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INPUT-OUTPUT MODEL EQUIVALENCE OF SPIN SYSTEMS: A CHARACTERIZATION USING LIE ALGEBRA HOMOMORPHISMS*

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Abstract. In this paper, we consider the problem of model equivalence for quantum systems. Two models are said to be (input-output) equivalent if they give the same output for every admissible input. In the case of quantum systems, we take as output the expectation value of a given observable or, more generally, a probability distribution for the result of a quantum measurement. We link the input-output equivalence of two models to the existence of a homomorphism of the underlying Lie algebra. In several cases, a Cartan decomposition of the Lie algebra $su(N)$ is useful to find such a homomorphism and to determine the classes of equivalent models. We consider in detail the important cases of two level systems with a Cartan structure and of spin networks. In the latter case, complete results are given generalizing previous results to networks of spin particles with arbitrary values of the spins. In treating this problem, we give independent proofs of some instrumental results on the subalgebras of $su(N)$.

Key words. quantum control systems, parameter identification, Lie algebraic methods, spin systems

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1. Introduction.

Structural properties of quantum systems recently have been the subject of investigation with methods of control theory. Appropriate definitions of controllability and observability of quantum systems have been given and practical conditions for checking these properties have been proposed (see, e.g., [1], [10], [17], [23]). In many cases, the tools used are those of Lie algebra and Lie group theory. Information on the properties of the dynamics is obtained by a study of the structure of a Lie algebra associated with the system and how this relates to the particular equations at hand. This geometric approach has proved useful not only to analyze the dynamics but also to design control laws (see, e.g., [3], [21], [22], [13]). This approach can also be used to study problems of parameter identification of quantum systems, and this is the subject of the present paper.

The problem we shall study is the classification of models of quantum systems whose behavior cannot be distinguished by an external observer. We shall call these models *(input-output) equivalent*. This problem is motivated by several experimental scenarios. In particular consider a molecule which is a network of particles with spin with all the other degrees of freedom neglected. A model Hamiltonian is associated with this system in which parameters modeling the interaction between particles as well as the interaction with an external electromagnetic field are unknown. Also, the initial state of the system might be unknown. In experimental scenarios such as nuclear magnetic resonance and electron paramagnetic resonance, it is possible to drive the system with a magnetic field and measure the expectation value of a given observable, for example, the total spin in a given direction. The question of

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fundamental and practical importance is to what extent, with this type of experiments, it is possible to distinguish between different models. As we shall see in this paper, this question is related to the existence of a particular Lie algebra homomorphism which maps one into the other the equations of the two models (definitions of Lie algebra theory are given in section 3). Further motivation for this research can be found in [27] where it was shown that thermodynamic methods commonly used to identify the parameters of spin networks such as in molecular magnets [5], [8] are not always adequate.

The main results of this paper are the solution of the model equivalence problem for a class of two level systems in Theorem 2 and Theorem 7 where we completely solve the problem of characterizing equivalent models for networks of spin. The latter result generalizes results previously obtained in [2] and [11], which were proven only for networks of spin $\frac{1}{2}$ and 1's, to networks of interacting spins of any value and where the spin itself is an unknown parameter to be identified. The generalization given in this paper is obtained through a Cartan decomposition technique recently presented in [12] which helps in determining the homomorphism between equivalent models in the form of a Cartan involution. In the process we shall prove a number of auxiliary results (Theorems 4–6) on the structure of the Lie algebra $su(N)$ and in particular on its subalgebras. These results could be formulated in terms of representation theory of Lie algebras (see, e.g., [18]), but we give here independent proofs which use only linear algebra arguments.

The paper is organized as follows. In section 2, we describe the problem of model equivalence for quantum systems. In section 3 we provide some background definitions of Lie algebra theory and describe how the quantum mechanical models we consider are related to mathematical notions in this theory. In section 4, we link the equivalence of two models to the existence of an appropriate Lie algebra homomorphism. This is the content of Theorem 1. In several cases the structure of the dynamics is related to a Cartan decomposition of $su(N)$ and suggests the form of such a homomorphism as well as of the classes of equivalent models. We give a two level example in section 5 and treat the case of general spin networks in section 6. Instrumental to the solution of the model equivalence problem for spin networks are some results of independent interest concerning the existence of subalgebras of $su(N)$ with specific features. The proofs of these results are presented in section 7. Concluding remarks are given in section 8.

2. The problem of model equivalence for quantum systems.

Consider a model Hamiltonian for a quantum system, $H(t) := H(u(t))$, where, in a semiclassical description, the dependence on time is due to the interaction with classical external fields, $u := u(t)$, which play the role of *controls*. For every t, $H(t)$ is a Hermitian operator on a Hilbert space $\mathcal{H}$. The state of a quantum system is described by a density matrix ρ, i.e., a positive, trace one, Hermitian operator on $\mathcal{H}$. The evolution of the state of the system, $\rho := \rho(t)$, is determined, other than by H, by the initial state $\rho(0) = \rho_0$. In particular, ρ is the solution of the *Liouville's equation*,

$$\dot{\rho} = [-iH, \rho], \tag{1}$$

with initial condition $\rho(0) = \rho_0$. Here and in the following, for two matrices A and B, the commutator $[A, B]$ is defined as $[A, B] := AB - BA$. According to the measurement postulate of quantum mechanics, with any measured quantity there is associated an observable S which is a Hermitian operator on $\mathcal{H}$. There are various types of measurements (see, e.g., [6]). Considering, for simplicity, a Von Neumann–Lüders measurement,[1] writing S in terms of orthogonal projections

$$S := \sum_j \lambda_j \Pi_j, \tag{2}$$

the probability of having a result λ_j, when the state is ρ, is given by

$$P_j := Tr(\Pi_j \rho). \tag{3}$$

As the probabilities P_j are the only information that can be gathered by an external observer, we are motivated to ask what classes of models $\{H, \rho_0\}$ will give the same probabilities, for any functional form of the control u. In other words, we ask what classes of models are indistinguishable by experiments that involve driving the system with controls, in a given set of functions, and measuring a given observable. These models will be called *(input-output) equivalent*.

Remark 2.1. The term *output* for the probabilities (3) or for the expectation value (4) below needs to be clarified. We have called output the information that can be gathered measuring a given observable S. In particular, consider a large number of identical systems. By measuring the observable S at a fixed time t and recording the various results, we obtain the probabilities (3). Two models that have the same probabilities (output) at any time t are exactly equivalent from the input-output point of view, because a measurement of S on any of them will give exactly the same result with exactly the same probability (or will have exactly the same expectation value if that is what interests us). Therefore, while it is convenient to call the functions (3) and (4) output and make a mathematical analogy with classical systems, the situation is not the same as for classical systems. In particular, for classical systems it is possible to monitor the output continuously. For quantum systems we consider measurements that in practice happen only at one instant of time. However, we can still ask what the classes of models would give *at any time* the same expectation value (output (4)) or the same result with the same probability (output (3)).[2]

It is appropriate to treat the case where the result of the measurement is the *expectation value* of the measurable S, i.e.,

$$y := Tr(S\rho). \tag{4}$$

Therefore, we take (4) as the *output* of the system. Not only is this the case in several experimental situations, such as nuclear magnetic resonance, but it is not a significant restriction as compared to the case where the probabilities (3) are considered. As the structure of the output (4) is the same as that of the outputs (3), the passage from the treatment for the expectation value to the one for probabilities corresponds to extending a single output treatment to a multiple output treatment. This can be accomplished without difficulties.

We need to assume some structure on the Hamiltonian H, in order to render the problem of characterizing the classes of equivalent models tractable. This corresponds to the passage from *unstructured uncertainty* to *parametric uncertainty,* often

[1] Natural extensions of what we shall say can be made to general measurements.

[2] Considering continuous measurements in quantum mechanics is possible and of interest in several experimental scenarios. In these cases, however, the equations of the dynamics (1) have to be modified to take into account the back-action of the measurement (see, e.g., [6]). These types of models will not be considered here.

discussed in identification theory (see, e.g., [26]). In particular, it is often the case that the Hamiltonian $H = H(u)$ has the *bilinear* form

$$H := H_0 + \sum_{j=1}^{m} H_j u_j(t) \tag{5}$$

for some control functions $u_1, \ldots, u_m$, and *internal Hamiltonian* H_0 and *interaction Hamiltonians* H_j's, $j = 1, \ldots, m$. In this paper we shall consider only *finite dimensional models*, and therefore H_0, H_j, $j = 1, \ldots, m$, and ρ are Hermitian matrices of finite dimension $N \times N$.

Remark 2.2. A classical problem in nonlinear control theory related to the one considered here is the *realization problem*. In the relevant literature, one considers a map from a space of input functions to a space of output functions. This map can be given in an abstract way [20], [28], or through Volterra [7], [9], [14], [19] or Fliess [15] series. Then conditions are given for the *existence* and *uniqueness* of a dynamical model which implements the given input-output relations. An algorithm for the construction of this model for bilinear systems on $\mathbb{R}^N$ is given, for example, in [24]. In our case, the input-output map is already given as realizable with a given class of models where only the parameters and the dimensions are unknown. The problem is to characterize the class of equivalence of models giving the specified input-output map. Therefore the problem considered here is essentially a *uniqueness* problem in realization theory while the existence is already assumed. In this sense the question treated here is more in the spirit of the work done in [4] for neural networks. The a priori assumptions on the structure of the system allow us to obtain stronger results. In particular, while in [20], [28] (under a suitable hypothesis) the realization is proved to be unique up to a diffeomorphism, in the results of sections 5 and 6 we shall give the explicit map between two different realizations of the same input-output map and therefore the explicit construction of all the input-output equivalent models. We notice that since the model (1), (5), (4) is bilinear, we could have followed a different approach by looking at the input-output map associated with the system, transforming the system into a system on $\mathbb{R}^{N^2}$, where N^2 is the dimension of the space of Hermitian matrices, and applying the results of [24]. This, however, does not seem to be the most natural approach. In fact, in doing this, we would have hidden some of the structure of the problem, as, for example, the fact that the linear map for the dynamics in (1) is given in terms of the commutator with a Hermitian matrix.

3. Lie algebra theory and modeling of quantum systems. In this paper we are interested in matrix *Lie algebras* over the real field, i.e., real vector spaces of matrices closed under the commutator. Particularly important Lie algebras for us are the Lie algebra of *skew-Hermitian* $N \times N$ matrices, which is denoted by $u(N)$, and the Lie algebra of *skew-Hermitian* $N \times N$ matrices with trace equal to zero, which is denoted by $su(N)$. Accordingly the spaces of Hermitian matrices and Hermitian matrices with zero trace will be denoted by $iu(N)$ and $isu(N)$, as their elements are obtained from those of $u(N)$ or $su(N)$ by multiplication by the imaginary unit $i := \sqrt{-1}$. In general, we shall often use the notation $i\mathcal{L}$ to denote a subspace of $iu(N)$ corresponding to a subspace $\mathcal{L}$ of $u(N)$ (or vice versa). All the spaces are inner product spaces when equipped with the inner product $\langle A, B\rangle := Tr(AB^*)$. A subalgebra $\mathcal{L}$ of $u(N)$ is a subspace of $u(N)$ which is also a Lie algebra. To every matrix Lie algebra $\mathcal{L}$ is associated a *Lie group* which is the group generated by elements e^A with A in $\mathcal{L}$ equipped with the structure of an analytic manifold. We shall denote this Lie group by $e^{\mathcal{L}}$. The Lie group associated with $u(N)$ ($su(N)$) is the Lie group of unitary matrices (with determinant equal to 1) and is denoted by $U(N)$ ($SU(N)$).

