[18] A. Papachristodoulou, M. M. Peet, and S. Lall, "Analysis of polynomial systems with time delays via the sum of squares decomposition," *IEEE Trans. Autom. Control*, vol. 54, no. 5, pp. 1058–1064, 2009.
[19] P. Parrillo, "Semidefinite programming relaxations for semialgebraic problems," *Math. Program. Ser. B*, vol. 96, no. 2, pp. 293–320, 2003.
[20] J. P. Richard, "Time-delay systems: An overview of some recent advances and open problems," *Automatica*, vol. 39, pp. 1667–1694, 2003.
[21] C. W. Scherer and C. W. J. Hol, "Matrix sum-of-squares relaxations for robust semi-definite programs," *Math. Program.*, vol. 107, no. 1–2, pp. 189–211, 2006.
[22] W. Tan and A. Packard, "Stability region analysis using polynomial and composite polynomial Lyapunov functions and sum-of-squares programming," *IEEE Trans. Autom. Control*, vol. 53, pp. 565–571, 2008.
[23] U. Topcu, A. Packard, and P. Seiler, "Local stability analysis using simulations and sum-of-squares programming," *Automatica*, vol. 44, pp. 2669–2675, 2008.

Hamiltonian Identification Through Enhanced Observability Utilizing Quantum Control

Zaki Leghtas, Gabriel Turinici, Herschel Rabitz, and Pierre Rouchon

***Abstract*—This note considers Hamiltonian identification for a controllable quantum system with nondegenerate transitions and a known initial state. We assume to have at our disposal a single scalar control input and the population measure of only one state at an (arbitrarily large) final time T. We prove that the quantum dipole moment matrix is locally observable in the following sense: for any two close but distinct dipole moment matrices, we construct discriminating controls giving two different measurements. This result suggests that what may appear at first to be very restrictive measurements are actually rich for identification, when combined with well designed discriminating controls, to uniquely identify the complete dipole moment of such systems.**

***Index Terms*—Hamiltonian identification, observability proof, quantum control.**

I. Introduction

Quantum control has been receiving increasing attention [1] and one of its promising applications is to Hamiltonian identification [2] by using the ability to actively control a quantum system as a means to gain information about the underlying Hamiltonian governing its dynamics. The underlying premise is that controls may be found which make the measurements not only robust to noise but also highly sensitive to the unknown parameters in the Hamiltonian. Hence, although the performance of laboratory measurements may be constrained, the ability to control a quantum system has the prospect of turning this data into a rich source of information on the system's Hamiltonian.

Manuscript received February 14, 2011; revised October 10, 2011; accepted January 26, 2012. Date of publication March 08, 2012; date of current version September 21, 2012. This work was supported by the U.S. Department of Energy, by the ANR, Projet Blanc EMAQS No. ANR-2011-BS01-017-01, by ANR, Projet C-QUID BLAN-3-139579, by the Agence Nationale de la Recherche (ANR), Projet Jeunes Chercheurs EPOQ2 ANR-09-JCJC-0070, and by the CNRS through a PICS grant. Recommended by Associate Editor M. R. James.

Z. Leghtas is with the INRIA Paris-Rocquencourt, Domaine de Voluceau, 78153 Le Chesnay Cedex, France. (e-mail: zaki.leghtas@inria.fr).
G. Turinici is with the CEREMADE, Université Paris Dauphine, 75775 Paris Cedex 16, France. (e-mail: Gabriel.Turinici@dauphine.fr).
H. Rabitz is with the Department of Chemistry, Princeton University, Frick Laboratory, Princeton, NJ 08544 USA (e-mail: hrabitz@princeton.edu).
P. Rouchon is with the Centre Automatique et Systèmes, Mines-ParisTech, 75272 Paris Cedex, France (e-mail: pierre.rouchon@mines-paristech.fr).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.
Digital Object Identifier 10.1109/TAC.2012.2190209

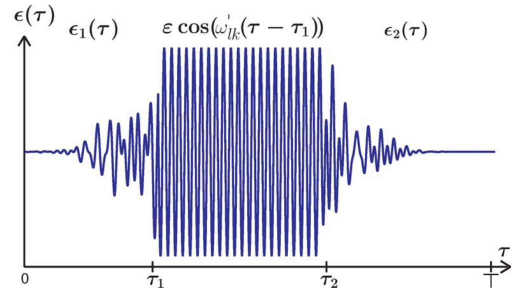

Fig. 1. A *good* control ϵ has three components (inspired from Ramsey interferometry) to enable the identification of μ_{lk}. The field ϵ_1 is defined over $[0, \tau_1]$ (analog of first Ramsey pulse) to steer the known initial state $|i\rangle$ to $|\psi_1\rangle = |l\rangle$: $|l\rangle = U(\tau_1, 0)|i\rangle$. The field ϵ_2 is defined over $[\tau_2, \mathsf{T}]$ (analog of second Ramsey pulse) is such that $|f\rangle = U(\mathsf{T}, \tau_2)|\psi_2\rangle$ where $|\psi_2\rangle = U(\tau_2, \tau_1)\left((|l\rangle + \imath|k\rangle)/\sqrt{2}\right)$ and the propagator $U(\tau_2, \tau_1)$ corresponds, for a long interval $\tau_2 - \tau_1$, to a large number of Rabi oscillations with the control $\varepsilon\cos(\omega'_{lk}(\tau-\tau_1))$ resonant with the $|l\rangle \leftrightarrow |k\rangle$ transition.

