

Model Identification for Spin Networks

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Abstract

We consider the problem of determining the unknown parameters of the Hamiltonian of a network of spin $\frac{1}{2}$ particles. In particular, we study experiments in which the system is driven by an externally applied electro-magnetic field and the expectation value of the total magnetization is measured. Under appropriate system theoretic assumptions, we prove that, if it is possible to prepare the system in a known initial state, the above experiment allows to identify the parameters of the Hamiltonian. In the case where the initial state is itself an unknown parameter, we characterize all the pairs Hamiltonian-Initial State which give the same value of the magnetization, for every form of the driving electro-magnetic field. The analysis is motivated by recent results on the isospectrality of Hamiltonians describing magnetic molecules.

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1 Introduction

In recent years, chemists have developed methods to synthesize large organometallic molecules which contain a core of magnetic transition metal ions interacting via electronic superexchange interactions [3], [4], [5]. One of the main advantages of this technology is that it makes it possible to arrange the molecules in regular van der Waals crystals in which the magnetic interactions among different molecules are negligible. Thus, every cluster of this kind behaves like an assembly of *identical* and *independent* nanosize magnets, each corresponding to one molecule. For this reason, these novel systems are now deemed ideal to

study *fundamental questions* concerning magnetism at the molecular level. In fact, even the simplest of these systems displays several new classical and quantum mechanical phenomena. One example is *macroscopic quantum tunneling of magnetization* [7], [8], a fascinating issue of relevance to a variety of mesoscopic systems and nanostructures. This paper is a mathematical study on the determination of the parameters for Hamiltonians describing *magnetic molecules*.

The determination of exchange constants for magnetic molecules has been traditionally obtained by measuring the temperature-dependent magnetic susceptibility or other thermodynamic properties. This technique relies on the assumption that there is a one to one correspondence between the spectrum of the Hamiltonian of the system in a static magnetic field, and its thermodynamic properties as well as the numerical values of the model parameters. However, a recent article [13] has shown that quantum Heisenberg spin systems, such as magnetic molecules, may have different coupling parameters but the same energy spectrum and hence the same thermodynamic properties. This raises the question of whether a *dynamic* technique could be used to identify the parameters of a spin network. In particular, as in NMR or EPR experiments, one could try to let the system evolve under the action of a driving time varying electro-magnetic field, measure the total magnetization and, from the measured value, infer the value of the parameters of the system. The question of whether these experiments allow to identify the unknown parameters can be tackled at different levels according to how much we assume known about the system under investigation; whether, for example, we assume the system prepared in a known initial state or the initial state itself a parameter to be identified. The question can also be cast in a more general framework concerning the application of concepts of systems and control to the problem of modeling Hamiltonians in quantum physics. From a *system theoretic viewpoint*, the above described experiment is an attempt of doing parameter identification [11] for a control system whose dynamics is governed by the Schrödinger equation with unknown parameters. The input magnetic field plays the role of the input *control variable* while the expectation value of the magnetization is the *output*. As in identification theory, the control theoretic concepts of *controllability* and *observability* (see e.g. [14]) play an important role in determining whether two different models may present the same input-output behavior.

In this paper, we restrict ourselves to the important case of networks of spin $\frac{1}{2}$ particles and present a positive answer to the above question. We prove that systems which give the same input-output behavior for any given state are the same. This shows that, if we can opportunely prepare an initial state, we can use the above scheme to identify the parameters of the system exactly. If the initial state of the system is unknown, we prove that there are only two possibilities (up to permutations of the spins) for two pairs Hamiltonian-Initial State to give the same input output behavior. They are either the same or the exchange constants have opposite signs and the initial states are related in a way we shall describe. So, in this case, the given experiments identify one of two possible systems giving the observed behavior. These results were announced in the conference paper [2] as an application of the observability theory for quantum systems [6]. The complete treatment with proofs is

presented in this paper.

The paper is organized as follows. In the next section, we present some preliminaries on spin networks, give the basic definitions and state the problem we want to solve in mathematical terms. In Section 3, we give the two results above described and prove the first one. This gives us the opportunity to elaborate on the control theoretic concepts of *observability* and *controllability* and their role in the parameter identification problem. The proof of the second result is much longer and it is given in Sections 4 and 5. Section 6 presents some conclusions and a discussion of the results.

2 Preliminaries and Statement of the Problem

Several elementary particles, such as electrons and nuclides, display a degree of freedom called ‘*spin*’. Although there is no classical counterpart to the spin of a particle, the operators describing it obey the same commutation relations as the angular momentum operators. When measured, the spin can assume one of $2j + 1$ values, where j is a positive integer or half integer which depends on the particle under consideration. In this paper, we shall restrict ourselves to the case of $j = \frac{1}{2}$. One of the earliest experiments of measurement of spin is the Stern-Gerlach experiment discussed in several textbook on quantum mechanics (see e.g. [12]). Interacting particles with spin, where all the other degrees of freedom are neglected, form a *spin network*, as for example in a molecule. Magnetic molecules, the systems which motivated the present research as discussed in the introduction, are examples of spin networks. The energy of a spin network is the sum of two main contributions one due to the interaction among the spins and one due to the interaction with an external time varying magnetic field. The state of a spin network is encoded in a density matrix ρ which evolves according to the Schrödinger equation

$$\dot{\rho}(t) = -i[H(t), \rho(t)]. \quad (1)$$

The Hamiltonian $H(t)$ is the matrix representation of the energy of the network. The solution of (1) varies as

$$\rho(t) = X(t)\rho(0)X^*(t), \quad (2)$$

where $X(t)$ is the unitary *evolution operator* solution of the Schrödinger equation

$$\dot{X} = -iH(t)X, \quad (3)$$

with initial condition equal to the identity.

We consider the Heisenberg spin model where $H(t)$ takes the form

$$H(t) := i(A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t)). \quad (4)$$

For a network of n spins we have

$$\begin{aligned} A &:= -i \sum_{k < l, k, l=1}^n J_{kl}(I_{kx, lx} + I_{ky, ly} + I_{kz, lz}), \\ B_v &:= -i(\sum_{k=1}^n \gamma_k I_{kv}), \quad \text{for } v = x, y, \text{ or } z. \end{aligned} \quad (5)$$

The matrices A and $B_x u_x(t) + B_y u_y(t) + B_z u_z(t)$ represent, respectively, the energy due to the interaction among spins and with an external magnetic field of components u_x , u_y and u_z , which plays the role of control. These controls are assumed to be piecewise continuous real functions. The real scalar parameter J_{kl} is the exchange constant between particle k and particle l and the real scalar parameter γ_k is the gyromagnetic ratio of particle k . The parameters J_{kl} and γ_k are the object of the identification problem treated in this paper. For a network of n spin $\frac{1}{2}$ particles, the matrix $I_{k_1 v_1, \dots, k_r v_r}$ is the Kronecker product of n matrices equal to the 2×2 identity except in the k_j -th ($j = 1, \dots, r$) position(s) occupied by the Pauli matrix σ_{v_j} , $v_j = x, y, z$. Recall (see e.g. [12]) that the Pauli matrices are defined as

$$\sigma_x := \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z := \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (6)$$

