Input-Output Equivalence of Spin Networks under Multiple Measurements

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Abstract

Two quantum control systems that are driven by an external field are said to be input-output equivalent if, for any control field, the measured value of a given observable is the same. Equivalent models cannot be distinguished by experiments involving state evolutions and measurements. In this paper, we characterize the equivalent models of networks of spin $\frac{1}{2}$'s driven by electro-magnetic fields for which the expectation value of the total magnetization is measured. Extending previous results and definitions that only dealt with the case of a single measurement, we describe the class of equivalent models under a *sequence* of Von Neumann measurements. The results are motivated by the problem of parameter identification for Heisenberg spin systems modeling molecular magnets.

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1 Input-output equivalence of quantum systems

In recent years, there has been a large amount of interest in studying quantum systems from the point of view of control theory. Quantum control systems are quantum systems whose dynamics depends on one or more functions of time that can be chosen. Physically these functions often represent externally applied electro-magnetic fields. They are the *inputs* or *controls* of the system. Measurements performed on the system return the expectation value of a given observable. They are the *outputs* of the system. Different types of measurements modify the state in different ways (see e.g. [6]). In modeling quantum systems, we can ask the question of whether using experiments involving evolutions and measurements we can identify the parameters of the model. In this context, two models are said to be *input-output equivalent* if, for any choice of the input field, they give the same output at any measurement. Equivalent models cannot be distinguished.

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Let us restrict ourselves to the case of closed systems under Von Neumann measurements. The dynamics is described by the Liouville's equation for the density matrix ρ:

$$i\frac{d}{dt}\rho = [H(u(t)), \rho]. \tag{1}$$

The Hermitian operator $H(u(t))$ is the Hamiltonian depending on the control function(s) $u(t)$. If the operator S represents the measured observable, the output $y(t)$ at time t is given by

$$y(t) := Tr\left(S\rho(t)\right). \tag{2}$$

After a measurement, the state is modified. In the case of Von Neumann measurement, if Π_k is the projection onto the eigenspace corresponding to the eigenvalue λ_k of the observable S, then the state is modified as

$$\rho \to \mathcal{P}(\rho), \tag{3}$$

where the map $\mathcal{P}$ is defined as

$$\mathcal{P}\left(F\right) := \sum_k \Pi_k F \Pi_k. \tag{4}$$

This measurement scheme is often referred to as *non-selective Von Neumann* measurement of the expectation value of S (see e.g. [6]).

Given an initial condition ρ_0 and a control u, we denote by $\rho(t; u, \rho_0)$, the density matrix solution of Liouville's equation (1) with control u and initial condition ρ_0. Given a sequence of times $0 < t_1 < \cdots < t_k$ and a corresponding sequence of control function u^j, defined for $j = 1, \ldots, k$ on $[0, t_j)$, we denote by $y^j(t_1, \ldots, t_j, u^1, \ldots, u^j, \rho_0)$, the corresponding output after the j-th measurement. Thus we have

$$\begin{array}{rcl} y^1(t_1, u^1, \rho_0) & = & Tr\left(S\rho(t_1; u^1, \rho_0)\right) \\ y^2(t_1, t_2, u^1, u^2, \rho_0) & = & Tr\left(S\rho(t_2; u^2, \mathcal{P}(\rho(t_1; u^1, \rho_0)))\right) \\ & \vdots & \\ y^k(t_1, .., t_k, u^1, .., u^k, \rho_0) & = & Tr\left(S\rho(t_k; u^k, \mathcal{P}(\rho(t_{k-1}; u^{k-1}, \mathcal{P}(\cdot\cdot\mathcal{P}(\rho(t_1; u^1, \rho_0))\cdot\cdot)))))\right). \end{array} \tag{5}$$

There are various definitions of input-output equivalence of two models that can be given. We shall adopt the following one in which we assume that the initial state ρ_0 as well as the parameters of the model are unknown and have to be detected by a sequence of evolutions and measurements. Therefore, if we denote by Σ the (unknown) model, we shall be concerned with the equivalence of pairs (Σ, ρ_0).

Definition 1.1 Consider two pairs model-initial state (Σ, ρ_0) and (Σ', ρ_0'). We mark with a prime $'$ all the symbols concerning system Σ'. We say that the two pairs (Σ, ρ_0) and (Σ', ρ_0') are *input-output equivalent* and we write

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

if for any sequence of times $0 < t_1 < \cdots < t_k$ and any corresponding sequence of controls u^j, defined on $[0, t_j)$, for $j = 1, \ldots, k$, we have

$$y^j(t_1, \ldots, t_j, u^1, \ldots, u^j, \rho_0) = y'^j(t_1, \ldots, t_j, u^1, \ldots, u^j, \rho_0'),$$

where y^j (and y'^j) are defined as in equation (5)

For the trivial case where all the eigenstates of S have the same probability namely the ensemble is a perfect mix of subsystems in the different states, the density matrix is a multiple of the identity operator and $Tr(S\rho(t)) = Tr(S\rho'(t)) \equiv \frac{1}{n}Tr(S)$, independently of the model (n is the dimension of the system). We shall exclude this degenerate case in the following. From a practical viewpoint the initial state ρ_0 may be considered different from the totally mixed state if $\rho_0 := \frac{1}{n}I + \Delta$ with $\Delta \neq 0$ and the measurement apparatus is able to detect a signal of the magnitude $\max_{X \in SU(n)} Tr(SX\Delta X^*)$.

