduce the possibility that the control is subject at each time to unknown perturbations. Since the actual control that acted on the system is unknown only a probability law of the observation can be recovered. We show that under technical conditions knowing this law allows to determine uniquely (up to phase factors) the free Hamiltonian and dipole moment (the observations are the populations of the quantum system).

The balance of the paper is as follows: in Section 2 we make explicit the model and assumptions used. The main theoretical results are given in Section 3 while a numerical application is presented in Section 4. Some closing remarks are present in Section 5.

1.1. Notations

We introduce the following notations

- $\mathbb{L}_{M_1,M_2,\cdots,M_m}$ is the Lie algebra spanned by matrices M_1, M_2, \cdots, M_m ;
- X^* is the adjoint of the matrix X; the adjoint is the transpose conjugate (and works for vectors too);

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- \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 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 (1) below;
- $\lambda_k(X), k = 1, ..., N$ are the eigenvalues of $X \in \mathcal{H}_N$ taken in increasing order; we also introduce $\phi_k(X)$
- k = 1, ..., N to be the eigenvectors of X (forming a basis of \mathbb{C}^N) corresponding to eigenvalues $\lambda_k(X)$;
- $\{e_k; k = 1, ..., N\}$ is the canonical basis of \mathbb{R}^N .

2. The model

We present the mathematical framework following closely the notations of the previous work [13].

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

$$\begin{cases} i\dot{\Psi} = (H + u(t)\mu)\Psi\\ \Psi(0) = \Psi_0, \end{cases}$$
(1)

where H is the internal ("'free"') Hamiltonian and μ the coupling operator between the control u(t) and the system. We work in a finite dimensional framework, therefore $H, \mu \in \mathcal{H}_N$. 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 [13] we allow in this work some time independent perturbations to appear in the control u(t). That is, in practice the nominal control intensity required by the experimentalist denoted $\epsilon(t)$ is perturbed by Y when the control is implemented which means that $u(t) = \epsilon(t) + Y$; here Y a discrete random variable with possible outcomes y_1, y_2, \ldots We assume that the law of the random variable Y is time independent. Such perturbation models have already been used in the quantum computing literature under the name "fixed systematic errors" or "low frequency noise" (see [10–12, 18]).

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 known the law of the measurements. From now on we will denote by $\mathcal{L}_Y Z$ the law of the random variable Z that depends on the randomness present in Y.

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

- (1) Setting (S1): The Hamiltonian H is known and the goal is to identify the dipole moment μ . The measurements concern the populations of the eigenstates $\phi_i(H)$ i.e., the law $\mathcal{L}_Y |\langle \Psi(t), \phi_k(H) \rangle|^2$ is known for all instants $t \geq 0$ and all k = 1, ..., N. This is performed with as many control amplitudes $\epsilon(t)$ as required.
- (2) Setting (S2): Neither H nor the dipole moment μ are known and have to be identified. Nevertheless, the eigenvalues of the Hamiltonian H are assumed to be known (this assumption is relevant in practice, see [13]). Here, we measure the law $\mathcal{L}_Y |\langle \Psi(t), e_k \rangle|^2$ of the populations along $\{e_k; k = 1, ..., N\}$ for all instants t > 0 and all control amplitudes $\epsilon(t)$.

Remark 2.1. In most of the experiments, the experimentalist only measures one observable (but can repeat the experiment many times). This means that no information is available on the joint distribution of, say, $|\langle \Psi(t), \phi_1 \rangle|^2$ and $|\langle \Psi(t), \phi_2 \rangle|^2$.

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 (and suppose that the model matches perfectly the observations).

3. Main results

3.1. Technical preliminaries: previous results

We recall the following two results from [13].

Theorem 3.1. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H \in \mathcal{H}_N$ (Hamiltonian) and $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$. We suppose that the following three assumptions hold true:

(A1): $\mathbb{L}_{iH,i\mu_1} = su(N).$

(A2): The transitions $(\lambda_j(H))_{j=1}^N$ are non-degenerate, i.e. $\lambda_{i_1}(H) - \lambda_{j_1}(H) \neq \lambda_{i_2}(H) - \lambda_{j_2}(H)$ for $i_1 \neq j_1$, $i_2 \neq j_2$ and $(i_1, j_1) \neq (i_2, j_2)$.

(A3): The diagonal part of the dipole moment μ_1 et μ_2 , when written in the eigenbasis of the Hamiltonian H, is zero: $\langle \phi_i(H) | \mu_1 | \phi_i(H) \rangle = 0$ et $\langle \phi_i(H) | \mu_2 | \phi_i(H) \rangle = 0 \forall i = 1, ..., N$. Suppose that the two states produce identical observations that is:

$$|\langle \Psi(t, H, \epsilon, \mu_1, \Psi_0^1) | \phi_i \rangle| = |\langle \Psi(t, H, \epsilon, \mu_2, \Psi_0^2) | \phi_i \rangle| \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+), \forall i = 1, .., N.$$

$$\tag{2}$$

Then there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that:

$$\forall i, j = 1, .., N, \quad (\mu_1)_{ij} = e^{i(\alpha_i - \alpha_j)} (\mu_2)_{ij}. \tag{3}$$

Remark 3.2. In general, (A1) is a sufficient condition for the controllability. However, under the hypothesis (A2) the hypothesis (A1) is equivalent to the controllability (see [1, 20, 21]) Moreover, (A1), (A2) and (A3) imply $\mathbb{L}_{iH,i\mu_2} = su(N)$.

Remark 3.3. The assumption (A3) can be made without loss of generality according to [13].

Theorem 3.4. Let $H_1, H_2 \in \mathcal{H}_N$ (Hamiltonians), $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$. Introduce the following assumption: (A4): $\lambda_k(H_1) = \lambda_k(H_2), \forall k = 1, ..., N$.

Suppose that the two states produce identical observations that is:

$$|\langle \Psi(t, H_1, \epsilon, \mu_1, \Psi_0^1) | e_i \rangle| = |\langle \Psi(t, H_2, \epsilon, \mu_2, \Psi_0^2) | e_i \rangle| \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathcal{L}^1_{loc}(\mathbb{R}_+), \forall i = 1, .., N,$$

$$\tag{4}$$

where $(e_i)_{1 \le i \le N}$ is the canonical basis of \mathbb{R}^N .

