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Optimal discrimination of multiple quantum systems: controllability analysis

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Abstract
A theoretical study is presented concerning the ability to dynamically discriminate between members of a set of different (but possibly similar) quantum systems. This discrimination is analysed in terms of independently and simultaneously steering about the wavefunction of each component system to a target state of interest using a tailored control (i.e. laser) field. Controllability criteria are revealed and their applicability is demonstrated in simple cases. Discussion is also presented in some uncontrollable cases.

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1. Introduction

Laser control of complex molecular and solid-state systems is becoming feasible, especially through the introduction of closed loop laboratory learning techniques [1, 2]. A specific chemical or physical goal is best achieved through the introduction of an optimally tailored laser field. Successful control may be expressed as a matter of high quality discrimination, whereby the control field steers the evolving quantum system dynamics out of the desired channel, while diminishing competitive flux into other undesirable channels. This discrimination is achieved through tailored field manipulation of constructive and destructive quantum wave interferences.

Building on the latter concepts and capabilities, a potential application of quantum control techniques is to the detection of specific molecules amongst others of similar chemical/physical characteristics. In this context, ordinary spectroscopies may be viewed as one-dimensional discrimination tools (i.e., in the frequency domain). Cases of special interest for discrimination include large polyatomic molecules of similar chemical nature, where their spectra can often mask each other. Molecules that appear as similar in a static (i.e., spectroscopic) sense may have dynamically very distinct behaviour, as revealed by their wavepackets evolving to become increasingly disparate for ready discrimination under the guidance of a suitable optimal laser control field.

The scenario outlined above describes a potentially valuable use of molecular optimal laser techniques for purposes of analytical detection. A simple application of this idea in a non-optimal framework for isotope separation has already been demonstrated in diatomic molecules [3]. A recent closed loop study discriminating two spectrally similar molecules in solution also indicates that this can be done [4]. Optimal control will be especially important for discriminating complex polyatomic molecules, and at the present time, the bounds of molecular discrimination have yet to be explored. A generic analysis would consist in applying a tailored laser field to a mixture of molecules, to stimulate wavepacket motion in such a fashion that a discriminating signal can be detected from one or more of the species present. Distinct control fields might aim at drawing out the presence of one molecular species over that of all others. In practice, such optimal fields would be deduced in the laboratory using closed loop learning control techniques [5].

Much work needs to be done to explore and develop the concept of coherent molecular discrimination, and a basic step in that direction is to establish the criteria for, in principle, independently controlling the dynamics of two or more molecular species with a single control field. This issue falls into the general category of controllability theory [6, 7], which aims at assessing the ability to steer a quantum system from an arbitrary initial state to an arbitrary final state, although other weaker forms of controllability may be defined. If a system is fully controllable, then, in principle, at least one field exists capable of steering the quantum system about in an arbitrary fashion. Discrimination of multiple molecules is a special case of this concept, where the full system consists of a set of subsystems (i.e., molecules of different type). In the simplest circumstances, the molecules may be taken as independent and non-interacting, such that the initial state $|\phi(0)\rangle = \prod_{\ell=1}^{L} |\phi_\ell(0)\rangle$ is a product of states $|\phi_\ell(0)\rangle$ for each of the $L \geqslant 2$ molecular species placed under simultaneous control. Full controllability would correspond to the ability to simultaneously and arbitrarily steer about each of the states $|\phi_\ell(0)\rangle \to |\phi_\ell(t)\rangle$, $t \geqslant 0$ under the influence of a single control laser electric field $\epsilon(t)$, where each molecule evolves under a separate Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t}|\phi_\ell(t)\rangle = \left[H_0^\ell - \mu^\ell \cdot \epsilon(t)\right]|\phi_\ell(t)\rangle. \tag{1}$$

Here, H_0^ℓ and μ^ℓ, respectively, are the free Hamiltonian and dipole of the ℓth molecule. Other more relaxed controllability criteria might also be specified. For example, a practical discrimination goal is that only a single molecular species ℓ^* be actively influenced by the field $\epsilon(t)$, while all other molecules $\ell \neq \ell^*$ evolve under just their associated free Hamiltonian H_0^ℓ. In the laboratory, the systems would generally be in an initial mixture of states specified by the temperature; such a case calls for extending the controllability concepts to consider the density matrix. The analysis here will be confined to the wavefunction.

The present paper aims at presenting the algorithmic concepts underlying quantum system controllability of an ensemble of L separate quantum systems in the presence of a single electric field $\epsilon(t)$. Section 2 of the paper reviews some of the essential components of quantum controllability, and then presents a formulation for exploring controllability of multiple quantum systems. We present in section 3 an algorithm that implements the theoretical results of section 2; section 4 gives some simple illustrations of the concepts, followed by a general discussion in section 5.