The contribution of this paper is a description of the equivalent pairs for the special but important case of Heisenberg spin $\frac{1}{2}$ systems. These systems are a model for molecular magnets (see e.g. [4], [5], [7]) and the problem of parameter identification is motivated by the results of [13]. In the latter paper, it was shown that standard thermodynamic methods, such as measurements of the magnetic susceptibility, may fail to determine the parameters of the Hamiltonian for these systems. In fact these methods are based on the assumption that spin systems with different (coupling) parameters will have different spectra which was proved in [13] not to be always the case. This raises the question of whether by driving the system with an appropriate field and detecting the value of the total magnetization it is possible to determine the parameters. This naturally leads to investigate the input-output equivalence above described. The input-output and control theoretic properties of Heisenberg spin systems where studied in [2] and [3]. In particular the latter paper contains the equivalence result for the case of a single measurement. The technical contribution of the present paper is an extension of this result to the case of multiple measurements.

The rest of the paper is organized as follows. In the next section, we describe Heisenberg spin networks from the view point of control theory and give the statement of our main result. In Section 3 we give the proof of our main result which is based on a lemma describing the properties of the map $\mathcal{P}$ in (4). The proof of this lemma is the main technical part of the present paper and it is given in sub-section 3.1. In Section 4, we present a discussion of the mathematical results and their practical significance.

2 Input-output equivalence of spin networks; Statement of the main result

An Heisenberg spin Hamiltonian, for n spin $\frac{1}{2}$'s, can be written as

$$H(u(t)) := (A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t)), \tag{6}$$

with

$$
\begin{aligned}
A &:= \textstyle\sum_{k<l,k,l=1}^{n} J_{kl}(I_{kx,lx} + I_{ky,ly} + I_{kz,lz}), \\
B_v &:= (\textstyle\sum_{k=1}^{n} \gamma_k I_{kv}), \qquad \text{for } \ v = x,\, y, \ \text{ or } \ z.
\end{aligned} \tag{7}
$$

Here the matrix I_{kv} ($I_{kv,lv}$) is the Kronecker product of n matrices equal to the 2×2 identity except in the $k-$th (k, l-th) position(s) occupied by the Pauli matrix σ_v, $v = x, y, z$. Recall (see e.g. [12]) that the Pauli matrices are defined as

$$
\sigma_x := \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z := \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8}
$$

J_{kl} is the coupling constant between the $k-$th and the $l-$th particle. We assume that it is possible to observe the expectation value of the total magnetization in the x, y, and z direction. Thus, we let the three observable matrices S_x, S_y, and S_z be

$$
S_v = \sum_{k=1}^{n} I_{kv}, \qquad \text{for } \ v = x, y, z. \tag{9}
$$

The system has three outputs given by $Tr(S_v \rho)$, $v = x, y, z$. We study the possibility of distinguishing the parameters of the Hamiltonian by multiple measurements of these outputs. Models that are equivalent with respect to these outputs are also equivalent with respect to *any* linear combination of them. Therefore, they always give the same total magnetization along *any* direction in space.

We can visualize the spin network with a graph whose vertices represent the particles. An edge in the graph connects the vertices representing the particles k and l if and only if J_{kl} is different from zero. If this graph is connected and the particles have different gyromagnetic ratios the system is controllable [2] namely it is possible to find a control which drives the unitary propagator to any matrix in the special unitary group $SU(2^n)$. Controllability implies observability of the quantum system [8] in a single measurement. It is reasonable to assume observability in problems of identification of the initial state since the unobservable dynamics does not contribute to the output which is our tool to identify the state. In the following we shall assume that we know a priori that, for the models under consideration, all the gyromagnetic ratios are different and the associated graph is connected and therefore we have controllability and observability. While, as mentioned above, the observability assumption is natural in our context, the assumption of different gyromagnetic ratios is mostly a technical one which was used in some of the proofs in [3] and that we need here as we will use the results of [3] (and only for this reason). This assumption is not directly related to the equivalence of two models as there may be two nonequivalent models and each of them having (possibly) gyromagnetic ratios with the same value. Alternatively, we could assume that it is possible to address each spin independently, as it is done in *selective Nuclear Magnetic Resonance*, and the arguments in the following will go through.