We suppose $N \ge 3$. Then under the assumptions (A1), (A2), (A3) and (A4) for both systems, there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the canonical basis, for all $1 \le i, j \le N$,

$$(\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk} \quad and \quad (H_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (H_2)_{jk}.$$
(5)

Remark 3.5. Under assumptions (A1), (A2), (A3) and (A4) for the first system, we also have $\mathbb{L}_{iH_2,i\mu_2} = su(N)$.

A simultaneous controllability result was proved recently in [4]:

Theorem 3.6. Let $\alpha_1, ..., \alpha_K \in \mathbb{R}$ be real constants such that $\alpha_i \neq \alpha_j \quad \forall i \neq j$. Consider the collection of control systems on SU(N):

$$\begin{cases} \frac{dX_{\ell}(t)}{dt} = \{A + (u(t) + \alpha_{\ell})B\}X_{\ell}(t), \\ X_{\ell}(0) = X_{\ell,0} \in SU(N). \end{cases}$$
(6)

Suppose that $\mathbb{L}_{[A,B],B} = su(N)$. Then there exists $T_{A,B,\alpha_1,...\alpha_K}$ such that the collection of system (7) is simultaneously controllable at any time $T \geq T_{A,B,\alpha_1,...\alpha_K}$, that is for any $\bar{X}_1,...,\bar{X}_K \in SU(N)$ there exists $u(t): [0,T] \to \mathbb{R}$ mesurable such that $X_\ell(T) = \bar{X}_\ell \ \forall \ell = 1,...,K$.

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.

3.2. Technical preliminaries: a correspondence lemma

We introduce here a technical tool that will be used throughout the paper. Let $O_a : \mathbb{C}^N \to \mathbb{R}$ a = 1, 2 and $h : \mathbb{R}^{d+1} \to \mathbb{R}$ be analytic functions.

Lemma 3.7. Let $A_a, B_a \in su(N), \epsilon \in L^1_{loc}(\mathbb{R}_+)$ and denote by X_a the solutions of

$$\begin{cases} \frac{dX_a(t,y_\ell,\epsilon)}{dt} = (A_a + h(\epsilon(t), y_\ell)B_a)X_a(t, y_\ell, \epsilon).\\ X_a(0, y_\ell, \epsilon) = Id \in SU(N) \end{cases}$$
(7)

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

 \mathbf{k}

$$\mathcal{L}_Y(O_1(X_1(t, Y, \epsilon))) = \mathcal{L}_Y(O_2(X_2(t, Y, \epsilon))) \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+)$$
(8)

Then for any $\ell \in \mathcal{I}$, there exists $\kappa_{O_1,O_2}(\ell) \in \mathcal{I}$ such that

$$O_1(X_1(t, y_\ell, \epsilon)) = O_2(X_2(t, y_{\kappa_{O_1, O_2}(\ell)}, \epsilon)) \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+)$$
(9)

Proof. The proof is divided in 4 steps. Fix an index ℓ . First, we find a κ depending on T, t and ϵ . Then, we prove that κ is independent of t, ϵ and T successively. Step 1:

Fix a time t and a control ϵ . We introduce the notation:

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

Then $\forall f \in \mathbf{C}^0$:

$$\sum_{k\in\mathcal{I}} f(v_1^k)\xi_k = \sum_{k'\in\mathcal{I}} f(v_2^{k'})\xi_{k'}.$$
(10)

Let us choose f_n to be the density of the normal distribution with mean v_1^{ℓ} and variance $\frac{1}{n^2}$, n = 1, 2, ... In particular $(f_n)_{n\geq 1}$ converges weakly to the Dirac measure $\delta_{v_1^{\ell}}$. So, when $n \to +\infty$, we have

$$\sum_{k \in \mathcal{I}/v_1^k = v_1^\ell} \xi_k = \sum_{k' \in \mathcal{I}/v_2^{k'} = v_1^\ell} \xi_{k'}.$$
(11)

Yet, $\ell \in \{k \in \mathcal{I}/v_1^k = v_1^\ell\}$. Then

$$\sum_{\substack{\nu \in \mathcal{I}/v_2^{k'} = v_1^\ell}} \xi_{k'} = \sum_{k \in \mathcal{I}/v_1^k = v_1^\ell} \xi_k \ge \xi_\ell > 0.$$

Therefore $\{k' \in \mathcal{I}/v_2^{k'} = v_1^\ell\} \neq \emptyset$. In addition, as $\sum_{k \in \mathbb{N}} \xi_k = 1$ and $\xi_k > 0$ for all k, there exists a n_0 such that $\sum_{k \geq n_0} \xi_k < \xi_\ell$. So we have $\{k' \in \mathcal{I}/v_2^{k'} = v_1^\ell\} \cap \{1, 2, ..., n_0\} \neq \emptyset$. As this is true for all t and ϵ , $\exists \kappa_1(t, \epsilon) \in \{1, 2, ..., n_0\}$ that $v_2^{\kappa_1(t, \epsilon)} = v_1^\ell$. The function κ_1 takes values in the set $\{k \in \mathcal{I}/v_2^k = v_1^\ell\} \cap \{1, 2, ..., n_0\}$. If the set has more than one element, any element can be chosen. We obtain for all t, ϵ :

$$O_1(X_1(t, y_{\ell}, \epsilon)) = O_2(X_2(t, y_{\kappa_1(t, \epsilon)}, \epsilon)).$$
(12)

Step 2:

Let $T = m \in \mathbb{N}^*$ and $n \in \mathbb{N}^*$. We consider the space $\mathcal{P}_{T,n}$ of piecewise constant controls $\mathcal{P}_{T,n} = \{f : [0,T] \to \mathbb{C}\}$