2. Theoretical controllability

The purpose of this section is to give theoretical criteria for the controllability of an ensemble of L separate quantum systems in the presence of a single electric field $\epsilon(t)$. The criteria will refer to a *finite-dimensional* setting where, for each ℓ, $0 \leqslant \ell \leqslant L$, the Hamiltonian H_0^ℓ and dipole operator μ^ℓ are expressed with respect to an eigenbasis of some relevant operator associated with the ℓth system. We will further suppose that the operators involved are developed in an eigenbasis of the internal Hamiltonians, as is typically the case in applications. More precisely, let $D^\ell = \left\{\phi_i^\ell(x); i = 1, \ldots, N_\ell\right\}$ be the set of the first N_ℓ, $N_\ell \geqslant 3$ eigenstates of the possibly infinite dimensional Hamiltonian H_0^ℓ, let M^ℓ be the linear space they generate, and let A^ℓ and B^ℓ be the matrices of the operators $-\mathrm{i}H_0^\ell$ and $-\mathrm{i}\mu^\ell$ respectively, with respect to this base. In order to exclude trivial control settings, it is supposed that $[A^\ell, B^\ell] \neq 0$, $\ell = 1, \ldots, L$.[5] From the definition of the basis D^ℓ and the fact that H_0^ℓ and μ^ℓ are Hermitian operators, it follows that A^ℓ is diagonal with purely imaginary elements and B^ℓ is skew-Hermitian. We will suppose moreover that

$$\forall \ell = 1, \ldots, L : \mathrm{Tr}(A^\ell) \neq 0 \qquad \mathrm{Tr}(B^\ell) = 0. \tag{2}$$

The assumption $\mathrm{Tr}(A^\ell) \neq 0$ is never restrictive in practice as eigenvalues of the internal Hamiltonian usually have common sign and are not all zero. The assumption $\mathrm{Tr}(B^\ell) = 0$ is also true for many realistic dipole interactions where the diagonal elements vanish (no self-interaction). As will be seen in section 2, the theoretical results can be extended to the case where this assumption is not satisfied.

Let us note that the results presented below remain valid when multiple $s > 1$ external fields are considered, which can be expressed by introducing multiple dipole moment operators μ_i^ℓ, $i = 1, \ldots, s$. Here i may label distinct spatial orientations.

With these notations, the wavefunction of the ℓth system can be written as $|\phi_\ell(t)\rangle = \sum_{i=1}^{N_\ell} c_i^\ell(t)\left|\phi_i^\ell\right\rangle$. The total wavefunction $\prod_{\ell=1}^{L} |\phi_\ell(t)\rangle$ will be represented as a column vector $c(t) = \left(c_1^1(t), \ldots, c_{N_1}^1(t), \ldots, c_1^L(t), \ldots, c_{N_L}^L(t)\right)^T$. Denote $N = \sum_{\ell=1}^{L} N_\ell$, A to be the $N \times N$ skew block-diagonal matrix obtained from A^ℓ, $\ell = 1, \ldots, L$ and B to be the skew block-diagonal matrix obtained from B^ℓ, $\ell = 1, \ldots, L$:

$$A = \begin{pmatrix} A^1 & 0 & \ldots & 0 \\ 0 & A^2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & A^L \end{pmatrix} \qquad B = \begin{pmatrix} B^1 & 0 & \ldots & 0 \\ 0 & B^2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & B^L \end{pmatrix}. \tag{3}$$

We will write this as $A = \mathrm{Diag}(A^\ell)_{\ell=1}^L$, $B = \mathrm{Diag}(B^\ell)_{\ell=1}^L$. With the scaling convention $\hbar = 1$, the dynamical equations read

$$\frac{\mathrm{d}}{\mathrm{d}t} c(t) = Ac(t) + \epsilon(t)Bc(t) \qquad c(0) = c_0. \tag{4}$$

Recalling that each individual wavefunction $|\phi_\ell(t)\rangle = \sum_{i=1}^{N_\ell} c_i^\ell(t)\left|\phi_i^\ell\right\rangle$ is L^2 unit normalized, we obtain in a discrete representation:

$$\sum_{i=1}^{N_\ell} \left|c_i^\ell(t)\right|^2 = 1 \qquad \forall t \geqslant 0 \qquad \forall \ell = 1, \ldots, L. \tag{5}$$

[5] The Lie bracket $[\cdot, \cdot]$ is defined as $[U, V] = UV - VU$.