Before stating our main result, we introduce some useful notations. Given a permutation π of the set $\{1, \ldots, n\}$, 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 $K_1,...,K_n$ we have

$$P_\pi(K_1\otimes K_2\otimes\cdots\otimes K_n)P_\pi^* = K_{\pi(1)}\otimes K_{\pi(2)}\otimes\cdots\otimes K_{\pi(n)}. \tag{10}$$

We denote by $\mathcal{I}_o$ ($\mathcal{I}_e$) the subspace of Hermitian matrices of dimension 2^n generated by Kronecker products that contain an odd (even) number of Pauli matrices and the rest identity matrices.

Now we state our main result.

Theorem 1 *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 Heisenberg spin models (equations (6), (7), and (9)). Assume that in both models all the γ_k and γ_k' are different from each other and that the associated graphs are connected. Then, the following are equivalent:*

(a) $(\Sigma,\rho_0)\sim(\Sigma',\rho_0')$, namely the two pairs are input-output equivalent,

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

1. *$\gamma_k=\gamma'_{\pi(k)}$,*
2. *denoting by $\pi^1_{lk}=\min\{\pi(l),\pi(k)\}$, and $\pi^2_{lk}=\max\{\pi(l),\pi(k)\}$, for $1\le l<k\le n$, then either:*

$$\begin{cases} J_{lk}=J'_{\pi^1_{lm}\pi^2_{lm}} & \forall 1\le l<k\le n,\\ P_\pi^*\rho_0'P_\pi=\rho_0; \end{cases} \tag{11}$$

or

$$\begin{cases} J_{lk}=-J'_{\pi^1_{lm}\pi^2_{lm}} & \forall 1\le l<k\le n,\\ \rho_o=\rho_o' \quad \text{and} & \rho_e=-\rho_e'; \end{cases} \tag{12}$$

where ρ_o and ρ_e (resp. ρ_o' and ρ_e') are the components of ρ_0 (resp. $P_\pi^*\rho_0'P_\pi$) in $\mathcal{I}_o$, $\mathcal{I}_e$, respectively.

Theorem 1 reads as the main result in [3] (see also next section, equation (13)). This is due to the fact that the classes of equivalent models do not vary by allowing more than one measurement. The difference between the two results is in the different definition of equivalent pairs. Theorem 1 implies, in particular, that models that have the same input output behavior after one measurement will have the same input-output behavior even if we allow several Von Neumann measurements.

3 Proof of Theorem 1

In this section we give the proof of Theorem 1. First, we state precisely the equivalence result when we allow only a single measurement. This result is proved in [3]. We need to define equivalence in a weaker sense (by allowing only one measurement).

Definition 3.1 We say that the two pairs (Σ, ρ_0) and (Σ', ρ_0') are *1-input-output equivalent* and we write

$$(\Sigma, \rho_0) \underset{1}{\sim} (\Sigma', \rho_0'),$$

if for any $t > 0$ and any control u, defined on $[0, t]$, we have

$$y^1(t, u, \rho_0) = y'^1(t, u, \rho_0'),$$

where y^1 (and y'^1) are defined as in equation (5)

Notice that if two models are equivalent then they are also 1-equivalent. But, in general, since after one measurement the state is modified, equivalence is stronger than 1-equivalence. However, for Heisenberg spin networks, Theorem 1 says that the two notions are indeed equivalent, since both of them are equivalent to condition (b) of Theorem 1. The equivalence result for $1-$equivalence is a weaker version of Theorem 1. It can be stated as [3]:

$$(\Sigma, \rho_0) \underset{1}{\sim} (\Sigma', \rho_0') \quad \Leftrightarrow \quad (b) \text{ of Theorem 1 holds .} \tag{13}$$

Now we begin to prove Theorem 1.

- $(a) \quad \Rightarrow \quad (b)$.

As observed before, models that have the same input-output behavior with several measurements have the same input-output behavior for one measurement, i.e. equivalent models are also 1-equivalent. Therefore this implication simply follows from (13).

- $(b) \quad \Rightarrow \quad (a)$.

Assume that condition (b) holds. To make notations simpler, we assume, without loss of generality, that we have already performed a change of coordinates in the second model so that the permutation π in (b) is the identity. Thus statement 1. of (b) becomes:

$$\gamma_k = \gamma_k', \quad \forall\, k \in \{1, \dots, n\}, \tag{14}$$

and equations (11) and (12) now read as:

$$\begin{cases} J_{lk} = J_{lk}' & \forall 1 \le l < k \le n, \\ \rho_0' = \rho_0; \end{cases} \tag{15}$$

or

$$\begin{cases} J_{lk} = -J_{lk}' \quad \forall 1 \le l < k \le n, \\ \rho_o = \rho_o' \quad \text{and} \quad \rho_e = -\rho_e'; \end{cases} \tag{16}$$

where ρ_o and ρ_e (resp. ρ_o' and ρ_e') are the components of ρ_0 (resp. ρ_0') in $\mathcal{I}_o$, $\mathcal{I}_e$, respectively.