 $\mathbb{R}|f = \alpha_1 \mathbf{1}_{[0,\frac{T}{n}]} + \alpha_2 \mathbf{1}_{]\frac{T}{n},\frac{2T}{n}]} + \dots + \alpha_n \mathbf{1}_{]\frac{(n-1)}{n}T,T]}, \alpha_1, \dots, \alpha_n \in \mathbb{R}\}. \text{ Denote } \alpha = (\alpha_1, \dots, \alpha_n). \text{ So that } \forall k \in \mathcal{I}, \text{ we can define the functions } g_k \text{ from } [0,T] \times \mathbb{R}^n \text{ to } \mathbb{R} \text{ by }$

$$g_k(t, \alpha) = O_2(X_2(t, y_k, \epsilon)) - O_1(X_1(t, y_\ell, \epsilon)).$$

We know that

$$X_a(t, y_k, \epsilon_\alpha) = e^{(A+h(\alpha_{\lfloor \frac{t}{n} \rfloor+1}, y_k)B_a)(t-\lfloor \frac{t}{n} \rfloor n)} \prod_{j=1}^{\lfloor \frac{t}{n} \rfloor} e^{(A+h(\alpha_j, y_k)B_a)\frac{T}{n}} \qquad a = 1, 2,$$
(13)

with A = -iH, $B_1 = -i\mu_1$ and $B_2 = -i\mu_2$. Therefore the functions X_a are analytic in t and α (the function h is analytic in α), and since O_a are analytic, the functions g_k are analytic. We denote $A_k = \{(t, \alpha) \in [0, T] \times \mathbb{R}^n/g_k(t, \alpha) = 0\}$. Each A_k is closed because g_k are continuous. In Step 1, it is proved that

$$\exists \kappa_T^{\mathcal{P}} : [0,T] \times \mathbb{R}^n \to \{1, 2, ..., n_0\} \quad \text{such that} \quad \forall (t,\alpha) \in [0,T] \times \mathbb{R}^n \quad g_{\kappa_T^{\mathcal{P}}(t,\alpha)}(t,\alpha) = 0.$$
(14)

So $\bigcup_{k \in \mathcal{I} \cap \{1, \dots, n_0\}} A_k = [0, T] \times \mathbb{R}^n$. By 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 $\forall m, n$, $\exists \kappa_2(m, n) \in \{1, 2, ..., n_0\} \cap \mathcal{I}$ such that $g_{\kappa_2(m, n)}(t, \epsilon) = 0$, $\forall t \in [0, m]$ and for any control $\epsilon \in \mathcal{P}_{m, n}$. Step 3:

Fix again m and take $n_l = 2^l$. Denote $B_l = \{k \in \mathcal{I} \cap \{1, 2, ..., n_0\}/g_k(t, \epsilon) = 0, \forall \epsilon \in \mathcal{P}_{m, n_\ell}\}$. In Step 2 it is proved that B_l is not empty for all l. Obviously $(B_l)_{l \in \mathbb{N}}$ is a decreasing sequence and B_l becomes stable from a certain term, thus $B_{\infty} \neq \emptyset$. This means $\forall m, \exists \kappa_3(m) \in \mathcal{I} \cap \{1, 2, ..., n_0\}$ such that $g_{\kappa_3(m)}(t, \epsilon) = 0, \forall t \in [0, m]$ and $\forall \epsilon \in \mathcal{P}_{m, n_\ell}$. Yet, $\bigcup_{\ell=1}^{\infty} \mathcal{P}_{m, 2^\ell}$ is dense in $L^1([0, m])$. So we have $\forall m, \exists \kappa_3(m) \in \mathcal{I} \cap \{1, 2, ..., n_0\}$ such that $g_{\kappa_3(m)}(t, \epsilon) = 0, \forall t \in [0, m]$ and for any control ϵ in $L^1([0, m])$.

Denote $C_m = \{k \in \mathcal{I} \cap \{1, 2, ..., n_0\}/g_k(t, \epsilon) = 0 \quad \forall \epsilon \in L^1_{loc}(\mathbb{R}_+), \forall t \in [0, m]\}$. The sequence $(C_m)_{n \in \mathbb{N}}$ is decreasing with $C_m \neq \emptyset \quad \forall m \in \mathbb{N}$. So we have $\cap_{k \geq 1} C_k \neq \emptyset$.

3.3. Setting (S1)

In this section and section 3.4, we suppose that d = 1, which means Y takes values in \mathbb{R} . The main result is the following:

Theorem 3.8. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H \in \mathcal{H}_N$ (Hamiltonian), $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$ and denote for $y \in \mathbb{R}$, $a = 1, 2 : \Psi_a(t, y) = \Psi(t, H, \epsilon(\cdot) + y, \mu_a, \Psi_0^a)$. Suppose that the observations of these two states follow the same law, that is:

$$\mathcal{L}_{Y}(\langle \Phi_{i}\Psi_{1}(t,Y)|\Psi_{1}(t,Y)\rangle) = \mathcal{L}_{Y}(\langle \Phi_{i}\Psi_{2}(t,Y)|\Psi_{2}(t,Y)\rangle) \quad \forall t \in \mathbb{R}_{+}, \forall \epsilon \in \mathrm{L}^{1}_{loc}(\mathbb{R}_{+})$$
(15)

 $\forall i = 1, ..., N$, with $\Phi_i = \phi_i(H)\phi_i(H)^*$ (the projector on $\phi_i(H)$). Then under the assumptions (A1),(A2) and (A3), there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the eigenbasis of H:

$$\forall j, k = 1, .., N, (\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}.$$
(16)

