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Parameter estimation of a 3-level quantum system with a single population measurement

Zaki Leghtas  Mazyar Mirrahimi  Pierre Rouchon

Abstract— An observer-based Hamiltonian identification algorithm for quantum systems has been proposed in [2]. The later paper provided a method to estimate the dipole moment matrix of a quantum system requiring the measurement of the populations on all states, which could be experimentally difficult to achieve. We propose here an extension to a 3-level quantum system, having access to the population of the ground state only. By a more adapted choice of the control field, we will show that a continuous measurement of this observable, alone, is enough to identify the field coupling parameters (dipole moment).

Keywords: Nonlinear systems, quantum systems, parameter estimation, nonlinear observers, averaging.

I. INTRODUCTION

For applications ranging from quantum computers to the synthesis of new molecules, an accurate estimation of the parameters involved in the dynamics of the quantum system is fundamental. Various methods have been engineered over the years like the maximum-likelihood methods [10], [8], [11], the maximum-entropy methods [4] and minimum Kullback entropy methods [13]. The optimal identification techniques via least-square criterias [6], [5], [12] and the map inversion techniques [14] are some other techniques explored in this area. In [9], a state-observer is presented for the state identification combined with a gradient method on the dipole moment. This result was then improved in [2] succeeding in simultaneously estimating the state of the system and its dipole moment using observers. In [12] a rigorous proof of the well-posedness of the problem is proposed. All these results required the knowledge of the populations on all energy levels. Experimentally, that is extremely difficult to achieve. Since in quantum mechanics, measuring an observable influences the system, the less information we need, the less we disturb the system, and the more likely our estimation is accurate. Our goal was to improve the result given in [2] in order to estimate the dipole moments of a quantum system measuring continuously the population on the first state only. We focus here on 3-level systems with a single population measure.

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In section III we explain the 3-level system and set the estimation problem attached to (1). In section III we present a 2-step estimation procedure based on two nonlinear asymptotic observers (3) and (4). Sections IV and V are devoted to local convergence proofs.

II. THE 3-LEVEL SYSTEM

A. Model and problem setting

Denote by $|k\rangle$, $k=1,2,3$ the 3 states of energies $E_k$ such that $|E_2-E_1| \neq |E_3-E_2|$. Throughout the paper we use the following notations for $k,l=1,2,3$: $\sigma^{kl} = |l\rangle \langle k| |l\rangle \langle l|$, $\sigma^{kk} = |l\rangle \langle k| |l\rangle \langle l|$, $\sigma^{kl} = |l\rangle \langle l| |k\rangle \langle k|$, $\sigma^{kk} = |l\rangle \langle k| |k\rangle \langle l|$, $P_k = |k\rangle \langle k|$ (projector on $|k\rangle$). Assume that the dynamics is described by the following Schrödinger equation:

$$
\frac{d}{dt} |\Psi\rangle = -\frac{i}{\hbar} (H_0 + A(t)H_1) |\Psi\rangle,
$$

where $|\Psi\rangle$ is the wave-function, $A(t) \in \mathbb{R}$ the electromagnetic field, $H_0 = \sum_1^3 E_k P_k$ the free Hamiltonian, $H_1 = \mu_{12} \sigma_{12}^2 + \mu_{23} \sigma_{23}^2$ the Hamiltonian matrix describing the coupling with the electromagnetic field (dipole moment) and $y$ the measurement output. Assuming the energies $E_k$ known, the goal consists in estimating the real coupling parameters $\mu_{12}$ and $\mu_{23}$ from the output $y$. We assume the electromagnetic field resonant with transitions $1-2$ and $2-3$:

$$
A(t) = \mu_{12} \bar{A}_{12} \sin \left( \frac{E_2-E_1}{\hbar} t \right) + \mu_{23} \bar{A}_{23} \sin \left( \frac{E_3-E_2}{\hbar} t \right)
$$

