Controllability, Observability and Parameter Identification of two coupled spin 1’s

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Abstract

In this paper, we study the control theoretic properties of a couple of interacting spin 1’s driven by an electro-magnetic field. In particular, we assume that it is possible to observe the expectation value of the total magnetization and we study controllability, observability and parameter identification of these systems. We give conditions for controllability and observability and characterize the classes of equivalent models which have the same input-output behavior. The analysis is motivated by the recent interest in three level systems in quantum information theory and quantum cryptography as well as by the problem of modeling molecular magnets as spin networks.

1 Introduction

In recent years, there have been several proposals to use three level systems, the so-called qutrits, in quantum information theory. The proposals concern the use of these systems as building blocks for protocols in quantum cryptography [12] and communication [7] as well as for the encoding of two logic qubits [16]. They also have been used to study fundamental questions in quantum mechanics such as entanglement measures [5], [9], [14]. A study of control of three level systems was considered in [6]. From a quantum control perspective, a system of two coupled three level systems represents the next more difficult case after the well studied system of coupled spin \(\frac{1}{2}\)’s [11], [19], [22]. Motivation to study these systems also comes from the problem of modeling molecular magnets. These novel materials [3], [4], [13], [20], [21] are of interest in many applications as nanosize magnets as well as for fundamental studies in quantum mechanics and biology. They are modeled as networks of interacting spins. Spin 1’s are a very common example of three level systems. Examples are the nuclear spins of the naturally occurring isotopes \(^6Li\), \(^2H\), \(^{14}N\).

We shall study the control-related properties, namely controllability, observability and parameter identifiability, for a pair of interacting spin 1’s particles. To be more specific, we shall consider an Heisenberg spin model with Hamiltonian given by

\[
H(t) := i(A + B_xu_x(t) + B_yu_y(t) + B_zu_z(t)),
\]  

(1)
with
\[ A := -iJ_{12}(\sum_{j=x,y,z} \bar{\sigma}_j \otimes \bar{\sigma}_j), \]  
\[ B_v := (\gamma_1 \bar{\sigma}_v \otimes \mathbf{1} + \gamma_2 \mathbf{1} \otimes \bar{\sigma}_v), \quad \text{for } v = x, y, \text{ or } z. \]  

Here \( J_{12} \) is the exchange constant, \( \gamma_1 \) and \( \gamma_2 \) are the gyromagnetic ratios of particle 1 and 2, respectively; \( u_{x,y,z} \) are the \( x, y, z \) time-varying components of the input electro-magnetic field; \( \mathbf{1} \) is the \( 3 \times 3 \) identity matrix. \( \bar{\sigma}_{x,y,z} \) are the spin matrices spanning the three dimensional representation of \( su(2) \) \[23\]

\[ \bar{\sigma}_x = \frac{i}{2} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} \end{pmatrix}, \]  
\[ \bar{\sigma}_y = \frac{i}{2} \begin{pmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i \end{pmatrix}, \]  
\[ \bar{\sigma}_z = -i \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \]

The total magnetization for the state \( \rho \) in the direction \( v = x, y, z \) is given by
\[ M_v = Tr(S_v^{TOT} \rho), \]  
where \( S_v^{TOT} = \bar{\sigma}_v \otimes \mathbf{1} + \mathbf{1} \otimes \bar{\sigma}_v, \quad v = x, y, z \). Recall that the density matrix (state) of the system \( \rho \) satisfies the Liouville’s equation \[23\]
\[ \dot{\rho} = -i[H(t), \rho]. \]

We are interested in the Heisenberg Hamiltonian (1) because we have in mind applications to spin Hamiltonians modeling the dynamics of molecular magnets \[3\], \[4\], \[13\], \[20\], \[21\]. However, the methods presented in this paper can be generalized to different types of coupled three level systems as for example two spins 1’s with interaction different from the one modeled in (2) or cases where one component of the magnetic field is held constant. The main tool is a Cartan decomposition of the Lie algebra \( su(3) \), described in Section 2, which gives a decomposition of higher dimensional Lie algebras constructed with tensor products of matrices in \( su(3) \). We begin by stating the definitions concerning controllability, observability and parameter identification with reference to the system we want to study.

**Definition 1.1** An \( n \)-level quantum system is controllable if it is possible to drive the evolution operator to any value in the special unitary group \( SU(n) \).