In the model Hamiltonian (5) it is often true that H_0 and the H_j's belong to two orthogonal complementary subspaces of $iu(N)$ corresponding to a Cartan decomposition [16] of $u(N)$. These are two orthogonal subspaces $i\mathcal{K}$ and $i\mathcal{P}$ such that the corresponding subspaces of $u(N)$, $\mathcal{K}$ and $\mathcal{P}$, satisfy[3]

$$u(N) = \mathcal{K} \oplus \mathcal{P} \tag{6}$$

and the commutation relations

$$[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}, \qquad [\mathcal{K}, \mathcal{P}] \subseteq \mathcal{P}, \qquad [\mathcal{P}, \mathcal{P}] \subseteq \mathcal{K}. \tag{7}$$

If $\mathcal{L}$ and $\mathcal{L}'$ are two (matrix) Lie algebras, a *homomorphism* ϕ is a linear map $\phi : \mathcal{L} \to \mathcal{L}'$, which preserves the commutation operation, i.e., $\phi([A, B]) = [\phi(A), \phi(B)]$, where the commutators on the left and right are calculated in $\mathcal{L}$ and $\mathcal{L}'$, respectively. If $\mathcal{L}$ and $\mathcal{L}'$ are two inner product spaces, associated with every linear map ϕ is a dual map ϕ^* which is a linear map $\mathcal{L}' \to \mathcal{L}$ defined by the property $\langle A, \phi(B)\rangle_{\mathcal{L}'} = \langle \phi^*(A), B\rangle_{\mathcal{L}}$, where the inner product $\langle \cdot, \cdot\rangle_{\mathcal{L}'}$ ($\langle \cdot, \cdot\rangle_{\mathcal{L}}$) is defined on $\mathcal{L}'$ ($\mathcal{L}$). A bijective homomorphism is called an *isomorphism*. An isomporphism is called an *automorphism* if $\mathcal{L} = \mathcal{L}'$. An automorphism θ is called a *Cartan involution* if θ^2 is the identity map. Associated with every Cartan decomposition satisfying (7) is a Cartan involution θ such that $\mathcal{K}$ and $\mathcal{P}$ are the $+1$ and -1 eigenspaces of θ. The following simple example illustrates these concepts.

Example 3.1. Consider the decomposition (6) of $u(N)$ where $\mathcal{K}$ and $\mathcal{P}$ are the subspaces of purely real and purely imaginary matrices, respectively. It is clear that the commutation relations (7) are verified. Moreover, the associated Cartan involution θ is the complex conjugation which leaves unchanged the elements in $\mathcal{K}$ and changes the sign of the elements in $\mathcal{P}$.

Another type of automorphism of (subalgebras of) $u(N)$ is a *conjugacy* which is defined as $\phi_P(A) := PAP^*$, where P is a unitary matrix and in particular such that $PP^* = P^*P = \mathbf{1}$, where $\mathbf{1}$ is the identity matrix. Notice that if $\mathcal{K}$ and $\mathcal{P}$ define a Cartan decomposition of $u(N)$ as in (6), $P\mathcal{K}P^*$ and $P\mathcal{P}P^*$ also define a decomposition.

Up to conjugacies, there are three types of Cartan decompositions of $u(N)$ labeled **AI**, **AII**, and **AIII**. In a decomposition **AI**, $\mathcal{K} = so(N)$ and $\mathcal{P} = (so(N))^{\perp}$ up to conjugacy. $so(N)$ is the subalgebra of $u(N)$ of real skew-symmetric matrices. This is the decomposition presented in Example 3.1. In a decomposition **AII**, N is even and $\mathcal{K} = sp(N/2)$ and $\mathcal{P} = (sp(N/2))^{\perp}$ up to conjugacy. $sp(N/2)$ is the subalgebra of $u(N)$ of symplectic matrices, namely, matrices A satisfying $AJ + JA^T = 0$, where J is the matrix

$$J := \begin{pmatrix} 0 & \mathbf{1}_{N/2\times N/2} \\ -\mathbf{1}_{N/2\times N/2} & 0 \end{pmatrix}.$$

The third type labeled **AIII** is not relevant here (see [16] for details).

[3]In the literature (see, e.g., [16]) Cartan decompositions are defined for general semisimple Lie algebras, and the results of Cartan parametrize all the possible decompositions for $su(N)$. From decompositions of $su(N)$ one can obtain decompositions of $u(N)$ by including multiples of the identity in one of the two subspaces $\mathcal{K}$ or $\mathcal{P}$. Although in the literature one often refers to decompositions of $su(N)$, we have preferred to define decompositions in terms of $u(N)$ to ease notation.

If the system is a multipartite system, every H_j, $j = 1, \ldots, m$, in (5) is a linear combination of Hamiltonians modeling the interaction of each individual system with the external field. In matrix notation, H_j is a linear combination of elements of the type $\mathbf{1} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes L \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}$, where L is a Hermitian matrix of appropriate dimensions and all the other places are occupied by identities $\mathbf{1}$. Also, H_0 is very often a linear combination of elements modeling the interaction between two subsystems, which can be written as tensor products of matrices equal to the identity, except in two locations. In these cases, using the Cartan decomposition (6) described in the recent paper [12] one finds that $iH_0 \in \mathcal{P}$ and $iH_j \in \mathcal{K}$, $j = 1, \ldots, m$. Also if S is a sum of observables on each individual subsystem, i.e., total spin angular momentum (see, e.g., [25]), it can always be written as a sum of tensor products all equal to the identity, except in one position. In these cases, $iS \in \mathcal{K}$ belongs to the subspace $\mathcal{K}$ of the above Cartan decomposition of [12].[4] We shall describe this structure in detail in section 6 because it is the main feature we use for the solution of the input-output equivalence problem.

According to the results in [1], [10], [17], [23], the controllability and observability properties of system (1), (4), (5) depend on the Lie algebra $\mathcal{L}$ generated by iH_0 and iH_j, $j = 1, \ldots, m$, i.e., the smallest subalgebra of $u(N)$ containing these matrices. In particular the set of states reachable from a density matrix ρ_0 is given by

$$\mathcal{O}_{\rho_0} := \{X\rho_0 X^* \mid X \in e^{\mathcal{L}}\}. \tag{8}$$

If, for every ρ_0, $\mathcal{O}_{\rho_0}$ is the set of all the density matrices with the same spectrum as ρ_0, the system is called *controllable*. This is the case if and only if $\mathcal{L} = u(N)$ or $\mathcal{L} = su(N)$. The system is *observable* if there are no pairs of states indistinguishable by input-output experiments. This is the case if and only if

$$isu(N) \subseteq \mathcal{O}_S := \{XSX^* \mid X \in e^{\mathcal{L}}\}. \tag{9}$$

Controllability implies observability for nonscalar S [10].

In the following, we shall consider, as a standing assumption, only finite dimensionality of the Hamiltonian H and the bilinear form (5) and will make precise the assumptions on the (Cartan) structure of the Hamiltonian when needed.

4. Model equivalence and Lie algebra homomorphisms. Consider two models with a Hamiltonian of the form (5) and an output of the form (4):

$$\dot{\rho} = \left[-i\left(H_0 + \sum_{j=1}^{m} H_j u_j\right), \rho\right], \quad \rho(0) = \rho_0, \quad y = Tr(S\rho), \tag{10}$$

$$\dot{\rho}' = \left[-i\left(H_0' + \sum_{j=1}^{m} H_j' u_j\right), \rho'\right], \quad \rho'(0) = \rho_0', \quad y' = Tr(S'\rho'). \tag{11}$$

The following theorem links the existence of an appropriate Lie algebra homomorphism to the equivalence of the two models.

THEOREM 1. *Let N and N' be the dimensions of the two models* (10)*,* (11)*, respectively. Let ϕ be a homomorphism, $\phi : u(N) \to u(N')$, and ϕ^* its dual with respect to the standard inner product $\langle A, B\rangle := tr(AB^*)$. Assume*

$$-iH_0' = \phi(-iH_0), \qquad -iH_j' = \phi(-iH_j), \qquad \phi^*(iS') = iS. \tag{12}$$

[4] Notice that the situation may be different if we consider the case of a single output given by the expectation value (4) and the case of several outputs given by the probabilities in (3).

Then if

$$i\rho_0' = \phi(i\rho_0), \tag{13}$$

the models are equivalent. Vice versa, if the models are equivalent and (11) *is observable, then* (13) *holds.*

Proof. Multiply (10) and (11) by i and then apply ϕ to the equation obtained from (10). Combining the two resulting equations, using the first two of (12), we obtain

$$\frac{d}{dt}(i\rho' - \phi(i\rho)) = \left[\phi(-iH_0) + \sum_j \phi(-iH_j)u_j,\, i\rho' - \phi(i\rho)\right]. \tag{14}$$

If (13) is verified, then $i\rho'(t) = \phi(i\rho(t))$ for every t and for every control. Therefore we have from the third one in (12),

$$Tr(S'\rho') = Tr(-iS'i(\rho')) = Tr(-iS'\phi(i\rho)) = Tr(\phi^*(-iS')i\rho) = Tr(S\rho), \tag{15}$$

and the two models are equivalent. Vice versa, assume that the two models are equivalent. From (15), we have

$$Tr(iS'(i\rho' - \phi(i\rho))(t)) = 0 \tag{16}$$

for every t. Writing the solution of (14) as $(i\rho' - \phi(i\rho))(t) = X(i\rho' - \phi(i\rho))(0)X^*$, where X is the solution of the *(Schrödinger) operator equation*

$$\dot{X} = \left(\phi(-iH_0) + \sum_j \phi(-iH_j)u_j\right)X, \qquad X(0) = \mathbf{1}, \tag{17}$$

we have

$$Tr\left(X^* iS' X\left(i\rho_0' - \phi(i\rho_0)\right)\right) = 0. \tag{18}$$

As the system (11) is observable, we have that $X^* iS' X$ span all of $su(n')$, which implies $i\rho_0' = \phi(i\rho_0)$. ◻

Summarizing, the theorem says that if the equation describing the dynamics is related through a Lie algebra homomorphism ϕ, and under an observability condition, then the two models are equivalent if and only if the initial states are related through the same Lie algebra homomorphism ϕ. As we shall show in the remainder of the paper (cf. also [2]), it is possible for cases of physical interest to give a stronger version of Theorem 1. In particular, it is possible to show that the existence of a homomorphism ϕ satisfying (12) is also necessary for equivalence of two models. Moreover, it is possible to construct such a homomorphism. This way, we can characterize the class of equivalent models. We shall do this for a two level example in the next section and for general spin networks in section 6. In both cases we exploit a Cartan decomposition underlying the dynamics of the models.

