Control of the evolution of Heisenberg spin systems

Francesca Albertini
Dipartimento di Matematica Pura ed Applicata,
Università di Padova,
via Belzoni 7,
35100 Padova, Italy.
Tel. (+39) 049 827 5966
email: albertin@math.unipd.it

Domenico D'Alessandro
Department of Mathematics
Iowa State University
Ames, IA 50011, USA
Tel. (+1) 515 294 8130
email: daless@iastate.edu

Abstract

In this paper, we give an algorithm for the control of the unitary evolution operator for the system of two spin $\frac{1}{2}$'s interacting through Heisenberg interaction. This algorithm allows for arbitrarily bounded control. The results extend previous ones that only concerned the control of a pure state. A Lie group decomposition technique is used to this goal and the problem is reduced to a two level problem with constraints. We also show how the control result allows to obtain information on the initial state through a series of evolutions and measurements.

The study of the Heisenberg spin model is motivated by applications in electron paramagnetic resonance and in molecular magnetism. For these systems, the drift which models the interaction between the spins is typically large and cannot be neglected in the control design but it has to be used to reach the objective.

1 Introduction and model to be studied

In a recent paper [16], an algorithm was given for the control of two spin $\frac{1}{2}$'s interacting through Heisenberg interaction. This algorithm allowed to control a pure state from an arbitrary value to an eigenstate of the free (uncontrolled) Hamiltonian. The algorithm consisted of a (theoretically) infinite sequence of two level problems that were solved with the use of an energy function technique [1]. In the present paper we improve this result in several aspects. We present an algorithm which allows to control *the unitary evolution operator.* This is more general than controlling the pure state only. Moreover, the control algorithm allows to drive the state to a desired value in *finite time* and it is possible to use *two controls only* rather than the three controls used in [16](see Remark 2.1 below). Our control algorithm, as the one [16], also allows to incorporate arbitrary bounds on the control in the control design. A further contribution of this paper is that we show how to use the control result for state determination. We still resort to a Lie algebraic decomposition as in [16], in order reduce the problem to a two level problem. However, instead of solving a sequence of two level problems, we solve a finite set of these problems with appropriate constraints.

We shall deal with an Heisenberg Hamiltonian H of the form

$$H(t) = H_0 + \sum_{j=x,y,z} H_j u_j. \tag{1}$$

The free Hamiltonian H_0 has the isotropic Heisenberg form $H_0 := J(S_x \otimes S_x + S_y \otimes S_y + S_z \otimes S_z)$ where J is the coupling constant and $S_{x,y,z}$ are the Pauli matrices defined by

$$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

The matrices H_j, $j = x, y, z$ are defined as $H_j(t) := (\gamma_1 S_j \otimes \mathbf{1} + \gamma_2 \mathbf{1} \otimes S_j)$, where γ_1 and γ_2 are the gyromagnetic ratios of particles 1 and 2, respectively. The controls $u_{x,y,z}$ are x, y and z components of the externally applied driving electro-magnetic field. The control problem is to steer the unitary evolution operator X solution of the Schrödinger equation,

$$\dot{X} = -iH(t)X, \qquad X(0) = I_{4\times 4}, \tag{3}$$

to any desired special unitary final value $X_f \in SU(4)$, in finite time. This problem has a solution if $\gamma_1 \neq \gamma_2$ since in this case (and only in this case) the system is controllable. This can be easily verified by evaluating the Lie algebra generated by $\{iH_0, iH_{x,y,z}\}$ [7], [8]. Following [3], [16], it will be convenient to rewrite equation (3), after a change of coordinates and re-scaling of the time and the control variables, as

$$\dot{X} = AX + B_x X u_x + B_y X u_y + B_z X u_z \qquad X(0) = I_{4\times 4}. \tag{4}$$

In (4), we have

$$A := diag(3i, -i, -i, -i), \tag{5}$$

$$B_x := \begin{pmatrix} 0 & 0 & 0 & r-1 \\ 0 & 0 & -(1+r) & 0 \\ 0 & (1+r) & 0 & 0 \\ 1-r & 0 & 0 & 0 \end{pmatrix}, \tag{6}$$

$$B_y := \begin{pmatrix} 0 & 0 & r-1 & 0 \\ 0 & 0 & 0 & r+1 \\ 1-r & 0 & 0 & 0 \\ 0 & -(1+r) & 0 & 0 \end{pmatrix}, \tag{7}$$

$$B_z := \begin{pmatrix} 0 & r-1 & 0 & 0 \\ 1-r & 0 & 0 & 0 \\ 0 & 0 & 0 & -(1+r) \\ 0 & 0 & 1+r & 0 \end{pmatrix}, \tag{8}$$

where $r := \frac{\gamma_2}{\gamma_1}$. To simplify formulas, we shall assume $r = 2$ in the following.