Denote by $\mathcal{S}_{\mathbb{C}}^{k-1}$ the complex unit sphere of $\mathbb{C}^k$.[6] Equation (5) reads

$$c(t) \in \mathcal{S} = \prod_{\ell=1}^{L} \mathcal{S}_{\mathbb{C}}^{N_\ell - 1} \qquad \forall t \geqslant 0. \tag{6}$$

Define the admissible control set $\mathcal{U}$ as the set of all piecewise continuous functions $\epsilon(t)$. With this definition, equation (4) has a (unique) solution for all $t \geqslant 0$. The system $\big((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\big)$ is said to be *controllable* if for any $c_i, c_f \in \mathcal{S}$ there exists a $t_f \geqslant 0$ (possibly depending on c_i, c_f) and $\epsilon(t) \in \mathcal{U}$ such that the solution of (4) with initial data $c(0) = c_i$ satisfies $c(t_f) = c_f$.

In order for the system $((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U})$ to be controllable each component system $(A^\ell, B^\ell, \mathcal{U})\ell = 1, \ldots, N$ has to be controllable, i.e. each system taken independently has to be controllable. However, requiring that all systems be controllable at the same time and with the same laser field is a more demanding condition; we will see later in section 4 an example of a pair of systems that are individually controllable but not jointly controllable. The goal of this paper is therefore to give practical criteria that allow for assessing simultaneous controllability of independent quantum systems.

In order to study the controllability properties of the system $\big((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\big)$ we introduce the following Lie algebra,

$$\begin{aligned} \mathcal{L} = \Big\{ X = \mathrm{Diag}(X^\ell)_{\ell=1}^L, X^\ell \in u(N_\ell), \ell = 1, \ldots, L; \\ (\mathrm{Tr}(X^\ell))_{\ell=1}^L = \lambda (\mathrm{Tr}\,(A^\ell))_{\ell=1}^L \text{ for some } \lambda \in \mathbb{R} \Big\} \end{aligned} \tag{7}$$

where $u(N)$ denotes the Lie algebra of N-dimensional skew-Hermitian matrices.

Note that no straightforward derivation of controllability criteria is possible from the classical results on the controllability of bilinear systems: the most natural Lie group to consider, i.e. the Lie group associated with the Lie algebra $\mathcal{L}(A, B)$ may not be closed hence compact. In fact, this Lie group is compact when the quotients $\frac{\mathrm{Tr}(A^{\ell_1})}{\mathrm{Tr}(A^{\ell_2})}$ are rational numbers (for all $\ell_1, \ell_2 = 1, \ldots, L$), which is an artificial requirement that does not add to the comprehension of the phenomena involved. A detailed analysis is therefore pursued in order to recover controllability criteria similar to those in [8] without the use of the technical condition above.

Since $A, B \in \mathcal{L}$, the Lie algebra generated by A and B is included in $\mathcal{L}$. Note that the dimension of $\mathcal{L}$ as a vector space over $\mathbb{R}$ is

$$\dim_{\mathbb{R}}(\mathcal{L}) = \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right) + 1. \tag{8}$$

Indeed, for any $\ell = 1, \ldots, L$, $\dim_{\mathbb{R}} u(N_\ell) = (N_\ell)^2$; the $L - 1$ additional constraints come from the requirement that $(\mathrm{Tr}(X^\ell))_{\ell=1}^L$ and $(\mathrm{Tr}(A^\ell))_{\ell=1}^L$ be proportional[7].

Denote

$$\mathcal{A}(c_0, T) = \{c(t) \text{ solution of (4)}, t \in [0, T], \epsilon \in \mathcal{U}\} \tag{9}$$

$$\mathcal{A}(c_0) = \bigcup_{t \geqslant 0} \mathcal{A}(c_0, t). \tag{10}$$

The set $\mathcal{A}(c_0)$ will be called the *set of points attainable from* c_0; the evolution system is controllable if (and only if) $\mathcal{A}(c_0) = \mathcal{S}$ for any $c_0 \in \mathcal{S}$.

[6] Here $\mathbb{C}$ denotes the set of complex numbers.

[7] The requirement $\lambda \in \mathbb{R}$ (and not in $\mathbb{C}$) does not bring any additional constraint as the trace of skew-Hermitian matrices is always purely imaginary.

Table 1. Criteria summary for the simultaneous controllability of independent quantum systems. Cases marked with a dash '–' denote situations not covered by the theory; in general these cases give rise to uncontrollable settings; cases marked with a 'N/A' denotes a combination of parameters that is impossible; note that $\dim_{\mathbb{R}} \mathcal{L}(A, B)$ cannot take values larger than $2 + \sum_{\ell=1}^{L}(N_\ell^2 - 1)$.