It is clear that, if equation (15) holds, than the two models, together with their initial states, are the same, and so they are obviously equivalent.

Thus we assume that (16) holds. We need to show that, for every sequence of controls, the outputs (see (5)) of the two models are always the same. Notice that we allow measurements of possibly different quantities $Tr(S_v\rho)$, $v = x, y, z$ at each step. Accordingly, the state will be modified (see (4)) by an automorphism $\mathcal{P}_v$, $v = x, y, z$, as $\rho \to \mathcal{P}_v(\rho)$ corresponding to the output $Tr(S_v\rho)$. By (13), we know that the two pairs give the same outputs at the first measurement (at time t_1). Moreover, if we let $\rho_o(t)$ and $\rho_e(t)$ (resp. $\rho_o'(t)$ and $\rho_e'(t)$) the components of $\rho(t; u^1, \rho_0)$ (resp. $\rho'(t; u^1, \rho_0'))$ in $\mathcal{I}_o$, $\mathcal{I}_e$, under the action of the first control u^1, it is proved in [3] that if (b) holds then, for all $0 \le t \le t_1$, we have:

$$\begin{cases} \rho_o(t) &= \rho_o^{'}(t) \\ \rho_e(t) &= -\rho_e^{'}(t). \end{cases} \tag{17}$$

After the first measurement, the state is modified according to equation (4). More precisely, we have that $\rho(t; u^1, \rho_0)$ (resp. $\rho'(t; u^1, \rho_0')$) is changed into $\mathcal{P}_v(\rho(t; u^1, \rho_0'))$ (resp. $\mathcal{P}_v(\rho'(t; u^1, \rho_0)))$. Now if we are able to prove that $\mathcal{P}_v(\mathcal{I}_o) \subseteq \mathcal{I}_o$ and $\mathcal{P}_v(\mathcal{I}_e) \subseteq \mathcal{I}_e$, then the components of the state $\rho(t)$ in $\mathcal{I}_o$ and $\mathcal{I}_e$ after the measurement will be $\mathcal{P}_v(\rho_o(t))$ and $\mathcal{P}_v(\rho_e(t))$, respectively. The components of the state $\rho'(t)$ in $\mathcal{I}_o$ and $\mathcal{I}_e$ after the measurement will be $\mathcal{P}_v(\rho_o'(t))$ and $\mathcal{P}_v(\rho_e'(t))$, respectively. Therefore, if (17) holds before the measurement it also holds after the measurement. Thus we can apply again (13), with the initial condition equal to the state after the first measurement, and conclude that the second measurement will give the same value for any control. It is clear now that we can use the same argument for the following measurements and conclude the input-output equivalence of the two pairs.

In view of the above all we are left with is to prove the following lemma.

Lemma 3.2 Let $\mathcal{P}_v$ be the automorphism defined by equation (4) and corresponding to the matrix $S_v = \sum_{k=1}^n I_{kv}$, $v = x$, y, and z. Then, for each Hermitian matrix F, it holds:

$$\begin{array}{l} \text{if } F \in \mathcal{I}_o \;\Rightarrow\; \mathcal{P}_v(F) \in \mathcal{I}_o \\ \text{if } F \in \mathcal{I}_e \;\Rightarrow\; \mathcal{P}_v(F) \in \mathcal{I}_e \end{array} \tag{18}$$

3.1 Proof of Lemma 3.2

We give the proof of Lemma 3.2 in the case $v = z$. The other two cases follow easily from this one. First we need to decompose S_z into its projection matrices. The matrix S_z has $n+1$ different eigenvalues. Each eigenvalue corresponds to the number of spins that are in the 'down' state. In particular we can have all the spin up, one down and the remaining ones up, two down and the remaining ones up and so on. The corresponding $n+1$ values of the total magnetization in the z direction which are the eigenvalues of S_z will be denoted by $\lambda_0, \ldots, \lambda_n$. The eigenvalue λ_k corresponds to the case in which k spins are down and $n-k$ are up. We define

$$U \;:=\; \tfrac{1}{2}id + \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$D \;:=\; \tfrac{1}{2}id - \sigma_z = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