There are several motivations to study Heisenberg spin systems. They model experiments in Electron Paramagnetic Resonance [14] and Nuclear Magnetic Resonance [6]. They are also a good model for magnetic molecules (see e.g. [15]) under the action of a time varying electro-magnetic field. The strategies to control these model have to be different from the ones used to control two spin $\frac{1}{2}$ coupled via Ising interaction as described in [2], [9]. The main difference is that, in this case the coupling parameter J is typically very large and it is in practice not possible to use very large controls in very short time so as to cancel the effect of the drift AX in equation (4). In this respect the technique of control we shall describe in this paper is closer in spirit to the techniques without 'hard pulses' described in [3], [12]. The technique uses the drift constructively in order to obtain control to the desired value for the unitary evolution operator.

In the following section, we describe our approach in more detail and show how the problem of control for system (4) can be reduced to a *finite number* of *two level problems with constraints*. We show how to solve this type of problems in Section 3. In Section 4, we consider an application of the control algorithm. In particular, we consider the problem of determining the initial state of the Heisenberg two spin system through a series of evolutions and Von Neumann measurements of the total magnetization. We show how the control result can be used to extract the maximum amount of information on the initial state. We present some conclusions in Section 5.

2 Reduction of the problem

Every matrix X_f in $SU(4)$ can be written as [11]

$$X_f = D(\alpha_1, \alpha_2, \alpha_3)U_{12}(\theta_1, \sigma_1)U_{13}(\theta_2, \sigma_2)U_{23}(\theta_3, \sigma_3)U_{14}(\theta_4, \sigma_4)U_{24}(\theta_5, \sigma_5)U_{34}(\theta_6, \sigma_6), \qquad (9)$$

where $D(\alpha_1, \alpha_2, \alpha_3)$ is a diagonal matrix $diag(e^{i\alpha_1}, e^{i\alpha_2}, e^{i\alpha_3}, e^{-i(\alpha_1+\alpha_2+\alpha_3)})$ for some real parameters $\alpha_1, \alpha_2, \alpha_3$ and the matrix $U_{kl}(\theta, \sigma)$ $(1 \leq k < l \leq 4)$ is equal to the identity except for the entries at the intersection of the $k-$th and $l-$th rows and columns which are occupied by the 2×2 submatrix

$$\bar{U}_{kl}(\theta, \sigma) = \begin{pmatrix} cos(\theta) & -sin(\theta)e^{-i\sigma} \\ sin(\theta)e^{i\sigma} & cos(\theta) \end{pmatrix}. \qquad (10)$$

The parameters $\alpha_{1,2,3}$, $\theta_{1,2,\ldots,6}$, $\sigma_{1,2,\ldots,6}$ completely parametrize $SU(4)$. The important feature of the decomposition (9), for our purposes, is that the parameters, and therefore the factors in (9) can be explicitly calculated using a very simple procedure. Starting with X_f, one first finds θ_6 and σ_6 so as to introduce a zero in the $(4,3)$ entry of the matrix $X_f U_{3,4}(-\theta_6, \sigma_6) = X_f[U_{3,4}(\theta_6, \sigma_6)]^{-1}$. Then one finds θ_5 and σ_5 in order to introduce a zero in the $(4,2)$ entry of $X_f U_{3,4}(-\theta_6, \sigma_6)U_{2,4}(-\theta_5, \sigma_5) = X_f U_{3,4}(-\theta_6, \sigma_6)[U_{2,4}(\theta_5, \sigma_5)]^{-1}$. This does not affect the zero previously introduced. Continuing this way, at each step one selects $[U_{kl}]^{-1}$ in order to introduce a zero in the $(l,k)-$th position. At the end of the procedure one obtains a diagonal matrix

$$X_f U_{34}^{-1} U_{24}^{-1} U_{14}^{-1} U_{23}^{-1} U_{13}^{-1} U_{12}^{-1} := D(\alpha_1, \alpha_2, \alpha_3), \tag{11}$$

from which the parameters $\alpha_{1,2,3}$ can be directly read. More details on this construction and extensions to the Lie groups $SU(n)$ and $U(n)$, for general n, can be found in [11].

We will, in the following, factorize X_f using matrices in the following Lie subgroups of $SU(4)$:

- $\mathbf{G}_x$, which is generated by matrices of the form

$$G_x := \begin{pmatrix} u & 0 & 0 & u \\ 0 & s & s & 0 \\ 0 & s & s & 0 \\ u & 0 & 0 & u \end{pmatrix}; \tag{12}$$

- $\mathbf{G}_y$, which is generated by matrices of the form

$$G_y := \begin{pmatrix} u & 0 & u & 0 \\ 0 & s & 0 & s \\ u & 0 & u & 0 \\ 0 & s & 0 & s \end{pmatrix}; \tag{13}$$

- $\mathbf{G}_z$, which is generated by matrices of the form

$$G_z := \begin{pmatrix} u & u & 0 & 0 \\ u & u & 0 & 0 \\ 0 & 0 & s & s \\ 0 & 0 & s & s \end{pmatrix}. \tag{14}$$

In the above definitions, the entries labeled by u form an arbitrary special unitary matrix in $SU(2)$. The entries labeled with s form an arbitrary orthogonal matrix in $SO(2)$. We shall use the following fact in the sequel.