We denote by \mathcal{R} the set of possible values for the density matrix, i.e. Hermitian, positive semidefinite matrices with trace one. Let $\rho(t, u_x, u_y, u_z, \rho_0)$, the density matrix solution of the Schrödinger equation (1) corresponding to the controls $u_x(t)$, $u_y(t)$, $u_z(t)$ and initial condition ρ_0 . We assume that it is possible to observe the expectation value of the total magnetization in the x , y , and z direction, namely:

$$M_v(t) := M_v(t; \rho_0, u_x, u_y, u_z) := \text{Tr}(S_v^{TOT} \rho(t, u_x, u_y, u_z, \rho_0)), \quad (7)$$

where

$$S_v^{TOT} = \sum_{k=1}^n I_{kv}, \quad \text{for } v = x, y, z.$$

We study the possibility of distinguishing the parameters by a single measurement of one of the above outputs. More precisely, we denote by $\Sigma \equiv \Sigma(n, J_{kl}, \gamma_k)$ a model described by the equations (4) and (5), and by $(\Sigma, \rho_0) \equiv (\Sigma(n, J_{kl}, \gamma_k), \rho_0)$ a model with fixed initial state ρ_0 . Thus, for given control functions u_x , u_y , and u_z , $M_v(t; \rho_0, u_x, u_y, u_z)$, for $v = x, y$, and z , are the corresponding output functions. The parameters J_{kl} and γ_k along with the number n of spins (and the value of the initial state ρ_0) characterize the model. The question of parameter identifiability through a single measurement of the magnetization can be posed by identifying the models (or set of parameters) that give the same input-output behavior. We have the following definition.

Definition 2.1 Consider two models Σ and Σ' . We mark with a prime ' all the symbols concerning system Σ' .

- Σ and Σ' are *equivalent* and we write

$$\Sigma \sim \Sigma'$$

if and only if $n = n'$ and for any given common initial condition ρ_0 and control functions u_x, u_y, u_z , we have

$$M_v(t; \rho_0, u_x, u_y, u_z) = M'_v(t; \rho_0, u_x, u_y, u_z), \quad \text{for } v = x, y, z.$$

- Two pairs model-initial state (Σ, ρ_0) and (Σ', ρ'_0) are equivalent and we write

$$(\Sigma, \rho_0) \sim (\Sigma', \rho'_0),$$

if for all control functions u_x , u_y , and u_z , we have

$$M_v(t; \rho_0, u_x, u_y, u_z) = M'_v(t; \rho'_0, u_x, u_y, u_z), \quad \text{for } v = x, y, z.$$

Definition 2.2 A model is *controllable* if, by varying opportunely the control functions (u_x, u_y, u_z) , it is possible to drive the evolution operator from the identity to any (special) unitary matrix.

For general quantum systems, controllability can be checked by verifying the so-called Lie algebra rank condition [10] which means that the matrices A and B 's characterizing the dynamics (cfr.(4)-(5)) generate the whole Lie Algebra $su(\tilde{n})$ (or $u(\tilde{n})$) where \tilde{n} is the dimension of the density matrix (2^n for the case of networks of spin $\frac{1}{2}$'s). To a network of spin $\frac{1}{2}$ one can associate a graph whose nodes represent the particles and an edge connects two nodes if and only if the corresponding exchange constant is different from zero. In the case of spin networks with different gyromagnetic ratios the system is controllable if and only if the graph associated to the network is connected, and sufficient controllability conditions can be given for the general case [1].

Definition 2.3 A model is *observable* if there are no two different states which give the same output for every set of control functions.

Observability can be checked by verifying that the *Observability Space* \mathcal{V} is equal to $su(\tilde{n})$ (\tilde{n} again is the dimension of the density matrix) [6]. Given the matrix that characterizes the output, S_v^{TOT} in (7) in our case, the observability space \mathcal{V} is the vector space spanned by the matrices,¹

$$ad_{B_{j_1}}^{k_1} ad_{B_{j_2}}^{k_2} \cdots ad_{B_{j_r}}^{k_r} iS_v^{TOT} \quad v = x, y, z, \quad (8)$$

where $j_k \in \{0, 1, 2, 3\}$ and $B_0 = A$, $B_1 = B_x$, $B_2 = B_y$, and $B_3 = B_z$. The following fact holds true [6].

Lemma 2.4 Controllability implies observability.

In parametric identification problems, it is reasonable to restrict ourselves to observable systems since the unobservable dynamics does not contribute to the output which is our tool to identify the system. Moreover, we want to check that observable systems which give the

¹ $ad_R^k T := [R, [R, \dots [R, T]]]$ where the Lie bracket is taken k times.

same input-output behavior, namely that are equivalent, have the same parameters. We can state the following two problems.

Problem 1 Characterize the classes of observable equivalent spin models.

Problem 2 Characterize the classes of observable equivalent pairs model-initial state.

We shall see that the equivalence classes in Problem 1 consist of a single element. We shall solve Problem 2 restricting ourselves to networks that have different gyromagnetic ratios (or for which the spins can be selectively addressed) and controllable.

3 Main Results

In the following, we shall always denote by $\rho(t)$ and $\rho'(t)$ two trajectories corresponding to the same controls u_x, u_y, u_z for the models Σ, Σ' , respectively. The following Proposition whose proof we relegate to Appendix A, will be used in the proof of both our main results. We notice here that the proof although presented for the case of spin Heisenberg systems can be adapted to any bilinear finite dimensional quantum control system.

Proposition 3.1 Let (Σ, ρ_0) and (Σ', ρ'_0) be the two fixed pairs. Then, the following are equivalent:

- (a) $(\Sigma, \rho_0) \sim (\Sigma', \rho'_0)$,
- (b) For all control functions $u_x(t)$, $u_y(t)$, and $u_z(t)$, we have:

$$\text{Tr}(F\rho(t)) = \text{Tr}(F'\rho'(t)), \quad (9)$$

for all $F \in \mathcal{V}$ and $F' \in \mathcal{V}'$, with F' constructed as F changing all B_i in B'_i (see (8)).

We now state the first of our two main results.

Theorem 1 Let $\Sigma(n, J_{kl}, \gamma_k) := \{A, B_x, B_y, B_z\}$ and $\Sigma'(n, J'_{kl}, \gamma'_k) := \{A', B'_x, B'_y, B'_z\}$ be two equivalent models. Assume one of them is observable. Then $A = A'$, $B_{x,y,z} = B'_{x,y,z}$.

Proof. From the equivalence of the models and specializing (9) of Proposition 3.1 to a common initial condition, we obtain

$$\text{Tr}(F\rho_0) = \text{Tr}(F'\rho_0), \quad (10)$$

for every $\rho_0 \in \mathcal{R}$. Therefore $F = F'$. From the observability assumption F (and F') span all of $su(2^n)$ (n here is the number of spins, which is assumed to be the same). Since F is a generic element of \mathcal{V} , we have $[A, F] = [A', F'] = [A', F]$ and therefore

$$[A - A', F] = 0. \quad (11)$$

Since F spans all of $su(2^n)$, $A - A'$ must be zero. Analogously one can prove $B_{x,y,z} = B'_{x,y,z}$. \square

Notice that, although presented for the case of spin networks, Theorem 1 holds for any finite dimensional quantum system and essentially says that two observable models with the same input-output behavior, for a every state, must be equal. The assumption of observability can be checked by checking controllability and applying Lemma 2.4. Conditions for controllability of spin networks are given in [1].