In this note, we consider the problem of identifying the dipole moment (which is assumed to be real) of an N–level quantum system, initialized to a known state (ground state), from a single population measurement at one arbitrarily large time T. We suppose an ability to freely control the system with a time dependent electric field $\epsilon(t)$. The measurements are obtained by: (i) initializing at time $t = 0$ the system's state at a known state $|i\rangle$, (ii) controlling in open loop and without measurement the system with an electric field $\epsilon_k(t)$ for $t \in [0, T]$ where $T > 0$, and (iii) measuring at final time T the population of one state $|f\rangle$. This may be repeated for many controls $(\epsilon_k)_k$. We prove the existence of controls which make the identification from one population measurement a well posed problem (theorem 1). These controls have a simple physical interpretation in analogy with Ramsey interferometry (see Fig. 1).

The perspective above combined with control theory is motivated by three practical arguments. First, measuring a state population at one time T is a technique which can have a very high signal-to-noise ratio (~ 100). Second, technological progress with spatial light modulators (SLM) permits generating a broad variety of controls in the laboratory. Third, ultrashort pulsed fields can be well measured in the laboratory [3]. Hence, we are able to design a variety of precisely known control inputs.

Le Bris *et al.* [4] prove the observability of the dipole moment when the population of all states are measured over an arbitrarily large interval of time. Algorithms to reconstruct the dipole from the measured data were proposed using nonlinear observers [5], [6]. A different setting is considered in [7], [8] where it is supposed that one can prepare and measure the system in a set of orthogonal states at various times, and the available data is the probability to measure the system in a certain state when it was prepared in another; Bayesian estimation is used to reconstruct the energy levels, the damping constants and the dipole moment from the measured data. We consider here the less demanding case where the only available measurement is the population of one state at one arbitrarily large time, and the initial state is known and coincides with the ground state.

The note is organized as follows. In Section II we state the main result in Theorem 1, and Section III gives the proof of the Theorem and an important lemma on which the main result is based. Finally concluding remarks are presented in Section IV.

II. Observability of the Quantum Dipole Moment

A. Problem Setting

We consider a quantum system in a pure state described by the wave function $|\psi\rangle \in \mathcal{S}$. Here $\mathcal{S}$ is the set of N dimensional complex vectors of unit norm. The system interacts with an electric field (the real control input) $\epsilon \in \mathcal{E}_T$ for some $T > 0$ with $\mathcal{E}_T \triangleq \{f : [0,T] \to \mathbb{R} \,|\, f \text{ piecewise continuous}\}$. For a given control ϵ we measure the population of the state $|f\rangle$ at time T denoted as $P_{if}(\epsilon)$. We denote by H_0 the free Hamiltonian (Hermitian matrix) and by μ the dipole moment operator, also a Hermitian matrix. The initial state $|i\rangle$ and the measured state $|f\rangle$ are eigenvectors of H_0. We consider a semiclassical model for the light-matter interaction, and the dynamics of $|\psi\rangle$ are given by the Schrodinger equation

$$\imath\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = (H_0 - \epsilon(t)\mu) |\psi(t)\rangle$$
$$|\psi(0)\rangle = |i\rangle, \quad P_{if}(\epsilon) = |\langle f|\psi(T)\rangle|^2 . \qquad (1)$$

For all $T > 0$, we suppose that we can create any field $\epsilon \in \mathcal{E}_T$ and that we can measure $P_{if}(\epsilon)$. For M different fields $\{\epsilon_1, \ldots, \epsilon_M\}$ we can collect the measurements $\{P_{if}(\epsilon_1), \ldots, P_{if}(\epsilon_M)\}$. Through (1), P_{if} is a function of μ and a functional of ϵ, and when necessary this explicit dependence will be written as $P_{if}(\epsilon, \mu)$. The aim of this note is to explore the feasibility of estimating the dipole moment μ from the measured data $\{P_{if}(\epsilon_1), \ldots, P_{if}(\epsilon_M)\}$ using well chosen controls $\{\epsilon_1, \ldots, \epsilon_M\}$. Below, $P_{if}(\epsilon, \mu)$ refers to the measurement achieved on the real system using a control ϵ, and for any $\hat\mu$, $P_{if}(\epsilon, \hat\mu)$ is the estimated measurement which is obtained by simulating system (1) with the control ϵ and coupling $\hat\mu$.

B. Main Result

For all $k \le N$ we denote $|k\rangle$ as the eigenvector of H_0 with associated eigenvalue E_k. Throughout the note, all matrices are written in the basis $(|1\rangle, \ldots, |N\rangle)$. The initial and measured states correspond to some indexes $i, f \in \{1, \ldots, N\}$. For all $k, l \le N$ we specify $\sigma_x^{lk} \triangleq |l\rangle\langle k| + |k\rangle\langle l|$. We define

$$\mathcal{M} \triangleq \mathrm{Span}\{\sigma_x^{lk} \backslash k, l \le N \text{ with } \mathrm{Tr}\left(\mu\sigma_x^{lk}\right) \ne 0\}$$

with Tr being the trace operation. When all nondiagonal elements of μ are nonnull $M = \dim(\mathcal{M}) = (N(N-1))/2$. The main result is as follows.

Theorem 1: Consider a real symmetric matrix μ with zero diagonal entries and a real diagonal matrix H_0 with nondegenerate transitions. Suppose that the system state in (1) *is controllable. Then for any positive constant α there exists a time $T > 0$ and M fields $(\epsilon_1, \ldots, \epsilon_M) \in \mathcal{E}_T{}^M$ such that the cost function*

$$J : \mathcal{M} \ni \hat\mu \to \sum_{k=1}^{M} \left(P_{if}(\epsilon_k, \hat\mu) - P_{if}(\epsilon_k, \mu)\right)^2$$

is in $\mathcal{C}^2(\mathcal{M}, \mathbb{R})$ and locally α-convex[1] around μ.