Fact: From the factorization (9), a factorization in terms of elements of $\mathbf{G}_x$, $\mathbf{G}_y$ and $\mathbf{G}_z$ only, can be derived. In fact, the factors in (9) can all be obtained as products of elements from $\mathbf{G}_x$, $\mathbf{G}_y$ and $\mathbf{G}_z$.

In order to see this, notice that $U_{12} \in \mathbf{G}_z$, $U_{13} \in \mathbf{G}_y$ and $U_{14} \in \mathbf{G}_x$, already. Moreover for $2 \leq k < l \leq 4$ we have

$$U_{1k}(\frac{\pi}{2}, 0) U_{1l}(\theta, \sigma) U_{1k}(-\frac{\pi}{2}, 0) = U_{kl}(\theta, \sigma). \tag{15}$$

The matrix $D(\alpha_1, \alpha_2, \alpha_3)$ can be obtained as a product of diagonal matrices from $\mathbf{G}_x$, $\mathbf{G}_y$ and $\mathbf{G}_z$.

In view of the above fact and the right invariance of system (4), the control problem of steering the state X from the identity to a desired X_f will be solved if we are able to steer X from the identity to any matrix in $\mathbf{G}_{x,y,z}$. In particular, we consider the controls that steer the identity to each matrix in the factorization of X_f, in the order from the right to the left. The control obtained by concatenating these controls, by right invariance, will steer the state to X_f. The technique of using Lie group decompositions for steering control has been discussed in several other papers (see e.g. [3], [9], [12]). Based on this technique, algorithms are known for several low dimensional quantum and classical systems. Decompositions are known for high dimensional Lie groups as well (see e.g. [11]) but their application to the control of high dimensional quantum system has proved more difficult. Typically one has less control power, as compared to the system degrees of freedom, and this makes it difficult to produce the basic factors of a decomposition.

We will now see that the problem of steering the state from the identity to an element of $\mathbf{G}_{x,y,z}$ is essentially a two level problem (namely a problem on $SU(2)$) with an additional (isoperimetric type of) constraint. The solution of this problem will be presented in the next section. We discuss this for a target state in $\mathbf{G}_x$. Everything we say can be said, with the obvious changes, for $\mathbf{G}_y$ and $\mathbf{G}_z$.

If we set all the components of the control except u_x equal to zero, then the state of system (4) varies on the connected Lie group associated to the Lie algebra generated by A and B_x. This Lie algebra $\mathcal{L}$ has the direct sum decomposition which corresponds to a Levi decomposition [5]

$$\mathcal{L} = \mathcal{S} \oplus \mathcal{A}_1 \oplus \mathcal{A}_2. \tag{16}$$

The simple Lie algebra $\mathcal{S}$ is spanned by matrices that have all the entries equal to zero except the entries at the intersection of first and fourth rows and columns, which are occupied by an arbitrary matrix in $su(2)$. The one dimensional Lie algebra $\mathcal{A}_1$ is spanned by $A_1 := diag(i, -i, -i, i)$ while the one dimensional Lie algebra $\mathcal{A}_2$ is spanned by

$$A_2 := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{17}$$

We also have

$$[\mathcal{S}, \mathcal{A}_1] = 0, \quad [\mathcal{S}, \mathcal{A}_2] = 0, \quad [\mathcal{A}_1, \mathcal{A}_2] = 0. \tag{18}$$

Moreover, the Lie algebra $\mathcal{S} \oplus \mathcal{A}_2$ is the Lie algebra of $\mathbf{G}_x$. It is convenient to rewrite equation (4) by separating, in the right hand side, the matrices in $\mathcal{S}$, $\mathcal{A}_1$ and $\mathcal{A}_2$. We obtain

$$\dot{X} = (2i\bar{S}_z - iu_x\bar{S}_y)X + A_1X - 3u_xA_2X. \tag{19}$$

Here $\bar{S}_{z,y}$ is the 4×4 matrix which has in the entries $(1,1)$, $(1,4)$, $(4,1)$ and $(4,4)$ the Pauli matrix $S_{z,y}$ in (2). For a given control u_x, it follows from (18) that the solution of (19) can be written as

$$X(t) = diag(e^{it}, e^{-it}, e^{-it}, e^{it}) \times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & cos(\theta(t)) & -sin(\theta(t)) & 0 \\ 0 & sin(\theta(t)) & cos(\theta(t)) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times X_1(t), \tag{20}$$

where $X_1(t)$ is the solution of

$$\dot{X}_1 = (2i\bar{S}_z - iu_x\bar{S}_y)X_1, \qquad X_1(0) = I_{4\times 4}, \tag{21}$$

and

$$\theta(t) := 3\int_0^t u_x(\tau)d\tau. \tag{22}$$

It follows from (20) that, in order to steer the state of the system to a value in $\mathbf{G}_x$, we have to find a control u_x to steer the state X_1 of (21) to a desired value. Moreover $\theta(t)$ in (22) has to be equal to a given value modulo a multiple of 2π, and the total time of transfer has to be a multiple of 2π in order for the first factor of (20) to be equal to the identity. Notice that the problem of control of system (21) is equivalent to the problem of control for the 2×2 system on $SU(2)$