U and D are the two dimensional projections onto the subspaces spanned by the spin up and spin down eigenstates, respectively. Let $\mathcal{H}^n$ be the set of matrices of the form $G = G_1 \otimes \cdots \otimes G_n$ where $G_j = U$ or $G_j = D$. Moreover, for $j = 0, \ldots, n$, denote by $\mathcal{H}_j^n$ the subset of $\mathcal{H}^n$ of those matrices $G = G_1 \otimes \cdots \otimes G_n$ with $|\{k \,|\, G_k = D\}| = j$. Notice that $\left|\mathcal{H}_j^n\right| = \left(\begin{array}{c} n \\ j \end{array}\right)$. Then, we let

$$\Pi_j \,:=\, \sum_{G \in \mathcal{H}_j^n} G. \tag{19}$$

We have

$$S_z = \sum_{j=0}^{n} \lambda_j \Pi_j.$$

Thus, for each matrix F, we have

$$\mathcal{P}_z(F) \,=\, \sum_{j=0}^{n} \Pi_j F \Pi_j \,=\, \sum_{j=0}^{n} \sum_{G, G' \in \mathcal{H}_j^n} G F G'.$$

Each matrix F can be written as $F = \sum_{j=1}^{s} \mu_j \sigma_{j1} \otimes \cdots \otimes \sigma_{jn}$ where $\sigma_{jk} \in \{\sigma_x,\, \sigma_y,\, \sigma_z,\, id.\}$. By linearity, it is sufficient to prove the lemma for matrices of the type $M^n := \sigma_1 \otimes \cdots \otimes \sigma_n$ where $\sigma_j \in \{\sigma_x,\, \sigma_y,\, \sigma_z,\, id,\}$, for $j = 1, ..., n$. For each $l = 0, \ldots, n$, we define

$$f_l(M^n) = \sum_{k=l}^{n} \sum_{G \in \mathcal{H}_{k-l}^n} \sum_{\tilde{G} \in \mathcal{H}_k^n} G M^n \tilde{G}. \tag{20}$$

Notice that

$$(f_l(M^n))^* = \sum_{k=l}^{n} \sum_{G \in \mathcal{H}_{k-l}^n} \sum_{\tilde{G} \in \mathcal{H}_k^n} \left(G M^n \tilde{G}\right)^* = \sum_{k=l}^{n} \sum_{G \in \mathcal{H}_{k-l}^n} \sum_{\tilde{G} \in \mathcal{H}_k^n} \tilde{G} M^n G. \tag{21}$$

Moreover, it holds

$$f_0(M^n) \,=\, \mathcal{P}_z(M^n). \tag{22}$$

We will prove, by induction on $n \geq 1$, that:

$$\text{if} \;\; M^n \in \mathcal{I}_o^c \;\; (\text{resp.} \;\; \mathcal{I}_e^c) \;\; \Rightarrow \;\; \forall\, l = 0, \ldots, n, \;\; f_l(M^n) \in \mathcal{I}_o^c \; (\text{resp.} \;\; \mathcal{I}_e^c), \tag{23}$$

where $\mathcal{I}_o^c$ and $\mathcal{I}_e^c$ are the complexifications of the vector spaces $\mathcal{I}_o$ and $\mathcal{I}_e$, respectively. In view of equality (22), and the fact that f_0 maps Hermitian matrices into Hermitian matrices, (23) implies Lemma 3.2.

To prove (23) we will use the following equalities that can be easily verified by direct calculation.

$$\begin{array}{llll} U id U = \frac{1}{2} id + \sigma_z & U \sigma_z U = \frac{1}{2}\sigma_z + \frac{1}{4} id & U \sigma_x U = 0 & U \sigma_y U = 0 \\ D id D = \frac{1}{2} id - \sigma_z & D \sigma_z D = \frac{1}{2}\sigma_z - \frac{1}{4} id & D \sigma_x D = 0 & D \sigma_y D = 0 \\ U id D = 0 & U \sigma_z D = 0 & U \sigma_x D = \frac{1}{2}\sigma_x + \frac{i}{2}\sigma_y & U \sigma_y D = \frac{1}{2}\sigma_y - \frac{i}{2}\sigma_x \\ D id U = 0 & D \sigma_z U = 0 & D \sigma_x U = \frac{1}{2}\sigma_x - \frac{i}{2}\sigma_y & D \sigma_y U = \frac{1}{2}\sigma_y + \frac{i}{2}\sigma_x \end{array} \tag{24}$$

If $n = 1$, we have:

$$f_0(M^1) = \mathcal{P}_z(M^1) = UM^1U + DM^1D,$$
$$f_1(M^1) = \sum_{G\in\mathcal{H}_0^1}\sum_{\tilde{G}\in\mathcal{H}_1^1} GM^1\tilde{G} = UM^1D.$$

Using the equalities given in (24), we can verify (23) for a basis of values of M^1, namely all the values in $\{id, \sigma_x, \sigma_y, \sigma_z\}$.