Proof. We renote for simplicity $\phi_k = \phi_k(H)$. The two observations have the same law, so $\forall f \in \mathcal{C}^0$

$$\sum_{k\in\mathcal{I}} f(\langle \Phi_i \Psi_1(t, y_k) | \Psi_1(t, y_k) \rangle) \xi_k = \sum_{k\in\mathcal{I}} f(\langle \Phi_i \Psi_2(t, y_k) | \Psi_2(t, y_k) \rangle) \xi_k$$
(17)

with $\xi_k = \mathbb{P}(Y = y_k)$. Recall that $\Psi_a(t, Y) = X_a(t, Y, \epsilon)\Psi_a(0, Y)$ with X_a solutions of (8), where $A_a = -iH$ and $B_a = -i\mu_a$, a = 1, 2. We apply the Lemma 3.7 to $O_a^i(X) = \langle \Phi_i X \Psi_0^a | X \Psi_0^a \rangle$, a = 1, 2 which are obviously analytic on Ψ , for all i = 1, ..., N and $h(\epsilon(t), y_\ell) = \epsilon(t) + y_\ell$. Then:

$$\langle \Phi_i \Psi_1(t, y_1) | \Psi_1(t, y_1) \rangle = \langle \Phi_i \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(1)}) | \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(1)}) \rangle.$$
(18)

We differentiate formula (18) with respect to time:

$$\begin{split} &(\epsilon(t)+y_1)\Im(\langle \mu_1\Psi_1(t,y_1)|\phi_i\rangle\langle \Psi_1(t,y_1)|\phi_i\rangle)\\ =&(\epsilon(t)+y_{\kappa_{O_1^i,O_2^i}(1)})\Im(\langle \mu_2\Psi_2(t,y_{\kappa_{O_1^i,O_2^i}(1)})|\phi_i\rangle\overline{\langle \Psi_2(t,y_{\kappa_{O_1^i,O_2^i}(1)})|\phi_i\rangle}), \end{split}$$

for all i = 1, 2, ..., N. Fix i, if $\exists \Psi$ such that

$$\Im(\langle \mu_1 \Psi | \phi_i \rangle \overline{\langle \Psi | \phi_i \rangle}) \neq 0,$$

then by controllability we can choose T > 0 and $\epsilon(t)$ such that $\Psi_1(T, y_1) = \Psi$. We can also choose $\epsilon(T) = -y_{\kappa_{O_1^i,O_2^i}(1)}$, which implies:

$$(-y_{\kappa_{O_1^i,O_2^i}(1)} + y_1)\Im(\langle \mu_1 \Psi | \phi_i \rangle \overline{\langle \Psi | \phi_i \rangle}) = 0.$$
⁽¹⁹⁾

Therefore $\kappa_{O_1^i,O_2^i}(1) = 1$. If $\forall i, \kappa_{O_1^i,O_2^i}(1) = 1$, then with a change of control $\epsilon(t) \to \epsilon(t) + y_1$, we can use Theorem 3.1. Now we suppose that $\exists j$ such that $\forall \Psi \in \mathbb{C}^N$,

$$\Im(\langle \mu_1 \Psi | \phi_j \rangle \overline{\langle \Psi | \phi_j \rangle}) = 0,$$

then ϕ_j is an eigenstate of μ_1 ; ϕ_j is a common eigenstate of H and μ_1 , so if we start with an initial state ϕ_j , one stays in the space of basis $\{\phi_j\}$ whatever the control, which contradicts the assumption of controllability.

Corollary 3.9. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H \in \mathcal{H}_N$ (Hamiltonian) and denote for a = 1, 2 by ρ_a the solution of:

$$\begin{cases} i\dot{\rho}_a(t,Y) = [H + (\epsilon(t) + Y)\mu_a, \rho_a(t,Y)] \\ \rho_a(0,Y) = \rho_0^a. \end{cases}$$
(20)

Suppose that the observations of these two states follow the same law:

$$\mathcal{L}_Y(Tr(\Phi_i\rho_1(t,Y)) = \mathcal{L}_Y(Tr(\Phi_i\rho_2(t,Y)) \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+)$$
(21)

for all i = 1, ..., N, with $\Phi_i = \phi_i(H)\phi_i(H)^*$. Then under the assumptions (A1), (A2) and (A3), there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the eigenbasis of H:

$$\forall j, k = 1, .., N, (\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}.$$
(22)

Remark 3.10. Recall that $\rho_a(t, y_\ell) = X_a(t, y_\ell, \epsilon)\rho_0^a X_a(t, y_\ell, \epsilon)^*$, a = 1, 2. For the proof of the corollary we apply Lemma 2.1 to $O_a^i(X) = Tr(\Phi_i X \rho_0^a X^*)$, a = 1, 2, for all i = 1, ..., N.

3.4. Setting (S2)

Theorem 3.11. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H_1, H_2 \in \mathcal{H}_N$ (Hamiltonian), $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$ and denote for $y \in \mathbb{R}$, $a = 1, 2 : \Psi_a(t, y) = \Psi(t, H_a, \epsilon(\cdot) + y, \mu_a, \Psi_0^a)$. Suppose that the observations of these two states follow the same law:

$$\mathcal{L}_Y(\langle E_i \Psi_1(Y, t) | \Psi_1(Y, t) \rangle) = \mathcal{L}_Y(\langle E_i \Psi_2(Y, t) | \Psi_2(Y, t) \rangle) \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+)$$
(23)

 $\forall i = 1, ..., N$, with $E_i = e_i e_i^*$ (the projector on e_i). We suppose $N \ge 3$. In this case, the assumption (A1) is replaced by a stronger assumption (A1'): (A1'): $\mathbb{L}_{[H_1,\mu_1],i\mu_1} = su(N)$ or $\mathbb{L}_{[H_2,\mu_2],i\mu_2} = su(N)$. Then under the assumptions (A1'),(A2), (A3) and (A4), there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the canonical basis, for all $1 \le i, j \le N$,

$$(\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)}(\mu_2)_{jk}$$
 and $(H_1)_{jk} = e^{i(\alpha_j - \alpha_k)}(H_2)_{jk}.$ (24)

Remark 3.12. The assumptions (A1) and (A2) do not implies (A1')(see Remark 1 in [4]). Assumption (A1)' is required for the simultaneous controllability, see Theorem 3.6.