with small amplitude magnitudes $\bar{A}_{12}$ and $\bar{A}_{23}$ and normalized slow modulations $|u_{12}|, |u_{23}| \in [0,1]$. We have $|\bar{A}_{12}\mu_{12}|, |\bar{A}_{23}\mu_{23}| \ll |E_2-E_1|, |E_3-E_2|$. In the interaction frame $|\Phi\rangle = e^{\frac{i\theta}{\hbar}} |\Psi\rangle$ and after neglecting highly oscillating terms (rotating wave approximation) we get the following model

$$
\frac{d}{dt} |\Phi\rangle = (u_{12} \Omega_{12} \sigma^{12} + u_{23} \Omega_{23} \sigma^{23}) |\Phi\rangle
$$

where $\Omega_{12} = \frac{\bar{A}_{12}\mu_{12}}{2\hbar}$ and $\Omega_{23} = \frac{\bar{A}_{23}\mu_{23}}{2\hbar}$ are Rabi amplitudes when $(u_{12},u_{23}) = (1,0)$ and $(u_{12},u_{23}) = (0,1)$.

In the sequel we will use the density operator $\rho = |\Phi\rangle \langle \Phi|$ instead of the wave function $|\Phi\rangle$. The estimation of the real parameters $\mu_{12}$ and $\mu_{23}$ is then equivalent to estimation of the two other real parameters $\Omega_{12}$ and $\Omega_{23}$ appearing in the dynamics of the projector $\rho$

$$
\frac{d}{dt} \rho = u_{12} \Omega_{12} \left[ \sigma^{12}, \rho \right] + u_{23} \Omega_{23} \left[ \sigma^{23}, \rho \right]
$$

(1)
via the output $y = \text{Tr}(P_t \rho)$ and using $u_{12}$ and $u_{23}$ as excitation real inputs. Remember that $\sigma^{12}$ and $\sigma^{23}$ are anti-symmetric and real matrices: if the entries of $\rho$ are initially real, they remain real; if $\rho$ is initially a projector and thus describes a pure quantum state, it remains a projector.

Since we are in the 3-level case, $\rho$ can be seen as a point on the two dimensional manifold $\mathbb{R}^2$, the projective space.

B. Identifiability

It is proved in [12] that it is possible to identify $\Omega_{12}$ and $\Omega_{23}$ by measuring all the populations, i.e., via the measurement outputs $\{\text{Tr}(P_t \rho), \text{Tr}(P_2 \rho)\} = \{1 - \text{Tr}(P_t \rho) - \text{Tr}(P_2 \rho)\}$. With just $y = \text{Tr}(P_t \rho)$, we provide here below arguments showing identifiability via adapted choices for inputs $u_{12}$ and $u_{23}$. With $u_{12} = 1$ and $u_{23} = 0$ we recover essentially a 2-level system with states $|1\rangle$ and $|2\rangle$ and we can identify $\Omega_{12}$ from $y$ following [2]. This corresponds to the first step that is treated in theorem 1.

Assume now that $\Omega_{12}$ is known. Set $u_{12} = 1$ and $u_{23} = \eta \cos \theta$ with $\frac{\theta}{2} = \Omega_{12}$ and $\eta$ a small positive parameter. With $\xi = e^{-\theta} \sigma^{12} P_{\epsilon} e^{\theta} \sigma^{12}$, the output map becomes

$$y(t) = \frac{\text{Tr}((P_t + P_2) \xi) + \cos(2\theta) \text{Tr}(\sigma^{12} \xi) + \sin(2\theta) \text{Tr}(\sigma^{12} \xi)}{2}$$

and $\xi$ obeys to

$$\frac{d}{dt} \xi = \eta \cos^2 \theta \Omega_{23}[\sigma^{23}, \xi] + \eta \cos \theta \sin \theta \Omega_{23}[\sigma^{23}, \xi]$$

Since $\eta \ll 1$ we can average its dynamics:

$$\frac{d}{dt} \xi = \frac{\eta \Omega_{23}}{2} [\sigma^{23}, \xi].$$

The average values of $y(t)(1 + 2 \cos(2\theta))$ and $y(t)(1 - 2 \cos(2\theta))$ are $\text{Tr}(P_t \xi)$ and $\text{Tr}(P_2 \xi)$, respectively. Thus in average all the populations are measured and according to [12], $\Omega_{23}$ is identifiable. This second step is treated in theorem 2.