$$\dot{X} = (2iS_z - iu_xS_y)X, \qquad X(0) = I_{2\times 2} \tag{23}$$

Moreover, notice that if we are able to steer the state of (23) to arbitrary values in $SU(2)$ we can do that in arbitrary time, as long as this time is larger than a prescribed one. In order to see this, we can concatenate every control to a control steering to

$$P_1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{24}$$

along with a control identically zero for time T and then a control steering to P_1^{-1} and then a control equal to zero for time T again. The net result is a matrix

$$e^{-iS_zT}P_1^{-1}e^{-iS_zT}P_1 = I_{2\times 2}, \tag{25}$$

which does not affect the state transfer but affects the time which we can adjust arbitrarily since T is arbitrary. Notice also that the above control sequence affects the integral (22) in a known way independent of T, since we set $u_x \equiv 0$ during time T which does not give contribution to the integral. Therefore the requirement on the first factor of (20) can be dropped and we can say that we solve the control problem to drive the state of (4) to any value in $\mathbf{G}_x$ if we can solve the following two level problem with constraints

Problem: Given an arbitrary $X_f \in SU(2)$ and $\gamma \in \mathbb{R}$, drive the state of the system

$$\dot{X} = (2iS_z - iu_xS_y)X, \qquad X(0) = I_{2\times 2}, \tag{26}$$

to X_f, in time t, with a control u_x satisfying

$$3\int_0^t u_x(\tau)d\tau = \gamma + 2k\pi, \qquad (27)$$

for some $k \in \mathbb{Z}$.

We shall solve this problem and therefore the whole control problem in the next section. Our solution will allow for arbitrarily bounded control. We conclude with the following remark

Remark 2.1 Notice that two of the subgroups $\mathbf{G}_{x,y,z}$ generate the other one. This implies, in view of the above described control procedure, that we can just use two of the controls $u_{x,y,z}$ and set the third one identically equal to zero.

3 Solution of a two level control problem with constraints

In this section, we will solve the two level problem with constraints given by equations (26) and (27). We will see that the problem can be solved even if we fix a bound on the control. Thus to get to the desired final state, we do not need very large controls. On the contrary the control can be chosen arbitrary small. More precisely the following holds.

> (P) Given any $X_f \in SU(2)$, any $\gamma \in \mathbb{R}$, and any $M > 0$, there exists a time $T > 0$ and a *piecewise constant control* $\bar{u}(\cdot)$, defined on $[0, T]$, such that:
>
> i) $||\bar{u}||_\infty \leq M$,
>
> ii) $\int_0^T \bar{u}(\tau)d\tau = \frac{\gamma}{3} + \frac{2}{3}k\pi$, for some $k \in \mathbb{Z}$.
>
> Moreover, if $X(t)$ is the solution of equation (26) with control $\bar{u}(\cdot)$, then $X(T) = X_f$.

Let $D(u) \in su(2)$ be the matrix defined by $D(u) := 2iS_z - iuS_y$. Equation (26) with control $u(t) \equiv u$ becomes:

$$\dot{X} = D(u)X = \begin{pmatrix} 2i & u \\ -u & -2i \end{pmatrix} X. \qquad (28)$$

A straightforward calculation shows that:

$$e^{D(u)t} = \begin{pmatrix} \cos(\lambda t) + \frac{2i}{\lambda}\sin(\lambda t) & \frac{u}{\lambda}\sin(\lambda t) \\ -\frac{u}{\lambda}\sin(\lambda t) & \cos(\lambda t) - \frac{2i}{\lambda}\sin(\lambda t) \end{pmatrix}, \qquad (29)$$

where $\lambda = \sqrt{4 + u^2}$. In particular,

$$e^{D(0)t} = e^{2iS_z t} = \begin{pmatrix} e^{2it} & 0 \\ 0 & e^{-2it} \end{pmatrix}. \qquad (30)$$

Now, any matrix $X_f \in SU(2)$ can be written as:

$$X_f = \begin{pmatrix} \cos(\theta)e^{i\sigma_1} & \sin(\theta)e^{i\sigma_2} \\ -\sin(\theta)e^{-i\sigma_2} & \cos(\theta)e^{-i\sigma_1} \end{pmatrix} \tag{31}$$

for some fixed parameters σ_1, σ_2, $\theta \in \mathbb{R}$. This is the classical Euler's decomposition as we have

$$X_f = e^{D(0)\frac{\sigma_1+\sigma_2}{4}} \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} e^{D(0)\frac{\sigma_1-\sigma_2}{4}} = e^{D(0)\frac{\sigma_1+\sigma_2}{4}} e^{-iS_y\theta} e^{D(0)\frac{\sigma_1-\sigma_2}{4}}. \tag{32}$$