$\mathcal{C}^k(A, B)$ denotes the set of k times continuously differentiable functions defined over A with values in B. In the Appendix we provide the definitions of controllability and a matrix with nondegenerate transitions. Here and throughout this note, the norm of matrix μ, noted $\|\mu\|$ refers to the max norm.

[1]The smallest eigenvalue of the Hessian $\nabla^2 J(\mu)$ is larger than α.

A direct consequence of Theorem 1 is the local observability of the dipole moment:

Corollary 1: Under the assumptions of Theorem 1, the dipole moment is locally observable in $\mathcal{M}$.

Proof: Take $\alpha > 0$. Theorem 1 implies that there exists a time $T > 0$ and M fields $(\epsilon_1, \ldots, \epsilon_M) \in \mathcal{E}_T{}^M$ such that the cost function J is $\mathcal{C}^2(\mathcal{M}, \mathbb{R})$ and locally α-convex around μ. Hence there $\exists r > 0$ such that for all $\hat\mu \in \mathcal{M}$ with $\|\hat\mu - \mu\| \le r$ and $\hat\mu \ne \mu$, $J(\hat\mu) > 0$, and hence there exists $\epsilon \in \{\epsilon_1, \ldots, \epsilon_M\}$ such that $P_{if}(\epsilon, \hat\mu) - P_{if}(\epsilon, \mu) \ne 0$. □

Remark 1: The local α–convexity is a property stronger than the mere possibility to identify the dipole matrix. It states that the distinction between a dipole candidate $\hat\mu$ and the true dipole μ can be observed (through the measurements aggregated in J) to first order in the distance $\|\mu - \hat\mu\|$. This first-order dependence of the measurement P_{if} with respect to the dipole μ is addressed in more detail in lemma 1. For well chosen controls, the J function has a very simple shape around μ and a simple gradient algorithm could be used to identify it.

The eigenvalues of H_0 are commonly measured through spectroscopy and can be found in reference tables [9] with precisions of order 10^{-7}. The result of Theorem 1 is also relevant for the problem of discriminating between two molecules with the same free Hamiltonian and different effective dipole operators. In that framework, $\hat\mu$ and μ would be the dipole operators of these two molecules (as opposed to one estimated and one true dipole, as considered in this note), and the aim is to find controls which produce different data sets for these two different but similar quantum systems. This was experimentally accomplished in [10] where a genetic algorithm is used to find these discriminating controls. A complementary theoretical controllability analysis can be found in [11].

Proofs

C. Existence of Discriminating Controls

We denote $\mu' = (1/\|\mu\|)\mu$ the normalized dimensionless dipole moment operator, $\mu'_{lk} \triangleq \mathrm{Tr}\left(\mu'\sigma_x^{lk}\right)$ and $(\partial P_{if}/\partial\mu'_{lk})(\epsilon)$ the partial derivative of $P_{if}(\epsilon)$ with respect to μ'_{lk}. Theorem 1 is based on the following lemma.

Lemma 1: Suppose that μ is real, symmetric and has only zeros on its diagonal and H_0 is real, diagonal, with nondegenerate transitions. Suppose system (1) *is controllable. Then for all (l,k) with $\mu_{lk} \ne 0$, there exists $\xi_0 > 0$ such that, for all $\xi \in]0, \xi_0[$, exist $T > 0$ and $\epsilon \in \mathcal{E}_T$ satisfying*

- $(\partial P_{if}/\partial\mu'_{lk})(\epsilon) = 1/2\xi + O(1)$
- $\forall\{m,n\} \ne \{l,k\}$ *with* $\mu_{mn} \ne 0$, $(\partial P_{if}/\partial\mu'_{mn})(\epsilon) = O(1)$,

where $O(1)$ corresponds to zero-order terms with respect to ξ around 0^+.

Proof of Theorem 1

To each pair of integers (l_p, k_p), $l_p < k_p$ such that $\mathrm{Tr}\left(\mu'\sigma_x^{l_p k_p}\right) \ne 0$ we associate a unique index $p \in \{1, \ldots, M\}$, and we define $\sigma_x^p \triangleq \sigma_x^{l_p k_p}$ along with $\mu'_p \triangleq \mathrm{Tr}\left(\mu'\sigma_x^p\right)$.

According to lemma 1, $\exists\xi_0 > 0$ such that $\forall\xi \in]0, \xi_0[$, $\exists\ T_1, \ldots, T_M$ and $(\epsilon_1, \ldots, \epsilon_M) \in \mathcal{E}_{T_1} \times \cdots \times \mathcal{E}_{T_M}$ such that: (i) $\forall p \in [1 : M]$ $(\partial P_{if}/\partial\mu'_p)(\epsilon_p) = 1/2\xi + O(1)$ and (ii) $\forall p' \ne p$ $(\partial P_{if}/\partial\mu'_{p'})(\epsilon_p) = O(1)$. We take $T = \max(T_1, \ldots, T_M)$ and for all $k \in \{1, \ldots, M\}$ we extend the definition of ϵ_k from $[0, T_k]$ to $[0, T]$ by taking $\epsilon_k(t) = 0$ for all $t \in]T_k, T]$. We will use $J : \mathcal{M} \to \mathbb{R}$ defined by:

$$J(\hat\mu) = \sum_{k=1}^{M} \left(P_{if}(\epsilon_k, \hat\mu) - P_{if}(\epsilon_k, \mu)\right)^2.$$