III. ESTIMATION ALGORITHMS AND SIMULATIONS

As explained above, we proceed in two steps. In a first step we set in (1), $u_{12} = 1$ and $u_{23} = 0$ and estimate from the output $y(t)$ the parameter $\Omega_{12}$ via the following nonlinear dynamical system (an invariant nonlinear observer inspired by [2], [1], [3]):

$$\frac{d}{dt} \hat{\rho} = \Omega_{12}[\sigma^{12}, \hat{\rho}] + ...$$

$$\frac{d}{dt} \Omega_{12} = \epsilon^2 \Gamma_1 \text{Tr}(\sigma^{12} [\sigma^{12}, \hat{\rho}]) \left(y(t) - \text{Tr}(P_t \hat{\rho})\right)$$

with $\Gamma_1, \Gamma_2$ positive parameters of order 1 and $\epsilon$ a small positive parameter. Local convergence is proved in theorem 1. The dynamics (3) respect two important features: if the entries $\hat{\rho}$ are initially real, they remain real for $t > 0$; if $\hat{\rho}$ is initially a projector and thus describes a pure quantum state, it remains a projector for $t > 0$.

Assuming $\Omega_{12}$ obtained via this first step, we take, as explained in previous section, $u_{12} = 1$ with $u_{23} = \eta \cos \theta$ ($\frac{d}{dt} \theta = \Omega_{12}$ and $\eta$ a small positive parameter) to estimate $\Omega_{23}$ via a second nonlinear dynamical system

$$\frac{d}{dt} \hat{\rho} = \Omega_{12}[\sigma^{12}, \hat{\rho}] + \eta \cos \theta \hat{\Omega}_{23}[\sigma^{23}, \hat{\rho}] + ...$$

$$\frac{d}{dt} \Omega_{23} = \epsilon^2 \eta \Gamma_2 \left(y(t) - \text{Tr}(\sigma^{12} [\sigma^{12}, \hat{\rho}])\right)$$

with $\Xi_{23}$ and $\gamma_{23}$ positive parameters of order 1 and $\epsilon$ is a small positive parameter. Local convergence is addressed in theorem 2.

![Fig. 1. Estimation of $\Omega_{12}$ in a first step ($t \in [0,50]$) via (1); estimation of $\Omega_{23}$ in a second step ($t > 50$) via (2) (no modeling and measure errors, $\Omega_{12}$ and $\Omega_{23}$ stand for $\Omega_{12}$ and $\Omega_{23}$).](image1)

![Fig. 2. Similar simulations to those of figure 1 but with 20% of Gaussian additive noise on the output $y(t)$ and 10% of Gaussian additive noise on the inputs $u_{12}$ and $u_{23}$.](image2)
\( \Gamma_{12} = \Gamma_{23} = 4, \ \gamma_{12} = \gamma_{23} = 1. \) Convergence of \( \hat{\Omega}_{12} \) is effective after \( t > 20 \) that corresponds to \( \frac{1}{4} \) Rabi periods associated to transition 1 \(-\) 2 for the average dynamics (3). Convergence of \( \hat{\Omega}_{23} \) is achieved for \( t \in [50, 200] \). The interval length corresponds to \( \frac{1}{4} \) Rabi periods associated to transition 2 \(-\) 3 for the average dynamics (3) since \( \frac{2\pi}{\Gamma_{23}} \approx 140 \). These convergence times are in good agreement with the convergence times that can be obtained from the linearized system (6) appearing during the proof of theorem 1. When additive noises are introduced on the inputs and output, the performance are not dramatically changed and the convergence times are almost the same.