The parameters of Euler's decomposition can be easily calculated by known methods (see e.g. [13]). From (32) it follows that if we solve the problem (P) with final state equal to $e^{-iS_y\theta}$, then we also solve the same problem with final state X_f. In fact, first notice that for $k \in \mathbb{Z}$, $e^{D(0)k\pi} = I_{2\times 2}$, thus we can assume that $t_1 = \frac{\sigma_1-\sigma_2}{4}$ and $t_2 = \frac{\sigma_1+\sigma_2}{4}$ are both positive. In fact, if this is not the case, we can add arbitrary multiple of π to make them positive. Assume that $\bar{u}(\cdot)$ is the control defined on some interval $[0, T]$, satisfying $i)$ and $ii)$ of (P), which drives the $I_{2\times 2}$ to $e^{-iS_y\theta}$, then a control $\tilde{u}(\cdot)$ satisfying $i)$ and $ii)$ of (P), which drives the $I_{2\times 2}$ to X_f can be constructed as follows. We first apply on $[0, t_1)$ the control $\tilde{u}(\cdot) \equiv 0$, then we apply on $[t_1, T + t_1)$ the control $\tilde{u}(\tau) = \bar{u}(\tau - t_1)$, finally we apply on $[T + t_1, T + t_1 + t_2]$, the control $\tilde{u}(\cdot) \equiv 0$. This control $\tilde{u}(\cdot)$ defined on $[0, T + t_1 + t_2]$ clearly satisfies again $i)$ and $ii)$ of (P), and, by right invariance, drives $I_{2\times 2}$ to X_f, as desired. Therefore to obtain (P), we will prove that:

> (Q) Given any $\theta \in \mathbb{R}$, any $\gamma \in \mathbb{R}$, and any $M > 0$, there exist $m \in \mathbb{N}$, t_1, $t_2 \in \mathbb{R}$, $t > 0$, and a value $0 < \bar{u} \leq M$ such that:
>
> $$e^{-iS_y\theta} = \left(e^{-iS_y\frac{\theta}{m}}\right)^m = \left(e^{D(0)t_2}e^{D(\bar{u})t}e^{D(0)t_1}\right)^m, \tag{33}$$
>
> and
>
> $$m\bar{u}t = \frac{\gamma}{3} + \frac{2}{3}k\pi, \tag{34}$$
>
> for some $k \in \mathbb{Z}$.

It is clear that, if (Q) holds, by using the decomposition (33) and arguing as before, we are able to find a piecewise constant control $u(\cdot)$ equal either to 0 or to $\bar{u}$ which drives $I_{2\times 2}$ to $e^{-iS_y\theta}$. Moreover, this control satisfies $i)$ since $\bar{u} \leq M$, and $ii)$ is exactly condition (34).

We have that:

$$e^{D(0)t_2}e^{D(u)t}e^{D(0)t_1} = \begin{pmatrix} e^{2i(t_2+t_1)}\left(\cos(\lambda t) + \frac{2i}{\lambda}\sin(\lambda t)\right) & e^{2i(t_2-t_1)}\left(\frac{u}{\lambda}\sin(\lambda t)\right) \\ e^{-2i(t_2-t_1)}\left(-\frac{u}{\lambda}\sin(\lambda t)\right) & e^{-2i(t_2+t_1)}\left(\cos(\lambda t) - \frac{2i}{\lambda}\sin(\lambda t)\right) \end{pmatrix}, \tag{35}$$

where $\lambda = \sqrt{4+u^2}$. Since t_1, $t_2 \geq 0$ can be chosen arbitrarily, (33) holds for $\bar{u} = u$ if and only if

$$\cos^2\left(\frac{\theta}{m}\right) = \cos^2(\lambda t) + \frac{4}{\lambda^2}\sin^2(\lambda t). \tag{36}$$

Notice that (34) holds if, for $u > 0$,

$$t = \left(\frac{\gamma}{3m} + \frac{2k\pi}{3m}\right)\frac{1}{u} := c_{km}\frac{1}{u}. \tag{37}$$

Formula (37) shows the dependence of the time t on the allowed magnitude of the control u. In particular, we can decrease the total time of the algorithm by increasing the allowed control magnitude. By substituting (37) into (36), we get:

$$\cos^2\left(\frac{\theta}{m}\right) = \cos^2\left(c_{km}\frac{\sqrt{4+u^2}}{u}\right) + \frac{4}{4+u^2}\sin^2\left(c_{km}\frac{\sqrt{4+u^2}}{u}\right). \tag{38}$$

For $u > 0$, we let

$$v = g(u) = \frac{\sqrt{4+u^2}}{u}. \tag{39}$$

The map g is a diffeomorphism from $(0, +\infty)$ to $(1, +\infty)$. Since $g' < 0$, saying $u \leq M$ means $v = g(u) \geq g(M)$. Moreover, if $v = g(u)$ then

$$\frac{\sqrt{4+u^2}}{u} = 1 - \frac{1}{v^2}. \tag{40}$$

In the variable v (38) becomes:

$$\cos^2\left(\frac{\theta}{m}\right) = \cos^2\left(c_{km}v\right) + \left(1 - \frac{1}{v^2}\right)\sin^2\left(c_{km}v\right) = 1 - \frac{\sin^2\left(c_{km}v\right)}{v^2}.$$

Thus to get (Q), it suffices to prove that

> for any $\theta \in \mathbb{R}$, any $\gamma \in \mathbb{R}$, and any $\alpha > 1$, there exist $m \in \mathbb{N}$, $k \in \mathbb{Z}$, and $\bar{v} \geq \alpha$ such that
>
> $$f(\bar{v}) = 1 - \frac{\sin^2\left(c_{km}\bar{v}\right)}{\bar{v}^2} = \cos^2\left(\frac{\theta}{m}\right), \tag{41}$$
>
> with $c_{km} = \left(\frac{\gamma}{3m} + \frac{2k\pi}{3m}\right) > 0$.