In general, more structure will have to be assumed to avoid trivial cases. For example, if $S = S'$ is a scalar matrix, then every two models are equivalent. To avoid this case, an appropriate extra assumption is the *observability* of the two models. Also, we need to assume that the initial states are not both perfect mixtures (i.e., multiples of the identity); otherwise, with $S = S'$, the output for any two equivalent models will be the same, independently of the dynamics. Moreover, $-iH_j$ and $-iH_j'$, $j = 0, \ldots, m$, may be generally assumed traceless, as the trace only adds an extra common phase factor to the dynamics, which cannot be detected. We shall use these assumptions in the following.

5. Model equivalence of two level systems. Consider a spin $\frac{1}{2}$ particle which is driven by an electromagnetic control field along the z axis, interacts with a constant unknown magnetic field along an (unknown) direction in the x-y plane, and has an unknown initial state. The practical question is to what extent, by driving the system with the control field and measuring the average value of the spin magnetization in the z direction, it is possible to obtain information about the unknown parameters of the system. This type of model has a Cartan structure which is shared by several other models of physical interest and is instrumental in finding a homomorphism between equivalent models. We describe this below.

The Lie algebra $su(2)$, which is the relevant Lie algebra in the two level case, has, up to conjugacy, only one Cartan decomposition which corresponds to the classical Euler decomposition of the Lie group $SU(2)$ [16]. This extends to a decomposition of $u(2)$ which can always be written as

$$u(2) = \mathcal{K} \oplus \mathcal{P}. \tag{19}$$

Here $\mathcal{K}$ and $\mathcal{P}$ satisfy the commutation relations in (7) and are given, up to conjugacy, by

$$\mathcal{K} := span\{i\sigma_z\}, \qquad \mathcal{P} := span\{i\sigma_x, i\sigma_y, i\mathbf{1}_{2\times 2}\}. \tag{20}$$

Here, $\mathbf{1}_{2\times 2}$ is the 2×2 identity matrix and σ_x, σ_y, and σ_z are the *Pauli matrices*

$$\sigma_x := \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \frac{1}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_z := \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{21}$$

which satisfy the commutation relations

$$[i\sigma_x, i\sigma_y] = i\sigma_z, \qquad [i\sigma_y, i\sigma_z] = i\sigma_x, \qquad [i\sigma_z, i\sigma_x] = i\sigma_y. \tag{22}$$

The dynamical and output equations, for the above model of a spin $\frac{1}{2}$ particle in an electromagnetic field, can be written as

$$\dot{\rho} = [A + i\sigma_z u(t), \rho], \quad y = Tr(\sigma_z \rho), \quad \rho(0) = \rho_0, \tag{23}$$

where ρ_0 is an unknown initial density matrix and $A := xi\sigma_x + yi\sigma_y$, with x and y unknown. This model has a *Cartan structure* in that A is in $\mathcal{P}$ and $i\sigma_z$ (the control and observation part) is in $\mathcal{K}$, with $\mathcal{K}$ and $\mathcal{P}$ defined as in (20). We assume $x^2+y^2 \neq 0$ which implies controllability and therefore observability [10] for this model. The following result characterizes all the classes of equivalent models in terms of Lie algebra homomorphisms.

THEOREM 2. *Consider two models*

$$\dot{\rho} = [A + i\sigma_z u(t), \rho], \quad y = Tr(\sigma_z \rho), \quad \rho(0) = \rho_0, \tag{24}$$

$$\dot{\rho}' = [A' + i\sigma_z u(t), \rho], \quad y = Tr(\sigma_z \rho'), \quad \rho'(0) = \rho_0', \tag{25}$$

with ρ_0 and ρ_0' not both equal to scalar matrices (representing perfect mixtures) and A and A' of the form

$$A := xi\sigma_x + yi\sigma_y \quad \textit{and} \quad A' := x'i\sigma_x + y'i\sigma_y \tag{26}$$

for real parameters x, y, x', y'. Assume

$$x^2 + y^2 \neq 0 \quad \textit{and} \quad x'^2 + y'^2 \neq 0. \tag{27}$$

Then the two models are equivalent if and only if there exists an automorphism $\phi : u(2) \to u(2)$ *with*

$$\phi^*(i\sigma_z) = i\sigma_z \tag{28}$$

and

$$A' = \phi(A), \quad \phi(i\sigma_z) = i\sigma_z, \quad i\rho_0' = \phi(i\rho_0). \tag{29}$$

Proof. It is clear that if the automorphism ϕ exists, satisfying (28) and (29), the two models are equivalent. This follows from a direct application of Theorem 1, with (28) and (29) replacing (12) and (13). To prove the opposite, first notice that, from the equivalence assumption, we have

$$y(t) := Tr(\sigma_z \rho(t)) = Tr(\sigma_z \rho'(t)) := y'(t) \tag{30}$$

for every $t \geq 0$ and every admissible control.

We consider an automorphism ϕ of the type

$$\phi(L) := e^{-i\alpha\sigma_z} L e^{i\alpha\sigma_z}, \quad L \in u(2), \tag{31}$$

as α varies in $\mathbb{R}$.

Clearly (28) and the second equation of (29) are verified for any $\alpha \in \mathbb{R}$. Moreover,

$$\phi(A) = \bar{x} i\sigma_x + \bar{y} i\sigma_y, \tag{32}$$

with

$$\begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix} = K_\alpha \begin{pmatrix} x \\ y \end{pmatrix}, \tag{33}$$

and

$$K_\alpha := \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix}. \tag{34}$$

Also, if we write

$$\begin{aligned} i\rho_0 &:= \rho_x i\sigma_x + \rho_y i\sigma_y + \rho_z i\sigma_z + \frac{1}{2} i\mathbf{1}, \\ i\rho_0' &:= \rho_x' i\sigma_x + \rho_y' i\sigma_y + \rho_z' i\sigma_z + \frac{1}{2} i\mathbf{1}, \end{aligned} \tag{35}$$

we have

$$\phi(i\rho_0) = \bar{\rho}_x i\sigma_x + \bar{\rho}_y i\sigma_y + \bar{\rho}_z i\sigma_z + \frac{1}{2} i\mathbf{1}, \tag{36}$$

with

$$\begin{pmatrix} \bar{\rho}_x \\ \bar{\rho}_y \end{pmatrix} = K_\alpha \begin{pmatrix} \rho_x \\ \rho_y \end{pmatrix}. \tag{37}$$

Using the equivalence assumption (30) at $t = 0$, we obtain

$$\rho_z = \rho_z'. \tag{38}$$

Moreover, differentiating (30), using the dynamical equations (24) and (25), we obtain

$$Tr(\rho[\sigma_z, A]) = Tr(\rho'[\sigma_z, A']). \tag{39}$$

Writing this at time $t = 0$ and using the definitions (26) and (35) along with the commutation relation for the Pauli matrices (22), we obtain

$$\rho_y x - \rho_x y = \rho'_y x' - \rho'_x y'. \tag{40}$$

Differentiating (39) and using the fact that the resulting equation has to be valid for every value of the control, we obtain the two equations

$$Tr(\sigma_z[A, [A, \rho]]) = Tr(\sigma_z[A', [A', \rho']]) \tag{41}$$

and

$$Tr(i\sigma_z[A, [\sigma_z, \rho]]) = Tr(i\sigma_z[A', [\sigma_z, \rho']]). \tag{42}$$

From (42), as for (40), we obtain

$$x\rho_x + y\rho_y = x'\rho'_x + y'\rho'_y. \tag{43}$$

From (41), we obtain

$$(x^2 + y^2)Tr(\sigma_z\rho) = (x'^2 + y'^2)Tr(\sigma_z\rho'). \tag{44}$$

Using the fact that $Tr(\sigma_z\rho)$ is not always zero (because of the controllability condition (27))[5] and (30), we have

$$x^2 + y^2 = x'^2 + y'^2. \tag{46}$$

Therefore, for some α, we can write

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = K_\alpha \begin{pmatrix} x \\ y \end{pmatrix}, \tag{47}$$

with K_α in (34), and this, compared with (33) and (32), gives the first term of (29). To obtain the third term (with the same ϕ), we recall from (27) that $x^2 + y^2 \neq 0$. Letting $J := \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ and using (47), we can write (40) and (43), respectively, as

$$[x, y]J[\rho_x, \rho_y]^T = [x, y]K_\alpha^T J[\rho'_x, \rho'_y]^T, \tag{48}$$

$$[x, y][\rho_x, \rho_y]^T = [x, y]K_\alpha^T[\rho'_x, \rho'_y]^T. \tag{49}$$

Since K_α^T commutes with J, we can write these as

$$\begin{pmatrix} [x, y]J \\ [x, y] \end{pmatrix} [\rho_x, \rho_y]^T = \begin{pmatrix} [x, y]J \\ [x, y] \end{pmatrix} K_\alpha^T[\rho'_x, \rho'_y]^T. \tag{50}$$

[5]From controllability (27), we cannot have

$$Tr(\sigma_z\rho(t)) \equiv Tr(\sigma_z\rho'(t)) \equiv 0 \tag{45}$$

for every control. This would mean that, for every reachable evolution operator X, the solution of the (Schrödinger) operator equation $\dot{X} = (A + i\sigma_z u)X$, with $X(0) = \mathbf{1}$, $X^*\sigma_z X$, would be orthogonal to ρ_0. However, because of controllability, X may attain all the values in $SU(2)$, and therefore $X^*\sigma_z X$ span, as X varies, may attain all of $isu(2)$. Therefore, $X^*\sigma_z X$ is always orthogonal to ρ_0 only if ρ_0 is a multiple of the identity, which we have excluded.

Since

$$x^2 + y^2 = -\det \begin{pmatrix} [x,y]J \\ [x,y] \end{pmatrix} \neq 0,$$

we can write

$$[\rho'_x, \rho'_y]^T = K_\alpha [\rho_x, \rho_y]^T, \tag{51}$$

and therefore

$$[\rho'_x, \rho'_y] = [\bar{\rho}_x, \bar{\rho}_y], \tag{52}$$

which along with $\rho'_z = \rho_z$ gives

$$i\rho' = \phi(i\rho). \tag{53}$$

This concludes the proof of the theorem. □

Remark 5.1. The proof of the above theorem also gives the explicit form of the homomorphism relating two equivalent models.