For a fixed $T > 0$ and $\epsilon \in \mathcal{E}_T$, since $\hat{\mu} \to P_{if}(\epsilon, \hat{\mu})$ is in $\mathcal{C}^2(\mathcal{M}, \mathbb{R})$, $J(\hat{\mu})$ is in $\mathcal{C}^2(\mathcal{M}, \mathbb{R})$. We find

$$\frac{\partial^2 J}{\partial \mu'_p \partial \mu'_{p'}}(\mu) = \sum_{k=1}^{M} \frac{\partial P_{if}}{\partial \mu'_p}(\epsilon_k, \mu) \frac{\partial P_{if}}{\partial \mu'_{p'}}(\epsilon_k, \mu)$$

so that for all $p \in \{1, \ldots, M\} : (\partial^2 J/\partial {\mu'_p}^2)(\mu) = 1/4\xi^2 + O(1/\xi)$ and when $p \neq p'$ $(\partial^2 J/\partial \mu'_p \partial \mu'_{p'})(\mu) = O(1/\xi)$. We have: $\nabla^2 J(\mu) = (1/4\xi^2)(I + O(\xi))$, where $\nabla^2 J(\mu)$ is the Hessian of J at μ and I is the identity matrix. The smallest eigenvalue of $\nabla^2 J(\mu)$ scales as $(1/4\xi^2)(1 + O(\xi))$, hence by taking ξ small enough it can be made larger than α thereby reaching the conclusion above. □

Proof of Lemma 1

We define the dimensionless time scale $\tau \triangleq (1/\hbar) \|H_0\| t$ and also $\top \triangleq (1/\hbar) \|H_0\| T$. For two times $\tau, \tau' \in [0, \top]$ we define the propagator $U(\tau', \tau)$ such that $|\psi(\tau')\rangle = U(\tau', \tau) |\psi(\tau)\rangle$. Rewriting (1) for $U(\tau, 0)$ we obtain

$$\imath \frac{\partial}{\partial \tau} U(\tau, 0) = \frac{1}{\|H_0\|}(H_0 - \epsilon(\tau)\mu) U(\tau, 0)$$
$$P_{if}(\epsilon) = |\langle f| U(\top, 0) |i\rangle|^2, U(0,0) = I. \quad (2)$$

The proof of lemma 1 has two parts I and II separately treated below.

Part I: Take two times $\tau_1, \tau_2, 0 < \tau_1 < \tau_2 < \top$. We can write (for any complex z we denote by $\bar{z}$ its complex conjugate): $P_{if}(\epsilon) = z\bar{z}$ where $z = \langle f| U(\top, \tau_2) U(\tau_2, \tau_1) U(\tau_1, 0) |i\rangle$.

Denote for any $m, n = 1, \ldots, M : \omega'_{mn} \triangleq (E_m - E_n)/\|H_0\|$ and consider the control defined on $[\tau_1, \tau_2]$

$$\epsilon(\tau) = \varepsilon \cos(\omega'_{lk}(\tau - \tau_1)) \quad (3)$$

where ε is a small strictly positive real parameter. Take $\xi = \|\mu\| \varepsilon / \|H_0\|$. The only remaining degree of freedom in the control over $[\tau_1, \tau_2]$ is ξ, which can be taken arbitrarily small. We define $H'_0 = (1/\|H_0\|) H_0$ and $\omega'_{mn} = \langle m| H'_0 |m\rangle - \langle n| H'_0 |n\rangle$. Note that $\omega'_{mn} = -\omega'_{nm}$. We have [12]

$$\frac{\partial}{\partial \mu'_{lk}} U(\tau_2, \tau_1) = \imath \frac{\|\mu\|}{\|H_0\|} U(\tau_2, \tau_1) \times \int_{\tau_1}^{\tau_2} \epsilon(\tau) U^\dagger(\tau, \tau_1) \sigma_x^{lk} U(\tau, \tau_1) d\tau. \quad (4)$$

We now rewrite (2) and (4) for the control given in (3) on the time interval $[\tau_1, \tau_2]$

$$\imath \frac{\partial}{\partial \tau} U(\tau, \tau_1) = (H'_0 - \xi \cos(\omega'_{lk}(\tau - \tau_1)) \mu') U(\tau, \tau_1) \quad (5)$$
$$\frac{\partial}{\partial \mu'_{lk}} U(\tau_2, \tau_1) = \imath \xi U(\tau_2, \tau_1) \times \int_{\tau_1}^{\tau_2} \cos(\omega'_{lk}(\tau - \tau_1)) U^\dagger(\tau, \tau_1) \sigma_x^{lk} U(\tau, \tau_1) d\tau. \quad (6)$$

The goal is to show that $(\partial/\partial \mu'_{lk}) U(\tau_2, \tau_1)$ can be made arbitrarily "large" while $(\partial/\partial \mu'_{mn}) U(\tau_2, \tau_1)$ stays bounded. Note that all the terms in the integrand of (6) are bounded, and a rough estimate of the norm of $(\partial/\partial \mu'_{lk}) U(\tau_2, \tau_1)$ gives a quantity proportional to $(\tau_2 - \tau_1)\xi$. Hence, we take $\tau_2 - \tau_1 = 1/\xi^2$, implying the need to have expressions for $U(\tau, \tau_1)$ over a time scale on the order of $1/\xi^2$. To this end we state lemma 2 which gives such an approximation.

Lemma 2: Consider (5). *There exists a Hermitian matrix K and $\xi_0 > 0$ such that, for any $\xi \in]0, \xi_0[$, we have*

$$\sup_{\tau \in [\tau_1, \tau_1 + \frac{1}{\xi^2}]} \left\| U(\tau, \tau_1) - e^{-\imath H'_0 (\tau - \tau_1)} e^{\imath (\xi \frac{\mu'_{lk}}{2} \sigma_x^{lk} + \xi^2 K)(\tau - \tau_1)} \right\| = O(\xi).$$

We continue with the proof of Lemma 1 and will come back to Lemma 2 in Section III-D.