Controllability can be checked \[18\] by verifying that the Lie Algebra generated by the matrices defining the dynamics \( (A, B_x, B_y, B_z \text{ in (1), (2)}) \) contains \( su(n) \) (in this case \( su(9) \)).
Definition 1.2 Denote by $\rho(t, \vec{u}, \rho_0)$ the trajectory corresponding to an initial state $\rho_0$ and control(s) $\vec{u}$. Let $S$ be the matrix corresponding to the output of the system $Tr(S\rho(t, \vec{u}, \rho_0))$ (in our case $S = S_{v}^{TOT}$, $v = x, y, z$ in (6)). Then the system is observable if $Tr(S\rho(t, \vec{u}, \rho_0)) = Tr(S\rho(t, \vec{u}, \rho'_0))$, for every $t$ and control $\vec{u}$, implies $\rho_0 = \rho'_0$.

This definition of observability refers to identification of the initial state by a measure of the expectation value of an observable. Observability for quantum mechanical systems in these terms was studied in [10]. If $L$ is the dynamical Lie Algebra (generated by $A, B_{x,y,z}$ above for our system), an $n$–level system with output $S$ (assumed w.l.g. traceless) ($S_{v}^{TOT}$ in our case) is observable if and only if

$$V := \oplus_{k=0}^{\infty} ad_{L}iS = su(n).$$

Here and in the following $\oplus$ denotes the sum of vector spaces (not necessarily direct sum). In the controllable case $su(n) \subset L$ and (8) is verified.

Now consider two models $\Sigma$ and $\Sigma'$ of Heisenberg spin 1's. These models may differ by the parameters $J_{12}$ and $\gamma_{1,2}$. They may also have different initial states say $\rho_0$ and $\rho'_0$. Therefore we often consider the pair $(\Sigma, \rho_0)$ and the pair $(\Sigma', \rho'_0)$. We investigate whether it is possible to distinguish state and parameters by an experiment involving control with an input field and a measurement of the output $S_{v}^{TOT}$. This problem is motivated by recent results on the isospectrality of Heisenberg Hamiltonians which showed the impossibility to distinguish the parameters in the Hamiltonian by a measure of thermodynamic properties [24]. We call $\rho(t) := \rho(t, u_x, u_y, u_z, \rho_0)$ a general trajectory for $(\Sigma, \rho_0)$ and $\rho'(t) := \rho(t, u_x, u_y, u_z, \rho'_0)$ the corresponding trajectory (with the same control) for $(\Sigma', \rho'_0)$. We give the following definition [1].

Definition 1.3 Two pairs $(\Sigma, \rho_0)$ and $(\Sigma', \rho'_0)$ are equivalent if

$$Tr(S_{v}^{TOT} \rho(t)) = Tr(S_{v}^{TOT} \rho'(t)),$$ 

for every trajectory $\rho$ and corresponding (with the same control) trajectory $\rho'$.

The question of whether or not it is possible to distinguish two models using a reading of the total magnetization will be posed by describing the classes of equivalent pairs model-initial state. If $\rho_0$ and $\rho'_0$ are scalar matrices so are $\rho(t)$ and $\rho'(t)$ for every $t$ so the outputs (9) are identically zero independently of the model. We shall exclude this degenerate case in the following treatment.

The rest of the paper is organized as follows. In the next section, we describe some properties and a decomposition of the Lie algebra $su(3)$ that will be used in the following. The question of controllability and observability is tackled in Section 3, where we prove that the system is controllable and observable if and only if $\gamma_1 \neq \gamma_2$ and $J_{12} \neq 0$. In Section 4 we give a description of the classes of equivalent pairs which, we prove, consist of only two elements. Some concluding remarks are presented in Section 5.
Properties of the Lie algebra $su(3)$

The Lie algebra $su(3)$ appears in several areas of quantum physics. As a result, it has been extensively studied in the mathematical physics literature (see e.g. [8], [15]). We describe here some properties that are important for our treatment. We consider a canonical, orthogonal basis of $su(3)$ given by the three matrices

$$
\sigma_x = \begin{pmatrix} 0 & i & 0 \\ i & 0 & i \\ 0 & i & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} -i & 0 & 0 \\ 0 & 0 & i \\ 0 & 0 & 0 \end{pmatrix},
$$

(compare with (3)-(5)), and the matrices

$$
R := \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad Q := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad T := \begin{pmatrix} i & 0 & 0 \\ 0 & -2i & 0 \\ 0 & 0 & i \end{pmatrix},
$$

(11)

$$
V := \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad U := \begin{pmatrix} 0 & i & 0 \\ i & 0 & -i \\ 0 & -i & 0 \end{pmatrix}.
$$