6. Model equivalence of spin networks.

6.1. A set of models of spin networks. We consider a network of n particles with spin that interact according to Heisenberg interaction. In particular, we denote the spin of the jth particle by l_j and by $N_j := 2l_j + 1$ the dimension of the Hilbert space for the state of the jth particle. The dimension of the Hilbert state space associated with the entire network is $N := \prod_{j=1}^n N_j$. The class of Hamiltonians we consider is of the form

$$H(t) := i\left(A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t)\right), \tag{54}$$

where A, modeling the *Heisenberg interaction* among the particles, and $B_{x,y,z}$, modeling the interaction with external fields, are given by

$$\begin{aligned} A &:= -i \sum_{k<l,\, k,l=1}^{n} J_{kl}(I_{kx,lx} + I_{ky,ly} + I_{kz,lz}), \\ B_v &:= -i\left(\sum_{k=1}^{n} \gamma_k I_{kv}\right) \quad \text{for} \quad v = x,\, y, \text{ or } z, \end{aligned} \tag{55}$$

respectively. Here and in the following we denote by $I_{k_1v_1,\dots,k_rv_r}$, for $1 \le k_1 < \cdots < k_r \le n$ and $v_j \in \{x,y,z\}$, the $N \times N$ matrix which is the Kronecker product of n matrices where in the jth position we have the $N_j \times N_j$ identity if $j \notin \{k_1,\dots,k_r\}$, while if $j = k_s$ we have the $N_j \times N_j$ representation of the v_s component of spin angular momentum for a particle with spin l_j. Such matrices are given by the Pauli matrices (21) in the case where $l_j = \frac{1}{2}$ and can be calculated for every value of the spin (see, e.g., [25, section 3.5]). For convenience of the reader, and since these matrices will be used several times in the following, we give their explicit form in Appendix B. With some abuse of notation, we shall continue denoting these matrices by σ_x, σ_y, and σ_z without explicit reference to the value of the spin. Therefore, for instance, we have that for a system of three spin,

$$I_{1x,3y} := \sigma_x \otimes \mathbf{1} \otimes \sigma_y \tag{56}$$

is the Kronecker product of three matrices. σ_x is the representation of the spin angular momentum in the x direction for the first spin (dimension $N_1 \times N_1$), σ_y is the representation of the spin angular momentum in the y direction for the third spin (dimension $N_3 \times N_3$), and the matrix $\mathbf{1}$ is the identity matrix for the second spin (dimension $N_2 \times N_2$). In all dimensions, the matrices σ_x, σ_y, and σ_z have several properties we shall use in the following. In particular, they satisfy the commutation relations (22) and

$$\sigma_x^2 + \sigma_y^2 + \sigma_z^2 = l_j(l_j+1)\mathbf{1}_{N_j \times N_j} \tag{57}$$

(see, e.g., formula (3.5.34a) in [25]).

The real scalar parameter J_{kl} in (55) is the *exchange constant* between particle k and particle l, and the real scalar parameter γ_k is the gyromagnetic ratio of particle k. We assume that the spins of the network have all nonzero and different gyromagnetic ratios. We can associate a graph with the model, where each node represents a particle and an edge connects two nodes if and only if the corresponding exchange constant is different from zero. It is not difficult to see that if the model is controllable, then, necessarily, this graph is connected. We shall assume this to be the case. Moreover, controllability implies observability for every output of the form (4) where S is a nonscalar matrix [10]. In our case, we presume to measure the expectation values of the total magnetization in the x, y, and z directions given as in (4), where S is one of the matrices:

$$S_v := \sum_{k=1}^{n} I_{kv} \quad \text{with} \quad v \in \{x, y, z\}. \tag{58}$$

Remark 6.1. We have chosen to model the interaction between spins with Heisenberg interaction of the form A in (55) because we have in mind applications to molecular magnets as described in [27], which was the first motivation for this research. The Heisenberg interaction is the most common model of interaction between spins when relativistic effects (and higher order terms) are neglected (see, e.g., [29]). However, other types of interaction can be more appropriate for modeling the interaction between spins for other systems. If we consider two-body interaction, the proof of Theorem 7 still holds in the first half but the computations in the second half use explicitly the form of the interaction.

A model of the type described above will be denoted by $\Sigma := \Sigma(n, l_j, J_{kl}, \gamma_k, \rho_0)$, where the parameters $n, l_j, J_{kl}, \gamma_k, \rho_0$, which determine the model, are unknown. We will assume to have two controllable models Σ and $\Sigma' := \Sigma'(n', l'_j, J'_{kl}, \gamma'_k, \rho'_0)$ which satisfy the previous requirements, and we look for necessary and sufficient conditions for these two models to be equivalent. We shall mark with a prime, $'$, all the quantities concerning the system Σ'.

6.2. Relevant homomorphism of $u(N)$. In [12] a method was described to construct a Cartan decomposition of the Lie algebra $su(N)$ for a multipartite system, starting from decompositions of the Lie algebras $su(N_j)$ associated with the single subsystems, each of dimension N_j, with $N := \prod_{j=1}^{n} N_j$. In particular, we have the following result.

THEOREM 3 (see [12, section 5]). *Consider a multipartite system with n subsystems of dimensions $N_1, \ldots, N_n$. Consider the Lie algebra $u(N_j)$ related to the jth subsystem and a Cartan decomposition*

$$u(N_j) = \mathcal{K}_j \oplus \mathcal{P}_j \tag{59}$$

of type **AI** *or* **AII**. *Denote by σ_j (S_j) a generic element of an orthogonal basis of $i\mathcal{K}_j$ ($i\mathcal{P}_j$). Let the (total) Lie algebra $u(N_1 N_2 \cdots N_n)$ be decomposed as*

$$iu(N_1 N_2 \cdots N_n) = \mathcal{I}_o \oplus \mathcal{I}_e. \tag{60}$$

$\mathcal{I}_o$ ($\mathcal{I}_e$) is the vector space spanned by matrices which are the tensor products of an odd (even) number of elements of type σ_j. Then $u(N_1 N_2 \cdots N_n) = i\mathcal{I}_o \oplus i\mathcal{I}_e$ is a Cartan decomposition, i.e.,

$$[i\mathcal{I}_o, i\mathcal{I}_o] \subseteq i\mathcal{I}_o, \qquad [i\mathcal{I}_o, i\mathcal{I}_e] \subseteq i\mathcal{I}_e, \qquad [i\mathcal{I}_e, i\mathcal{I}_e] \subseteq i\mathcal{I}_o. \tag{61}$$

The decomposition (60) is called a decomposition of the *odd-even type*.

Associated with Cartan decomposition (61) is a Cartan involution ϕ which is the identity on $i\mathcal{I}_o$ and multiplication by -1 on $i\mathcal{I}_e$. The structure of system (54) and (55) suggests that it is possible to choose this Cartan involution as a homomorphism mapping the equations of two equivalent models as in (12). In fact, assume that there is the same number of subsystems (spin particles) in the two models and that corresponding subsystems have the same dimensions (namely, the same spin). If we can display a decomposition (59) of type **AI** or **AII** for every (spin) $u(N_j)$ such that $i\sigma_{x,y,z} \in \mathcal{K}_j$, then, for every value of the parameters, it holds that $B_{x,y,z}(') \in i\mathcal{I}_o$ and $A(') \in i\mathcal{I}_e$. As shown in Theorems 4–6 following, decompositions of this type exist. We shall see in the following subsection that the Cartan involution associated with an odd-even type of Cartan decomposition is the correct homomorphism to describe classes of equivalent spin networks. In fact, not only are models which are related by such a homomorphism equivalent (according to Theorem 1) but the opposite is true as well. In other words, two equivalent models are either exactly the same or are related through such a homomorphism.

The following three theorems show the existence of a decomposition (59) of $u(N_j)$ of type **AI** or **AII** where the subalgebra $\mathcal{K}_j$ contains the matrices $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$. Equivalently, they show the existence of a subalgebra of $sp(\frac{N_j}{2})$ (type **AII**) or $so(N_j)$ (type **AI**) conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$. The proofs are presented in the following section. We shall see that the situation is different for integer and half-integer spins.

THEOREM 4. *If the dimension N_j of the system is even (half-integer spin (Fermions)), there exists a subalgebra of $sp(\frac{N_j}{2})$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$.*

THEOREM 5. *If the dimension N_j of the system is odd (integer spin (Bosons)), there exists a subalgebra of $so(N_j)$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$.*

THEOREM 6. *If the dimension N_j of the system is even (half-integer spin (Fermions)), there is no subalgebra of $so(N_j)$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$.*

6.3. Necessary and sufficient conditions for model equivalence. In this subsection we shall prove the equivalence result concerning models of spin networks. This is given by the following theorem.

THEOREM 7. *Let $\Sigma := \Sigma(n, l_j, J_{kl}, \gamma_k, \rho_0)$ and $\Sigma' := \Sigma(n', l'_j, J'_{kl}, \gamma'_k, \rho'_0)$ be two given models (see* (54), (55)*). Assume that both models are controllable, that for model Σ (Σ'), all the γ_k (γ'_k) are nonzero and different from each other, and that ρ_0 and ρ'_0 are not both scalar matrices. Then Σ is equivalent to Σ' i.e.,*

$$y_v(t) := Tr(S_v \rho(t)) \equiv y'_v(t) := Tr(S'_v \rho'(t)) \quad \textit{for} \quad v \in \{x, y, z\} \tag{62}$$

and for every control u_x, u_y, u_z, if and only if the following condition holds:

Condition $(*)$:

1. $n = n'$,

   Up to a permutation of the set $\{1, \dots, n\}$ (i.e., a permutation of the indices for the particles), the following three conditions hold:

2. $$\gamma_k = \gamma_k',$$

3. $$l_k = l_k', \tag{63}$$

   and

4. *one of the following two conditions holds:*

   (a) $$A = A' \text{ and } \rho_0 = \rho_0'. \tag{64}$$

   (b) *Given the Cartan involution ϕ associated with the decomposition of the odd-even type as from Theorem* 3 *(see also Remark* 6.2 *below),*

   $$A' = \phi(A) \text{ and } i\rho_0' = \phi(i\rho_0). \tag{65}$$

Remark 6.2. The simplest way to describe the Cartan involution ϕ associated with the odd-even decomposition is in terms of its action on the subspaces $i\mathcal{I}_o$ and $i\mathcal{I}_e$ defined in Theorem 3; that is, ϕ leaves unchanged the elements of $i\mathcal{I}_o$ and multiplies by -1 the elements of $i\mathcal{I}_e$. $\mathcal{I}_o$ and $\mathcal{I}_e$ are defined in terms of the Cartan decompositions on the single subsystems. In our case, this is done according to Theorems 4 and 5. In particular consider the jth subsystem and assume that it has even dimension. Then with the unitary transformation U defined in (87), $u(N_j)$ has the Cartan decomposition (59) of type **AII**, with $\mathcal{K}_j$, given by $\mathcal{K}_j := U^* sp(N_j/2)U$ and $\mathcal{P}_j = U^* sp(N_j/2)^\perp U$. Analogously if the jth system has odd dimension, one considers the unitary transformation U defined in (92). Then $u(N_j)$ has the Cartan decomposition (59) of the type **AI**, with $\mathcal{K}_j$, given by $\mathcal{K}_j := U^* so(N_j)U$, and $\mathcal{P}_j = U^* so(N_j)^\perp U$. According to Theorems 4 and 5, in both cases $i\sigma_{x,y,z}$ are in $\mathcal{K}_j$. If we call σ_j a generic element of $i\mathcal{K}_j$, $\mathcal{I}_o$ ($\mathcal{I}_e$) is spanned by an odd (even) number of σ_j's. Notice in particular that in the model (55), $A \in i\mathcal{I}_e$ and $B_v \in i\mathcal{I}_o$, so that ϕ changes the sign of A and leaves the B_v's unchanged.