Using the expression of $U(\tau, \tau_1)$ given in lemma 2, the integrand in (6) is

$$\cos(\omega'_{lk}(\tau - \tau_1)) U^\dagger(\tau, \tau_1) \sigma_x^{lk} U(\tau, \tau_1) = e^{-\imath (\xi (\mu'_{lk}/2) \sigma_x^{lk} + \xi^2 K)(\tau - \tau_1)} (\cos(\omega'_{lk}(\tau - \tau_1)) e^{\imath H'_0 (\tau - \tau_1)} \sigma_x^{lk} e^{-\imath H'_0 (\tau - \tau_1)}) e^{\imath (\xi (\mu'_{lk}/2) \sigma_x^{lk} + \xi^2 K)(\tau - \tau_1)} + O(\xi).$$

In order to compute (6), we need the following result:

$$\cos(\omega'_{lk}(\tau - \tau_1)) e^{\imath H'_0 (\tau - \tau_1)} \sigma_x^{lk} e^{-\imath H'_0 (\tau - \tau_1)} = \frac{1}{2} \sigma_x^{lk} + \frac{1}{2} \cos(2\omega'_{lk}(\tau - \tau_1)) \sigma_x^{lk} + \frac{1}{2} \sin(2\omega'_{lk}(\tau - \tau_1)) \sigma_y^{lk} \quad (7)$$

where we denote $\sigma_y^{lk} = +\imath |l\rangle \langle k| - \imath |k\rangle \langle l|$. In (7), the terms oscillating at frequency $2\omega'_{lk}$ independent of ξ will only contribute to $O(\xi)$ in (6). We now focus on the contribution of the term with σ_x^{lk} in (6) which calls for (see the Appendix) $\forall \tau$

$$e^{-\imath (\xi (\mu'_{lk}/2) \sigma_x^{lk} + \xi^2 K)(\tau - \tau_1)} \sigma_x^{lk} e^{\imath (\xi (\mu'_{lk}/2) \sigma_x^{lk} + \xi^2 K)(\tau - \tau_1)} = \sigma_x^{lk} + O(\xi). \quad (8)$$

Introducing (8) into (6), we find

$$\frac{\partial}{\partial \mu'_{lk}} U(\tau_2, \tau_1) = \imath \xi U(\tau_2, \tau_1) \left(\frac{\tau_2 - \tau_1}{2} \sigma_x^{lk} + O(1) + (\tau_2 - \tau_1) O(\xi) \right).$$

From now on, we take $\tau_2 = \tau_1 + 1/\xi^2$ and obtain

$$\frac{\partial}{\partial \mu'_{lk}} U(\tau_2, \tau_1) = \imath U(\tau_2, \tau_1) \left(\frac{1}{2\xi} \sigma_x^{lk} + O(1) \right). \quad (9)$$

We define $|\psi_1\rangle \triangleq |l\rangle$ and $|\psi_2\rangle \triangleq (1/\sqrt{2}) U(\tau_2, \tau_1)(|l\rangle + \imath |k\rangle)$. Since the system is controllable there exists a time τ_1 and a field $\epsilon_1 \in \mathcal{E}_{\tau_1}$ such that $U(\tau_1, 0) |i\rangle = |\psi_1\rangle$, and there exists a time $\top$ and a field ϵ_2 defined over $[\tau_2, \top]$ such that $U^\dagger(\top, \tau_2) |f\rangle = |\psi_2\rangle$. Since the state space is compact (here it is a sphere), we know that if the system is controllable, it is controllable in bounded time, and with bounded controls (see [13, Th. 6.5]). Hence, $\top - \tau_2$ can be chosen bounded for all ξ. Therefore $(\partial/\partial \mu_{lk}) U(0, \tau_1)$ and $(\partial/\partial \mu_{lk}) U(\tau_2, \top)$ are bounded. Thus, we have

$$\frac{\partial}{\partial \mu'_{lk}} P_{if}(\epsilon) = 2\Re(\langle f| U(\top, \tau_2) \frac{\partial}{\partial \mu'_{lk}} U(\tau_2, \tau_1) U(\tau_1, 0) |i\rangle \langle i| U^\dagger(\tau_1, 0) U^\dagger(\tau_2, \tau_1) U^\dagger(\top, \tau_2) |f\rangle) + O(1).$$

We now utilize $U(\tau_1, 0) |i\rangle = |\psi_1\rangle$ and $U^\dagger(\top, \tau_2) |f\rangle = |\psi_2\rangle$ where $|\psi_1\rangle$ and $|\psi_2\rangle$ are defined above, and replace $(\partial/\partial \mu'_{lk}) U(\tau_2, \tau_1)$ by its expression in (9) to find: $(\partial/\partial \mu'_{lk}) P_{if}(\epsilon) = 1/2\xi + O(1)$. This expression holds for the control defined as (see Fig. 1)

$$\epsilon(\tau) = \begin{cases} \epsilon_1(\tau), & \text{if } \tau \in [0, \tau_1] \\ \frac{\|H_0\|}{\|\mu\|} \xi \cos(\omega'_{lk}(\tau - \tau_1)), & \text{if } \tau \in]\tau_1, \tau_2[\\ \epsilon_2(\tau), & \text{if } \tau \in [\tau_2, \top] \end{cases}. \quad (10)$$