The matrices $\sigma_{x,y,z}$ span a Lie algebra isomorphic to $su(2)$ which we denote by $S$. In particular we have

$$
[\sigma_x, \sigma_y] = 2\sigma_z, \quad [\sigma_y, \sigma_z] = \sigma_x, \quad [\sigma_z, \sigma_x] = \sigma_y.
$$

(13)

The matrices $R, Q, T, V, U$ along with multiples of the $3 \times 3$ identity $1$ span the orthogonal complement of $S$ in $u(3)$, which we denote by $S^\perp$. The following tables summarize the remaining commutation relation for $su(3)$ in terms of the basis elements we have defined

$$
\begin{array}{|c|c|c|c|c|}
\hline
| & R & Q & T & V \\
\hline
Q & -2\sigma_z & & & \\
T & 0 & 0 & & \\
V & \sigma_x & \sigma_y & 3\sigma_x & \\
U & \sigma_y & -\sigma_x & -3\sigma_y & 2\sigma_z \\
\hline
\end{array}
$$

(14)

$$
\begin{array}{|c|c|c|c|c|}
\hline
| & R & Q & T & V & U \\
\hline
\sigma_x & -V & U & -3V & 2T + 2R & -2Q \\
\sigma_y & -U & -V & 3U & 2Q & -2T + 2R \\
\sigma_z & 2Q & -2R & 0 & -U & V \\
\hline
\end{array}
$$

(14)

From these tables, it follows

$$
[S, S] = S, \quad [S^\perp, S] = S^\perp / \text{span}\{i1\} \quad [S^\perp, S^\perp] = S.
$$

(15)

We also have that for any matrix in the set $\{R, Q, T, V, U\}$, say $L$

$$
\bigoplus_{k=0}^{\infty} ad_S L = S^\perp / \text{span}\{i1\}.
$$

(16)
The anticommutation relations are summarized in the following tables

\[
\begin{array}{cccccc}
-i\{,\} & R & Q & T & V & U \\
R & \frac{2}{3}i1 + \frac{2}{3}T & 0 & 2R & -U & -V \\
Q & 0 & \frac{2}{3}i1 + \frac{2}{3}T & 4i1 - 2T & -V & -U \\
T & 2R & 2Q & 4i1 - 2T & \frac{2}{3}i1 - \frac{2}{3}T + 2R & \frac{2}{3}i1 - \frac{2}{3}T - 2R \\
V & V & -U & -V & \frac{2}{3}i1 - \frac{2}{3}T + 2R & \frac{2}{3}i1 - \frac{2}{3}T - 2R \\
U & -U & -V & -U & \frac{2}{3}i1 - \frac{2}{3}T - 2R & \frac{2}{3}i1 + \frac{2}{3}T \\
\end{array}
\]  

We have
\[
i\{S,S\} = S^\perp, \quad i\{S_\perp,S\} = S \quad i\{S_\perp,S_\perp\} = S^\perp.
\]  

In the following, we denote by \(\sigma\) a generic element of \(iS\) and by \(S\) a generic element of \(iS^\perp\). Therefore, \(\sigma\) and \(S\) are Hermitian matrices. The decomposition of \(u(3)\) which we have introduced in this section has consequences for decompositions of higher dimensional spaces. We shall use this in the following sections, in particular in Section 4.

### 3 Controllability and Observability

The system of two interacting spin 1’s, if the gyromagnetic ratios are equal, has dynamical Lie algebra isomorphic to \(su(2)\) or \(u(2)\) according to whether or not \(J_{12}\) is equal to zero. In the case \(J_{12} = 0\) we also have a Lie algebra isomorphic to \(su(2)\) even in the case of different \(\gamma\)’s. The only nontrivial case is when \(\gamma_1 \neq \gamma_2\) and \(J_{12} \neq 0\). In this case, we have the following Theorem.

**Theorem 1** If \(\gamma_1 \neq \gamma_2\) and \(J_{12} \neq 0\), the system is controllable namely the dynamical Lie algebra is equal to \(su(9)\).