Proof. Suppose that $\mathbb{L}_{[H_2,\mu_2],i\mu_2} = su(N)$. We apply the Lemma 3.7 to $O_a^i(X) = \langle E_i X \Psi_0^a | \Psi_0^a \rangle$, a = 1, 2, which are analytic, for all i = 1, ..., N. Hence:

$$\langle E_i \Psi_1(t, y_\ell) | \Psi_1(t, y_\ell) \rangle = \langle E_i \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)}) | \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)}) \rangle$$
(25)

for all i = 1, 2, ..., N and all $l \in \mathcal{I}$. By replacing $\epsilon(t) + y_{\ell}$ by $\epsilon(t)$, we obtain that for any $\epsilon(t)$, any $\ell, n \in \mathcal{I}$ and $t \ge 0$:

$$\langle E_i \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)} - y_\ell) | \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)} - y_\ell) \rangle = \langle E_i \Psi_1(t, 0) | \Psi_2(t, 0) \rangle = \langle E_i \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(n)} - y_n) | \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(n)} - y_n) \rangle$$

$$(26)$$

If $y_{\kappa_{O_1^i,O_2^i}(\ell)} - y_\ell \neq y_{\kappa_{O_1^i,O_2^i}(n)} - y_n$, then according to the Theorem 3.6, we know that

 \mathbf{k}

$$\begin{cases} i\dot{X}_{\ell}(t) = (H_2 + (\epsilon(t) + y_{\kappa_{O_1^i,O_2^i}}(\ell) - y_{\ell})\mu_2)X_{\ell}(t) \\ X_{\ell}(0) = X_{\ell}^0 \end{cases}$$
(27)

and

$$\begin{cases} i\dot{X}_n(t) = (H_2 + (\epsilon(t) + y_{\kappa_{O_1^i,O_2^i}(n)} - y_n)\mu_2)X_n(t) \\ X_n(0) = X_n^0 \end{cases}$$
(28)

are simultaneously controllable. Thus there exists T > 0 such that $\Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)} - y_\ell) = e_i$ and $\Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(n)} - y_n) = e_j$, which contradicts the equation (25). Thus $\exists C_i \in \mathbb{R}$ such that $y_{\kappa_{O_1^i, O_2^i}(\ell)} = y_\ell + C_i \ \forall l \in \mathcal{I}$. Recall equation (10) in the Lemma 3.7:

$$\sum_{\in \mathcal{I}/v_1^k = v_1^\ell} \xi_k = \sum_{k' \in \mathcal{I}/v_2^{k'} = v_1^\ell} \xi_{k'}$$
(29)

Lemma 3.7 proves that for any control ϵ , $v_1^{\ell} = v_2^{\kappa_{O_1^i,O_2^i}(\ell)}$. Now for any $\eta > 0$, there exists n_{η} such that $\sum_{k>n_{\eta}} \xi_k \leq \eta$. According to Theorem 1.4, there exists a control ϵ and a time T > 0 such that $X_{\kappa_{O_1^i,O_2^i}(\ell)}(T) = e_i$ and $X_k = e_j$ for all $k \leq n_{\eta}$ and $k \neq \kappa_{O_1^i,O_2^i}(\ell)$. So for this ϵ ,

$$\xi_{\ell} \leq \sum_{\substack{\kappa_{O_{1}^{i},O_{2}^{i}}(\ell)\\k \in \mathcal{I}/v_{1}^{k} = v_{2}}} \xi_{k} = \sum_{\substack{k' \in \mathcal{I}/v_{2}^{k'} = v_{2}}} \xi_{k'} \leq \xi_{\kappa_{O_{1}^{i},O_{2}^{i}}(\ell)} + \sum_{k > n_{\eta}} \xi_{k} \leq \xi_{\kappa_{O_{1}^{i},O_{2}^{i}}(\ell)} + \eta$$
(30)

Then for all $\eta > 0$, $\xi_{\kappa_{O_1^i,O_2^i}(\ell)} + \eta \ge \xi_{\ell}$ which means $\xi_{\kappa_{O_1^i,O_2^i}(\ell)} \ge \xi_{\ell}$. In addition, $\sum_{k \in \mathcal{I}} \xi_k = 1$. If $C_i \ne 0$, then $1 = \sum_{k \in \mathcal{I}} \xi_k \ge \sum_{m=1}^{\infty} \mathbb{E}(\{Y = y_l + mC_i\}) \ge \sum_{m=1}^{\infty} \xi_\ell = \infty$, which is absurd. Therefore $C_i = 0$. Now we are in the case of Theorem 3.4.

Corollary 3.13. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H_1, H_2 \in \mathcal{H}_N$ (Hamiltonians) and for a = 1, 2 denote by ρ_a the solution of:

$$\begin{cases} i\dot{\rho}_{a}(t,Y) = [H_{a} + (\epsilon(t) + Y)\mu_{a}, \rho_{a}(t,Y)] \\ \rho_{a}(0,Y) = \rho_{0}^{a} \end{cases}$$
(31)

Suppose that the observations of these two states follow the same law:

$$\mathcal{L}_Y(Tr(E_i\rho_1(Y,t))) = \mathcal{L}_Y(Tr(E_i\rho_2(Y,t))) \quad \forall t \in \mathbb{R}_+, \forall \epsilon \in \mathrm{L}^1_{loc}(\mathbb{R}_+)$$
(32)

and for all i = 1, ..., N, with $E_i = e_i e_i^*$. We suppose $N \ge 3$. Then under the assumptions (A1'),(A2), (A3) and (A4) and, there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the canonical basis, for all $1 \le i, j \le N$,

$$(\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}$$
 and $(H_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (H_2)_{jk}.$ (33)

3.5. The polynomial case in setting (S1)

In this section d > 1 and we suppose that the value set \mathcal{V} is bounded and not a subset of $\mathbb{R} \times \{(\underbrace{0, \cdots, 0}_{d-1})\}$.

Here Y takes values in $\mathcal{V} \subset \mathbb{R}^d$ so we can denote $(Y)_0, \cdots, (Y)_{d-1}$ the components of Y.