Let $n > 1$, and write an element of the basis of $\mathcal{I}_o^c \oplus \mathcal{I}_e^c$ as $M^n = \sigma_1 \otimes \cdots \otimes \sigma_n = \sigma_1 \otimes N^{n-1}$. We first obtain an expression for $f_l(M^n)$ for $l = 0, \ldots, n-1$ and then for the case $l = n$. We notice that for $j = 0, \ldots, n$:

$$G \in \mathcal{H}_j^n \quad \Rightarrow \quad \begin{array}{lll} i) & G = U \otimes G_1 & \text{with } \ G_1 \in \mathcal{H}_j^{n-1}, \\ \text{or} & & \\ ii) & G = D \otimes G_1 & \text{with } \ G_1 \in \mathcal{H}_{j-1}^{n-1}, \end{array} \tag{25}$$

where if $j = 0$ then necessarily we are in case $i)$, while if $j = n$ then necessarily we are in case $ii)$.

Now we rewrite $f_l(M^n)$ by using the decomposition given by (25) both for G and $\tilde{G}$, and we get:

$$f_l(M^n) = \sum_{k=l}^{n} \Big(\sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} U\sigma_1U \otimes GN^{n-1}\tilde{G} + \sum_{G\in\mathcal{H}_{k-l-1}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_{k-1}^{n-1}} D\sigma_1D \otimes GN^{n-1}\tilde{G} +$$
$$+ \sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_{k-1}^{n-1}} U\sigma_1D \otimes GN^{n-1}\tilde{G} + \sum_{G\in\mathcal{H}_{k-l-1}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} D\sigma_1U \otimes GN^{n-1}\tilde{G}\Big).$$

In this formula, sets of the type $\mathcal{H}_a^b$ which have not been defined ($(a > b)$ or $a < 0$) have to be considered empty. We can rewrite the previous equation as:

$$f_l(M^n) =$$
$$= (U\sigma_1U) \otimes \left(\sum_{k=l}^{n} \sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} GN^{n-1}\tilde{G} \right) + (D\sigma_1D) \otimes \left(\sum_{k=l}^{n} \sum_{G\in\mathcal{H}_{k-l-1}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_{k-1}^{n-1}} GN^{n-1}\tilde{G} \right)$$
$$+ U\sigma_1D \otimes \left(\sum_{k=l}^{n} \sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_{k-1}^{n-1}} GN^{n-1}\tilde{G} \right) + D\sigma_1U \otimes \left(\sum_{k=l}^{n} \sum_{G\in\mathcal{H}_{k-l-1}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} GN^{n-1}\tilde{G} \right)$$

In the above formula, the coefficients of $U\sigma_1U$ and $D\sigma_1D$ are the same. In order to see this, notice that

$$\sum_{k=l}^{n} \sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} GN^{n-1}\tilde{G} = \sum_{k=l}^{n-1} \sum_{G\in\mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G}\in\mathcal{H}_k^{n-1}} GN^{n-1}\tilde{G},$$

since $\mathcal{H}_n^{n-1}$ is the empty set. Moreover this is the same as the coefficient of $D\sigma_1D$ if we notice that the part of the sum corresponding to $k = l$ is zero and make a change of index

$k \to h := k-1$. Neglecting terms in the sum that are zero one can simplify the coefficient of $D\sigma_1 U$ as well. In conclusion, one can rewrite $f_l(M^n)$ as

$$f_l(M^n) = (U\sigma_1 U + D\sigma_1 D) \otimes \left(\sum_{k=l}^{n-1} \sum_{G \in \mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_k^{n-1}} G N^{n-1} \tilde{G} \right) + \tag{26}$$

$$+ U\sigma_1 D \otimes \left(\sum_{k=l}^{n} \sum_{G \in \mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_{k-1}^{n-1}} G N^{n-1} \tilde{G} \right) + D\sigma_1 U \otimes \left(\sum_{k=l+1}^{n-1} \sum_{G \in \mathcal{H}_{k-(l+1)}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_k^{n-1}} G N^{n-1} \tilde{G} \right)$$

Notice that

$$\sum_{k=l}^{n-1} \sum_{G \in \mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_k^{n-1}} G N^{n-1} \tilde{G} \; = \; f_l(N^{n-1}), \quad \forall \, l = 0, \ldots, n-1. \tag{27}$$

Moreover

$$\sum_{k=l}^{n} \sum_{G \in \mathcal{H}_{k-l}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_{k-1}^{n-1}} G N^{n-1} \tilde{G} = \left\{ \begin{array}{c} \left(\sum_{k=l-1}^{n-1} \sum_{G \in \mathcal{H}_{k-(l-1)}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_k^{n-1}} G N^{n-1} \tilde{G} \right) = f_{l-1}(N^{n-1}) \\ \forall \, l = 1, \ldots, n-1 \\ \left(\sum_{k=1}^{n-1} \sum_{G \in \mathcal{H}_k^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_{k-1}^{n-1}} G N^{n-1} \tilde{G} \right) = (f_1(N^{n-1}))^* \\ l = 0, \end{array} \right\} \tag{28}$$

where, in the second equation, we have used (21). Also

$$\sum_{k=l+1}^{n-1} \sum_{G \in \mathcal{H}_{k-(l+1)}^{n-1}} \sum_{\tilde{G} \in \mathcal{H}_k^{n-1}} G N^{n-1} \tilde{G} \; = \; f_{l+1}(N^{n-1}) \;\; \forall \, l = 0, \ldots, n-2. \tag{29}$$

Thus, by using equations (27), (28), and (29), we can rewrite (26) as follows.