**Proof.** We have to prove that, by calculating (repeated) Lie brackets of the matrices \(A, B_{x,y,z}\), we can obtain all the matrices of the form \(iC \otimes D\) where \(C\) and \(D\) vary in the orthogonal basis of \(u(3)\) described in the previous section, except the \(9 \times 9\) identity. By repeated Lie brackets of the \(B_{x,y,z}\) and using a determinant of Vandermonde type of argument similar to the one in Lemma 4.1 of [2], we obtain all the matrices of the form \(i\sigma \otimes 1\) and \(i1 \otimes \sigma\). Then, using the Lie bracket of these matrices with \(A\) several times, we obtain also all the matrices of the form \(i\sigma_1 \otimes \sigma_2\). To obtain the other elements we proceed as follows: We calculate \([i\sigma_z \otimes \sigma_x, i\sigma_z \otimes \sigma_y]\) (see Table (17)). This gives a multiple of \(i1 \otimes \sigma_z\) (which is already in the dynamical Lie algebra) plus a multiple of \(T \otimes \sigma_z\), with \(T\) defined in (11). From this, taking the Lie brackets with elements of the type \(i1 \otimes \sigma\) and \(i\sigma \otimes 1\), using (16) we obtain all the matrices of the form \(iS \otimes \sigma\) and analogously we can obtain all the matrices of the type...
To conclude the proof of controllability we only have to prove that we can obtain all the matrices \(iS \otimes S\) except the \(9 \times 9\) identity. Notice that since \(su(3)\) is a simple Lie algebra \([su(3), su(3)] = su(3)\). Therefore given \(C\) in \(su(3)\) we can choose two matrices \(M\) and \(N\) such that \([M, N] = C\). Using the well known fact (see e.g. [23]) that \(\sum_{j=x, y, z} (-i\sigma_j)^2 = 2 \times 1\), we calculate

\[
\sum_{j=x, y, z} [M \otimes -i\sigma_j, N \otimes -i\sigma_j] = \sum_{j=x, y, z} C \otimes (-i\sigma_j)^2 = 2C \otimes 1.
\] (19)

Analogously we can see that we can generate all the matrices \(1 \otimes C\) with \(C \in su(3)\). Now, since \(C\) is a general matrix in \(su(3)\) we can obtain all the elements of the type \(K \otimes Y\) with \(Y \in su(3)\) (or \(K \in su(3)\)) and \(K\) (or \(Y\)) in the orbit \(\oplus_{k=0}^{\infty} ad_{su(3)}^k iS\). However this orbit is equal to \(su(3)\) (it is a nonzero ideal in \(su(3)\) and therefore it must be \(su(3)\) itself since \(su(3)\) is simple). This concludes the proof. \(\square\)

In the case \(\gamma_1 \neq \gamma_2\) \(J_{12} \neq 0\) the system being controllable is also observable. In all the other cases, the space \(\mathcal{V}\) defined in (8) is different from \(su(9)\). In these cases, initial density matrices which differ by a matrix in \(\mathcal{V}^\perp\) cannot be distinguished and the system is not observable.

### 4 Parameter Identification

We now characterize the classes of equivalent pairs model-initial state. In other terms, we investigate what can be said concerning the parameters of the system by experiments involving control with an external electro-magnetic field and measurement of the total magnetization. We shall assume that we are in the controllable (and therefore observable) case, namely we know that \(\gamma_1 \neq \gamma_2\) and \(J_{12} \neq 0\). We state and prove the main result of this section in the following Theorem 2, where we characterize the classes of equivalent models. In the following we mark with a prime \(\prime\) every symbol concerning system \(\Sigma\). We first give three preliminary results that can be proved as in the case of networks of spin \(1/2\)'s treated in [1]. For completeness we give self contained proofs and some additional considerations in the Appendix.

**Lemma 4.1** If, for every trajectory of \(\Sigma\), \(\rho\), and corresponding trajectory of \(\Sigma'\), \(\rho'\), we have

\[
Tr(S\rho) = Tr(S'\rho'), \quad v = x, y, z,
\] (20)

for some pair of matrices \(S\) and \(S'\), then for every \(F, F := ad_{B_{j_1}} ad_{B_{j_2}} \cdots ad_{B_{j_r}} S\), and corresponding \(F', F' := ad_{B'_{j_1}} ad_{B'_{j_2}} \cdots ad_{B'_{j_r}} S'\), \((j_1, ..., j_r \in \{x, y, z\}\) or \(B_j = A)\), we have

\[
Tr(F\rho) = Tr(F'\rho'),
\] (21)

for every pair of trajectories \(\rho\) and \(\rho'\).
Lemma 4.2 Let \((\Sigma, \rho_0)\) and \((\Sigma', \rho'_0)\) be two equivalent models. Then up to a permutation of the indices
\[
\gamma_{1,2} = \gamma'_{1,2},
\]
and for every \(\sigma \in iS\)
\[
Tr(\sigma \otimes 1\rho(t)) = Tr(\sigma \otimes 1\rho'(t)), \quad Tr(1 \otimes \sigma\rho(t)) = Tr(1 \otimes \sigma\rho'(t)).
\]