We can assume, without loss of generality, that $\sin(2\pi\alpha) \neq 0$. In fact, if $\sin(2\pi\alpha) = 0$, we may choose any $\tilde{\alpha} > \alpha$, for which $\sin(2\pi\tilde{\alpha}) \neq 0$, and we will find a value $\bar{v} \geq \tilde{\alpha}$ (so also $\bar{v} \geq \alpha$) for which (41) holds. Fix $k = 3m$. Notice that we have

$$\lim_{m\to+\infty} \cos\left(\frac{\theta}{m}\right) = 1, \tag{42}$$

$$\lim_{m\to+\infty,\, k=3m} c_{km} = 2\pi, \tag{43}$$

and, by continuity of the map f, we also have

$$\lim_{m\to+\infty,\, k=3m} f(\alpha) = 1 - \frac{\sin^2(2\pi\alpha)}{\alpha^2} := 1 - \delta < 1. \tag{44}$$

Now, to get (41), it is enough to observe that

- If we choose $\epsilon < \delta/2$, we have that there exists $\bar{m}$ such that for all $m \geq \bar{m}$:

$$1 - \epsilon \leq \cos^2\left(\frac{\theta}{m}\right), \tag{45}$$

  and

$$f(\alpha) \leq 1 - \delta/2 \leq 1 - \epsilon. \tag{46}$$

- f assume the value 1 at all the points $v_l := \frac{l\pi}{c_{km}}$ whose limit as $l \to +\infty$ is $+\infty$. Thus, in particular, $f(\beta) = 1$ for some $\beta > \alpha$.

Since f is a continuous function it assumes all values in the interval $[1-\delta/2, 1]$ for $v \in [\alpha, \beta]$. Thus, there exists a $\bar{v} \geq \alpha$ for which equality (41) holds.

In conclusion, in order to find the value the control for given θ, γ, and $\alpha := g(M)$, we proceed as follows. First, we set $k = 3m$ in (41), then we choose an arbitrary $\tilde{\alpha} \geq \alpha$, with $\delta := \frac{\sin^2(2\pi\tilde{\alpha})}{\tilde{\alpha}^2} > 0$. Now given any arbitrary $\epsilon \leq \frac{\delta}{2}$, one chooses m so that equations (45) and (46) are verified. Plugging this m into (41), one obtains an equation in the variable v only. This equation, by the above argument, has a solution greater than $\tilde{\alpha}$, thus also greater than α. Solving this nonlinear equation one obtains the value of $\bar{v}$ and plugging this for $\bar{v}$ into (40) one obtains the value of $\bar{u}$. The time t is obtained from equation (37).

4 Applications of the control algorithm: Determination of the initial state

One of the most important problems in experiments with quantum systems is the determination of their state from appropriate measurements. Techniques of state determination go under the name of *quantum state tomography* and a review can be found in [10]. In [4] the problem was looked at from the point of view of control theory. In particular it was investigated whether it is possible to obtain information on the *initial* state by alternating appropriate evolutions and Von Neumann measurements. Such a method assumes that we are able to use control to drive the unitary evolution to any desired target. In [4] it was assumed that we measured the mean value of a nondegenerate observable and a general algorithm was given to determine the parameters of the initial density matrix. In the case of non degenerate observable at most $n-1$ independent parameters of the initial density matrix can be determined.

We consider now the problem of initial state determination for the spin Heisenberg system of this paper. We assume that we are measuring the mean value of the total magnetization in the z-direction given by the matrix (in the original coordinates)

$$S_z^{TOT} := S_z \otimes \mathbf{1} + \mathbf{1} \otimes S_z, \tag{47}$$

where $\mathbf{1}$ is the 2×2 identity matrix and S_z is the Pauli matrix defined in (2). After a Von Neumann measurement of the mean value of S_z^{TOT}, the density matrix ρ is modified as

$$\rho \to \mathcal{P}(\rho) = \sum_{j=1}^{3} \Pi_j \rho \Pi_j. \tag{48}$$

Here the projection Π_j projects onto the eigenspace of the j-th eigenvector of S_z^{TOT}. These matrices are given by $\Pi_1 := diag(1,0,0,0)$, $\Pi_2 := diag(0,1,1,0)$, and $\Pi_3 := (0,0,0,1)$. In our case, the observable S_z^{TOT} is degenerate since the eigenvalue zero has multiplicity 2. Therefore we cannot directly apply the results of [4]. All the matrices of the form $\mathcal{P}(F)$ have a block diagonal structure of the type $diag(A_{11}, A_{22}, A_{33})$ where A_{11} and A_{33} are 1×1 and A_{22} is 2×2. The value of the output at the $k-$th measurement, y_k is given by