Theorem 3.14. Let $\mu_1, \mu_2 \in \mathcal{H}_N$ (dipole moments), $H_1 \in \mathcal{H}_N$ (Hamiltonian), $\Psi_0^1, \Psi_0^2 \in \mathcal{S}_N$ and denote for $a = 1, 2, y \in \mathcal{V}$ by $\Psi_a(t, y) = \Psi(t, H_a, \sum_{n=0}^{d-1} (y)_n \epsilon(t)^n, \mu_a, \Psi_0^a)$. Suppose that the observations of these two states follow the same law:

$$\mathcal{L}_{Y}(\langle \Phi_{i}\Psi_{1}(t,Y)|\Psi_{1}(t,Y)\rangle) = \mathcal{L}_{Y}(\langle \Phi_{i}\Psi_{2}(t,Y)|\Psi_{2}(t,Y)\rangle) \quad \forall t \in \mathbb{R}_{+}, \forall \epsilon \in \mathrm{L}^{1}_{loc}(\mathbb{R}_{+}), \forall i = 1, \cdots, N,$$
(34)

with $\Phi_i = \phi_i(H)\phi_i(H)^*$. Suppose also $\exists y_{\ell_0} \in \mathcal{V} \setminus (\mathbb{R} \times \{\underbrace{(0, \cdots, 0)}_{d-1}\})$ with $-y_{\ell_0} \notin \mathcal{V}$. Then under the assumptions (A1), (A2) and (A3) for both systems, there exists $(\alpha_i)_{i=1}^N \in \mathbb{R}^N$ such that, in the eigenbasis of H:

$$\forall j, k = 1, .., N, (\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}.$$
(35)

Proof. We use the similar arguments as in the proof of Theorem 3.8. For all $i = 1, 2, \dots, N$ and all $\ell \in \mathcal{I}$ such that $y_{\ell} \in \mathcal{V} \setminus (\mathbb{R} \times \{\underbrace{(0, \cdots, 0)}_{d-1}\}):$

$$\begin{split} &\sum_{n=0}^{d-1} (y_{\ell})_n \epsilon(t)^n \Im(\langle \mu_1 \Psi_1(t, y_{\ell}) | \phi_i \rangle \overline{\langle \Psi_1(t, y_{\ell}) | \phi_i \rangle}) \\ &= &\sum_{n=0}^{d-1} (y_{\kappa_{O_1^i, O_2^i}(\ell)})_n \epsilon(t)^n \Im(\langle \mu_2 \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)}) | \phi_i \rangle \overline{\langle \Psi_2(t, y_{\kappa_{O_1^i, O_2^i}(\ell)}) | \phi_i \rangle}) \end{split}$$

 $\text{Fix } i \text{, then we denote } m_{\mu_1} = \max_{\Psi \in \mathcal{S}^{N-1}(\mathbb{C})} |\Im(\langle \mu_1 \Psi | \phi_i \rangle \overline{\langle \Psi | \phi_i \rangle})| \text{ and } m_{\mu_2} = \max_{\Psi \in \mathcal{S}^{N-1}(\mathbb{C})} |\Im(\langle \mu_2 \Psi | \phi_i \rangle \overline{\langle \Psi | \phi_i \rangle})|.$ Hypothesis (A1) assure that for any $a = 1, 2, \forall y_{\ell} \in \mathcal{V} \setminus (\mathbb{R} \times \{\underbrace{(0, \cdots, 0)}_{d-1}\})$, the system (1) for $u(t) = \sum_{n=0}^{d-1} (y_{\ell})_n \epsilon(t)^n$

is controllable, see [19]. Thus there exists Ψ^0 such that

$$|\Im(\langle \mu_1 \Psi^0 | \phi_i \rangle \langle \Psi^0 | \phi_i \rangle)| = m_{\mu_1},$$

then by controllability we can choose T > 0 and $\epsilon(t)$ such that $\Psi_1(T, y_1) = \Psi^0$ and $\epsilon(T)$ be equal to any predefined value. So we have for any $\epsilon(T)$:

$$\left|\sum_{n=0}^{d-1} (y_{\ell})_n \epsilon(T)^n\right| \le \frac{m_{\mu_2}}{m_{\mu_1}} \left|\sum_{n=0}^{d-1} (y_{\kappa_{O_1^i,O_2^i}(\ell)})_n \epsilon(T)^n\right|.$$
(36)

Similarly, we also have $\forall \epsilon(T)$

$$\left|\sum_{n=0}^{d-1} (y_{\ell})_{n} \epsilon(T)^{n}\right| \ge \frac{m_{\mu_{2}}}{m_{\mu_{1}}} \left|\sum_{n=0}^{d-1} (y_{\kappa_{O_{1}^{i},O_{2}^{i}}(\ell)})_{n} \epsilon(T)^{n}\right|.$$
(37)

The inequalities (36) and (37) imply that $y_{\kappa_{O_1^i,O_2^i}(\ell)} = \gamma_{\ell,i}y_\ell$ with $\gamma_{\ell,i} = \pm \frac{m_{\mu_1}}{m_{\mu_2}}$. By changing the role of μ_1 and μ_2 we can suppose that $\frac{m_{\mu_1}}{m_{\mu_2}} \ge 1$. If $\frac{m_{\mu_2}}{m_{\mu_1}} > 1$ then for $\ell = \ell_0$, $|y_{\kappa_{O_1^i,O_2^i}(\ell_0)}| = (\frac{m_{\mu_1}}{m_{\mu_2}})^n |y_{\ell_0}| \to +\infty$ when $n \to +\infty$, which contradicts the fact that the value set \mathcal{V} is bounded. Here $\kappa^{(n)} = \underbrace{\kappa \circ \cdots \circ \kappa}_{n \text{ times}}$. So we can conclude that

 $\frac{m_{\mu_1}}{m_{\mu_2}} = 1$. As $-y_{\ell_0} \notin \mathcal{V}$, we have $\gamma_{\ell_0,i} = 1$ for all $i = 1, 2, \cdots, N$.