Lemma 4.3 Assume two models \((\Sigma, \rho_0)\) and \((\Sigma', \rho'_0)\) are equivalent. For every pair of matrices \(S\) and \(S'\) such that
\[
Tr(S\rho) = Tr(S'\rho'),
\]
we also have
\[
Tr([S, \sigma \otimes 1]\rho) = Tr([S', \sigma \otimes 1]\rho') \quad Tr([S, 1 \otimes \sigma]\rho) = Tr([S', 1 \otimes \sigma]\rho').
\]

We define now two orthogonal subspaces of \(isu(9)\): \(I\) which is spanned by elements of the type \(\sigma_1 \otimes \sigma_2\) and \(S_1 \otimes S_2\) (namely the factors of the tensor product are both in \(iS\) or both in \(iS^\perp\)), except the identity, and \(I^\perp\) which is spanned by mixed type of elements namely elements of the type \(\sigma \otimes S\) and \(S \otimes \sigma\). We shall use this decomposition of \(isu(9)\) (which induces a decomposition of \(su(9)\)) in the following treatment. The induced decomposition of \(su(9)\) is a Cartan type (see e.g. [17]) of decomposition as stated in the following Lemma.

Lemma 4.4
\[
su(9) = iI \oplus iI^\perp,
\]
with
\[
[iI^\perp, iI^\perp] \subseteq iI^\perp, \quad [iI^\perp, iI] \subseteq iI, \quad [iI, iI] \subseteq iI^\perp.
\]

Proof. To verify (27), we consider a Lie bracket \([\sigma_1 \otimes S_1, \sigma_2 \otimes S_2]\) and prove that it is orthogonal to elements of the form \(\sigma_3 \otimes \sigma_4\) as well as to elements of the form \(S_3 \otimes S_4\). To do this, we rewrite \([\sigma_1 \otimes S_1, \sigma_2 \otimes S_2]\) as
\[
[\sigma_1 \otimes S_1, \sigma_2 \otimes S_2] = \sigma_1\sigma_2 \otimes S_1S_2 - \sigma_2\sigma_1 \otimes S_2S_1.
\]
We can decompose \(\sigma_1\sigma_2 \otimes S_1S_2\) as
\[
\sigma_1\sigma_2 \otimes S_1S_2 = \frac{1}{4}(\{\sigma_1, \sigma_2\} + \{\sigma_1, \sigma_2\}) \otimes ([S_1, S_2] + \{S_1, S_2\}).
\]
From this expression, using (15) and (18), the only term that is not perpendicular to \(\sigma_3 \otimes \sigma_4\) is \([\sigma_1, \sigma_2] \otimes [S_1, S_2]\). Doing the same thing for the second term on the right hand side of (30), one obtains that the only term which is not perpendicular to \(\sigma_3 \otimes \sigma_4\) is \([\sigma_2, \sigma_1] \otimes [S_2, S_1]\). But these two terms cancel. Analogously one proves orthogonality to matrices of the type \(S_3 \otimes S_4\). To conclude the proof of (27) one has to prove orthogonality of terms of the form \([\sigma_1 \otimes S_1, S_2 \otimes \sigma_2]\). This is obtained using similar arguments. Also similar arguments, considering all the sub-cases, prove (28) and (29). \(\square\)
Remark 4.5 The argument in the above Lemma can be generalized to deal with decompositions of $su(3^n)$, for every $n \geq 1$. One can define a subspace of $isu(3^n)$ of tensor products of matrices of the form $\sigma \otimes S \otimes \cdots \otimes \sigma$ with an odd number of $\sigma$’s and a complementary space with an even number of $\sigma$’s. Call these subspaces $I_o$ and $I_e$ respectively. Then one can show, by induction on $n$ that

$$[iI_o,iI_o] \subseteq iI_o, \quad [iI_o,iI_e] \subseteq iI_e, \quad [iI_e,iI_e] \subseteq iI_o,$$

and

$$\{I_o,I_o\} \subseteq I_e, \quad \{I_o,I_e\} \subseteq I_o, \quad \{I_e,I_e\} \subseteq I_e.$$

In fact for $n = 1$ (32) and (33) follow immediately from (15) and (18). For $n > 1$, (32) follows by writing

$$[A \otimes B, C \otimes D] = \frac{1}{2}([A, C] \otimes [B, D] + [A, C] \otimes \{B, D\}),$$

and applying the inductive assumption to all the factors in this expression and considering all the sub-cases. Analogously one can prove (33).

The following is the main theorem of this section.