$$y_k = Tr(S_z^{TOT} X_k \mathcal{P}(X_{k-1} \mathcal{P}(\cdots \mathcal{P}(X_1 \rho_0 X_1^*) \cdots) X_{k-1}^*) X_k^*), \tag{49}$$

where X_j, $j = 1, ..., k$, is the evolution between the $(j-1)$-th and $j-$th measurements. Using elementary properties of the trace, we obtain

$$\begin{aligned} y_k = {} & Tr(S_z^{TOT} X_k \mathcal{P}(X_{k-1} \mathcal{P}(\cdots \mathcal{P}(X_1 \rho_0 X_1^*) \cdots) X_{k-1}^*) X_k^*) = \\ & Tr(X_k^* S_z^{TOT} X_k \mathcal{P}(X_{k-1} \mathcal{P}(\cdots \mathcal{P}(X_1 \rho_0 X_1^*) \cdots) X_{k-1}^*)) = \\ & Tr(\mathcal{P}(X_k^* S_z^{TOT} X_k) X_{k-1} \mathcal{P}(\cdots \mathcal{P}(X_1 \rho_0 X_1^*) \cdots) X_{k-1}^*) = \\ & Tr(X_{k-1}^* \mathcal{P}(X_k^* S_z^{TOT} X_k) X_{k-1} \mathcal{P}(\cdots \mathcal{P}(X_1 \rho_0 X_1^*) \cdots)) = \\ & \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \cdot \\ & \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \cdot \\ & \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \cdot \end{aligned} \tag{50}$$

$$Tr(\mathcal{P}(X_2^* \mathcal{P}(\cdots \mathcal{P}(X_{k-1}^* \mathcal{P}(X_k^* S_z^{TOT} X_k) X_{k-1}) \cdots) X_2) X_1 \rho_0 X_1^*). \tag{51}$$

We notice, from the last line, that the output only depends on the elements of $X_1 \rho_0 X_1^*$ in the 1×1, 2×2 and 1×1 blocks corresponding to the blocks of the range of $\mathcal{P}(\cdot)$. Therefore at most $1^2 + 2^2 + 1^2 - 1 = 5$ independent parameters of the matrix $\tilde{\rho} := X_1 \rho_0 X_1^*$ can be detected. Our goal in the following is to give an algorithm to obtain these 5 parameters. In particular, we shall give 4 unitary evolutions X_2, X_3, X_4, X_5 so that y_1, y_2, y_3, y_4 and y_5 calculated as in (51) are linearly independent functions of the parameters of $\tilde{\rho}$. Therefore we will have an algorithm to obtain the maximum number of parameters of $\tilde{\rho}$. We remark that this is a new result as compared to [4] because, in our case, we have a degenerate observable. Moreover, this algorithm can be performed in view of the results of the previous sections, since we have now a method to generate arbitrary evolutions X_1, X_2, X_3, X_4, X_5.

Finding the above evolutions $X_2, ..., X_5$ for linearly independent outputs is equivalent to finding evolutions $X_2, ..., X_5$ so that the matrices

$$S_1 := S_z^{TOT}, \quad S_2 := \mathcal{P}(X_2^* S_z^{TOT} X_2), \quad S_3 := \mathcal{P}(X_2^* \mathcal{P}(X_3^* S_z^{TOT} X_3) X_2),$$

$$S_4 := \mathcal{P}(X_2^* \mathcal{P}(X_3^* \mathcal{P}(X_4^* S_z^{TOT} X_4) X_3) X_2),$$

and

$$S_5 := \mathcal{P}(X_2^*\mathcal{P}(X_3^*\mathcal{P}(X_4^*\mathcal{P}(X_5^* S_z^{TOT} X_5)X_4)X_3)X_2)$$

span all of $\mathcal{P}(isu(4))$, where $isu(4)$ is the vector space of Hermitian matrices with zero trace. Equivalently, we must have that if $\Gamma \in \mathcal{P}(isu(4))$ is such that

$$Tr(\Gamma S_j) = 0, \quad j = 1, ..., 5, \tag{52}$$

then $\Gamma = 0$. Using elementary properties of the trace and the fact that $\mathcal{P}(\Gamma) = \Gamma$ we rewrite explicitly (52) as

$$Tr(\Gamma S_z^{TOT}) = 0, \tag{53}$$

$$Tr(X_2 \Gamma X_2^* S_z^{TOT}) = 0, \tag{54}$$

$$Tr(X_3 \mathcal{P}(X_2 \Gamma X_2^*) X_3^* S_z^{TOT}) = 0, \tag{55}$$

$$Tr(X_4 \mathcal{P}(X_3 \mathcal{P}(X_2 \Gamma X_2^*) X_3^*) X_4^* S_z^{TOT}) = 0, \tag{56}$$

$$Tr(X_5 \mathcal{P}(X_4 \mathcal{P}(X_3 \mathcal{P}(X_2 \Gamma X_2^*) X_3^*) X_4^*) X_5^* S_z^{TOT}) = 0. \tag{57}$$