IV. ESTIMATION OF \( \Omega_{12} \)

Theorem 1: Take system (1) with inputs \( u_{12} = 1, u_{23} = 0 \) and consider the estimation of \( \rho \) and \( \Omega_{12} \) via (3). Take \( \Gamma_{12}, \gamma_{12} > 0 \) and assume that \( \rho(0) \) and \( \hat{\rho}(0) \) are real projectors with \( \text{Tr}((P_1 + P_2)\rho(0)) \leq 0 \). Then, for \( \epsilon > 0 \) small enough, exists \( \sigma > 0 \) such that, if \( 1 - \text{Tr}(\hat{\rho}(0)\rho(0)) \leq \sigma \) and \( |\hat{\Omega}_{12}(0) - \Omega_{12}| \leq \sigma, \) then \( \lim_{t \to +\infty}\hat{\rho}(t) = \rho(t) = 0 \) and \( \lim_{t \to +\infty}\hat{\Omega}_{12}(t) = \Omega_{12}. \) Moreover the convergence is exponential.

Proof: Since \( \rho \) and \( \hat{\rho} \) remain real projectors for \( t > 0 \), they can be seen as points on the two dimensional manifold \( \mathbb{R}^2, \) a projective space. In particular (1) is a dynamical system with only 2 degrees of freedom whereas the space of 3 \( \times \) 3 symmetric real matrices where the dynamics is expressed is dimension 9. We have to try use less variables but averaging computations performed here below are too much complicated. In fact calculations based on 3 \( \times \) 3 symmetric real matrices and thus with more variables than necessary simplify notably the analysis.

Set \( \hat{\theta} = \theta \) and consider the unitary and real transformation \( (P_2 = \{3\} \{3\}) \)

\[
U(t) = \exp(\theta(t)\sigma^{12}) = P_3 + \cos(\theta(t))(P_1 + P_2) + \sin(\theta(t))\sigma^{12}
\]

and the attached change of frame \( \xi = U^\dagger \rho U, \) \( \hat{\xi} = U^\dagger \hat{\rho} U. \) Since

\[
U^\dagger P_1 U = \frac{P_1 + P_2}{2} + \frac{\cos(2\theta)}{2} \sigma^{12} + \frac{\sin(2\theta)}{2} \sigma^{12}
\]

and

\[
U^\dagger \sigma^{12} U = \cos(2\theta)\sigma^{12} + \sin(2\theta)\sigma^{12}
\]

system (3) reads

\[
\frac{d}{dt} \hat{\xi} = \epsilon\hat{\Omega}_{12}[\sigma^{12}, \hat{\xi}] + ... \]

\[
...\epsilon\frac{\Gamma_{12}}{4}\text{Tr} \left( \left( P_1 + P_2 \right) + \frac{\cos(2\theta)}{2} \sigma^{12} + \frac{\sin(2\theta)}{2} \sigma^{12} \right) (\xi - \hat{\xi}) \right) + ...
\]

\[
\left( \cos(2\theta)\sigma^{12} + \sin(2\theta)\sigma^{12} \right) \dot{\xi} + \hat{\xi} \left( \cos(2\theta)\sigma^{12} + \sin(2\theta)\sigma^{12} \right) - 2\text{Tr} \left( \left( \cos(2\theta)\sigma^{12} + \sin(2\theta)\sigma^{12} \right) (\xi - \hat{\xi}) \right) \dot{\xi}
\]

\[
\frac{d}{dt} \hat{\Omega}_{12} = \epsilon\gamma_{12} \text{Tr} \left( \left( \cos(2\theta)\sigma^{12} + \sin(2\theta)\sigma^{12} \right) [\sigma^{12}, \hat{\xi}] \right) + ...
\]

with \( \epsilon\hat{\Omega}_{12} = \hat{\Omega}_{12} - \Omega_{12}. \) Since \( \frac{d}{dt} \xi = 0, \) for \( \epsilon \) small enough we can consider the average system:

\[
\frac{d}{dt} \xi = \epsilon\hat{\Omega}_{12}[(\sigma^{12}, \hat{\xi}) + ... \]

\[
...\epsilon\frac{\Gamma_{12}}{4}\text{Tr} \left( \left( \sigma^{12}\right)^{12} \xi + \hat{\xi} \sigma^{12} - 2\text{Tr} \left( \sigma^{12} \xi \right) \hat{\xi} \right) + ...
\]

\[
...\frac{\Gamma_{12}}{4}\text{Tr} \left( \left( \sigma^{12}(\xi - \hat{\xi}) \right) \xi + \hat{\xi} \sigma^{12} - 2\text{Tr} \left( \sigma^{12} \xi \right) \hat{\xi} \right)
\]