(a)

$$f_0(M^n) = (U\sigma_1 U + D\sigma_1 D) \otimes f_0(N^{n-1}) + U\sigma_1 D \otimes \left(f_1(N^{n-1}) \right)^* + D\sigma_1 U \otimes f_1(N^{n-1}),$$

(b) for $l = 1, \ldots, n-2$,

$$f_l(M^n) = (U\sigma_1 U + D\sigma_1 D) \otimes f_l(N^{n-1}) + U\sigma_1 D \otimes f_{l-1}(N^{n-1}) + D\sigma_1 U \otimes f_{l+1}(N^{n-1}),$$

(c)

$$f_{n-1}(M^n) = (U\sigma_1 U + D\sigma_1 D) \otimes f_{n-1}(N^{n-1}) + U\sigma_1 D \otimes f_{n-2}(N^{n-1}).$$

To complete the picture, we consider the case $l = n$, which is particularly simple. In this case, from the definition of $f_n(M^n)$ in (20), we have

(d)

$$f_n(M^n) = U\sigma_1 D \otimes \cdots \otimes U\sigma_n D.$$

Now, assume $M^n \in \mathcal{I}_o^c$. Then for $f_0(M^n)$ we consider the three elements in the sum (a) above. If σ_1 is the identity, then N^{n-1} is in $\mathcal{I}_o^c$ and so are by the inductive assumption $f_0(N^{n-1})$, $f_1(N^{n-1})$ and $f_1(N^{n-1})^*$. Moreover it follows from (24) that $U\sigma_1 U + D\sigma_1 D = id$ and $U\sigma_1 D = D\sigma_1 U = 0$, which shows that $f_0(M^n) \in \mathcal{I}_o^c$. If σ_1 is a Pauli matrix, then, from the inductive assumption $f_0(N^{n-1})$, $f_1(N^{n-1})$ and $f_1(N^{n-1})^*$ are in $\mathcal{I}_e^c$ while from (24) $U\sigma_1 U + D\sigma_1 D$ is either zero or σ_z and $U\sigma_1 D$ and $D\sigma_1 U$ are linear combinations of Pauli matrices. Analogously, using the inductive assumption and (24), one can verify $f_0(M^n) \in \mathcal{I}_e^c$ if $M^n \in \mathcal{I}_e^c$. Analogously one can verify (23) for $n \geq l > 0$, using (b), (c) and (d) above. The crucial fact, beside the inductive assumption, is that $U\sigma D$, $D\sigma U$ and $U\sigma U + D\sigma D$ are in $\mathcal{I}_o^c$ if $\sigma = \sigma_x$, σ_y, or σ_z, while they are in $\mathcal{I}_e^c$ if $\sigma = id$. This completes the proof of the Lemma.

4 Discussion

The notion of input-output equivalence for quantum control systems is relevant to modelling and parameter identification. This notion can be extended to consider cases where we perform several evolutions and measurements. In these cases, the dynamics have to be modified to incorporate the effect of the measurement on the state. Motivated by problems of model identification for molecular magnets, we have considered in the input-output equivalence of networks of spin $\frac{1}{2}$ where the total magnetization is measured. According to the main result of [3] if we drive a spin network with an electromagnetic field and measure the total magnetization the results will always be the same for networks with parameters and initial states related by equations (11) or (12). This raised the question of whether it is possible to distinguish the cases (11) and (12) by performing several Von Neumann measurements and this paper has given a negative answer to this question.