 $\frac{1}{m_{\mu_2}} = 1.165$ $g_{\ell_0} \neq 1$, we have $p_{0,\ell}$ According to [19], for any polynomial P of degree ≥ 1 , the set of attainable states

$$\left\{ \Psi\left(t, \begin{pmatrix} H & 0\\ 0 & H \end{pmatrix}, v, \begin{pmatrix} \mu_1 & 0\\ 0 & \mu_2 \end{pmatrix}, \begin{pmatrix} \Psi_1^0\\ \Psi_2^0 \end{pmatrix} \right) \middle| t \ge 0, v \in \mathcal{L}^1_{loc} \right\},$$
(38)

is the same as the set of attainable states

$$\left\{ \Psi\left(\tau, \begin{pmatrix} H & 0\\ 0 & H \end{pmatrix}, P(w), \begin{pmatrix} \mu_1 & 0\\ 0 & \mu_2 \end{pmatrix}, \begin{pmatrix} \Psi_1^0\\ \Psi_2^0 \end{pmatrix} \right) \middle| \tau \ge 0, w \in \mathcal{L}^1_{loc} \right\}.$$
(39)

Here the polynomial is $P(X) = \sum_{n=0}^{d-1} (y_{\ell_0})_n X^n$. Since $\Psi(\tau, H, P(w), \mu_1, \Psi_1^0)$ and $\Psi(\tau, H, P(w), \mu_2, \Psi_2^0)$ have the same observations, the states $\Psi(t, H, v, \mu_1, \Psi_1^0)$ and $\Psi(t, H, v, \mu_2, \Psi_2^0)$ will have the same observations for any $t \ge 0$ and $v \in L^1_{loc}$. So now we can apply the Theorem 3.1 to $\hat{\Psi}_1$ and $\hat{\Psi}_2$.

Remark 3.15. The theorem is also true when \mathcal{V} is symmetric with respect to the origin but the ensemble of two systems (H, μ_1) and $(H, -\mu_1)$ is simultaneously controllable (for instance when the graph of μ_1 is not bipartite, see [17]). In this situation, one concludes as follows: $\forall y_{\ell} \in \mathcal{V} \setminus (\mathbb{R} \times \{(0, \dots, 0) \in \mathbb{R}^{d-1}\})$, if for example $\gamma_{\ell,i} = 1$ and $\gamma_{\ell,j} = -1$, then we control the system (H, μ_1) to ϕ_i and the system $(H, -\mu_1)$ to ϕ_j at time T; we obtain $\langle \Phi_i \Psi_1(T, y_\ell) | \Psi_1(T, y_\ell) \rangle = 1$ and $\langle \Phi_i \Psi_1(T, y_\ell) | \Psi_1(T, y_\ell) \rangle = 1$ which is impossible. In this case the conclusion is

$$\forall j, k = 1, .., N, (\mu_1)_{jk} = e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}.$$
(40)

or

$$\forall j, k = 1, ..., N, (\mu_1)_{jk} = -e^{i(\alpha_j - \alpha_k)} (\mu_2)_{jk}.$$
(41)

When d = 1, $(Y)_0 \equiv 0$ and $(Y)_1$ is symmetric with respect to the origin, we see that for any $\epsilon(t)$, the laws of the observables corresponding to (H,μ) and $(H,-\mu)$ are the same. Therefore, the alternative (41) can not be eliminated.

4. NUMERICAL APPLICATION

The tests are made for the setting (S2). We consider the 4-level system (N = 4) in [7] and want to recover the Hamiltonian matrix H_{real} and the dipole moment matrix μ_{real} :

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

Note that:

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

As previously discussed, 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}_{real} . The law of the perturbation Y is known :

$$\mathcal{L}_Y = \begin{pmatrix} 0.000156 & 0.000211 & 0.000975 & 0.000740 & 0.000679 & 0.000816 & 0.000224 & 0.001025 & 0.000066 & 0.000400 \\ 0.01818 & 0.03636 & 0.05454 & 0.07272 & 0.09090 & 0.10909 & 0.12727 & 0.14545 & 0.16363 & 0.18181 \end{pmatrix}.$$

The first row represents the value set and the second row is the probability. The values are chosen at random uniformly in $[0, 0.1 * \frac{||H||_{l^{\infty}}}{||\mu||_{l^{\infty}}} = 0.0012]$ and the probability at random (uniformly) then rescaled to 1. The control fields are of the form of $\epsilon(t) = \exp\left(-40(t-T/2)^2/T^2\right) \sum_{i\neq j} A_{ij}\sin(\omega_{ij}t + \theta_{ij})$. Here $\omega_{ij} = \lambda_j(H) - \lambda_i(H)$ are the transition frequencies between the eigenstates of H. The total simulation time is T = 3200 which means about 10 periods of the smallest frequency. We choose N_{ϵ} controls $\epsilon(t)$ drawing θ_{ij} uniformly in $[0, 2\pi]$ and A_{ij} uniformly in [0, 0.0012] and we define the functional to be minimized:

$$\mathcal{J}(\mathcal{P},\mu) = \sum_{i=1}^{N_{\epsilon}} \sum_{j=1}^{N} \mathcal{T}_{2}(\mathcal{L}_{Y}(|(\Psi(T, e^{\mathcal{P}} De^{-\mathcal{P}}, \epsilon_{i}, \mu, \Psi_{1}^{0}), \mathcal{L}_{Y}(|(\Psi(T, H_{real}, \epsilon_{i}, \mu_{real}, \Psi_{real}^{0}))).$$
(42)

Here we use the bounded Lipschitz distance (see page 34-35 in [22]) \mathcal{T}_2 between two laws $L_Y Z_1$ and $L_Y Z_2$ defined as $\mathcal{T}_2(L_Y Z_1, L_Y Z_2) = \sqrt{\int_0^1 |(F_{Z_1}^{-1}(x) - G_{Z_2}^{-1}(x)|^2 dx}$ with F(respectively G) the cumulative distribution function of Z_1 (respectively Z_2)(see page 73-75 in [22] for details). Here N = 4 and $N_{\epsilon} = 36$. We start with a 10% relative error on μ and \mathcal{P} and we use a classical unconstrained nonlinear optimization to minimize $\mathcal{J}(\mathcal{P}, \mu)$ (we used the Gnu Octave [8,16] 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 a 0.003% relative error on μ and a 0.001% relative error on \mathcal{P} . We note that the histograms of the real law and the final law are nearly the same. See figures 1 and 2 for details.