	$\dim_{\mathbb{R}} \mathcal{L}(A, B) = \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right)$	$\dim_{\mathbb{R}} \mathcal{L}(A, B) = 1 + \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right)$	$\dim_{\mathbb{R}} \mathcal{L}(A, B) = 2 + \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right)$
All dipoles have zero trace All Hamiltonians have zero trace	Controllable	N/A	N/A
All dipoles have zero trace At least one Hamiltonian has nonzero trace	–	Controllable	N/A
The vector of all dipole traces $(\mathrm{Tr}(B^\ell))_{\ell=1}^L$ and the vector of all Hamiltonian traces $(\mathrm{Tr}(A^\ell))_{\ell=1}^L$ are linearly dependent	–	Controllable	N/A
The vector of all dipole traces $(\mathrm{Tr}(B^\ell))_{\ell=1}^L$ and the vector of all Hamiltonian traces $(\mathrm{Tr}(A^\ell))_{\ell=1}^L$ are linearly independent	–	–	Controllable

We are now ready to give the main controllability criterion. Denote by $\mathcal{L}(A, B)$ the Lie sub-algebra of $\mathcal{L}$ generated by A and B.

Theorem 1. *If*

$$\dim_{\mathbb{R}} \mathcal{L}(A, B) = 1 + \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right) \tag{11}$$

then the system $\left((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\right)$ *is controllable (the dimension of* $\mathcal{L}(A, B)$ *is computed over the scalar field* $\mathbb{R}$*). Moreover, when the system is controllable, there exists a time* $T > 0$ *such that all targets can be attained before or at time* T*, i.e. for any* $c_0 \in \mathcal{S}$, $\mathcal{A}(c_0, T) = \mathcal{S}$.

Proof. See the appendix. □

Complementary results can also be obtained for the case of non-zero dipole moment traces or traceless internal Hamiltonians. We summarize below the controllability criteria that are useful in situations where the assumption in equation (2) is broken for some $\ell \in \{1, \dots, L\}$.

Theorem 2.

(a) If the vectors $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ *and* $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ *are linearly dependent and* $\dim_{\mathbb{R}} \mathcal{L}(A, B) = 1 + \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right)$*, then the system* $\left((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\right)$ *is controllable.*
(b) If the vectors $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ *and* $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ *are linearly independent and* $\dim_{\mathbb{R}} \mathcal{L}(A, B) = \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right) + 2$*, then the system* $\left((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\right)$ *is controllable.*
(c) If the vectors $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ *and* $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ *are both zero and* $\dim_{\mathbb{R}} \mathcal{L}(A, B) = \sum_{\ell=1}^{L} \left(N_\ell^2 - 1\right)$*, then the system* $\left((A^\ell, B^\ell)_{\ell=1}^L, \mathcal{U}\right)$ *is controllable.*

Proof. See the appendix. □

3. Algorithmic considerations

The controllability criteria given in section 2 are summarized in table 1. Starting from the table we can establish the following four-step algorithm to assess controllability in a given setting:

(i) The proper representation bases $D^\ell, \ell = 1, \dots, L$ are identified such that the internal Hamiltonian matrices are diagonal; the matrices A and B are constructed as in equaton (3).

(ii) The traces $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ of the internal Hamiltonians and the traces of the dipole moments $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ are computed.

(iii) The dimension $d = \dim_{\mathbb{R}} \mathcal{L}(A, B)$ (as real vector space) of the Lie algebra $\mathcal{L}$ generated by A and B is computed.

(iv) If the following criteria are satisfied

(a) the dimension d equals $2 + \sum_{\ell=1}^L \left(N_\ell^2 - 1\right)$

or

(b) all traces $\mathrm{Tr}\, A^\ell, \ell = 1, \dots, N$ and $\mathrm{Tr}\, B^\ell, \ell = 1, \dots, N$ are zero and d equals $\sum_{\ell=1}^L \left(N_\ell^2 - 1\right)$

or

(c) the vectors $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ and $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ are linearly dependent and d equals $1 + \sum_{\ell=1}^L \left(N_\ell^2 - 1\right)$

then the system is controllable; all other cases not satisfying the criteria may correspond to non-controllable settings (but the present theory gives no definite assessment).

Note that the situation (iva) of the algorithm only happens when the vectors $(\mathrm{Tr}\, A^\ell)_{\ell=1}^L$ and $(\mathrm{Tr}\, B^\ell)_{\ell=1}^L$ are linearly independent and thus in particular non-null (also see the caption to table 1).