We now consider a more difficult problem since we assume to have much less knowledge of the model to be identified. We assume not to know its dimension nor the initial condition. We perform black-box type of experiments on two pairs model-initial state and we obtain the same results. We investigate what can be said about the two models. We assume that all the gyromagnetic ratios γ_k , (γ'_k) are different. This fact implies that the (mild) assumption that the graph associated to the spin network is connected is equivalent to controllability [1]. We shall assume this. Under this assumption, we can easily rule out the case in which the responses of the systems are both identically zero. In this case (and only in this case) the corresponding initial density matrices are scalar matrices and nothing more can be said about two equivalent models. So we will assume that the two initial states are not scalar matrices.

Before stating the result, we need to introduce some more notation. We denote by \mathcal{I}_o (\mathcal{I}_e) the subspace of the Hermitian matrices of dimension 2^n generated by Kronecker products that contain an odd (even) number of Pauli matrices (and the rest 2×2 identity matrices). Moreover, if π is a permutation of the set $\{1, \dots, n\}$, we denote by P_π the matrix which transforms Kronecker products of n 2×2 matrices according to the permutation π (cfr. [9] pg. 260), namely for every n -ple of 2×2 matrices K_1, \dots, K_n we have

$$P_\pi(K_1 \otimes K_2 \otimes \dots \otimes K_n)P_\pi = K_{\pi(1)} \otimes K_{\pi(2)} \otimes \dots \otimes K_{\pi(n)}. \quad (12)$$

Theorem 2 *Let $(\Sigma, \rho_0) \equiv (\Sigma(n, J_{kl}, \gamma_k), \rho_0)$ and $(\Sigma', \rho'_0) \equiv (\Sigma'(n', J'_{kl}, \gamma'_k), \rho'_0)$ be two fixed models whose dynamics and output are given by equations (4), (5), and (7). Assume that both models are controllable, that all the γ_k and γ'_k different from each other, and that ρ_0 and ρ'_0 are not scalar matrices. Then the following are equivalent:*

(a) $(\Sigma, \rho_0) \sim (\Sigma', \rho'_0)$,

(b) $n = n'$ and there exists a permutation π of the set $\{1, \dots, n\}$ such that

1. $\gamma_k = \gamma'_{\pi(k)}$,
2. denoting by $\pi_{lk}^1 = \min\{\pi(l), \pi(k)\}$, and $\pi_{lk}^2 = \max\{\pi(l), \pi(k)\}$, for $1 \leq l < k \leq n$, then either:
$$\begin{cases} J_{lk} = J'_{\pi_{lk}^1 \pi_{lk}^2} & \forall 1 \leq l < k \leq n, \\ P_\pi \rho'_0 P_\pi = \rho_0; \end{cases} \quad (13)$$

or

$$\begin{cases} J_{lk} = -J'_{\pi_{l_1}^1 \pi_{l_m}^2} & \forall 1 \leq l < k \leq n, \\ \rho_1 = \rho'_1 & \text{and} \quad \rho_2 = -\rho'_2; \end{cases} \quad (14)$$

where ρ_1 and ρ_2 (resp. ρ'_1 and ρ'_2) are the components of ρ_0 (resp. $P_\pi \rho'_0 P_\pi$) in \mathcal{I}_o , \mathcal{I}_e , respectively.

Equations (13), (14) say that, up to a permutation of the spins, the exchange constants are all the same or all opposite. In one case the initial conditions are the same in the other case the components in \mathcal{I}_o are the same while the components in \mathcal{I}_e are opposite. The next two sections are devoted to the proof of Theorem 2. We recall that we have two standing assumptions in all the treatment. The models we are dealing with have different γ 's and are controllable.

4 Preliminary Results

In order to prove the implication (a) \Rightarrow (b) we shall need some properties of equivalent pairs. We present them in this section with all the proofs in Appendix B. The following proposition says that equivalent pairs (Model-Initial State) must have the same dimension.

Proposition 4.1 Let (Σ, ρ_0) and (Σ', ρ'_0) be the two fixed models. If they are equivalent, then $n = n'$ and there exists a permutation π of the set $\{1, \dots, n\}$ such that:

1. $\gamma_k = \gamma'_{\pi(k)}$ for all $k \in \{1, \dots, n\}$,
2. $Tr(I_{kv}\rho(t)) = Tr(I_{\pi(k)v}\rho'(t))$ for all $t \geq 0$, all $k \in \{1, \dots, n\}$, all $v \in \{x, y, z\}$, and all possible trajectories $\rho(t)$ of (Σ, ρ_0) and corresponding $\rho'(t)$ of (Σ', ρ'_0) .

The proof of the next lemma is not presented in the Appendix since it is just a notational modification of the proof of Proposition 3.1.

Lemma 4.2 Let W and W' be two Hermitian matrices of dimensions 2^n and $2^{n'}$, respectively. If, for every trajectory $\rho(t)$ of (Σ, ρ_0) and corresponding trajectory $\rho'(t)$ of (Σ', ρ'_0) we have

$$Tr(W\rho(t)) = Tr(W'\rho'(t)), \quad (15)$$

then for every F , $F := ad_{B_{j_1}} ad_{B_{j_2}} \cdots ad_{B_{j_r}} W$, and corresponding F' , $F' := ad_{B'_{j_1}} ad_{B'_{j_2}} \cdots ad_{B'_{j_r}} W'$, with $r \geq 0$ and $j_1, \dots, j_r \in \{0, 1, 2, 3\}$, we also have

$$Tr(F\rho(t)) = Tr(F'\rho'(t)). \quad (16)$$

Lemma 4.3 Let W and W' be two Hermitian matrices of dimensions 2^n and $2^{n'}$, respectively. If, for every trajectory $\rho(t)$ of (Σ, ρ_0) and corresponding trajectory $\rho'(t)$ of (Σ', ρ'_0) we have

$$Tr(W\rho(t)) = Tr(W'\rho'(t)), \quad (17)$$

then, for every K , $K := ad_{B_{j_1}} ad_{B_{j_2}} \cdots ad_{B_{j_r}} B_{j_0}$, and corresponding K' , $K' := ad_{B'_{j_1}} ad_{B'_{j_2}} \cdots ad_{B'_{j_r}} B'_{j_0}$, with $r \geq 0$ and $j_0, \dots, j_r \in \{0, 1, 2, 3\}$, we also have

$$Tr([W, K]\rho(t)) = Tr([W', K']\rho'(t)). \quad (18)$$

Lemma 4.4 Let (Σ, ρ_0) and (Σ', ρ'_0) be two fixed models. Assume that they are equivalent and let π be the permutation given by Proposition 4.1. If W and W' are two given Hermitian matrices such

$$Tr(W\rho(t)) = Tr(W'\rho'(t)), \quad (19)$$

for every pair of corresponding trajectories $\rho(t)$ and $\rho'(t)$, then it also holds

$$Tr([W, I_{kv}]\rho(t)) = Tr([W', I_{\pi(k)v}]\rho'(t)), \quad \forall k \in \{1, \dots, n\}. \quad (20)$$