Theorem 2 Two controllable pairs Model-Initial State $\Sigma(n, J_{12}, \gamma_1, \gamma_2, \rho_0)$, $\Sigma'(n', J'_{12}, \gamma'_1, \gamma'_2, \rho'_0)$ are equivalent if and only if (up to a permutation of the indices)

1. $\gamma_1 = \gamma'_1$
2. $\gamma_2 = \gamma'_2$
3. $|J_{12}| = |J'_{12}|$
4. If $J_{12} = J'_{12}$ then $\rho_0 = \rho'_0$. If $J_{12} = -J'_{12}$, denote by $\rho_1$ ($\rho'_1$) the component of $\rho$ ($\rho'$) in $I^\perp$ and $\rho_2$ ($\rho'_2$) the component of $\rho$ ($\rho'$) in $I$ then $\rho_1(0) = \rho'_1(0)$ and $\rho_2(0) = -\rho'_2(0)$.

Proof. Assume first that the two pairs are equivalent. We have, from Lemma 4.2, that, up to a permutation of the indices, $\gamma_{1,2} = \gamma'_{1,2}$.

Consider now the following procedure to generate a basis of $su(9)$. Start with $A$, $i \mathbf{1} \otimes \sigma$ and $i \sigma \otimes \mathbf{1}$ at Step 0. At step $n$ take the Lie brackets of the matrices obtained at step $n - 1$ with $A$, $i \mathbf{1} \otimes \sigma$ and $i \sigma \otimes \mathbf{1}$. By controllability, the procedure generates a basis of $su(9)$. Moreover every element we calculate belongs to either $iI$ or $iI^\perp$ and there are no combinations. This follows by induction on the step and applying Lemma 4.4. We can repeat the same procedure starting with $A'$, $i \mathbf{1} \otimes \sigma$ and $i \sigma \otimes \mathbf{1}$. Let $F$ and $F'$ be two corresponding matrices obtained at a step $d \geq 1$. We have $F = J^k_{12} \bar{F}$ and $F' = J^k_{12} \bar{F}$ for the same $\bar{F}$ and with $k$ odd for $F(F') \in iI$ and even (not zero) for $F(F') \in iI^\perp$. This is true at Step 1 and follows by induction for elements obtained at the following steps by applying Lemma 4.4. Now notice that elements obtained from Step 1 on also span all of $su(9)$ as
is the Lie algebra generated by \( \{ su \} \). The same argument holds with \( \{ R \} \), where \( R \) is the set \( \{ A, i1 \otimes \sigma, i\sigma \otimes 1 \} \). It follows from an application of the Jacobi identity that this is equal to \( \oplus_{k=0}^{\infty} ad_{T_1}^{k} ad_{T_2}^{k} \cdots ad_{T_r}^{k} R_1 \), where \( T_1, T_2, \ldots, T_r \) are in the set \( \{ A, i1 \otimes \sigma, i\sigma \otimes 1 \} \). It follows from an application of the Jacobi identity that this is equal to \( \oplus_{k=0}^{\infty} ad_{\mathcal{L}}^{k} R_1 \), where \( \mathcal{L} \) is the Lie algebra generated by \( \{ A, i1 \otimes \sigma, i\sigma \otimes 1 \} \) which by controllability is \( su(9) \). So this is equal to \( \oplus_{k=0}^{\infty} ad_{su(9)}^{k} R_1 \) which is a nonzero ideal in \( su(9) \) and therefore \( su(9) \) itself since \( su(9) \) is a simple Lie algebra. The same argument holds with \( A' \) replacing \( A \). In conclusion we have, by applying Lemmas 4.1, 4.2 and 4.3, for any \( F \in \mathcal{I} \)

\[
J_{12}^k Tr(F\rho) = J_{12}^k Tr(F\rho'),
\]

with \( k \) odd and, for any \( F \in \mathcal{I}^\perp \),

\[
J_{12}^k Tr(\bar{F}\rho) = J_{12}^k Tr(\bar{F}\rho'),
\]

with \( k \) even. In particular, by applying (36) for \( F = 1 \otimes \sigma \) and comparing with (23) of Lemma 4.2 we obtain \( |J_{12}| = |J_{12}'| \).

The proof goes now in an analogous way to the case of spin \( \frac{1}{2} \) treated in [1]. We have two cases: If \( J_{12} = J_{12}' \), we have \( A = A', B_{x,y,z} = B'_{x,y,z} \). In this case since the systems are observable and we have the same input-output behavior then we must have \( \rho_0 = \rho_0' \). If \( J_{12} = -J_{12}' \), then from the above discussion we have

\[
Tr(G\rho_0) = Tr(G\rho_0'), \quad \forall G \in \mathcal{I}^\perp,
\]

and

\[
Tr(G\rho_0) = -Tr(G\rho_0'), \quad \forall G \in \mathcal{I},
\]

so the components of \( \rho_0 \) and \( \rho_0' \) in \( \mathcal{I}^\perp \) are equal while the components in \( \mathcal{I} \) are opposite.