4. Applications

Armed with the theoretical results of the previous sections we will now consider some applications to illustrate the basic concepts.

We begin with a simple case of two ($L = 2$) three-level systems $N_1 = 3$, $N_2 = 3$ having the same Hamiltonian but different dipole moments:

$$A^1 = A^2 = -\mathrm{i}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 5 \end{pmatrix} \qquad B^1 = -\mathrm{i}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \qquad B^2 = -B^1. \tag{12}$$

Each system A^1, B^1 and A^2, B^2 is controllable, which can be checked by the Lie algebra criterion of [8] (the dimension of the Lie algebra is found to be 9). Denoting by $\left(c_1^1, c_2^1, c_3^1\right)$ and by $\left(c_1^2, c_2^2, c_3^2\right)$ respectively the coefficients of the wavefunction of the first system and the second system, the dynamical equations are

$$\begin{aligned}
\mathrm{i}\frac{\partial}{\partial t} c_1^1(t) &= c_1^1 + \epsilon(t) c_2^1 \\
\mathrm{i}\frac{\partial}{\partial t} c_2^1(t) &= 2c_2^1 + \epsilon(t) c_1^1 + 2\epsilon(t) c_3^1 \\
\mathrm{i}\frac{\partial}{\partial t} c_3^1(t) &= 5c_3^1 + 2\epsilon(t) c_2^1 \\
\mathrm{i}\frac{\partial}{\partial t} c_1^2(t) &= c_1^2 - \epsilon(t) c_2^2 \\
\mathrm{i}\frac{\partial}{\partial t} c_2^2(t) &= 2c_2^2 - \epsilon(t) c_1^2 - 2\epsilon(t) c_3^2 \\
\mathrm{i}\frac{\partial}{\partial t} c_3^2(t) &= 5c_3^2 - 2\epsilon(t) c_2^2.
\end{aligned} \tag{13}$$

Let us analyse now this system with the theoretical tools presented above; this system corresponds to the second line of table 1. We expect that the Lie algebra will have dimension $3^2 + 3^2 - 1 = 17$ but the computation shows that the dimension of this algebra is 9. Although we cannot directly deduce from here that the system is not controllable (the criterion in table 1 is only sufficient, but not also necessary), we are warned by this test and we can analyse it further. The analysis of this system reveals a dynamical invariant (conservation law) that can be written as: for any evolution (i.e., for any $\epsilon(t)$)

$$L(t) = \overline{c_1^1(t)}c_1^2(t) + \overline{c_3^1(t)}c_3^2(t) - \overline{c_2^1(t)}c_2^2(t) = \text{constant} \tag{14}$$

where the overbar denotes complex conjugation. The presence of dynamical invariants implies that the system is not controllable because, for instance, starting with both systems in ground state i.e. $\left(c_1^1(0), c_2^1(0), c_3^1(0)\right) = (1, 0, 0)$, $\left(c_1^2(0), c_2^2(0), c_3^2(0)\right) = (1, 0, 0)$ one cannot steer both to their respective first excited state $\left(c_1^1(T), c_2^1(T), c_3^1(T)\right) = (0, 1, 0)$, $\left(c_1^2(T), c_2^2(T), c_3^2(T)\right) = (0, 1, 0)$. The reason is that in the ground states the dynamical invariant takes the value $L(0) = 1 + 0 - 0 = 1$ while for the first excited states the dynamical invariant is equal to $L(T) = 0 + 0 - 1 = -1$.

We continue this section with additional examples on how to use the algorithm presented above and we will then consider the more physically relevant goal of discriminating among similar systems.

Consider two three-level systems ($L = 2$, $N_1 = 3$, $N_2 = 3$) given by

$$A^1 = -\mathrm{i}\begin{pmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 3.0 \end{pmatrix} \qquad A^2 = -\mathrm{i}\begin{pmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 4.0 \end{pmatrix} \tag{15}$$

$$B^1 = -\mathrm{i}\begin{pmatrix} 0.0 & 1.0 & 0.0 \\ 1.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{pmatrix} \qquad B^2 = -\mathrm{i}\begin{pmatrix} 0.0 & 2.0 & 0.0 \\ 2.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{pmatrix}. \tag{16}$$

The dimension of the Lie algebra $\mathcal{L}(A, B)$ was computed with the online software from [9] (that implements an algorithm similar to that in [10]) and was found to be $17 = 1 + (3^2 - 1) + (3^2 - 1)$. We are thus in situation (ivc) of the algorithm; it follows that the two systems can be simultaneously controlled.