5 Proof of Theorem 2

Let (Σ, ρ_0) and (Σ', ρ'_0) be the two given equivalent models. Assume that both models are controllable and that all the γ_k and γ'_k are different from each other. We already know that $n = n'$ and 1 and 2 of Proposition 4.1 hold. To simplify the notations, we assume, without loss of generality, that we have performed a change of coordinates in the second model so that the permutation π of Proposition 4.1 is the identity. Thus we can write

$$\gamma_k = \gamma'_k, \quad \forall k \in \{1, \dots, n\}, \quad (21)$$

and

$$Tr(I_{kv}\rho(t)) = Tr(I_{kv}\rho'(t)) \quad \forall k \in \{1, \dots, n\}. \quad (22)$$

Equations (13) and (14) now read as:

$$\begin{cases} J_{lk} = J'_{lk} & \forall 1 \leq l < k \leq n, \\ \rho'_0 = \rho_0; \end{cases} \quad (23)$$

or

$$\begin{cases} J_{lk} = -J'_{lk} & \forall 1 \leq l < k \leq n, \\ \rho_1 = \rho'_1 \quad \text{and} \quad \rho_2 = -\rho'_2; \end{cases} \quad (24)$$

where ρ_1 and ρ_2 (resp. ρ'_1 and ρ'_2) are the components of ρ_0 (resp. ρ'_0) in $\mathcal{I}_o, \mathcal{I}_e$, respectively. We shall need the following two lemmas whose proofs are presented in Appendix C.

Lemma 5.1 Assume that for all $t \geq 0$, all possible trajectories $\rho(t)$ of (Σ, ρ_0) and corresponding $\rho'(t)$ of (Σ', ρ'_0) , for fixed values $1 \leq k_1, \dots, k_r \leq n$, and fixed $v_j \in \{x, y, z\}$ we have:

$$Tr(I_{k_1 v_1, \dots, k_r v_r} \rho(t)) = Tr(I_{k_1 v_1, \dots, k_r v_r} \rho'(t)), \quad (25)$$

Then:

1. equation (25) holds for any possible choice of the values of $v_j \in \{x, y, z\}$;

2.

$$Tr \left(\left[\left[iI_{\bar{v}_l}, [iI_{\bar{k}v_{\bar{k}}}, A] \right], I_{k_1v_1, \dots, k_rv_r} \right] \rho(t) \right) = Tr \left(\left[\left[iI_{\bar{v}_l}, [iI_{\bar{k}v_{\bar{k}}}, A] \right], I_{k_1v_1, \dots, k_rv_r} \right] \rho'(t) \right), \quad (26)$$

for every values $1 \leq \bar{l} \neq \bar{k} \leq n$ and every $\{v_{\bar{l}} \neq v_{\bar{k}}\} \in \{x, y, z\}$.

Lemma 5.2 Assume that for all $t \geq 0$, all possible trajectories $\rho(t)$ of (Σ, ρ_0) and corresponding $\rho'(t)$ of (Σ', ρ'_0) , for fixed values $1 \leq k_1, \dots, k_r \leq n$, $v_j \in \{x, y, z\}$ and for given constants α and α' , we have:

$$\alpha Tr(I_{k_1v_1, \dots, k_rv_r} \rho(t)) = \alpha' Tr(I_{k_1v_1, \dots, k_rv_r} \rho'(t)), \quad (27)$$

Then

1. For any pair of indices $\bar{k}, \bar{l} \in \{1, \dots, n\}$ with $\bar{k} \in \{k_1, \dots, k_r\}$ and $\bar{l} \notin \{k_1, \dots, k_r\}$,

$$\alpha J_{\bar{k}\bar{l}} Tr(I_{k_1v_1, \dots, k_rv_r, \bar{l}\bar{v}} \rho(t)) = \alpha' J'_{\bar{k}\bar{l}} Tr(I_{k_1v_1, \dots, k_rv_r, \bar{l}\bar{v}} \rho'(t)), \quad (28)$$

for any value $\bar{v} \in \{x, y, z\}$.

2. For any pair of indices \bar{k}, \bar{l} both in $\{k_1, \dots, k_r\}$, (for example $\bar{k} = k_1, \bar{l} = k_2$) then

$$\alpha J_{\bar{k}\bar{l}} Tr(I_{k_1v_1, k_3v_3, \dots, k_rv_r} \rho(t)) = \alpha' J'_{\bar{k}\bar{l}} Tr(I_{k_1v_1, k_3v_3, \dots, k_rv_r} \rho'(t)). \quad (29)$$

5.1 (a) \Rightarrow (b)

Fix any $1 \leq k_1 < k_2 \leq n$, then, by applying statement 1. of Lemma 5.2, i.e. equation (28) with $\bar{k} = k_1, \bar{l} = k_2$ to equation (22) with $k = k_1$, we have:

$$J_{k_1k_2} Tr(I_{k_1v_1, k_2v_2} \rho(t)) = J'_{k_1k_2} Tr(I_{k_1v_1, k_2v_2} \rho'(t)), \quad \forall v_1, v_2 \in \{x, y, z\}. \quad (30)$$

Now, to the previous equality, we apply statement 2. of Lemma 5.2, i.e. equation (29) with $\bar{k} = k_1$ and $\bar{l} = k_2$ to get:

$$J_{k_1k_2}^2 Tr(I_{k_1v_1} \rho(t)) = J_{k_1k_2}'^2 Tr(I_{k_1v_1} \rho'(t)),$$

which, by equation (22), implies:

$$J_{k_1k_2}^2 = J_{k_1k_2}'^2. \quad (31)$$

Therefore the exchange constants are equal up to the sign. Now we prove, by the way of contradiction that they are either all equal or all opposite i.e.

$$\{J_{kl} = J'_{kl} \forall 1 \leq k < l \leq n\} \quad \text{or} \quad \{J_{kl} = -J'_{kl} \forall 1 \leq k < l \leq n.\} \quad (32)$$

Assume, by contradiction, that (32) does not hold. By the controllability assumption and the results of [1] we know that the graph associated to the network is connected. From this fact it is not difficult to see that if (32) is false, there must exist 3 indices l, k_1 , and k_2 (here,

to simplify notations, we assume $1 \leq l < k_1 < k_2 \leq n$, the other cases can be treated using exactly the same arguments) such that:

$$J_{lk_1} = J'_{lk_1}, \quad \text{and} \quad J_{lk_2} = -J'_{lk_2}. \quad (33)$$