But \( \xi = \xi \) and \( \hat{\Omega}_{12} = \Omega_{12} = 0 \) is a steady state of this average system. Assume we have proved that this equilibrium is exponentially stable. Then the averaging theorem (see, e.g., [7, theorem 4.1.1, page 168]) ensures that the above time-periodic system admits a unique periodic orbit exponentially stable near \( (\xi, 0). \) Since \( (\xi, 0) \) is also an equilibrium of this time-periodic system, this exponentially stable orbit coincides with this equilibrium and the theorem is proved.

Let us prove now that \( (\xi, 0) \) is a hyperbolically stable equilibrium of the average system. We have \( \text{Tr}(\sigma^{12}[\sigma^{12}, \xi] \hat{\xi}) = \text{Tr}(\sigma^{12}, \sigma^{12}, \xi) \) and \( [\sigma^{12}, \sigma^{12}] = -2\sigma^{12}. \) Thus \( \text{Tr}(\sigma^{12}[\sigma^{12}, \xi] \hat{\xi}) = \text{Tr}(\sigma^{12} \sigma^{12} \xi \hat{\xi}) \) and \( \text{Tr}(\sigma^{12} \sigma^{12} \xi \hat{\xi}) = -2\text{Tr}(\sigma^{12} \sigma^{12} \xi \hat{\xi}) \) Thus the average system reads

\[
\frac{d}{dt} \xi = \epsilon\hat{\Omega}_{12}[\sigma^{12}, \xi] + ...
\]

\[
...\epsilon\frac{\Gamma_{12}}{4}\text{Tr} \left( \left( \sigma^{12}(\xi - \hat{\xi}) \right) \xi + \hat{\xi} \sigma^{12} - 2\text{Tr} \left( \sigma^{12} \xi \right) \hat{\xi} \right) + ...
\]

\[
...\frac{\Gamma_{12}}{4}\text{Tr} \left( \left( \sigma^{12}(\xi - \hat{\xi}) \right) \xi + \hat{\xi} \sigma^{12} - 2\text{Tr} \left( \sigma^{12} \xi \right) \hat{\xi} \right)
\]

Assumption \( \text{Tr}((P_1 + P_2)\rho(0)) > 0 \) implies that \( \text{Tr}((P_1 + P_2)\xi) > 0 \). We can choose the initial value of \( \theta \) such that \( \text{Tr}(P_1 \xi) > 0 \). Then \( (P_1 + P_2)\xi > 0 \) and \( (P_2 + P_2)\xi = 0 \). \( \xi \) and \( \hat{\xi} \) belong to \( \mathbb{R}^2 \) and around \( \xi \) the variables \( \hat{\xi} = \text{Tr}(\sigma^{12} \xi) \) and \( \hat{\xi} = \text{Tr}(P_2 \xi) \) form local coordinates for \( \hat{\xi} \): when \( \hat{\xi} = \xi, \hat{\xi} = 0 \) and \( \hat{\xi} = a \) with \( a \in [0, 1] \). Some standard computations yield to the following linearized dynamics:

\[
\frac{d}{dt} \hat{x} = -2\epsilon a\hat{\Omega}_{12} - \frac{\epsilon a\Gamma_{12}}{2} \hat{\xi}
\]

\[
\frac{d}{dt} \hat{\xi} = \frac{\epsilon a(1 - a)\Gamma_{12}}{2} \hat{\xi}
\]

(6)

with \( \hat{x} = \hat{x} \) and \( \hat{\xi} = \hat{\xi} - a \). This linearized system is exponentially stable.
Remark 1: The stability of the above average system (5) is more than local. It admits the following Lyapunov function:

\[ \frac{4}{\gamma_{12}}(\Omega_{12})^2 + \text{Tr}(\sigma_1^{12}(\xi - \hat{\xi})^2) + \text{Tr}(\sigma_2^{12}(\xi - \hat{\xi})^2) \]

Even if theorem 4 is a local stability result, the proposed estimator 3 should have a large attraction region. This is corroborated by simulations of figure 1.