Theorem 7 says that, under appropriate controllability assumptions, two equivalent models for spin networks are equivalent if and only they have the same number of particles, corresponding particles have the same spin, and their dynamical models and initial states are either exactly the same or are related through the Cartan involution associated with a decomposition of the odd-even type. In practical terms, given a general spin network, by driving the network with an external electromagnetic field and measuring the total spin in the x, y, and z direction, it is, in principle, possible to identify the number of particles, their spin, the gyromagnetic ratios of every spin, and the exchange constants only up to a common sign factor, if the initial state is not known. The proof that Condition $(*)$ implies equivalence is an application of the general property of Theorem 1. The proof that equivalence implies Condition $(*)$ is considerably longer. However, several results can be obtained with proofs that are formal modifications of the ones presented in [2] for the special case of spin $\frac{1}{2}$ particles. We shall focus on the new part of the proof needed to generalize to the case of unknown spins:

Condition $(*)$ implies equivalence.

It is clear that if Condition $(*)$ holds with (64), then the two models differ possibly only by a permutation of the indices of the particles. So they are equivalent. Assume now that Condition $(*)$ holds with (65) and assume for simplicity (and without loss of generality) that the permutation of indices is the trivial permutation. Let ϕ be the Cartan involution associated with the decomposition of the odd-even type. We notice that

$$\phi^*(iS_v) = iS_v = iS'_v, \quad v = x, y, z. \tag{66}$$

In fact, given any $C \in u(N)$, we can write $C = C_o + C_e$, with $C_o \in i\mathcal{I}_o$ and $C_e \in i\mathcal{I}_e$. It holds that

$$Tr(\phi^*(iS_v)C) := Tr((iS_v)\phi(C)) = Tr((iS_v)(C_o - C_e)) = Tr((iS_v)C_o) = Tr((iS_v)C),$$

which, since it has to hold for every C, gives (66). Equations (65) and (66) imply that (12) of Theorem 1 holds. Since we also have (13), from (65) we conclude that the two models are equivalent using Theorem 1 as follows.

Equivalence implies Condition $(*)$.

The technique used in [2] to prove this result for networks of spin $\frac{1}{2}$ particles extends to the general case treated here. However, further analysis is required in this case, in particular to prove that equivalent spin networks have the same values of the spins, while in [2] it was assumed that the networks were composed by all spin $\frac{1}{2}$'s. The main reason why the proof in [2] can be extended to this case is that the basic commutation relations, which were the essential ingredient of the proofs in [2], still hold. More precisely, the matrices σ_x, σ_y, and σ_z still satisfy, for every value of the spin, the commutation relations (22). This fact implies that it also holds that

$$\left[I_{k_1v_1,\ldots,k_rv_r}, I_{\bar{k}v_{\bar{k}}}\right] = \begin{cases} 0 & \text{if } \bar{k} \notin \{k_1,\ldots,k_r\}, \\ 0 & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} = v_j, \\ iI_{k_1v_1,\ldots,k_j[v_jv_{\bar{k}}],\ldots,k_rv_r} & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} \neq v_j \end{cases} \tag{67}$$

independently of the values of the spins.[6]

Assume now that the two models Σ and Σ' are equivalent. Then, using exactly the same arguments as in the proof of Proposition 4.1 of [2], we obtain that the number of the spin particle must be the same, namely, $n = n'$, and, up to a permutation of the indices, $\gamma_k = \gamma'_k$ for all $k \in \{1,\ldots,n\}$, which is parts 1 and 2 of Condition $(*)$. Moreover, as in Proposition 4.1 of [2], we obtain

$$Tr(I_{kv}\rho(t)) = Tr(I'_{kv}\rho'(t)) \;\; \forall k \in \{1,\ldots,n\}, \; \forall v \in \{x,y,z\}. \tag{68}$$

[6] In the notation used here $[v\bar{v}]$ give a result in agreement with the commutator of $i\sigma_v$ and $i\sigma_{\bar{v}}$ (cf. (22)). Therefore, for example, $[xy] := z$. Moreover, $I_{k_1v_1,\ldots,k_j(-v_j),\ldots,k_rv_r} := -I_{k_1v_1,\ldots,k_j(v_j),\ldots,k_rv_r}$.

Here I'_{kv} is defined as I_{kv} but for Σ' and, at this point, it may be different from I_{kv} since we have not shown yet that corresponding spins must be equal. To prove this fact, we shall use Lemma 8 below. The proof of this lemma is a generalization of the proof of Lemma 5.2 in [2], where we use the general property (57) instead of the corresponding property for spin $\frac{1}{2}$'s. We postpone this proof to Appendix A.

LEMMA 8. *Assume that for all $t \geq 0$, all possible trajectories $\rho(t)$ of Σ, and corresponding $\rho'(t)$ of Σ', for fixed values $1 \leq k_1, \ldots, k_r \leq n$, $v_j \in \{x, y, z\}$ and for given constants β and β', we have*

$$\beta Tr\left(I_{k_1 v_1,\ldots,k_r v_r}\rho(t)\right) = \beta' Tr\left(I'_{k_1 v_1,\ldots,k_r v_r}\rho'(t)\right). \tag{69}$$

Then

1. *for any pair of indices $\bar{k}, \bar{d} \in \{1, \ldots, n\}$ with $\bar{k} \in \{k_1, \ldots, k_r\}$ and $\bar{d} \notin \{k_1, \ldots, k_r\}$,*

$$\beta J_{\bar{k}\bar{d}} Tr\left(I_{k_1 v_1,\ldots,k_r v_r,\bar{d}\bar{v}}\rho(t)\right) = \beta' J'_{\bar{k}\bar{d}} Tr\left(I'_{k_1 v_1,\ldots,k_r v_r,\bar{d}\bar{v}}\rho'(t)\right) \tag{70}$$

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

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

$$\begin{aligned} &\beta(l_{\bar{d}}(l_{\bar{d}}+1)) J_{\bar{k}\bar{d}} Tr\left(I_{k_1 v_1,k_3 v_3,\ldots,k_r v_r}\rho(t)\right) \\ &= \beta'(l'_{\bar{d}}(l'_{\bar{d}}+1)) J'_{\bar{k}\bar{d}} Tr\left(I'_{k_1 v_1,k_3 v_3,\ldots,k_r v_r}\rho'(t)\right). \end{aligned} \tag{71}$$

In other words, formula (71) means that from (69), it is possible to derive a new formula as follows. Select two indices in the set $\{k_1, \ldots, k_r\}$, $\bar{k}$ and $\bar{d}$. One of the two indices (say, $\bar{d}$) disappears from the subscript in the matrices I and corresponding I'. However, a coefficient $l_{\bar{d}}(l_{\bar{d}}+1)$ and $l'_{\bar{d}}(l_{\bar{d}}+1)$ appears in the left- and right-hand side, respectively, as well as a coefficient $J_{\bar{k}\bar{d}}$ and $J'_{\bar{k}\bar{d}}$.

Analogously, for formula (70) one selects two indices $\bar{k}$ and $\bar{d}$ corresponding to two given particles, with $\bar{k} \in \{k_1, \ldots, k_r\}$ and $\bar{d} \notin \{k_1, \ldots, k_r\}$. $J_{\bar{k}\bar{d}}$ and $J'_{\bar{k}\bar{d}}$ denote the coupling constants between the $\bar{k}$th and $\bar{d}$th particle in the two models. Formula (70) is in fact three formulas, one for each value of $\bar{v} = x, y, z$.

We shall now prove that, under the assumption of equivalence, the squares of the exchange constants J_{dk} and J'_{dk} must be proportional, with a proportionality factor common to all pairs of indices d and k, and this will also be instrumental in the proof of part 3 of Condition $(*)$.

Fix any $1 \leq k_1 < k_2 \leq n$. Then, by applying statement 1 of Lemma 8, i.e., (70) with $\bar{k} = k_1$, $\bar{d} = k_2$, to (68) with $k = k_1$, we have

$$J_{k_1 k_2} Tr\left(I_{k_1 v_1,k_2 v_2}\rho(t)\right) = J'_{k_1 k_2} Tr\left(I'_{k_1 v_1,k_2 v_2}\rho'(t)\right) \quad \forall\ v_1, v_2 \in \{x, y, z\}. \tag{72}$$

Now, to the previous equality we apply statement 2 of Lemma 8, i.e., (71) with $\bar{k} = k_1$ and $\bar{d} = k_2$, to get

$$(l_{k_2}(l_{k_2}+1)) J^2_{k_1 k_2} Tr\left(I_{k_1 v_1}\rho(t)\right) = (l'_{k_2}(l'_{k_2}+1)) J'^2_{k_1 k_2} Tr\left(I'_{k_1 v_1}\rho'(t)\right),$$

which, by (68), implies

$$(l_{k_2}(l_{k_2}+1)) J^2_{k_1 k_2} = (l'_{k_2}(l'_{k_2}+1)) J'^2_{k_1 k_2}. \tag{73}$$

Using the facts that the two indices k_1 and k_2 above are arbitrary and that the graph associated with the network is connected, by the controllability assumption (cf. the discussion at the end of subsection 6.1) it is easy to see that there exists a positive constant $\alpha \in \mathbb{R}$ such that, for all $1 \leq d < k \leq n$,

$$J_{dk}^2 = \alpha^2 {J'}_{dk}^2 \quad \text{and} \quad l_k(l_k+1) = \frac{1}{\alpha^2} l'_k(l'_k+1). \tag{74}$$

Using (74), we can now prove part 3 of Condition $(*)$. We will do this using some lemmas and arguing by contradiction. First, notice that from (74), we have that if there exists a $\bar{k} \in \{1, \dots, n\}$ such that $l_{\bar{k}} = l'_{\bar{k}}$, then necessarily $\alpha^2 = 1$, and thus $l_j = l'_j$ for all $j = 1, \dots, n$, namely, all the particles have the same spin. So if we assume that (63) does not hold, without loss of generality, we can assume $l_1 > l'_1$. Using (74), we get that $l_j > l'_j$ for all $j = 1, \dots, n$, and thus also $N_j > N'_j$. Let $R := \frac{N}{N_1} = \prod_{j=2}^n N_j$ and $R' := \frac{N'}{N'_1} = \prod_{j=2}^n N'_j$.