Using equation (30) we get:

$$J_{lk_1} \text{Tr}(I_{lv, k_1 v_1} \rho(t)) = J'_{lk_1} \text{Tr}(I_{lv, k_1 v_1} \rho'(t)),$$

for all $v, v_1 \in \{x, y, z\}$ and all corresponding trajectories $\rho(t)$ and $\rho'(t)$. By applying to the previous equality statement 1. of Lemma 5.2, i.e. equation (28) with $\bar{k} = l$ and $\bar{l} = k_2$, we get:

$$J_{lk_1} J_{lk_2} \text{Tr}(I_{lv, k_1 v_1, k_2 v_2} \rho(t)) = J'_{lk_1} J'_{lk_2} \text{Tr}(I_{lv, k_1 v_1, k_2 v_2} \rho'(t)) \quad (34)$$

for all $v, v_1, v_2 \in \{x, y, z\}$ and all corresponding trajectories $\rho(t)$ and $\rho'(t)$. Now we apply to equation (34) statement 2. of Lemma 5.2, i. e. equation (29) with $\bar{k} = k_1$ and $\bar{l} = l$ to get:

$$J_{lk_1}^2 J_{lk_2} \text{Tr}(I_{k_1 v_1, k_2 v_2} \rho(t)) = J_{lk_1}^2 J'_{lk_2} \text{Tr}(I_{k_1 v_1, k_2 v_2} \rho'(t)). \quad (35)$$

On the other hand, we can apply to equation (34) again statement 2. of Lemma 5.2, i. e. equation (29) this time with $\bar{k} = k_2$ and $\bar{l} = l$ to get:

$$J_{lk_1} J_{lk_2}^2 \text{Tr}(I_{k_1 v_1, k_2 v_2} \rho(t)) = J'_{lk_1} J_{lk_2}^2 \text{Tr}(I_{k_1 v_1, k_2 v_2} \rho'(t)). \quad (36)$$

Since $J_{lk_1}^2 J_{lk_2} = -J_{lk_1}^2 J'_{lk_2}$ while $J_{lk_1} J_{lk_2}^2 = J'_{lk_1} J_{lk_2}^2$ (by (33)), equations (35) and (36) imply $\text{Tr}(I_{k_1 v_1, k_2 v_2} \rho(t)) = 0$ for all $v_1, v_2 \in \{x, y, z\}$ and all trajectories $\rho(t)$. This fact contradicts the controllability assumption, thus equation (32) holds.

If $J_{kl} = J'_{kl}$ for every pair $1 \leq k < l \leq n$, from the observability of the model, we must have $\rho_0 = \rho'_0$, thus equation (23) holds.

On the other hand, if $J'_{kl} = -J_{kl}$ for every pair $1 \leq k < l \leq n$, we argue as follows. First, we prove, by induction on $1 \leq r \leq n$ that:

$$\text{Tr}(I_{k_1 v_1, \dots, k_r v_r} \rho(t)) = (-1)^{r-1} \text{Tr}(I_{k_1 v_1, \dots, k_r v_r} \rho'(t)), \quad \forall v_j \in \{x, y, z\}, \quad 1 \leq k_1 < \dots < k_r \leq n, \quad (37)$$

and for all corresponding trajectories $\rho(t)$ and $\rho'(t)$.

For $r = 1$ the previous equation is equation (22), thus the result holds for $r = 1$. Assume that (37) holds for $1 < r < n$, and consider an arbitrary set of indices $1 \leq k_2 < \dots < k_{r+1}$. By the inductive assumption we have:

$$\text{Tr}(I_{k_1 v_1, \dots, k_r v_r} \rho(t)) = (-1)^{r-1} \text{Tr}(I_{k_1 v_1, \dots, k_r v_r} \rho'(t)).$$

Since the graph associated to the network is connected, for each node k_j , $j = 1, \dots, r$, there exists a path joining the node k_j with the node k_{r+1} . Let \bar{j} be the index for which this path is the shortest one, and denote by l_1, \dots, l_d the intermediate nodes. By the way we have chosen \bar{j} , it is easy to see that $\{k_1, \dots, k_r\} \cap \{l_1, \dots, l_d\} = \emptyset$. To fix notations, we may assume without loss of generality (being all the other cases the same) that $1 \leq k_1 < \dots <$

$k_r < l_1 < \dots < l_d < k_{r+1}$. By applying statement 1. of Lemma 5.2, equation (28) with $\bar{k} = \bar{j}$ and $\bar{l} = l_1$, since $J_{\bar{j}l_1} = -J'_{\bar{j}l_1}$, we have:

$$Tr(I_{k_1 v_1, \dots, k_r v_r, l_1 w_1} \rho(t)) = (-1)(-1)^{r-1} Tr(I_{k_1 v_1, \dots, k_r v_r, l_1 w_1} \rho'(t)),$$

for any $w_1 \in \{x, y, z\}$. By applying again statement 1. of Lemma 5.2, equation (28) another $d-1$ -times with $\bar{k} = l_i$ and $\bar{l} = l_{i+1}$, $i = 1, \dots, d-1$, and then another time with $\bar{k} = l_d$ and $\bar{l} = k_{r+1}$, we end up with:

$$Tr(I_{k_1 v_1, \dots, k_r v_r, l_1 w_1, \dots, l_d w_d, k_{r+1} v_{r+1}} \rho(t)) = (-1)^d (-1)^r Tr(I_{k_1 v_1, \dots, k_r v_r, l_1 w_1, \dots, l_d w_d, k_{r+1} v_{r+1}} \rho'(t)). \quad (38)$$

Now we apply to equation (38), statement 2. of Lemma 5.2, i.e. equation (29) $d-1$ -times with $\bar{k} = l_{i+1}$ and $\bar{l} = l_i$, $i = 1, \dots, d-1$, to get:

$$Tr(I_{k_1 v_1, \dots, k_r v_r, l_d w_d, k_{r+1} v_{r+1}} \rho(t)) = (-1)^{d-1} (-1)^d (-1)^r Tr(I_{k_1 v_1, \dots, k_r v_r, l_d w_d, k_{r+1} v_{r+1}} \rho'(t)).$$

Finally, by applying again statement 2. of Lemma 5.2, i.e. equation (29) with $\bar{k} = k_{r+1}$ and $\bar{l} = l_d$, we end up with:

$$Tr(I_{k_1 v_1, \dots, k_r v_r, k_{r+1} v_{r+1}} \rho(t)) = (-1)^r Tr(I_{k_1 v_1, \dots, k_r v_r, k_{r+1} v_{r+1}} \rho'(t)),$$

as desired. Thus equation (37) holds.

Now, denoting by ρ_1 and ρ_2 (resp. ρ'_1 and ρ'_2) the components of ρ_0 (resp. ρ'_0) in \mathcal{I}_o , \mathcal{I}_e , by using (37), we have:

$$Tr((I_o(\rho_0 - \rho'_0))) = 0, \quad Tr((I_e(\rho_0 + \rho'_0))) = 0, \quad (39)$$

for all elements $I_o \in \mathcal{I}_o$ and $I_e \in \mathcal{I}_e$. Equation (39) implies that the components of ρ_0 and ρ'_0 in \mathcal{I}_o coincide while the components in \mathcal{I}_e are opposite to each other. Thus equation (24) holds.

5.2 (b) \Rightarrow (a)

Let (Σ, ρ_0) and (Σ', ρ'_0) be two models, which are both controllable, with all the γ_k and γ'_k different from each other.

In the case where equation (23) holds (i.e. same model and same initial condition), obviously that:

$$\rho'(t) = \rho(t),$$

for all $t \geq 0$. Thus the two models are equivalent.