V. ESTIMATION OF \( \Omega_{23} \)

Theorem 2: Take system 1 with inputs \( u_{12} = 1, u_{23} = \eta \cos \theta \) where \( \eta \) is constant and \( \frac{\partial}{\partial \theta} \Omega_{12} \). Consider the estimation of \( \rho \) and \( \Omega_{23} \) via (4). Take \( \Gamma_{23} > 0 \) and \( \gamma_{23} > 0 \). Assume \( \rho \) is a real projector with \( \text{Tr}((P_1 + P_2)\rho(0)) > 0 \).

Then for \( \epsilon \), \( \eta \) positive and small enough, exists \( \sigma > 0 \) such that, if \( \hat{\rho}(0) \) is a real projector such that \( 1 - \text{Tr}(\hat{\rho}(0)\rho(0)) \leq \sigma \) and \( \Omega_{23}(0) = \Omega_{23} \leq \sigma \), then \( \lim_{t \to +\infty} \hat{\rho}(t) - \rho(t) = 0 \) and \( \lim_{t \to +\infty} \Omega_{23}(t) = \Omega_{23} \).

Proof: The unitary real transformation \( U = e^{i\theta \sigma^{12}} \) reads \( P_1 + \cos \theta (P_1 + P_2) + \sin \theta \sigma^{12} \). Consider the attached change of frames \( \xi = U^\dagger \rho U, \hat{\xi} = U^\dagger \hat{\rho} U \). Since \( U^\dagger \sigma^{23} U = \cos \theta \sigma^{23} - \sin \theta \sigma^{13}, \xi \) obeys to

\[
\frac{d}{dt} \dot{\xi} = \eta \cos \theta \Omega_{23}[\sigma^{23}, \xi] + \eta \cos \theta \sin \theta \Omega_{23}[\sigma^{13}, \xi] + ...
\]

and 4 becomes

\[
\frac{d}{dt} \dot{\xi} = \eta \cos \theta \Omega_{23}[\sigma^{23}, \xi] + \eta \cos \theta \sin \theta \Omega_{23}[\sigma^{13}, \xi] + ...
\]

In average,

\[
\text{Tr}\left( (I_{12} + \cos(2\theta)\sigma_1^{12} + \sin(2\theta)\sigma_2^{12}) (\xi - \hat{\xi}) \right) \left( 1 - 2\cos(2\theta) \right)
\]

is equal to \( \text{Tr}\left( P_2(\xi - \hat{\xi}) \right) \). After neglecting the highly oscillating terms, we obtain:

\[
\frac{d}{dt} \xi = \eta \frac{1}{2} \Omega_{23}(\sigma^{23}, \xi) \]

of the above average system converges locally exponentially towards \( (\xi, \Omega_{23}) \). Since \( (\xi, \Omega_{23}) = (\xi, \Omega_{23}) \) is also solution of the original system 4, this implies that, for \( \eta \) small enough, \( (\xi, \Omega_{23}) \) converges locally towards \( (\xi, \Omega_{23}) \). This convergence is exponential.

VI. CONCLUSION

For a 3-level system 1 with only a single population measurement we have proposed an algorithm in two steps for the estimation of \( \Omega_{12} \) and \( \Omega_{23} \). Simulations show the robustness to additive noise of this algorithm relying on nonlinear asymptotic observers preserving the usual symmetries (change of frames). Theorems 1 and 2 ensure the local and exponential convergence. We can imagine switching periodically between estimation of \( \Omega_{12} \) via 4 and estimation of \( \Omega_{23} \) via 3 in order to produce estimations of \( \Omega_{12} \) and \( \Omega_{23} \) in real-time.

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