Lemma 9. *For all $t \in \mathbb{R}$ and all the admissible trajectories ρ and corresponding trajectories ρ', we have*

$$\begin{aligned} &Tr\left((e^{i\sigma_z t} \otimes \mathbf{1}_{R\times R}) I_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R\times R}) \rho(s)\right) \\ &= Tr\left((e^{i\sigma_z t} \otimes \mathbf{1}_{R'\times R'}) I'_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R'\times R'}) \rho'(s)\right) \end{aligned} \tag{75}$$

for all $s \geq 0$.

Proof. First, we notice that from the Campbell–Baker–Hausdorff formula, we have

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R\times R}) I_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R\times R}) = \sum_{k=0}^{\infty} \left(ad^k_{i\sigma_z \otimes \mathbf{1}_{R\times R}} I_{1v}\right) \frac{t^k}{k!} \quad \forall v \in \{x, y, z\} \tag{76}$$

and an analogous equation for Σ'. Moreover, by applying Lemma 11 in Appendix A, with $W = I_{1v}$, $W' = I'_{1v}$, and $k = 1$, $v = z$, we have

$$Tr\left(ad_{i\sigma_z \otimes \mathbf{1}_{R\times R}} I_{1v} \rho(s)\right) = Tr\left(ad_{i\sigma_z \otimes \mathbf{1}_{R'\times R'}} I'_{1v} \rho'(s)\right).$$

Now we can apply again Lemma 11 to the previous equality to get

$$Tr\left(ad^2_{i\sigma_z \otimes \mathbf{1}_{R\times R}} I_{1v} \rho(s)\right) = Tr\left(ad^2_{i\sigma_z \otimes \mathbf{1}_{R'\times R'}} I'_{1v} \rho'(s)\right).$$

By applying this procedure repeatedly we obtain

$$Tr\left(ad^k_{i\sigma_z \otimes \mathbf{1}_{R\times R}} I_{1v} \rho(s)\right) = Tr\left(ad^k_{i\sigma_z \otimes \mathbf{1}_{R'\times R'}} I'_{1v} \rho'(s)\right)$$

for all $k \geq 0$. Using this in (76), equation (75) follows. ∎

The proof of the following lemma is given in Appendix A.

Lemma 10. *The following formula holds:*

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R\times R}) I_{1x} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R\times R}) := P_{N_1}(t) \otimes \mathbf{1}_{R\times R}, \tag{77}$$

where the matrix $P_{N_1}(\cdot)$ is periodic with period 2π. Moreover,

$$P_{N_1}(\pi) = -P_{N_1}(0) = -\sigma_x. \tag{78}$$

Using Lemmas 9 and 10, we can now conclude the proof that the spins are the same. Let $\bar{\rho}(s) \otimes \mathbf{1}_{R\times R}$ (resp., $\bar{\rho}'(s) \otimes \mathbf{1}_{R'\times R'}$) be the orthogonal component of $\rho(s)$

(resp., $\rho'(s)$) along $\sigma_x \otimes \mathbf{1}_{R\times R}$ (resp., $\sigma_x \otimes \mathbf{1}_{R'\times R'}$). Using (77), equality (75) with $v = x$ can be written as

$$Tr\left(P_{N_1}(t)\bar{\rho}(s)\right) R = Tr\left(P_{N_1'}(t)\bar{\rho}'(s)\right) R'. \tag{79}$$

Since we have assumed by contradiction $R > R'$, from (79) we have for every t,

$$Tr\left(P_{N_1}(t)\bar{\rho}(s)\right) < Tr\left(P_{N_1'}(t)\bar{\rho}'(s)\right). \tag{80}$$

Now we will derive a contradiction by evaluating the previous inequality at $t = 0$ and $t = \pi$ and using (78). In fact we have

$$Tr\left(P_{N_1}(0)\bar{\rho}(s)\right) < Tr\left(P_{N_1'}(0)\bar{\rho}'(s)\right),$$

and thus

$$Tr\left(P_{N_1}(\pi)\bar{\rho}(s)\right) = -Tr\left(P_{N_1}(0)\bar{\rho}(s)\right) > -Tr\left(P_{N_1'}(0)\bar{\rho}'(s)\right) = Tr\left(P_{N_1'}(\pi)\bar{\rho}'(s)\right).$$

The previous inequality contradicts (80). Thus we conclude that $l_1 = l_1'$, which implies that (63) holds.

Since the two equivalent models Σ and Σ' have the same spin, the positive constant α in (74) is equal to one. Therefore, for every pair $d, k \in \{1, \ldots, n\}$, J_{dk} and J'_{dk} only differ possibly by the sign factor. Using the same argument as in the main theorem of [2] we can in fact conclude that there are only two possible cases: The case where $J_{dk} = J'_{dk}$ for every pair d, k, and the case where $J_{dk} = -J'_{dk}$ for every pair d, k. If we are in the first case, then from the observability (which follows from controllability) of the model, we must have $\rho_0 = \rho_0'$, and thus (64) holds. This is case (a) of part 4 of Condition $(*)$. On the other hand, if $J'_{kd} = -J_{kd}$ for every pair $1 \le k < d \le n$, we may conclude using Theorem 1. In fact we consider the homomorphism ϕ given by the Cartan involution associated with the odd-even decomposition as in the previous part of the proof. Conditions (12) hold, and thus, since the models are equivalent and observable, we get that

$$i\rho_0' = \phi(i\rho_0),$$

and thus (65) holds. This concludes the proof of the theorem.

7. Proofs of Theorems 4–6.

In the proofs of Theorems 4 and 5, we shall use the following two types of elementary $k \times k$ matrices:

$$C_k = \mathrm{diag}(-1, 1, -1, \ldots, (-1)^k), \quad T_k = \mathrm{adiag}(1, 1, 1, \ldots, 1) = \begin{pmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & \cdots & 0 \end{pmatrix}. \tag{81}$$

Thus, the matrix C_k is diagonal with alternating elements while T_k is antidiagonal with all ones on the secondary diagonal and zeros everywhere else. Obvious properties of these matrices are the following:

$$C_k^2 = T_k^2 = \mathbf{1}_{k\times k}, \qquad T_k = T_k^T. \tag{82}$$

We are interested in the action of these matrices by similarity transformation on diagonal and tridiagonal $k \times k$ matrices.[7] In particular, let us denote by D a generic, real, diagonal, $k \times k$ matrix and by F a generic, real, $k \times k$, tridiagonal matrix which is also symmetric and has zero diagonal; thus F will be of the type

$$F = \begin{pmatrix} 0 & a_1 & 0 & 0 & \cdots & 0 \\ a_1 & 0 & a_2 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & a_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{k-2} & 0 & a_{k-1} \\ 0 & 0 & \cdots & 0 & a_{k-1} & 0 \end{pmatrix}.$$

If M^a denotes the antitransposed of M, namely, the matrix obtained by reflecting about the secondary diagonal, we can easily verify the following properties:

1.
$$C_k D C_k = D, \qquad C_k F C_k = -F, \tag{83}$$

2.
$$T_k D T_k = D^a, \qquad T_k F T_k = F^a. \tag{84}$$

Remark 7.1. In the proofs of Theorems 4 and 5 below we do not need to write explicitly the matrices σ_x, σ_y, and σ_z, which are the representation of the x, y, and z components of spin angular momentum; nevertheless we need to write their structure. This structure is given by (85) and (86) for half-integer spin and by (90) and (91) for integer spin (see, e.g., [25, section 3.5] and Appendix B). In both proofs we make the explicit computation only for $i\sigma_x$ and $i\sigma_z$; this is possible since the third of the commutation relations (22) gives $i\sigma_y = [i\sigma_z, i\sigma_x]$.

Now we are ready to prove Theorems 4 and 5.

Proof of Theorem 4. The matrices $i\sigma_z$ and $i\sigma_x$ have (for every value of the spin) the following structure:

$$i\sigma_z = i\begin{pmatrix} D & 0 \\ 0 & -D^a \end{pmatrix}, \tag{85}$$

$$i\sigma_x = i\begin{pmatrix} F & P \\ P^T & F^a \end{pmatrix}, \tag{86}$$

where F and D have the structure above specified with $k := \frac{N_j}{2}$, and P is a $k \times k$ real matrix of all zeros except in the $(k, 1)$st position. Now use

$$U := \begin{pmatrix} C_k & 0 \\ 0 & T_k \end{pmatrix}, \tag{87}$$

which is orthogonal and therefore unitary.

We calculate, using the first terms of (83) and (84),

$$i\tilde{\sigma}_z := U i\sigma_z U^* = i\begin{pmatrix} D & 0 \\ 0 & -D \end{pmatrix}. \tag{88}$$

[7] A matrix F is tridiagonal if $f_{ij} = 0$ when $|i - j| > 1$.

Moreover, using the second terms of (83) and (84), we have

$$i\tilde{\sigma}_x := Ui\sigma_x U^* = i\begin{pmatrix} -F & C_k P T_k \\ T_k P C_k & F \end{pmatrix}. \tag{89}$$

It is easily seen that $i\tilde{\sigma}_z$ and $i\tilde{\sigma}_x$ are symplectic by observing that $C_k P T_k$ is a real symmetric matrix (only the (k,k)th element is different from zero). Therefore $\mathrm{sp}(\frac{N_j}{2})$ contains a subalgebra conjugate to the one spanned by $i\sigma_x$ and $i\sigma_z$, and therefore $i\sigma_y$ and the theorem is proved. $\square$

We now proceed to the proof of Theorem 5.

Proof of Theorem 5. In this case we set $k := \frac{N_j - 1}{2}$. The matrix $i\sigma_z$ has the form

$$i\sigma_z := i\begin{pmatrix} -D & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D^a \end{pmatrix}, \tag{90}$$

with D of dimension $k \times k$. Moreover, $i\sigma_x$ has the form

$$i\sigma_x := i\begin{pmatrix} F & v & 0 \\ v^T & 0 & w^t \\ 0 & w & F^a \end{pmatrix}, \tag{91}$$

where F is as above and v (w) is a vector of dimension k with only the last (the first) component different from zero, and the components different from zero are equal for v and w. We use the unitary matrix

$$U := \begin{pmatrix} \frac{i}{\sqrt{2}} C_k & 0 & (-1)^k \frac{i}{\sqrt{2}} T_k \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} T_k & 0 & \frac{1}{\sqrt{2}} C_k \end{pmatrix}, \tag{92}$$

which is easily seen to be unitary by (81) and (82). We calculate

$$\begin{aligned} i\tilde{\sigma}_z &:= Ui\sigma_z U^* \\ &= i\begin{pmatrix} \frac{1}{2}(T_k D^a T_k - C_k D C_k) & 0 & \frac{i}{2}((-1)^k T_k D^a C_k - C_k D T_k) \\ 0 & 0 & 0 \\ \frac{i}{2}(T_k D C_k - (-1)^k C_k D^2 T_k) & 0 & \frac{1}{2}(C_k D^a C_k - T_k D T_k) \end{pmatrix}. \end{aligned} \tag{93}$$

Using the first terms of (83) and (84), we find that the diagonal blocks are zero. Moreover, the remaining elements of the matrix are real so that $i\tilde{\sigma}_z$ is real. Analogously, we calculate

$$\begin{aligned} i\tilde{\sigma}_x &:= Ui\sigma_x U^* \\ &= i\begin{pmatrix} \frac{1}{2}(C_k F C_k + (-1)^{2k} T_k F^a T_k) & \frac{i}{\sqrt{2}}(C_k v + (-1)^k T_k w) & \frac{i}{2}(C_k F T_k + (-1)^k T_k F^a C_k) \\ * & 0 & \frac{1}{\sqrt{2}}(v^T T_k + w^T C_k) \\ * & * & \frac{1}{2}(T_k F T_k + C_k F^a C_k) \end{pmatrix}, \end{aligned} \tag{94}$$

where we have denoted by $*$ the components that can be obtained from the requirement that the matrix is skew-Hermitian. Now the $(1,1)$ and $(3,3)$ blocks are zero from the second terms of properties (83) and (84), while the $(2,3)$ block is zero because of the structure of the vectors v and w. All the other blocks are purely real matrices so that $i\tilde{\sigma}_x$ is also in $so(N)$, and this completes the proof. $\square$

We now give the proof of the negative result in Theorem 6.