Part II: We now need to prove that $(\partial/\partial\mu'_{mn})P_{if}(\epsilon) = O(1)$ for $\{m,n\} \neq \{l,k\}$, where ϵ is the control found above in (10). As in (6), we have

$$\frac{\partial}{\partial\mu'_{mn}}U(\tau_2,\tau_1) = \imath\xi U(\tau_2,\tau_1) \times \int_{\tau_1}^{\tau_2}\cos(\omega'_{lk}(\tau-\tau_1))U^\dagger(\tau,\tau_1)\sigma_x^{mn}U(\tau,\tau_1)d\tau \quad (11)$$

and again the result of lemma 2 is employed. Equation (11) calls for

$$\begin{aligned}2\cos(\omega'_{lk}(\tau-\tau_1))&e^{\imath H'_0(\tau-\tau_1)}\sigma_x^{mn}e^{-\imath H'_0(\tau-\tau_1)}\\ &= \cos((\omega'_{lk}-\omega'_{mn})(\tau-\tau_1))\sigma_x^{mn}\\ &\quad -\sin((\omega'_{lk}-\omega'_{mn})(\tau-\tau_1))\sigma_y^{mn}\\ &\quad +\cos((\omega'_{lk}+\omega'_{mn})(\tau-\tau_1))\sigma_x^{mn}\\ &\quad +\sin((\omega'_{lk}+\omega'_{mn})(\tau-\tau_1))\sigma_y^{mn}. \end{aligned} \quad (12)$$

Considering that H_0 has nondegenerate transitions (see definition in the Appendix) implies that $\omega'_{lk}-\omega'_{mn} \neq 0$ and $\omega'_{lk}+\omega'_{mn} \neq 0$. As the expression in (12) oscillates at frequencies independent of ξ, it therefore contributes to $O(\xi)$ in (11). Hence, for $\tau_2-\tau_1 = 1/\xi^2$ we can directly conclude that $(\partial/\partial\mu'_{mn})P_{if}(\epsilon) = O(1)$. □

Proof of Lemma 2

This proof relies on three consecutive changes of frame that aim to cancel the oscillating terms of order 0 and 1 with respect to ξ. We then derive a specific form of the averaging Theorem (see [14, Th. 4.3.6] for a general form of the averaging theorem). For the sake of clarity and with no loss of generality, we take $\tau_1 = 0$ and note $U(\tau) \triangleq U(\tau,\tau_1)$. Equation (5) may be written in the interaction frame $U_I(\tau) \triangleq e^{\imath H'_0\tau}U(\tau)$

$$\frac{\partial}{\partial\tau}U_I(\tau) = \imath\xi\left(\frac{\mu'_{lk}}{2}\sigma_x^{lk} + \frac{\partial}{\partial\tau}H_I(\tau)\right)U_I(\tau)$$

where

$$\frac{\partial}{\partial\tau}H_I(\tau) = \frac{1}{2}\sum_{(m,n)\neq(k,l)}\mu'_{mn}e^{\imath(-\omega'_{kl}+\omega'_{mn})\tau}|m\rangle\langle n| + \frac{1}{2}\sum_{(m,n)\neq(l,k)}\mu'_{mn}e^{\imath(-\omega'_{lk}+\omega'_{mn})\tau}|m\rangle\langle n|$$

and the average of H_I is zero. The average of a time dependent operator $C(\tau)$ is defined as follows (see [14, def. 4.2.4]): $\overline{C} = \lim_{\theta\to+\infty}(1/\theta)\int_0^\theta C(\tau)d\tau$. We now take $U'_I(\tau) = (I-\imath\xi H_I(\tau))U_I(\tau)$. Since $(\partial/\partial\tau)H_I$ is almost periodic[2], then H_I is also almost periodic and hence bounded for all τ. Hence, there exists $\xi_0 > 0$, $\forall\xi < \xi_0$, $I-\imath\xi H_I(\tau)$ has an inverse and $(I-\imath\xi H_I(\tau))^{-1} = I+\imath\xi H_I(\tau)+O(\xi^2)$. We find

$$\frac{\partial}{\partial\tau}U'_I(\tau) = \imath\left(\xi\frac{\mu'_{lk}}{2}\sigma_x^{lk} - \imath\xi^2\left(\frac{\mu'_{lk}}{2}[H_I(\tau),\sigma_x^{lk}] + H_I(\tau)\frac{\partial}{\partial\tau}H_I(\tau)\right) + O(\xi^3)\right)U'_I(\tau).$$

Notice that, with $K = -\imath\overline{H_I(\partial/\partial\tau)H_I}$ independent of ξ and $\tilde{K}(\tau)$ almost periodic with zero average, we also have

$$\frac{\mu'_{lk}}{2}[H_I(\tau),\sigma_x^{lk}] + H_I(\tau)\frac{\partial}{\partial\tau}H_I(\tau) = \imath\left(K + \frac{\partial}{\partial\tau}\tilde{K}(\tau)\right).$$

[2]Can be written as $\sum_{k=1}^{M}e^{i\omega_k\tau}A_k$

It is important to note that

$$\frac{1}{2}\overline{\frac{\partial}{\partial\tau}H_I^2} = 0 = \overline{H_I\frac{\partial}{\partial\tau}H_I} + \overline{\left(\frac{\partial}{\partial\tau}H_I\right)H_I} = \imath(K-K^\dagger).$$

Hence $K = K^\dagger$ is Hermitian.