Suppose now that the first value on the diagonal of A^1 is changed from 0.0 to $(-\mathrm{i})(-5.0)$ and the first value on the diagonal of A^2 is changed from 0.0 to $(-\mathrm{i})(-6.0)$. The dimension of the Lie algebra $\mathcal{L}(A, B)$ is computed as $d = 16 = (3^2 - 1) + (3^2 - 1)$; the set of systems remains controllable because we are in situation (ivb) of the algorithm. Finally, consider the matrices A^1 and A^2 in equation (15) but change the first diagonal element of B^1 from 0.0 to $(-\mathrm{i})1.0$. The computation of d gives $d = 18 = 2 + (3^2 - 1) + (3^2 - 1)$; we are thus in the case (iva) of the algorithm and we conclude that the systems are again controllable; in particular the vectors of traces $(\mathrm{Tr}(A^1), \mathrm{Tr}(A^2)) = (-\mathrm{i})(5, 6)$ and $(\mathrm{Tr}(B^1), \mathrm{Tr}(B^2)) = (-\mathrm{i})(1, 0)$ are independent.

In order to investigate the degree of discrimination possible when similar systems are considered, theorem 1 was applied for various finite-level quantum systems. Consider [11] two four-level systems ($L = 2$, $N_1 = 4$, $N_2 = 4$):

$$A^1 = -\mathrm{i}\begin{pmatrix} 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 4.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 6.0 \end{pmatrix} \qquad A^2 = -\mathrm{i}\begin{pmatrix} 0.0052 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.007 & 0.0 & 0.0 \\ 0.0 & 0.0 & 3.9943 & 0.0 \\ 0.0 & 0.0 & 0.0 & 5.99 \end{pmatrix}$$

$$B^1 = -\mathrm{i}\begin{pmatrix} 0.0 & 1.6 & 0.3 & 0.7 \\ 1.6 & 0.0 & 0.8 & 0.2 \\ 0.3 & 0.8 & 0.0 & 0.9 \\ 0.7 & 0.2 & 0.9 & 0.0 \end{pmatrix} \qquad B^2 = -\mathrm{i}\begin{pmatrix} 0.0 & 1.5896 & 0.2977 & 0.6996 \\ 1.5896 & 0.0 & 0.8011 & 0.1985 \\ 0.2977 & 0.8011 & 0.0 & 0.894 \\ 0.6996 & 0.1985 & 0.894 & 0.0 \end{pmatrix}.$$

The dimension of the Lie algebra $\mathcal{L}(A, B)$ was found to be $31 = 1 + (4^2 - 1) + (4^2 - 1)$. By the alternative (ivc) of the algorithm in section 2 it follows that the two systems can be simultaneously controlled.

A further example drawn from an optimal control treatment was studied consisting of $L = 3$ similar quantum systems with each having $N_1 = N_2 = N_3 = 10$ levels. See footnote[8] for the matrix entries which indicate that the three species are quite similar. The computation of the dimension of the Lie algebra $\mathcal{L}(A, B)$ was pursued with the same software package [9] and is $298 = 1 + (10^2 - 1) + (10^2 - 1) + (10^2 - 1)$. From the alternative (ivc) of the algorithm we conclude that the three systems can be simultaneously controlled. This result is consistent with the numerical optimal control studies which showed excellent quality discrimination amongst these three species [11].

Finally consider the case

$$\begin{aligned} A^1 &= -\mathrm{i}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \qquad A^2 = -\mathrm{i}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 6 \end{pmatrix} \\ B^1 &= -\mathrm{i}\cdot\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \qquad B^2 = -\mathrm{i}\begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \end{aligned} \tag{17}$$

Each system A^1, B^1 and A^2, B^2 is controllable, but their union is not (the dimension of the Lie algebra generated by $\mathrm{Diag}(A^1, A^2)$ and $\mathrm{Diag}(B^1, B^2)$ is 9). In this case dynamical invariants exist, but due to the intricate form of their expression we omit presenting them here.