Proof of Theorem 6. Assume that there exists a matrix $X \in SU(N_j)$ such that

$$X i\sigma_x X^* := \tilde{R}_x, \tag{95}$$

$$X i\sigma_y X^* := \tilde{R}_y, \tag{96}$$

$$X i\sigma_z X^* := \tilde{R}_z, \tag{97}$$

with $\tilde{R}_x$, $\tilde{R}_y$, and $\tilde{R}_z$ in $so(N_j)$. Then we can use the **AI** Cartan decomposition of $SU(N_j)$ [16] to write X as

$$X = K_1 A K_2, \tag{98}$$

with K_1 and K_2 in $SO(N_j)$ and A diagonal, i.e.,

$$A := \operatorname{diag}\left(e^{i\phi_1}, \ldots, e^{i\phi_{\frac{N_j}{2}}}\right). \tag{99}$$

Therefore we can write

$$K_1 A K_2 i\sigma_{x,y,z} K_2^T \bar{A} K_1^T = \tilde{R}_{x,y,z}, \tag{100}$$

or, defining $R_{x,y,z} := K_1^T \tilde{R}_{x,y,z} K_1$, which is also real skew-symmetric, we can write

$$K_2 i\sigma_{x,y,z} K_2^T = \bar{A} R_{x,y,z} A. \tag{101}$$

The real matrices $R_{x,y,z}$ must satisfy the same basic commutation relations (22) of $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$ and have the same eigenvalues of $i\sigma_x$, $i\sigma_y$, and $i\sigma_z$, namely, for a (half-integer) spin $j, \pm ji, \pm(j+1)i, \ldots, \pm\frac{1}{2}i$. We now study the structure of $R_{x,y,z}$ in (101) and get a contradiction with these facts.

First notice that, since A is diagonal as in (99), the action of A on the right-hand side of (101), namely, $R \to \bar{A}RA$, changes the (real) element r_{jk} of R into $r_{jk}e^{-i(\phi_j-\phi_k)}$. Since the entries on the left-hand side of (101) are either all purely imaginary or all purely real, if $\phi_j - \phi_k$ is not a multiple of $\frac{\pi}{2}$, then we must have $r_{jk} = 0$. Consider the indices $1, \ldots, N_j$ and let $\mathcal{O}$ be the set of indices k such that $\phi_1 - \phi_k$ is an odd multiple of $\frac{\pi}{2}$ and $\mathcal{E}$ the set of indices k such that $\phi_1 - \phi_k$ is an even multiple of $\frac{\pi}{2}$, and $\mathcal{N}$ the set of indices k such that $\phi_1 - \phi_k$ is not an integer multiple of $\frac{\pi}{2}$.

From (101) it follows that since $i\sigma_y$ is real, the terms r_{jk} of R_y, where j and k belong to different sets, must be zero because in that case $e^{i(\phi_j-\phi_k)}$ in (99) has a nonzero imaginary part. Therefore only the elements r_{jk}, where both j and k belong to $\mathcal{O}$ or $\mathcal{E}$ or $\mathcal{N}$, are possibly different from zero. Therefore after possibly reordering rows and columns, which corresponds to a similarity transformation by a permutation matrix, R_y must be of block diagonal form, and without loss of generality and for simplicity we shall assume only two blocks (rather than three). Therefore we write

$$R_y := \begin{pmatrix} Y_{11} & 0 \\ 0 & Y_{22} \end{pmatrix}, \tag{102}$$

where Y_{11} has dimensions $n_o \times n_o$ with n_o the cardinality of $\mathcal{O}$, and Y_{22} has dimension $(N_j - n_o) \times (N_j - n_o)$. Both Y_{11} and Y_{22} are skew-symmetric matrices. An analogous argument shows that, after possibly the same reordering of column and row indices, R_z can be written as

$$R_z := \begin{pmatrix} 0 & Z_{12} \\ -Z_{12}^T & 0 \end{pmatrix}, \tag{103}$$

where Z_{12} is a general matrix of dimensions $n_o \times (N_j - n_o)$.

Now consider the possible values for n_o. n_o odd is to be excluded because this would cause $\det Y_{11} = 0$ in (102), and this contradicts the fact that R_y has no zero eigenvalues. Moreover, $n_o \neq (N_j - n_o)$ (i.e., $n_o \neq \frac{N_j}{2}$) would cause R_z to have a determinant equal to zero. This can be easily verified by calculating

$$\det(R_z^2) = (\det R_z)^2 = \det \begin{pmatrix} -Z_{12}Z_{12}^T & 0 \\ 0 & -Z_{12}^T Z_{12} \end{pmatrix} \tag{104}$$

since, in this case, at least one of the matrices on the diagonal blocks does not have full rank. These considerations already exclude the cases where $\frac{N_j}{2}$ is an odd number as for spins $\frac{1}{2}$, $\frac{5}{2}$, $\frac{9}{2}$, etc., and we can assume R_y and R_z of the form (102) and (103) with $n_o = \frac{N_j}{2}$. To obtain a contradiction in this case too, we first notice that, since Y_{11} and Y_{22} have even dimension and are skew-symmetric, we can apply a similarity transformation $T := \left(\begin{smallmatrix} T_1 & 0 \\ 0 & T_2 \end{smallmatrix}\right)$, with T_1 and T_2 orthogonal so that TR_yT^T is block diagonal,

$$TR_yT^T = \left(D_1, D_2, \dots, D_{\frac{N_j}{2}}\right), \tag{105}$$

where the 2×2 block D_k has the form

$$D_k := \begin{pmatrix} 0 & l_k \\ -l_k & 0 \end{pmatrix}, \tag{106}$$

where each l_k corresponds to a pair of complex conjugate eigenvalues of R_y so that $l_k = \frac{p}{2}$ with p odd corresponds to the pair $\pm\frac{p}{2}i$. Moreover, we choose T so that the first $\frac{N_j}{4}$ blocks are ordered according to the increasing value of l_k, and the same holds for the last $\frac{N_j}{4}$ blocks. We shall therefore assume this structure of R_y in the remainder of the proof. We notice also that the transformation TR_zT^T does not change the structure of R_z, as Z_{12} in (103) was chosen to be a general $\frac{N_j}{2} \times \frac{N_j}{2}$ real matrix. Express Z_{12} in terms of 2×2 blocks L_{fk}, $f, k = 1, \dots, \frac{N_j}{4}$, $k = \frac{N_j}{4}+1, \dots, \frac{N_j}{2}$, which is possible since $\frac{N_j}{2}$ is an even number. Now, we impose the fact that R_y and R_z have to satisfy the same commutation relations as $i\sigma_y$ and $i\sigma_z$. In particular, we must have

$$[[R_y, R_z], R_y] = R_z. \tag{107}$$

This equation gives the following for the L_{fk} block:

$$2D_f L_{fk} D_k - L_{fk} D_k^2 - D_f^2 L_{fk} = L_{fk}. \tag{108}$$

If we write the generic L_{fk} as

$$L_{fk} := \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}, \tag{109}$$

and recall the structure of D_f and D_k,

$$D_f := \begin{pmatrix} 0 & l_f \\ -l_f & 0 \end{pmatrix}, \qquad D_k := \begin{pmatrix} 0 & l_k \\ -l_k & 0 \end{pmatrix}, \tag{110}$$

we obtain the following equations for a_2 and a_3 (and analogous equations for a_1 and a_4):

$$2l_k l_f a_3 = (1 - l_f^2 - l_k^2)a_2, \tag{111}$$

$$2l_k l_f a_2 = (1 - l_f^2 - l_k^2)a_3. \tag{112}$$

Combining these, we obtain

$$4l_k^2 l_f^2 a_3 = (1 - l_k^2 - l_f^2)^2 a_3, \tag{113}$$

which shows, taking the square root of both sides, that the only possible ways to have a_3 and therefore a_2 different from zero are the cases $l_f + l_k = \pm 1$. In these cases we can easily see that

$$a_3 = -a_2. \tag{114}$$

Similarly, one finds that we have a_4 and a_1 in (109) different from zero if and only if $l_f + l_k = \pm 1$, and in these cases we have

$$a_1 = a_4. \tag{115}$$

In conclusion, all the blocks L_{fk} are zero except the ones corresponding to indices f and k with neighboring values of l_f and l_k, which have the structure

$$L_{fk} := \begin{pmatrix} x & y \\ -y & x \end{pmatrix}. \tag{116}$$

Therefore R_z has the form in (103) where the fth block row of Z_{12} has at most two blocks different from zero and with the structure in (116). We denote these blocks by P_f and S_f, where P (S) stands for "predecessor" ("successor") and corresponds to the index k such that $l_k = l_f - 1$ and $l_k = l_f + 1$, respectively. Now, we argue that a matrix R_z with this structure must necessarily have all the (purely imaginary) eigenvalues with multiplicity at least two, and this gives the desired contradiction because R_z should have the same spectrum of $i\sigma_{x,y,z}$, which consists of all simple eigenvalues. In order to see this fact, reconsider the block structure of R_y in (105). If the blocks corresponding to eigenvalues $\pm\frac{1}{2}i$ and $\pm\frac{3}{2}i$ belong to the same half, then the corresponding matrix R_z will have a two-dimensional block row (or column) equal to zero, and therefore 0 will be an eigenvalue with multiplicity at least 2. Therefore we can assume that these two blocks belong to two different halves, and by the ordering we have imposed they must be the first ones of each half. Assume that the block corresponding to $\pm\frac{1}{2}i$ is in the first half. If this is not the case, consider the transpose of R_z and repeat the arguments that follow. It is possible to choose a block diagonal similarity transformation

$$U := \text{diag}\left(G_1, G_2, \ldots, G_{\frac{N_j}{4}}, F_1, F_2, \ldots, F_{\frac{N_j}{4}}\right), \tag{117}$$