Assume now that equation (24) holds. Thus,

$$A' = -A, \quad \text{and} \quad B'_v = B_v \quad \forall v \in \{x, y, z\}.$$

and

$$\rho_1 = \rho'_1 \quad \text{and} \quad \rho_2 = -\rho'_2.$$

We have:

$$\dot{\rho}(t) = [A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho(t)], \quad (40)$$

while

$$\dot{\rho}'(t) = [-A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho'(t)]. \quad (41)$$

It is easily verified (cfr. Lemmas 5.1 and 5.2) that:

$$\begin{aligned} [B, I_o] &\in \mathcal{I}_o, & [A, I_o] &\in \mathcal{I}_e, & \forall I_o \in \mathcal{I}_o, \\ [B, I_e] &\in \mathcal{I}_e, & [A, I_e] &\in \mathcal{I}_o, & \forall I_e \in \mathcal{I}_e. \end{aligned} \quad (42)$$

Thus, we can write the differential equations for $\rho_1(t)$ and $\rho_2(t)$ as:

$$\begin{aligned} \dot{\rho}_1(t) &= [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho_1(t)] + [A, \rho_2(t)] \\ \dot{\rho}_2(t) &= [A, \rho_1(t)] + [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho_2(t)] \end{aligned} \quad (43)$$

and similarly the differential equation for $\rho'_1(t)$ and $\rho'_2(t)$ as:

$$\begin{aligned} \dot{\rho}'_1(t) &= [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho'_1(t)] - [A, \rho'_2(t)] \\ \dot{\rho}'_2(t) &= -[A, \rho'_1(t)] + [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho'_2(t)] \end{aligned} \quad (44)$$

Combining equations (43) and (44), we obtain a differential equation for $\rho_1(t) - \rho'_1(t)$ and for $\rho_2(t) + \rho'_2(t)$. In particular, we have

$$\begin{aligned} \dot{\rho}_1(t) - \dot{\rho}'_1(t) &= [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho_1(t) - \rho'_1(t)] + [A, \rho_2(t) + \rho'_2(t)] \\ \dot{\rho}_2(t) + \dot{\rho}'_2(t) &= [A, \rho_1(t) - \rho'_1(t)] + [B_x u_x(t) + B_y u_y(t) + B_z u_z(t), \rho_2(t) + \rho'_2(t)] \end{aligned} \quad (45)$$

From equations (45) 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 controls $u_x(t)$, $u_y(t)$, and $u_z(t)$. In particular, since $\text{Tr}(S_v^{TOT} \rho(t)) = \text{Tr}(S_v^{TOT} \rho_1(t))$ for all $v \in \{x, y, z\}$ and $\rho_1(t) \equiv \rho'_1(t)$ the two models are equivalent.

6 Conclusions

In this paper, we have investigated methods of dynamic parameter identification for networks of spin $\frac{1}{2}$ particles. We have shown that by driving the network with an appropriate electromagnetic field and measuring the total magnetization in a given (arbitrary) direction it is possible to identify the parameters. Moreover, if the initial state is not known, it is possible to obtain combined information about the initial state and the parameter values. We have assumed that all the gyromagnetic ratios of the spins are different or that it is possible to address each spin separately. In the opposite case, where all the gyromagnetic ratios are the same, the unitary evolution $X(t)$, solution of Schrödinger operator equation, has the form $X(t) = e^{At}\Phi(t)$ where $\Phi(t)$ depends only on the controls u_x, u_y, u_z and A is defined in (4), (5). In this case, we have that A commutes with Φ and S_v^{TOT} , $v = x, y, z$, and therefore the output $\text{Tr}(S_v^{TOT} e^{At}\Phi(t)\rho_0\Phi^*(t)e^{-At})$ is equal to $\text{Tr}(e^{-At}S_v^{TOT}e^{At}\Phi(t)\rho_0\Phi^*(t)) =$

$Tr(S_v^{TOT}\Phi(t)\rho_0\Phi^*(t))$. The output is therefore independent of A . This implies that it is not possible to identify the parameters in A by a reading of the total magnetization.

In our approach, the system theoretic concepts of controllability and observability as well as previously known results on the controllability of spin networks have played an important role. This is usually the case in the theory of parameter identification and we believe this approach will be useful for other classes of quantum systems. Extensions of the results presented here are possible and will be object of further research. For example, the hypothesis of controllability of the models can be weakened. If a spin network is not controllable and has different gyromagnetic ratios the associated graph has several connected components. The dynamical Lie Algebra associated to the system is the direct sum of Lie Algebras isomorphic to $su(2^{n_j})$ where n_j is the number of nodes (spins) in the j -th component [1]. Another important research problem is the actual design of control algorithms for parameter identification for which the research presented here is a preliminary step.

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Appendix A: Proof of Proposition 3.1

Proof. It is clear that (b) implies (a), since $iS_v^{TOT} \in \mathcal{V}$ ($iS_v'^{TOT} \in \mathcal{V}'$) for $v = x, y, z$. We will prove the converse implication by induction on the depth $s = \sum_{i=1}^r k_i$ in (8) of the matrix $F \in \mathcal{V}$. If $s = 0$ then $F = iS_v^{TOT}$ for $v = x, y$ or z , thus equation (9) holds by definition of equivalence. Assume that equation (9) holds for matrices in \mathcal{V} of depth $\leq s$ and let $F \in \mathcal{V}$ with depth equal $s + 1$. Then

$$F = ad_{B_{\bar{t}}} G, \quad \text{with } G \in \mathcal{V},$$

and the depth of G is equal to s . Assume, by contradiction, that there exist control functions $u_x(\cdot)$, $u_y(\cdot)$, and $u_z(\cdot)$, and $\bar{t} \geq 0$ such that equation (9) does not hold, i.e.

$$Tr(F\rho(\bar{t})) \neq Tr(F'\rho'(\bar{t})). \quad (46)$$

On the other hand, since by the inductive assumption, equation (9) holds for the matrix G , we have:

$$\frac{d}{dt} Tr(G\rho(t)) = \frac{d}{dt} Tr(G'\rho'(t)),$$

for all $t \geq 0$. This implies:

$$\begin{aligned} & Tr([G, B_0]\rho(t)) + Tr([G, B_1]\rho(t))u_x(t) + Tr([G, B_2]\rho(t))u_y(t) + \\ & Tr([G, B_3]\rho(t))u_z(t) = Tr([G', B'_0]\rho'(t)) + Tr([G', B'_1]\rho'(t))u_x(t) + \\ & + Tr([G', B'_2]\rho'(t))u_y(t) + Tr([G', B'_3]\rho'(t))u_z(t) \end{aligned} \quad (47)$$

Define:

$$u_v^0(t) = \begin{cases} u_v(t) & \text{for } t < \bar{t} \\ 0 & \text{for } t \geq \bar{t}. \end{cases}$$

Then, clearly the trajectories $\rho(t)$ and $\rho'(t)$ corresponding to the two sets of controls $u_v(\cdot)$ and $u_v^0(\cdot)$ are equal up to time \bar{t} . Thus evaluating (47) at $t = \bar{t}$, using controls u_v^0 , we get:

$$\text{Tr}([G, B_0]\rho(\bar{t})) = \text{Tr}([G', B'_0]\rho'(\bar{t})), \quad (48)$$

which contradicts (46) if $\bar{i} = 0$. Assume $\bar{i} \neq 0$. First notice that, by repeating the same argument as above for a generic $t \geq 0$, the previous equality (48) must hold for all $t \geq 0$. To get a contradiction we use the control functions $u_v^{\bar{i}}$ given by²:

$$u_v^{\bar{i}}(t) = \begin{cases} u_v(t) & \text{for } t < \bar{t} \\ \delta_{\bar{i},v} & \text{for } t \geq \bar{t}. \end{cases}$$