5. Discussion and conclusions

In an attempt to analyse the simultaneous controllability of a set of finite level independent quantum systems, this paper provides sufficient results for controllability using Lie group analysis specific to bilinear control settings. The criteria presented are tested with generic

[8] The representations are chosen such that the internal Hamiltonians $-\mathrm{i}A_1$, $\mathrm{i}A_2$ and $-\mathrm{i}A_3$ are diagonal with elements (2.9923, 5.9973, 8.6744, 10.9953, 13.0022, 14.6376, 15.9601, 16.9411, 17.5713, 17.8630), (2.9902, 5.9976, 8.6823, 11.0114, 13.0021, 14.6465, 15.9688, 16.9445, 17.5772, 17.8689) and (2.9998, 6.0064, 8.6842, 11.0037, 12.9945, 14.6543, 15.9689, 16.9349, 17.5775, 17.8607), respectively. The dipole matrices $-\mathrm{i}B_1$, $-\mathrm{i}B_2$ and $-\mathrm{i}B_3$ are symmetric and therefore we only give the lower triangular part of each one: we begin with the entry at line 2 column 1, continue until the entry at line 10 column 1 (9 entries in all) then go to column 2 (only 8 entries) etc. For $-\mathrm{i}B_1$ we have: 0.09760, −0.03660, 0.49041, 0.00640, −0.06500, 0.60770, −0.00140, 0.01328, −0.09290, 0.70360, 0.00040, −0.00347, 0.02174, −0.12250, 0.80120, −0.00010, 0.00100, −0.00620, 0.03187, −0.15560, 0.88880, 0.00000, −0.00038, 0.00210, −0.01010, 0.04340, −0.18831, 0.97425, 0.00000, 0.00010, −0.00080, 0.00360, −0.01490, 0.05690, −0.22170, 1.06240, 0.00000, −0.00006, 0.00030, −0.00140, 0.00588, −0.02100, 0.07307, −0.25970, 1.13400. For $-\mathrm{i}B_2$ we have: 0.09780, −0.03640, 0.48750, 0.00641, −0.06400, 0.60753, −0.00140, 0.01320, −0.09360, 0.70980, 0.00041, −0.00350, 0.02160, −0.12373, 0.80130, −0.00010, 0.00100, −0.00629, 0.03210, −0.15525, 0.89710, 0.00000, −0.00030, 0.00210, −0.01010, 0.04400, −0.18780, 0.97550, −0.00002, 0.00010, −0.00080, 0.00360, −0.01499, 0.05742, −0.22100, 1.06040, 0.00001, 0.00000, 0.00030, −0.00140, 0.00590, −0.02110, 0.07360, −0.25880, 1.13120. For $-\mathrm{i}B_3$ we have: 0.09695, −0.03650, 0.48710, 0.00640, −0.06468, 0.60530, −0.00148, 0.01310, −0.09290, 0.70920, 0.00040, −0.00340, 0.02160, −0.12460, 0.80316, −0.00013, 0.00107, −0.00620, 0.03150, −0.15390, 0.89069, 0.00005, −0.00030, 0.00212, −0.01009, 0.04373, −0.18690, 0.97970, 0.00000, 0.00015, −0.00081, 0.00369, −0.01480, 0.05780, −0.22302, 1.05500, 0.00000, 0.00000, 0.00034, −0.00150, 0.00580, −0.02114, 0.07240, −0.25955, 1.12540.

online software tools [9]. Even if the conditions are not necessary for controllability, examples are presented to show that when criteria are not fulfilled the systems become uncontrollable. Additional examples of quantum system discrimination are presented in another work [11] on optimal control of multiple quantum systems.

The present work extends the existing controllability analysis capabilities [8] to provide a new tool to assess the feasibility of achieving full quantum dynamic discrimination amongst similar systems modelled as finite dimensional. Although such finite dimensional model systems are often simplifications, they can provide insights and guidance for control algorithm development [11] to aid in the execution of laboratory studies on realistic systems. Applications can range from the analytical discrimination of similar molecules or the control of similar quantum dots with a single control field.

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Appendix. Mathematical considerations

Proof of theorem 1. The proof relies on the following lemmas: □

Lemma 1. *For any $c \in \mathcal{S}$ denote by $T_c\mathcal{S}$ the tangent space in c to $\mathcal{S}$. Then $\mathcal{L}c = T_c\mathcal{S}$, where $\mathcal{L}c = \{Mc; M \in \mathcal{L}\}$.*

Proof. Since $\prod_{\ell=1}^{L} su(N_\ell) \subset \mathcal{L} \subset \prod_{\ell=1}^{L} u(N_\ell)$ it follows that

$$\left(\prod_{\ell=1}^{L} su(N_\ell)\right) c \subset \mathcal{L}c \subset \left(\prod_{\ell=1}^{L} u(N_\ell)\right) c.$$

Since in addition $\left(\prod_{\ell=1}^{L} su(N_\ell)\right)c = T_c\mathcal{S}$ and $\left(\prod_{\ell=1}^{L} u(N_\ell)\right)c = T_c\mathcal{S}$ the conclusion of the lemma follows. □