5. Perspectives and concluding remarks

Previous results were obtained under technical assumptions concerning the systems to identify and some demanding assumptions on the observables. A related question is whether it is enough to only measure one



FIGURE 1. The logarithm of $\mathcal{J}(\text{left})$, the relative error on $\mathcal{P}(\text{middle})$ and the relative error on $\mu(\text{right})$ as a function of the iteration index.

observable (and not N of them) at some final time T. We expect that if T is large enough and the system is controllable this assertion is true.

Also interesting would be to consider time-dependent perturbations and more elaborate noise models (not polynomial) and, of course, perturbations that can take values in an uncountable set (in the same spirit of [3,14]).

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References

- Claudio Altafini. Controllability of quantum mechanical systems by root space decomposition of su(N). J. Math. Phys., 43(5):2051–2062, 2002.
- [2] Lucie Baudouin and Alberto Mercado. An inverse problem for Schrodinger equations with discontinuous main coefficient. *Applicable Analysis*, 87(10-11):1145–1165, 2008.
- [3] Karine Beauchard, Jean-Michel Coron, and Pierre Rouchon. Controllability issues for continuous-spectrum systems and ensemble controllability of Bloch equations. Comm. Math. Phys., 296(2):525–557, 2010.
- [4] Mohamed Belhadj, Julien Salomon, and Gabriel Turinici. Simultaneous controllability and discrimination of collections of perturbed bilinear control systems on the Lie group SU(N). preprint HAL 00866229, http://hal.archives-ouvertes.fr/hal-00866229.
- [5] S. Bonnabel, M. Mirrahimi, and P. Rouchon. Observer-based hamiltonian identification for quantum systems. Automatica, 45(5):1144 – 1155, 2009.
- [6] Constantin Brif, Raj Chakrabarti, and Herschel Rabitz. Control of quantum phenomena: past, present and future. New Journal of Physics, 12(7):075008, 2010.
- [7] Ashley Donovan and Herschel Rabitz. Exploring the hamiltonian inversion landscape. Phys. Chem. Chem. Phys., 16:15615– 15622, 2014.
- [8] John W. Eaton, David Bateman, and Soren Hauberg. GNU Octave version 3.0.1 manual: a high-level interactive language for numerical computations. CreateSpace Independent Publishing Platform, 2009. ISBN 1441413006.
- [9] J. M. Geremia and H. Rabitz. Optimal hamiltonian identification: The synthesis of quantum optimal control and quantum inversion. The Journal of Chemical Physics, 118(12):5369–5382, 2003.
- [10] D. Hocker, C. Brif, M. D. Grace, A. Donovan, T.-S. Ho, K. W. Moore Tibbetts, R. Wu, and H. Rabitz. Characterization of control noise effects in optimal quantum unitary dynamics. ArXiv e-prints, May 2014. Version 1.



FIGURE 2. The optimization algorithm iterates from the initial guess (\mathcal{P}_0, μ_0) and constructs a sequence of estimations (\mathcal{P}_k, μ_k) . We plot here severals histograms of the laws $\mathcal{L}_Y(|(\Psi_1^{\epsilon_i}(T,Y))_j|^2)$ for various choices of k and $i = 1, \dots, 5$ and j = 1, 2, 3, 4. In the top picture are the histograms of the observations for the real law, in the middle picture are the histograms for the initial guess k = 0 and in the bottom image the histograms for the final iteration k = 277. The optimization worked well as there is an obvious match between the top and the bottom histograms.

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- [11] Kaveh Khodjasteh and Lorenza Viola. Dynamical quantum error correction of unitary operations with bounded controls. Phys. Rev. A, 80:032314, Sep 2009.
- [12] Kaveh Khodjasteh and Lorenza Viola. Dynamically error-corrected gates for universal quantum computation. Phys. Rev. Lett., 102:080501, Feb 2009.
- [13] Claude Le Bris, Mazyar Mirrahimi, Herschel Rabitz, and Gabriel Turinici. Hamiltonian identification for quantum systems: well-posedness and numerical approaches. ESAIM Control Optim. Calc. Var., 13(2):378–395, 2007.
- [14] J.-S. Li and N. Khaneja. Control of inhomogeneous quantum ensembles. Phys. Rev. A, 73:030302, 2006.
- [15] Y. Maday and J. Salomon. A greedy algorithm for the identification of quantum systems. In Decision and Control, 2009 held jointly with the 2009 28th Chinese Control Conference. CDC/CCC 2009. Proceedings of the 48th IEEE Conference on, pages 375–379, Dec 2009.
- [16] Octave community. GNU Octave 3.8.1, 2014.
- [17] Herschel Rabitz and Gabriel Turinici. Controlling quantum dynamics regardless of laser beam spatial profile and molecular orientation. Physical review A: Atomic, Molecular and Optical Physics, 75(4):043409, 2007.
- [18] Alexandre M. Souza, Gonzalo A. Álvarez, and Dieter Suter. Experimental protection of quantum gates against decoherence and control errors. Phys. Rev. A, 86:050301, Nov 2012.
- [19] Gabriel Turinici. Beyond bilinear controllability : applications to quantum control. In Control of coupled partial differential equations, volume 155 of Internat. Ser. Numer. Math., pages 293–309, Oberwolfach, Allemagne, 2007. Birkhauser.
- [20] Gabriel Turinici and Herschel Rabitz. Quantum wavefunction controllability. Chemical Physics, 267(1-3):1 9, 2001.
- [21] Gabriel Turinici and Herschel Rabitz. Wavefunction controllability in quantum systems. Journal of Physics A: Mathematical and Theoretical, 36:2565–2576, 2003.
- [22] Cédric Villani. Topics in optimal transportation. Graduate studies in mathematics. American Mathematical Society, cop., Providence (R.I.), 2003.
- [23] Wusheng Zhu and Herschel Rabitz. Potential surfaces from the inversion of time dependent probability density data. The Journal of Chemical Physics, 111(2):472–480, 1999.