Again the trajectories corresponding to the two set of controls $u_v(\cdot)$ and $u_v^{\bar{i}}(\cdot)$ are equal up to time \bar{t} , thus evaluating (47) at $t = \bar{t}$ using controls $u_v^{\bar{i}}$ we get:

$$\text{Tr}([G, B_0]\rho(\bar{t})) + \text{Tr}([G, B_{\bar{i}}]\rho(\bar{t}))u_{\bar{i}}(\bar{t}) = \text{Tr}([G', B'_0]\rho'(\bar{t})) + \text{Tr}([G', B'_{\bar{i}}]\rho'(\bar{t}))u_{\bar{i}}(\bar{t})$$

which, since the first terms are equal as observed before, contradicts (46), and ends the proof. \square

Appendix B: Proofs of the preliminary results in section 4

Proof of Proposition 4.1

Proof. It is not difficult to see that, for all $l \geq 0$, if $F^l = \sum_{k=1}^n \gamma_k^l I_{kv} \in \mathcal{V}$, then the corresponding matrix in \mathcal{V}' is $F'^l = \sum_{k=1}^{n'} \gamma_k'^l I_{kv}$. By Proposition 3.1, it holds that:

$$\text{Tr}(F^l \rho(t)) = \text{Tr}(F'^l \rho'(t)).$$

for all $t \geq 0$ and all possible trajectories. Thus we have:

$$\sum_{k=1}^n \gamma_k^l \text{Tr}(I_{kv} \rho(t)) = \sum_{k=1}^{n'} \gamma_k'^l \text{Tr}(I_{kv} \rho'(t)). \quad (49)$$

Fix v and let $\alpha_k(t) = \text{Tr}(I_{kv} \rho(t))$ and $\alpha'_k(t) = \text{Tr}(I_{kv} \rho'(t))$, then we rewrite equation (49) as:

$$\sum_{k=1}^n \gamma_k^l \alpha_k(t) - \sum_{k=1}^{n'} \gamma_k'^l \alpha'_k(t) = 0 \quad (50)$$

² $\delta_{1x} \equiv \delta_{2y} \equiv \delta_{3z} \equiv 1$, $\delta_{iv} \equiv 0$ otherwise.

The matrix $M \in \mathcal{R}^{(n+n') \times (n+n')}$ given by:

$$M = \begin{pmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ \gamma_1 & \dots & \gamma_n & \gamma'_1 & \dots & \gamma'_{n'} \\ \gamma_1^2 & \dots & \gamma_n^2 & \gamma_1'^2 & \dots & \gamma_{n'}'^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \gamma_1^{n+n'} & \dots & \gamma_n^{n+n'} & \gamma_1'^{n+n'} & \dots & \gamma_{n'}'^{n+n'} \end{pmatrix},$$

is a Vandermonde type of matrix. Notice that the coefficients γ_k , $k = 1, \dots, n$ and also γ'_k , $k = 1, \dots, n'$, are all different. Moreover, the coefficients $\alpha_k(t)$ and $\alpha'_k(t)$ are not identically zero. In fact, if $\alpha_k(t)$ was identically zero we would have $Tr(A\rho(t)) = 0$, for every $A \in su(2^n)$ (by the controllability assumption) which would imply ρ_0 equal to a multiple of the identity matrix which we have excluded. Thus, from equation (50), we conclude that there exist two indices \bar{k} and $\pi(\bar{k})$ such that

$$\gamma_{\bar{k}} = \gamma'_{\pi(\bar{k})}.$$

We can rewrite equation (50), as

$$\gamma_{\bar{k}}^l (\alpha_{\bar{k}}(t) - \alpha'_{\pi(\bar{k})}(t)) + \sum_{k=1, k \neq \bar{k}}^n \gamma_k^l \alpha_k(t) - \sum_{k=1, k \neq \pi(\bar{k})}^{n'} \gamma_k^l \alpha'_k(t) = 0 \quad (51)$$

Now we can repeat the same argument and, unless $n = 1$ or $n' = 1$, we will find two more indices \bar{j} and $\pi(\bar{j})$ whose corresponding values of $\gamma_{\bar{j}}$ and $\gamma'_{\pi(\bar{j})}$ are equal. We may assume without loss of generality that $n' \geq n$ and repeat this procedure n -times. Thus we find a permutation π from the set $\{1, \dots, n\}$ to the set $\{1, \dots, n'\}$ and we rewrite equation (51) as:

$$\sum_{k=1}^n \gamma_k^l (\alpha_k(t) - \alpha'_{\pi(k)}(t)) - \sum_{\substack{k \neq \pi(j) \\ j=1, \dots, n}}^{n'} \gamma_k^l \alpha'_k(t) = 0. \quad (52)$$

Now, we can apply again the same argument, using the Vandermonde matrix N constructed with all the coefficients γ_k and the coefficients γ'_k for those indices that are not in the image of π . Since the coefficients $\alpha'_k(t)$ are not identically zero, we can conclude that all the coefficients γ'_k , for those indices that are not in the image of π , must be zero. Thus, in particular $n = n'$, the map π is a permutation and :

$$\gamma_k = \gamma'_{\pi(k)}, \quad \alpha_k(t) - \alpha'_{\pi(k)}(t) = 0, \quad \forall t \geq 0,$$

which concludes the proof. \square

Proof of Lemma 4.3

Proof. We will prove the result by induction on the depth r of K and K' . If $r = 0$, the result follows from Lemma 4.2. Now assume that for every pair K and K' of depth r , and every pair of matrices W and W' , (17) implies (18). From the inductive assumption we have

$$\text{Tr}([W, K]\rho(t)) = \text{Tr}([W', K']\rho'(t)), \quad (53)$$

and

$$\text{Tr}([W, B_j]\rho(t)) = \text{Tr}([W', B'_j]\rho'(t)). \quad (54)$$

Applying the inductive assumption with W (W') replaced by $[W, K]$ and $[W, B_j]$ ($[W', K']$ and $[W', B'_j]$) we obtain

$$\text{Tr}([[W, K], B_j]\rho(t)) = \text{Tr}([[W', K'], B'_j]\rho'(t)), \quad (55)$$

$$\text{Tr}([[W, B_j], K]\rho(t)) = \text{Tr}([[W', B'_j], K']\rho'(t)). \quad (56)$$

Combining (55) and (56) using the Jacobi identity, we obtain

$$\text{Tr}([W, [K, B_j]]\rho(t)) = \text{Tr}([W', [K', B'_j]]\rho'(t)), \quad (57)$$

which proves the lemma. \square

Proof of Lemma 4.4

Proof. For any $l \geq 0$ let $F_l := \sum_{k=1}^n \gamma_k^l I_{kv} \in \mathcal{V}$; then its corresponding matrix in \mathcal{V}' is $F'_l := \sum_{k=1}^n \gamma_{\pi(k)}^l I_{\pi(k)v}$. By applying Lemma 4.3, with $K = F_l$ and $K' = F'_l$, we obtain

$$\sum_{k=1}^n \gamma_k^l \text{Tr}([I_{kv}, W]\rho(t)) = \sum_{k=1}^n \gamma_{\pi(k)}^l \text{Tr}([I_{\pi(k)v}, W']\rho'(t)). \quad (58)$$