$X_2, ..., X_5$ will be expressed in terms of elementary planar rotations $U_{kl}(\theta, \sigma)$ which have been defined at the beginning of Section 2 (see (10)). We choose, $X_2 := U_{12}(\frac{\pi}{4}, 0)$, $X_3 := U_{13}(\frac{\pi}{4}, 0)$, $X_4 := U_{12}(\frac{\pi}{4}, 0)U_{23}(\frac{\pi}{4}, \frac{\pi}{2})$ and $X_5 := U_{12}(\frac{\pi}{4}, 0)U_{23}(\frac{\pi}{4}, 0)$. With this choice, and denoting by γ_{jk} the $jk-$th element of the matrix Γ, the first three equations above, (53)-(55), become, respectively

$$\gamma_{11} - \gamma_{44} = 0, \tag{58}$$

$$\gamma_{11} + \gamma_{22} - 2\gamma_{44} = 0, \tag{59}$$

$$\gamma_{11} + \gamma_{22} + 2\gamma_{33} - 4\gamma_{44} = 0. \tag{60}$$

These, along with

$$\gamma_{11} + \gamma_{22} + \gamma_{33} + \gamma_{44} = 0, \tag{61}$$

imply

$$\gamma_{11} = \gamma_{22} = \gamma_{33} = \gamma_{44} = 0. \tag{62}$$

Using this and the fact that $\gamma_{32} = \gamma_{23}^*$, equation (56) becomes

$$Im(\gamma_{23}) = 0. \tag{63}$$

Using (63), equation (57) becomes

$$Re(\gamma_{23}) = 0. \tag{64}$$

5 Conclusions

Heisenberg spin systems frequently occur in electron paramagnetic resonance experiments, as models of molecular magnets as well as in other applications. In many cases the coupling between the two spins is strong and cannot be neglected in the design of control fields. This motivates control algorithms that constructively use the coupling to drive the system to a desired configuration. In this paper, we have presented an algorithm for the control of the unitary evolution operator for two coupled Heisenberg systems to an arbitrary configuration. In this algorithm, the control fields can be considered as perturbations and in fact arbitrarily bounded control fields can be used. We have shown how the capability of obtaining any desired evolution can be used to extract (maximum) information on the initial state of the system by a sequence of evolutions and Von Neumann measurements of the total magnetization.

Acknowledgment D. D'Alessandro would like to thank I. Mezić and U. Vaidya for helpful discussions on the topic of this paper.
D. D'Alessandro's research was supported by NSF Career Grant ECS-ECS0237925.
F. Albertini's research was partially supported by M.I.U.R., project "Viscosity, metric, and control theoretic methods for nonlinear partial differential equations."

References

[1] K. J. RAström and K. Furuta, Swinging up a pendulum by energy control, *Automatica* **36**, 2000, pp. 287-295.

[2] D. D'Alessandro, Algorithms for quantum control based on decompositions of Lie groups, in Proceedings 39-th Conference on Decision and Control, Sydney, Australia, Dec. 2000.

[3] D. D'Alessandro, Controllability of one spin and two interacting spins, *Mathematics of Control Signals and Systems*, Vol 16: 1-25, (2003)

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

[5] W. A. de Graaf, *Lie Algebras, Theory and Algorithms*, North Holland Mathematical Library, **56**, Amsterdam, 2000.

[6] R. R. Ernst, G. Bodenhausen and A. Wokaun, *Principles of Nuclear Magnetic Resonance in one and two dimensions*, Oxford Science Publications, New York 1987.

[7] G. M. Huang, T. J. Tarn and J. W. Clark, On the controllability of quantum mechanical systems, *J. Math. Phys.*, **24**, 11, November 1983, pg. 2608-2618.

[8] V. Jurdjević and H. J. Sussmann, Control systems on Lie groups, *Journal of Differential Equations*, **12**, 1972, 313-329.

[9] N. Khaneja, R. Brockett, S. J. Glaser, Time Optimal Control of Spin Systems, *Physical Review A*, **63**, 2001, 032308.

[10] U. Leonhardt, *Measuring the Quantum State of Light*, Cambridge University Press, New York, 1997.

[11] F. D. Murnaghan, *The Orthogonal and Symplectic Groups*, Communications of the Dublin Institute for Advanced Studies. Series A, No. 13.

[12] V. Ramakrishna, R. J. Ober, K. L. Flores and H. Rabitz, Control of a coupled two spin system without hard pulses, Phys. Rev. A 65, 063405 (2002), http://arXiv, quant-ph 0012019.

[13] K. N. S. Rao, *Linear Algebra and Group Theory for Physicists*, New Age International, New Delhi, 1996.

[14] A. Raymond, Electron Paramagnetic Resonance; Techniques and Applications, *Interscience Publishers*, New York 1968

[15] 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.

[16] U. Vaidya, D. D'Alessandro and I. Mezić, Control of Heisenberg spin systems; Lie algebraic decompositions and action-angle variables, Proceedings. 42nd IEEE Conference on Decsion and Control, Volume: 4 , 9-12 Dec. 2003 Pages:4174 - 4178.