As a simple example of the situation (12) described in Theorem 1, consider an Heisenberg network of two spins $\frac{1}{2}$ and consider the two initial states

$$\rho_0 = \frac{1}{4} id \otimes id - \sigma_z \otimes \sigma_z, \rho_0' = \frac{1}{4} id \otimes id + \sigma_z \otimes \sigma_z. \tag{30}$$

These are both physically admissible density matrices as they are Hermitian, trace one and positive semidefinite. In particular ρ_0 represents a mixture with equal weights of two pure states representing respectively spin 1 up and spin 2 down and spin one down and spin 2 up, i.e. in Dirac notation

$$\rho_0 = \frac{1}{2} | \uparrow\downarrow >< \uparrow\downarrow | + \frac{1}{2} | \downarrow\uparrow >< \downarrow\uparrow |. \tag{31}$$

With the same notation ρ_0' represent the mixture

$$\rho_0' = \frac{1}{2} | \uparrow\uparrow >< \uparrow\uparrow | + \frac{1}{2} | \downarrow\downarrow >< \downarrow\downarrow |. \tag{32}$$

These two states are related as in (12). From, the results of this paper it follows that by driving the system with an electro-magnetic field and measuring the total magnetization, it is not possible to decide whether we are in the initial state (31) and the coupling constant is positive or we started from an initial state (32) and the coupling constant is negative. And this is not possible even if we allow multiple Von Neumann measurements.

The results presented here concern the input output behavior of different models and are preliminary to algorithms for state and model identifications. These algorithms might simplify if we assume preliminary knowledge. For example, if the model is known, they are just algorithms for quantum state determination, which are currently under intensive research. Some references and analysis from a control theoretic perspective can be found in [8]. It should be mentioned that, opposite to classical systems, identification algorithms for quantum systems will require several copies of the same system, as the measurement will in general modify the state.

The fact that input-output equivalence under one measurement or multiple measurements are the same for Heisenberg spin systems is a special property of the class of models considered here and it is not true for other class of models. For example, if we consider a class of pairs model-initial state where the model is the same and the initial states can possibly change the notion of input-output equivalence is the same as the notion of indistinguishability for states. According to the results of [8] states are indistinguishable in k measurements if and only if they have the same components on the observability space $\mathcal{V}_k$ (defined in [8] in terms of commutators depending on the output and the model). As the sequence of observability spaces $\mathcal{V}_k$ is typically strictly increasing (for small k) there exists states that are indistinguishable in one measurement but can be distinguished in be distinguished in more than one measurement. More examples of systems where 1-equivalence is not the same as multiple equivalence can be constructed by considering *generalized measurement* i.e. measurement not necessarily of the Von Neumann type [6]. In these cases the state will be modified according to

$$\rho \to \mathcal{F}(\rho) := \sum_{m \in \mathcal{M}} \Phi_m(\rho), \tag{33}$$

where $\mathcal{M}$ is the set of possible outcomes and Φ_m is a set of positive linear operators which take different form according to the measurement we are considering (e.g. unsharp measurements, indirect measurements). The operation $\mathcal{F}$ is a generalization of $\mathcal{P}$ in (3) (4) and does not in general satisfy the property of Lemma (3.2).

Input-output equivalence will be investigated for different models and for open systems in future research.

References

[1] F. Albertini and D. D'Alessandro, Notions of controllability for multilevel bilinear quantum mechanical systems, *IEEE Transactions on Automatic Control*, Vol. 48, No. 8, pg.

1399-1403. See also (longer version) F. Albertini and D. D'Alessandro, Notions of controllability for quantum mechanical systems, Preprint arXiv:quant-ph/0106128, 2001.

[2] F. Albertini and D. D'Alessandro, The Lie Algebra structure and controllability of spin systems, *Linear Algebra and its Applications*, 350, (2002), 213-235.

[3] F. Albertini and D. D'Alessandro, Model identification for spin networks, ArXiv: quant-ph/0307128. To appear.

[4] D. D. Awschalom and D. P. DiVincenzo, Complex dynamics of mesoscopic magnets, *Physics Today*, April 1995, pp. 43-48.

[5] B. Barbara and L. Gunther, Magnets, molecules and quantum mechanics, *Physics World*, March 1999, pp. 35-39.

[6] H-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, New York 2002.

[7] G. Christou, D. Gatteschi, D. N. Hendrickson and R. Sessoli, Single-Molecule magnets, *MRS Bulletin*, November 2000, pp. 66-71.

[8] D. D'Alessandro, On quantum state observability and measurement, *Journal of Physics A: Mathematical and General* **36** (2003) 9721-9735

[9] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis*, Cambridge University Press, 1991.

[10] G. M. Huang, T. J. Tarn and J. W. Clark, On the controllability of quantum mechanical systems, *Journal of Mathematical Physics*, **24** (11) (1983) 2608-2618.

[11] L. Ljung and T. Soderstrom, *Theory and Practice of Recursive Identification*, MIT Press, Cambridge, Massachusetts, 1983.

[12] J. J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley Pub. Co., Reading, Mass. 1994.

[13] H-J Schmidt and M. Luban, Continuous families of isospectral Heisenberg spin systems and the limits of inference from measurements, *J. Phys. A: Math. Gen.* **34** (2001), 2839-2858.

[14] E. Sontag, *Mathematical Control Theory; Deterministic, Finite Dimensional Systems*, Springer, New York, 1990.