To prove the converse of the theorem, the only nontrivial case is when \( J_{12} = -J_{12}' \). In this case let us write the equation for \( \rho \) as

\[
\dot{\rho} = [A + B(t), \rho],
\]

and the equation for \( \rho' \) as

\[
\dot{\rho}' = [-A + B(t), \rho'].
\]

We can write \( \rho (\rho') \) as \( \rho := \rho_1 + \rho_2, \rho' := \rho_1' + \rho_2' \) with \( \rho_1' \in \mathcal{I}^\perp \) and \( \rho_2' \in \mathcal{I} \). Using relations (27), (28), (29) of Lemma 4.4 and noticing that \( A \in i\mathcal{I} \) while \( B(t) \in i\mathcal{I}^\perp \), for every \( t \), we can write the differential equations for \( \rho_1 \) and \( \rho_2 \) as

\[
\dot{\rho}_1 = [B(t), \rho_1] + [A, \rho_2],
\]

and the differential equation for \( \rho_1' \) and \( \rho_2' \) as

\[
\dot{\rho}_1' = [B(t), \rho_1'] + [A, \rho_2']
\]

\[
\dot{\rho}_2' = [A, \rho_1'] + [B(t), \rho_2'].
\]
Combining these equations we obtain a differential equation for $\rho_1 - \dot{\rho}_1$ and $\rho_2 + \dot{\rho}_2$. In particular, we have

$$\begin{align*}
\dot{\rho}_1 - \dot{\rho}_1 &= [B(t), \rho_1 - \dot{\rho}_1] + 2[A, \rho_2 + \dot{\rho}_2] \\
\dot{\rho}_2 + \dot{\rho}_2 &= 2[A, \rho_1 - \dot{\rho}_1] + [B(t), \rho_2 + \dot{\rho}_2].
\end{align*}$$

(43)

From equations (43), it follows that if $\rho_1(0) = \rho_1'(0)$ and $\rho_2(0) = -\rho_2'(0)$, then $\rho_1(t) = \rho_1'(t)$ and $\rho_2(t) = -\rho_2'(t)$, for every $t$, and for every control $B(t)$. In particular, since $Tr(S_v^{TOT} \rho) = Tr(S_v^{TOT} \rho_1)$ and $\rho_1 \equiv \rho_1'$, the two models are equivalent.

\[\square\]

5 Conclusions

We have presented a control theoretic analysis of a system of two coupled spin 1’s. In particular, this concerns the controllability, observability and identifiability properties of this model. A Cartan decomposition of the Lie algebra $su(3)$ induces a decomposition of the Lie algebra $su(9)$ which plays a fundamental role in the control theoretic properties of this system. A similar situation was found in [1] for general networks of spin $\frac{1}{2}$ and it is likely to appear for other type of networks of spins not necessarily equal to $\frac{1}{2}$ or 1. We believe that the methods of analysis developed in this paper can be generalized to include for example different forms of the interaction, models where one or more components of the input field are held constant, networks with more than two spins (cfr. Remark 4.5). We have proved that if (and only if) the gyromagnetic ratios are different and the coupling constant is not zero the system is controllable and observable. In this case, we have characterized the set of equivalent models that give the same input output behavior. Our results are motivated by the problem of identifying the unknown parameters in molecular magnets through experiments involving driving the system with an input field and measuring the total magnetization. The analysis is also instrumental to the design of controls which will be considered in further research.

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Appendix: Proofs of Lemmas 4.1, 4.2, 4.3

Proof of Lemma 4.1

Proof. The proof can be obtained by induction on the depth of $F$ and $F'$ defined as the number of the operations $ad$ in its calculation. For depth 0 (21) is the same as (20). Now assuming that $F$ has depth $d - 1$, we can write for every $\tau$ and $t$ (considering a trajectory corresponding to controls identically zero from a certain instant on)

$$Tr(Fe^{At}\rho(\tau)e^{-At}) = Tr(F'e^{A't}\rho'(\tau)e^{-A't}),$$

which taking the derivative with respect to $t$ at zero gives

$$Tr([A,F]\rho(\tau)) = Tr([A',F']\rho'(\tau)).$$

(45)

Analogously one can obtain (with appropriate constant control)

$$Tr([A+B_{x,y,z},F]\rho(\tau)) = Tr([A'+B'_{x,y,z},F']\rho'(\tau)),$$

which combined with (45) gives

$$Tr([B_{x,y,z},F]\rho(\tau)) = Tr([B'_{x,y,z},F']\rho'(\tau)).$$

(47)

Lemma (4.1) can be generalized as follows. For $\Sigma$ and $\Sigma'$ we can construct a basis for the dynamical Lie algebra starting from $A, B_{x,y,z}$ or $A', B'_{x,y,z}$ and at each step calculating
the Lie brackets of the elements obtained at the previous step by $A, B_x, y, z$ or $A', B'_x, y, z$.