Let us recall [12, 13] the following definition: a point $c \in \mathcal{S}$ is said to be Poisson stable (with respect to the vector field A) if for any neighbourhood V of c and every $T > 0$ there exist $t_1 > T$, $t_2 > T$ such that $\exp(t_1 A)(c) \in V$, $\exp(-t_2 A)(c) \in V$. With this definition we can state the following

Lemma 2. *All points $c \in \mathcal{S}$ are Poisson stable (with respect to the vector field A).*

Proof. Let c be any point of $\mathcal{S}$, $T > 0$ and $\epsilon > 0$. Consider now the set $E = \{\exp(nTA)c; n \in \mathbb{N}\}$.[9] Since E is a subset of the bounded set $\mathcal{S}$ it follows that there exist $n_2 > n_1 > 0$ such that $\|\exp(n_1TA)c - \exp(n_2TA)c\| \leqslant \epsilon$. Note that $\|\exp(n_1TA)c - \exp(n_2TA)c\| = \|\exp((n_2-n_1)TA)c - c\| = \|\exp((n_1-n_2)TA)c - c\|$. We have thus proved that for any $\epsilon > 0$ there exists $t_1 = t_2 = (n_2-n_1)T > T$ such that $\|\exp(t_1A)c - c\| \leqslant \epsilon$, $\|\exp(-t_2A)c - c\| \leqslant \epsilon$, which concludes the proof. □

Note that under the hypothesis of the theorem if follows from equation (8) that $\mathcal{L}(A, B) = \mathcal{L}$; therefore for any $c \in \mathcal{S} : \mathcal{L}(A, B)c = T_c\mathcal{S}$. In order to prove the first part of the theorem we apply the following version of a known result (see theorem 1 in [14] page 384

[9] Here $\mathbb{N}$ is the set of all non-negative integers.

or proposition 3.4 [12] page 715): if the set of Poisson stable points is dense in $\mathcal{S}$ and $\mathcal{L}(A, B)c = T_c\mathcal{S}$ for any $c \in \mathcal{S}$ then the system is controllable.

In order to prove the last part of the theorem, note that since the system is controllable we have, for any $c \in \mathcal{S}$: $\mathcal{A}(c) = \mathcal{S}$; note also that

$$\forall t > 0 \qquad \forall U \in \prod_{\ell=1}^{L} U(N_\ell) : \mathcal{A}(Uc, t) = U\mathcal{A}(c, t) \tag{A.1}$$

as $Uc(t)$ is the solution of (4) with initial data $Uc(0) = Uc$.

Let c be any point of $\mathcal{S}$; from $\mathcal{A}(c) = \mathcal{S}$ it follows that $\bigcup_{t\geqslant 0} \mathcal{A}(c, t) = \mathcal{S}$; since $\mathcal{A}(c, t)$ are increasing it follows that there exists $t' > 0$ such that $\mathcal{A}(c, t')$ has at least one interior point, denote it by c'. Denote for any $t > 0$ by $W(t)$ the interior of $\mathcal{A}(c, t)$. We will prove that $\bigcup_{t\geqslant 0} W(t) = \mathcal{S}$; to this effect, let c'' be an arbitrary point in $\mathcal{S}$. Then there exists $U \in \prod_{\ell=1}^{L} U(N_\ell)$ such that $c'' = Uc'$, which implies that c'' is an interior point of $\mathcal{A}(Uc, t')$. Since the system is controllable there exists $t''' > 0$ such that $Uc \in \mathcal{A}(c, t''')$ which implies that c'' is interior to $\mathcal{A}(c, t' + t''')$. Thus we have proved that $\bigcup_{t\geqslant 0} W(t) = \mathcal{S}$; since $W(t)$ are increasing it follows that there exists $T > 0$ such that $W(T) = \mathcal{S}$ and therefore $\mathcal{A}(c, T) = \mathcal{S}$. The conclusion of the theorem follows then from equation (A.1).

Proof of theorem 2. The proof is as for theorem 1 but now the Lie algebra is

$$\mathcal{L}' = \Big\{X = \mathrm{Diag}(X^\ell)_{\ell=1}^L, X^\ell \in u(N_\ell), \ell = 1, \ldots, L; \\ (\mathrm{Tr}(X^\ell))_{\ell=1}^L = \lambda(\mathrm{Tr}(A^\ell))_{\ell=1}^L + \nu(\mathrm{Tr}(B^\ell))_{\ell=1}^L, \lambda, \nu \in \mathbb{R}\Big\}. \qquad \square$$

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