with all the G_f's and F_f's being 2×2 orthogonal matrices so that UR_zU^T has the same structure as before, but all the matrices P_j and S_j are *scalar* matrices. We construct the matrix U proceeding by block rows. The first block row contains only S_1, as $\frac{1}{2}$ has no predecessors. All the zero blocks remain zero and S_1 is transformed into

$$G_1 S_1 F_1^T. \tag{118}$$

We choose $F_1 = \mathbf{1}_{2\times 2}$ and G_1, which has the general form

$$G_1 := \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}, \tag{119}$$

so that $\sin(\theta)x + \cos(\theta)y = 0$ if $S_1 := \left(\begin{smallmatrix} x & y \\ -y & x \end{smallmatrix}\right)$. This will give a scalar matrix. At the generic fth block row, we have at most two nonzero blocks P_{fk} and S_{fb}, where we now use an extra index k and b to indicate the block column to which they belong. They transform into

$$P_{fk} \to G_f P_{fk} F_k^T \tag{120}$$

and

$$S_{fb} \to G_f S_{fb} F_b^T, \tag{121}$$

respectively, while all the other blocks remain zero. If F_k has not been chosen before, we set $F_k = \mathbf{1}_{2\times 2}$. In any case, we choose G_f as before to make $G_f P_{fk} F_k^T$ a scalar matrix. We then choose F_b to make $G_f S_{fb} F_b^T$ a scalar matrix. G_f and F_b had not been chosen at previous steps. This is obvious for G_f and follows by an induction argument for F_b since all the F matrices chosen before the fth step correspond to predecessors and successors with (column) indices strictly less than b (recall that in the two halves of the matrix R_y the blocks are arranged in increasing order of (absolute value of) eigenvalue). In conclusion, modulo the similarity transformation defined by U in (117), we can assume that R_z has the form

$$R_z = K \otimes I_{2\times 2}, \tag{122}$$

where K is a skew-symmetric $\frac{N_j}{2} \times \frac{N_j}{2}$ matrix. By known results on the eigenvalues of the Kronecker products of two matrices, it follows that the eigenvalues of R_z are the same as those of K, each with multiplicity at least 2. This gives the desired contradiction and concludes the proof of the theorem. ∎

8. Conclusions. This paper has presented a collection of mathematical results concerning the input-output equivalence of quantum systems. Models that are equivalent cannot be distinguished by an external observer and therefore the determination of parameters in a quantum Hamiltonian can be obtained only up to equivalent models. Motivated by recent results on the isospectrality of quantum Hamiltonians [27] in molecular magnets, we have completely characterized the classes of spin networks which are equivalent. In several cases, the characterization of equivalent models can be obtained through a Lie algebra homomorphism, which is suggested by a Cartan structure of the underlying dynamics.

We believe many of the results and the concepts presented in this paper for quantum systems could be generalized to classes of systems relevant in other applications with both dynamics and output linear in the state. This will be the subject of further research.

Appendix A: Additional results and proofs. The proof of the following lemma can be obtained with a formal modification of the proof of Lemma 4.4 in [2] and is therefore omitted.

LEMMA 11. *Let Σ and Σ' be two equivalent models. If W and W' are two given Hermitian matrices such that*

$$Tr(W\rho(t)) = Tr(W'\rho'(t)) \tag{123}$$

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

$$Tr([W, I_{kv}]\rho(t)) = Tr([W', I'_{(k)v}]\rho'(t)) \quad \forall k \in \{1, \dots, n\},\ \forall v \in \{x, y, z\}, \tag{124}$$

up to a permutation of the indices.[8]

Proof of Lemma 8. We first state a lemma whose proof can be obtained from the proof of Lemma 5.1 in [2] and then proceed to the proof of Lemma 8.

LEMMA 12. *Assume that for all $t \geq 0$, all the possible trajectories $\rho(t)$ of Σ and corresponding $\rho'(t)$ of Σ', for fixed values $1 \leq k_1, \dots, k_r \leq n$, and fixed $v_j \in \{x, y, z\}$, we have*

$$Tr\left(I_{k_1v_1,\dots,k_rv_r}\rho(t)\right) = Tr\left(I'_{k_1v_1,\dots,k_rv_r}\rho'(t)\right). \tag{125}$$

Then

1. *equation* (125) *holds for any possible choice of the values of $v_j \in \{x, y, z\}$;*
2. $$\begin{aligned} &Tr\left(\left[\left[iI_{\bar{d}v_{\bar{d}}}, [iI_{\bar{k}v_{\bar{k}}}, A]\right], I_{k_1v_1,\dots,k_rv_r}\right]\rho(t)\right) \\ &= Tr\left(\left[\left[iI'_{\bar{d}v_{\bar{d}}}, [iI'_{\bar{k}v_{\bar{k}}}, A']\right], I'_{k_1v_1,\dots,k_rv_r}\right]\rho'(t)\right) \end{aligned} \tag{126}$$

   for all the indices $1 \leq \bar{d} \neq \bar{k} \leq n$ and every $\{v_{\bar{d}} \neq v_{\bar{k}}\} \in \{x, y, z\}$.

We now proceed to the proof of Lemma 8. First notice that from Lemma 12, it is enough to prove (70) and (71) for a particular choice of $\{v_j\}$ and $\bar{v}$. Moreover, we have, for $\bar{d} > \bar{k}$,

$$[iI_{\bar{d}z}, [iI_{\bar{k}x}, A]] = -J_{\bar{k}\bar{d}}iI_{\bar{k}z,\bar{d}x}. \tag{127}$$

1. By applying Lemma 12 (equation (126)) to (69) and using (127) we get:

$$\beta Tr\left(\left[-J_{\bar{k}\bar{d}}iI_{\bar{k}z,\bar{d}x}, I_{k_1v_1,\dots,k_rv_r}\right]\rho(t)\right) = \beta' Tr\left(\left[-J'_{\bar{k}\bar{d}}iI'_{\bar{k}z,\bar{d}x}, I'_{k_1v_1,\dots,k_rv_r}\right]\rho'(t)\right). \tag{128}$$

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

$$-J_{\bar{k}\bar{d}}\left[I_{\bar{k}z,\bar{d}x}, I_{k_1v_1,\dots,k_rv_r}\right] = J_{\bar{k}\bar{d}}iI_{k_1v_1,\dots,k_jy,\dots,k_rv_r,\bar{d}x}.$$

Combining the previous equality with (128), equation (70) follows easily.

2. Using the same procedure, we obtain again (128), but now both indices $\bar{k}$ and $\bar{d}$ are in $\{k_1, \dots, k_r\}$. Assume, for example that $k_1 = \bar{k}$ and $k_2 = \bar{d}$, and take $v_{k_1} = v_{k_2} = x$.

[8] This permutation is the same and fixed for all the results in which it is mentioned.

Now we have

$$[I_{k_1z,k_2x}, I_{k_1x,k_2x,\dots,k_rv_r}] = I_{k_1y,k_2x^2,k_3v_3,\dots,k_rv_r}, \tag{129}$$

where, with this notation, we mean that in the k_2th position we have the matrix σ_x^2. Thus, combining (128) and (129), we get

$$\beta J_{k_1k_2} Tr\left(I_{k_1y,k_2x^2,k_3v_3,\dots,k_rv_r}\rho(t)\right) = \beta' J'_{k_1k_2} Tr\left(I'_{k_1y,k_2x^2,k_3v_3,\dots,k_rv_r}\rho'(t)\right). \tag{130}$$

Using the same procedure, we conclude that

$$\beta J_{k_1k_2} Tr\left(I_{k_1y,k_2y^2,k_3v_3,\dots,k_rv_r}\rho(t)\right) = \beta' J'_{k_1k_2} Tr\left(I'_{k_1y,k_2y^2,k_3v_3,\dots,k_rv_r}\rho'(t)\right) \tag{131}$$

and

$$\beta J_{k_1k_2} Tr\left(I_{k_1y,k_2z^2,k_3v_3,\dots,k_rv_r}\rho(t)\right) = \beta' J'_{k_1k_2} Tr\left(I'_{k_1y,k_2z^2,k_3v_3,\dots,k_rv_r}\rho'(t)\right). \tag{132}$$

Adding together (130), (131), and (132) and using (57), we get

$$\beta(l_{k_2}(l_{k_2}+1))J_{k_1k_2} Tr\left(I_{k_1y,k_3v_3,\dots,k_rv_r}\rho(t)\right) = \beta'(l'_{k_2}(l'_{k_2}+1))J'_{k_1k_2} Tr\left(I'_{k_1y,k_3v_3,\dots,k_rv_r}\rho'(t)\right),$$

as desired.

Proof of Lemma 10. We recall the formulas (77) and (78) to be proved, i.e.,

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R\times R}) I_{1x} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R\times R}) := P_{N_1}(t) \otimes \mathbf{1}_{R\times R}, \tag{133}$$

where the matrix $P(\cdot)$ is periodic with period 2π, and

$$P_{N_1}(\pi) = -P_{N_1}(0) = \sigma_x. \tag{134}$$

The proof can be done directly by computing the matrix above. This is simplified by the fact that the matrix σ_z is always a diagonal matrix. We will give an outline of the argument when l_1 is a half-integer spin. The idea is to use the representations for the matrices σ_z and σ_x given by (85) and (86). The case of integer spin can be derived similarly starting with the representations given by (90) and (91).

Using (85) and (86), we obtain

$$e^{i\sigma_z t} i\sigma_x e^{-i\sigma_z t} = \begin{pmatrix} e^{iDt}Fe^{-iDt} & e^{iDt}Pe^{iD^a t} \\ e^{iD^a t}P^T e^{-iDt} & e^{-iD^a t}F^a e^{iD^a t}\end{pmatrix}. \tag{135}$$

The properties of the matrices D, P, and F are described in section 7. Moreover, $D = \text{diag}(j, j-1, \dots, \frac{1}{2})$ for a half-integer spin j. By using these properties, it follows that all the time-dependent terms in (135) are of the form e^{it}. Thus matrix (135) is periodic of period 2π. The fact that the dependence is of type e^{it}, in turn, implies that (133) and (134) hold.

Appendix B: Matrix elements of spin angular momentum operator. For a spin l, the matrices $\sigma_{x,y,z}$ are of dimensions $2l+1$. It is convenient to label the rows and columns by the index $-l, -l+1, \dots, l-1, l$. With this convention we have that σ_z is diagonal, and in particular,

$$(\sigma_z)_{m,s} := m\delta_{ms}, \qquad m, s = -l, -l+1, \dots, l-1, l.$$

σ_x and σ_y are defined through the matrices J_+ and J_- as

$$\sigma_x := \frac{J_+ + J_-}{2}, \qquad \sigma_y := \frac{J_+ - J_-}{2i}$$

with

$$(J_+)_{m,s} := \sqrt{(l-m)(l+m+1)}\delta_{s(m+1)}, \qquad m,s = -l, -l+1, \ldots, l-1, l,$$

$$(J_-)_{m,s} := \sqrt{(l+m)(l-m+1)}\delta_{(s+1)(m)}, \qquad m,s = -l, -l+1, \ldots, l-1, l.$$

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