We now take $U''_I(\tau) = (I-\imath\xi^2\tilde{K}(\tau))U'_I(\tau)$. Since $\tilde{K}(\tau)$ is bounded for all τ, then for a sufficiently small ξ, $I-\imath\xi^2\tilde{K}(\tau)$ has an inverse and $(I-\imath\xi^2\tilde{K}(\tau))^{-1} = I+\imath\xi^2\tilde{K}(\tau)+O(\xi^4)$. U''_I satisfies the following equation:

$$\frac{\partial}{\partial\tau}U''_I(\tau) = \imath\left(\xi\frac{\mu'_{lk}}{2}\sigma_x^{lk} + \xi^2K + O(\xi^3)\right)U''_I(\tau) \quad (13)$$

and we define U_{av} to be the solution to the averaged dynamics ($U_{av}(0) = I$)

$$\frac{\partial}{\partial\tau}U_{av}(\tau) = \imath\left(\xi\frac{\mu'_{lk}}{2}\sigma_x^{lk} + \xi^2K\right)U_{av}(\tau). \quad (14)$$

We can directly solve (14): $U_{av}(\tau) = e^{\imath(\xi(\mu'_{lk}/2)\sigma_x^{lk}+\xi^2K)\tau}$. Subtracting (13) from(14), we find, using Gronwall's lemma, that for all $\tau < 1/\xi^2$ one has $U''_I(\tau) = U_{av}(\tau)+O(\xi)$. Also note that to go from U_I to U''_I we have used two consecutive changes of variables which are close to the identity, hence, $\forall\tau$ $U''_I(\tau) = U_I(\tau)+O(\xi)$. Finally, since $e^{-\imath H'_0\tau}$ is an isometry, we have

$$U(\tau) = e^{-\imath H'_0\tau}e^{\imath(\xi(\mu'_{lk}/2)\sigma_x^{lk}+\xi^2K)\tau} + O(\xi) \text{ for all } \tau \leq \frac{1}{\xi^2}.$$

□

III. Conclusion

Identification of the real dipole moment matrix is shown to be well posed for a controllable finite dimensional quantum system with nondegenerate transitions and using as measurements only one population at a final time T. The results also provide a theoretical foundation to optimal discrimination experiments.

Appendix

Definition 1: We say that system (1) *is controllable[15] if for all* $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{S}$ *there exists a time* t *and a control* $\epsilon \in \mathcal{E}_t$ *such that for* $|\psi(0)\rangle = |\psi_1\rangle$, (1) *leads to* $|\psi(t)\rangle = |\psi_2\rangle$.

Definition 2: Let H_0 *and* μ *be* $N\times N$ *Hermitian matrices. We denote* $E_1,\ldots,E_N$ *the eigenvalues of* H_0 *and* $|1\rangle,\ldots,|N\rangle$ *its corresponding eigenvectors. We say that* H_0 *has nondegenerate transitions [16] if* $\forall(l,k)\neq(m,n)$, $l\neq k$ *and* $m\neq n$, *such that* $\langle l|\mu|k\rangle \neq 0$ *and* $\langle m|\mu|n\rangle \neq 0$, *we have* $E_l-E_k \neq E_m-E_n$.

Definition 3: Take system (1). *Let us denote* $\mathcal{M}$ *as the space to which* μ *belongs. We say that* μ *is locally observable in* $\mathcal{M}$ *if there exists* $r > 0$ *such that for all* $\hat{\mu} \in \mathcal{M}$ *with* $0 < \|\hat{\mu}-\mu\| \leq r$ and $\hat{\mu} \neq \mu$, *there exists* $T > 0$ *and* $\epsilon \in \mathcal{E}_T$ *such that* $P_{if}(\epsilon,\hat{\mu}) \neq P_{if}(\epsilon,\mu)$.

Computation: Here, we compute

$$\Sigma_x^{lk}(\tau) = e^{-i(\xi(\mu'_{lk}/2)\sigma_x^{lk}+\xi^2K)(\tau-\tau_1)}\sigma_x^{lk}e^{i(\xi(\mu'_{lk}/2)\sigma_x^{lk}+\xi^2K)(\tau-\tau_1)}.$$

We have $\mu'_{lk} \neq 0$ and $\sigma_x^{lk}+\xi(2K/\mu'_{lk})$ is Hermitian. Hence, there exists a unitary matrix P_ξ and a real diagonal matrix Δ_ξ such that $\sigma_x^{lk}+\xi(2K/\mu'_{lk}) = P_\xi\Delta_\xi P_\xi^\dagger$. The function $\xi \in [0,\xi_0] \to \sigma_x^{lk}+\xi(2K/\mu'_{lk})$ is analytic, therefore the eigenvectors of $\sigma_x^{lk}+\xi(2K/\mu'_{lk})$ can be continued analytically as a function of ξ (see [17, Th. 6.1 in ch.

II, Sec. 6 section 1 and 2]). Hence, $P_\xi = P_0 + O(\xi)$ where P_0 is such that $P_0^\dagger \sigma_x^{lk} P_0 = \sigma_z^{lk}$ is real and diagonal. $\sigma_z^{lk} = |l\rangle\langle l| - |k\rangle\langle k|$. We find $\forall\tau$: $\Sigma_x^{lk}(\tau) = \sigma_x^{lk} + O(\xi)$, where $O(\xi)$ is a first-order term in ξ and a bounded function of τ.

Acknowledgment

The authors thank M. Mirrahimi and A. Goun for discussions.

References

[1] C. Brif, R. Chakrabarti, and H. Rabitz, "Control of quantum phenomena: past, present and future," *New J. Phys.*, vol. 12, no. 7, p. 075008, 2010.

[2] W. S. Warren, H. Rabitz, and M. Dahleh, "Coherent control of quantum dynamics: the dream is alive," *Science*, vol. 259, pp. 1581–1589, 1993.

[3] C. Iaconis and I. Walmsley, "Spectral phase interferometry for direct electric-field reconstruction of ultrashort optical pulses," *Opt. Lett.*, vol. 23, no. 10, pp. 792–794, 1998.