Consider the depth of the element of the basis as the number of Lie brackets calculated. The generalization consists of noticing that if (20) holds for some $S$ and $S'$ it also holds for $[L, S]$ and $[L', S']$ where $L$ and $L'$ are elements of the basis of the dynamical Lie Algebra obtained the same way just replacing the $A, B_x, y, z$ with $A', B'_x, y, z$. This is true for every element of depth 0 from Lemma 4.1. Now assume it is true for elements $L$ and $L'$ of depth $d - 1$. From the Jacobi identity we have

$$
Tr([[B, L], S]\rho) + Tr([[L, S], B]\rho) + Tr([[S, B], L]\rho) = 0,
$$

for some $B$ in the set $A, B_x, y, z$ and corresponding $B'$. Now the second terms of the two sides are equal by applying the inductive assumption and Lemma 4.1. The same thing is true for the third term where we apply first Lemma 4.1 to obtain $Tr([S, B]\rho) = Tr([S', B']\rho')$ and then the inductive assumption on $L$ (with $S$ replaced by $[S, B]$). Therefore the first terms are also equal. This facilitates the proofs of Lemmas 4.2 and 4.3.

Proof of Lemma 4.2

Proof. By performing (repeated) Lie brackets of $B_x, B_y$ and $B_z$, it is possible to obtain all the matrices of the form $\gamma^1_k i\sigma \otimes 1 + \gamma^2_k i \otimes \sigma$, with $k = 1, 2, \ldots$ (cfr. Lemma 4.1. in [2]). The corresponding matrices for $\Sigma'$ are $\gamma^1_k i\sigma \otimes 1 + \gamma^2_k i \otimes \sigma$. Now, starting from

$$
Tr(S^\text{TOT}_v) = Tr(S^\text{TOT}_v'),
$$

and taking the Lie bracket with the matrices above obtained, we have

$$
\gamma^1_k Tr(\sigma \otimes 1\rho) + \gamma^2_k Tr(1 \otimes \sigma\rho) = \gamma^1_k Tr(\sigma \otimes 1\rho') + \gamma^2_k Tr(1 \otimes \sigma\rho'), \quad k = 0, 1, 2, \ldots
$$

(50)

Since $Tr(\sigma \otimes 1\rho)$ is not zero for every trajectory $\rho$ (unless $\rho$ is a scalar matrix which is a case we exclude), the only possibility for (50) to be verified is that the determinant

$$
D = \begin{vmatrix}
1 & 1 & 1 & 1 \\
\gamma^1_1 & \gamma^1_2 & \gamma^1_1' & \gamma^1_2' \\
\gamma^2_1 & \gamma^2_2 & \gamma^2_1' & \gamma^2_2' \\
\gamma^3_1 & \gamma^3_2 & \gamma^3_1' & \gamma^3_2'
\end{vmatrix},
$$

(51)

is equal to zero. But this is a Vandermonde determinant, therefore we need two of the $\gamma$’s and $\gamma'$’s to be equal. Up to a permutation we can choose $\gamma_1 = \gamma_1'$. We can now use the same Vandermonde determinant type of argument starting from

$$
\gamma^1_1(Tr(\sigma \otimes 1\rho) - Tr(\sigma \otimes 1\rho')) + \gamma^2_2 Tr(1 \otimes \sigma\rho) - \gamma^2_2 Tr(1 \otimes \sigma\rho') = 0,
$$

(52)

to conclude that $\gamma_2 = \gamma_2'$ and that (23) holds.

Proof of Lemma 4.3

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Proof. As in the previous Lemma we obtain

\[ \gamma_1^k (\text{Tr}(\rho[S, \sigma \otimes 1]) - \text{Tr}(\rho'[S', \sigma \otimes 1])) + \gamma_2^k (\text{Tr}(\rho[S, 1 \otimes \sigma]) - \text{Tr}(\rho'[S', 1 \otimes 1])) = 0, \quad k = 1, 2, \ldots \]  

(53)

This since \( \gamma_1 \neq \gamma_2 \), we obtain (25). \( \square \)