Using the fact that $\gamma_k = \gamma_{\pi(k)}$, we can rewrite equation (58) as

$$\sum_{k=1}^n \gamma_k^l \left(\text{Tr}([I_{kv}, W]\rho(t)) - \text{Tr}([I_{\pi(k)v}, W']\rho'(t)) \right) = 0.$$

Since the coefficients γ_k are all different and the previous equality holds for every $l \geq 0$, using a Vandermonde determinant type of argument, we obtain

$$\text{Tr}([I_{kv}, W]\rho(t)) - \text{Tr}([I_{\pi(k)v}, W']\rho'(t)) = 0, \quad (59)$$

as desired. \square

Appendix C: Proofs of the lemmas in Section 5

Proof of Lemma 5.1

Proof.

1. This fact follows easily by applying Lemma 4.4 with $W = W' = I_{k_1 v_1, \dots, k_r v_r}$, since, if $v_j \neq w_j$, it holds:

$$[I_{k_1 v_1, \dots, k_r v_r}, I_{k_j w_j}] = i I_{k_1 v_1, \dots, k_j [v_j w_j], \dots, k_r v_r}. \quad (60)$$

Here we have used the notation $[v_j w_j] = v$ if $[\sigma_{v_j}, \sigma_{w_j}] = \pm i \sigma_v$, and agreed to multiply (60) by -1 if the minus sign appears.

2. By applying Lemma 4.2 to equation (25), we have:

$$Tr([A, I_{k_1 v_1, \dots, k_r v_r}] \rho(t)) = Tr([A', I_{k_1 v_1, \dots, k_r v_r}] \rho'(t)). \quad (61)$$

Now, we apply Lemma 4.4 to the previous equation to get:

$$Tr([A, I_{k_1 v_1, \dots, k_r v_r}], I_{\bar{k} v_{\bar{k}}}] \rho(t)) = Tr([A', I_{k_1 v_1, \dots, k_r v_r}], I_{\bar{k} v_{\bar{k}}}] \rho'(t)). \quad (62)$$

Using the Jacobi identity, we have:

$$[A, I_{k_1 v_1, \dots, k_r v_r}], I_{\bar{k} v_{\bar{k}}}] = [A, [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}]] + [I_{k_1 v_1, \dots, k_r v_r}, [A, I_{\bar{k} v_{\bar{k}}}]] \quad (63)$$

We have

$$[I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}] = \begin{cases} 0 & \text{if } \bar{k} \notin \{k_1, \dots, k_r\} \\ 0 & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} = v_j \\ i I_{k_1 v_1, \dots, k_j [v_j v_{\bar{k}}], \dots, k_r v_r} & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} \neq v_j. \end{cases} \quad (64)$$

Using the fact that (61) holds for any choice of values v_k , and (64) we get:

$$Tr([A, [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}]] \rho(t)) = Tr([A', [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}]] \rho'(t)).$$

Thus combining the previous equality with (62) and (63) we get:

$$Tr([A, I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}] \rho(t)) = Tr([A', I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}}] \rho'(t)). \quad (65)$$

Notice that equation (65) is of the same type as equation (61); it is enough to replace A with $[A, I_{\bar{k} v_{\bar{k}}}]$ (resp. A' with $[A', I_{\bar{k} v_{\bar{k}}}]$). Thus by applying first Lemma 4.4 and then the Jacobi identity we get:

$$\begin{aligned} & Tr([A, I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{l} v_{\bar{l}}}] \rho(t)) + Tr([I_{k_1 v_1, \dots, k_r v_r}, [A, I_{\bar{k} v_{\bar{k}}}], I_{\bar{l} v_{\bar{l}}}] \rho(t)) = \\ & = Tr([A', I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{l} v_{\bar{l}}}] \rho'(t)) + Tr([I_{k_1 v_1, \dots, k_r v_r}, [A', I_{\bar{k} v_{\bar{k}}}], I_{\bar{l} v_{\bar{l}}}] \rho'(t)). \end{aligned} \quad (66)$$

On the other hand, using (64) and (65), we get:

$$Tr([A, I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{l} v_{\bar{l}}}] \rho(t)) = Tr([A', I_{\bar{k} v_{\bar{k}}}], [I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{l} v_{\bar{l}}}] \rho'(t)).$$

Thus:

$$Tr([I_{k_1 v_1, \dots, k_r v_r}, [A, I_{\bar{k} v_{\bar{k}}}], I_{\bar{l} v_{\bar{l}}}] \rho(t)) = Tr([I_{k_1 v_1, \dots, k_r v_r}, [A', I_{\bar{k} v_{\bar{k}}}], I_{\bar{l} v_{\bar{l}}}] \rho'(t));$$

which implies (26), as desired. \square

Proof of Lemma 5.2

Proof. Both statements are a consequence of Lemma 5.1 (equation (26)). First notice that, again by Lemma 5.1, it is enough to prove (28) and (29) for a particular choice of $\{v_j\}$ and \bar{v} . We have, for $\bar{l} > \bar{k}$,

$$[iI_{\bar{l}z}, [iI_{\bar{k}x}, A]] = -J_{\bar{k}\bar{l}} iI_{\bar{k}z, \bar{l}x}. \quad (67)$$

1. By applying Lemma 5.1 (equation (26)) to (27) and using (67) we get:

$$\alpha Tr \left(\left[-J_{\bar{k}\bar{l}} iI_{\bar{k}z, \bar{l}x}, I_{k_1 v_1, \dots, k_r v_r} \right] \rho(t) \right) = \alpha Tr \left(\left[-J'_{\bar{k}\bar{l}} iI_{\bar{k}z, \bar{l}x}, I_{k_1 v_1, \dots, k_r v_r} \right] \rho'(t) \right). \quad (68)$$

We may assume, without loss of generality, that $\bar{k} = k_j$ and $v_j = x$. In this case we have:

$$-J_{\bar{k}\bar{l}} \left[I_{\bar{k}z, \bar{l}x}, I_{k_1 v_1, \dots, k_r v_r} \right] = J_{\bar{k}\bar{l}} iI_{k_1 v_1, \dots, k_j y, \dots, k_r v_r, \bar{l}x}.$$

Combining the previous equality with (68), equation (28) follows easily.

2. Using the same procedure, we end up again with equation (68), but now both indices \bar{k} and \bar{l} are in $\{k_1, \dots, k_r\}$. Assume, for example that $k_1 = \bar{k}$ and $k_2 = \bar{l}$, and take $v_{k_1} = v_{k_2} = x$, then equation (29) follows since it holds:

$$[I_{k_1 z, k_2 x}, I_{k_1 x, k_2 x, \dots, k_r v_r}] = 1/4 I_{k_1 y, k_3 v_3, \dots, k_r v_r}.$$

□