[4] C. LeBris, M. Mirrahimi, H. Rabitz, and G. Turinici, "Hamiltonian identification for quantum systems: well-posedness and numerical approaches," *ESAIM*, vol. 13, no. 2, pp. 378–395, 2007.

[5] Z. Leghtas, M. Mirrahimi, and P. Rouchon, "Parameter estimation of a 3-level quantum system with a single population measurement," in *Proc. IEEE. 48th CDC*, 2009, pp. 3816–3820.

[6] S. Bonnabel, M. Mirrahimi, and P. Rouchon, "Observer-based Hamiltonian identification for quantum systems," *Automatica*, vol. 45, no. 5, pp. 1144–1155, 2009.

[7] S. Schirmer and F. Langbein, "Quantum system identification: Hamiltonian estimation using spectral and Bayesian analysis," in *Proc. ISCCSP*, 2010, pp. 1–5.

[8] S. Schirmer and D. Oi, "Quantum system identification by Bayesian analysis of noisy data: Beyond Hamiltonian tomography," *Laser Phys.*, vol. 20, pp. 1203–1209, 2010.

[9] E.g See National Institute of Standards and Technology (NIST) Data Sheets.

[10] J. Petersen *et al.*, "How shaped light discriminates nearly identical biochromophores," *Phys. Rev. Lett.*, vol. 105, p. 073003, 2010.

[11] G. Turinici, V. Ramakhrishna, B. Li, and H. Rabitz, "Optimal discrimination of multiple quantum systems: controllability analysis," *J. Phys. A*, vol. 37, no. 1, p. 273, 2004.

[12] V. Beltrani, J. Dominy, T. Ho, and H. Rabitz, "Photonic reagent control of dynamically homologous quantum systems," *J. Chem. Phys*, vol. 126, no. 094105, 2007.

[13] V. Jurdjevic and H. J. Sussmann, "Control systems on Lie groups," *J. Diff. Eq.*, vol. 12, pp. 313–329, 1972.

[14] J. Sanders, F. Verhulst, and J. Murdock, *Averaging Methods in Nonlinear Dynamical Systems*. New York: Springer, 2007.

[15] D. D'Alessandro, *Introduction to Quantum Control and Dynamics*. London, U.K.: Chapman and Hall/CRC, 2008.

[16] G. Turinici and H. Rabitz, "Wavefunction controllability for finite-dimensional bilinear quantum systems," *J. Phys. A*, vol. 36, no. 10, p. 2565, 2003.

[17] T. Kato, *Perturbation Theory for Linear Operators*. New York: Springer, 1966.

Robust Control of Constrained Linear Systems With Bounded Disturbances

Reza Ghaemi, Jing Sun, *Fellow, IEEE*, and Ilya V. Kolmanovsky, *Fellow, IEEE*

***Abstract*—This technical note develops a novel robust control algorithm for linear systems subject to additive and bounded disturbances. The approach is based on the constraint tightening method. While this problem can be tackled using existing robust model predictive control techniques, the proposed method has an advantage in that it is computationally efficient and avoids the need to solve repeatedly an online optimization problem, while the optimization problem solved at initialization is a simple linear programming problem. The algorithm elaborated in this technical note guarantees convergence to a minimal disturbance invariant set, and the terminal predicted state constraint set is allowed to be larger than the minimal disturbance invariant set. As an illustration, the developed algorithm is applied to constrained roll control of a ship operating in a wave field. Simulation results show that the proposed approach reduces the ship roll motion while the input and dynamic stall constraints are satisfied.**

***Index Terms*—Model predictive control (MPC).**

I. Introduction

In this technical note, we consider a control problem for constrained discrete-time linear systems that are subject to bounded additive disturbances. Our goal is to provide a control method that enforces specified state and input constraints in the presence of disturbances and steers state trajectories to a given target set.

This problem has been studied employing invariant set methods (see [1], [2] and references therein) and optimization based control strategies such as model predictive control (MPC) [3]. In the MPC literature, one approach relies on sufficient contractivity of the open-loop system [4]. MPC strategies in which a deterministic control sequence is optimized, may result in a small domain of attraction hence another approach has been proposed in which optimization is performed over feedback policies [5]. However, optimization over arbitrary feedback policies, in the presence of constraints, may be especially difficult. As an alternative, affine feedback policies were employed where the state feedback gain(s) are calculated off-line and optimization was performed over constant offset terms [6]–[8].

Many robust MPC schemes are based on tightening the constraints (on states and controls) over the prediction horizon. This method was proposed initially in [9] as well as in [6], [10]–[12]. Based on constrained tightening approach, a robust MPC for nonlinear systems subject to bounded disturbances has been introduced in [13], that guarantees convergence to an ellipsoidal disturbance invariant set. An alter-

Manuscript received January 09, 2011; revised June 22, 2011; accepted March 14, 2012. Date of publication April 19, 2012; date of current version September 21, 2012. This work is supported in part by the National Science FoundationNSF ECS-0501284 and ONR N00014-05-1-0537. Recommended by Associate Editor T. Zhou.

R. Ghaemi is with the Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 USA (e-mail: ghaemi@mit.edu).

J. Sun is with the Department of Naval Architecture and Marine Engineering, The University of Michigan, Ann Arbor, MI 48109 USA (e-mail: jingsun@umich.edu).

I. V. Kolmanovsky is with the Department of Aerospace Engineering, The University of Michigan, Ann Arbor, MI 48109 USA (e-mail: ilya@umich.edu; ikolmano@ieee.org).

Color versions of one or more of the figures in this technical note are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/TAC.2012.2192362