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Controllability of Symmetric Spin Networks

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We consider a network of n spin $\frac{1}{2}$ systems which are pairwise interacting via Ising interaction and are controlled by the same electro-magnetic control field. Such a system presents symmetries since the Hamiltonian is unchanged if we permute two spins. This prevents full (operator) controllability, in that not every unitary evolution can be obtained. We prove however that controllability is verified if we restrict ourselves to unitary evolutions which preserve the above permutation invariance. For low dimensional cases, $n = 2$ and $n = 3$, we provide an analysis of the Lie group of available evolutions and give explicit control laws to transfer between two arbitrary permutation invariant states. This class of states includes highly entangled states such as GHZ states and W states, which are of interest in quantum information.

Keywords: Controllability of Spin Networks, Permutation Invariant States, Lie Algebraic Methods in Quantum Control.

I. INTRODUCTION

The *controllability* of a control system describes the set of states which can be reached for that system by opportunely changing the external controls. For finite dimensional quantum systems, controllability is usually assessed by calculating the Lie algebra generated by the Hamiltonians of the system [2]. Such a Lie algebra is called the *dynamical Lie algebra*. If the dynamical Lie algebra of a system of dimension d is the full Lie algebra $u(d)$ ($su(d)$) of $d \oplus d$ skew-Hermitian matrices (with zero trace) then the set of available evolutions is the full Lie group of $d \oplus d$ unitary matrices $U(d)$ (with determinant equal to 1, $SU(d)$) and the system is said to be *operator controllable* (the term 'completely controllable' is also used to denote this situation [7]). More in general the set of the available evolutions is dense in the Lie group associated with the dynamical Lie algebra and it is equal to such a Lie group in the case where such a Lie group is compact. Although controllability is the generic situation [14], often in reality symmetries in the system's dynamics restrict the type of available evolutions. In this paper, we analyze one of these situations for a system of interest in the implementation of quantum information processing and the generation of entangled states.

We consider a network of $n \to 2$ spins controlled in parallel by an electromagnetic field. Such a system was also considered in [1] and allows one to perform quantum information processing and generate entangled states without the need to address the spins individually. A common control field is used to control all spins *simultaneously*. The Hamiltonian (cf. (6) below) is symmetric in the sense that is invariant under permutation. As a consequence, starting from the ground state where all the spin are in state $|0\rangle$ the possible states of the spin network will also be permutation invariant. Examples of such states are the GHZ states introduced in [8]

$$|GHZ\rangle := \frac{1}{\sqrt{2}}(|00\cdots0\rangle + |11\cdots1\rangle), \tag{1}$$

and the W states

$$|W\rangle := \frac{1}{\sqrt{n}}(|100\cdots0\rangle + |010\cdots0\rangle + |001\cdots0\rangle + \cdots + |000\cdots1\rangle), \tag{2}$$

considered in [6]. We do not restrict ourselves to transfer to or from these states as in [1] but consider the control problem on the full subspace of permutation invariant states. A basis for such a subspace is given by the $n+1$ orthonormal states, for $m = 0, 1, ..., n$,

$$|\phi_m\rangle = \frac{1}{\sqrt{\binom{n}{m}}} \sum_k |k\rangle. \tag{3}$$

In formula (3), for each m the sum runs for all the elements in the computational basis which have m 1's and $n - m$ 0's. For instance, $|GHZ\rangle$ in (1) corresponds to $\frac{1}{\sqrt{2}}(|\phi_0\rangle + |\phi_n\rangle)$, while $|W\rangle$ in (2) corresponds to $|\phi_1\rangle$.

We **present the following results:**

1. We prove the controllability of the system in the sense that the dynamical Lie algebra $\mathcal{P}$ is the full Lie subalgebra of $u(2^n)$ consisting of matrices which have zero trace and are permutation invariant. The corresponding Lie group is compact and therefore the set of possible available evolutions is equal to such a Lie group $e^{\mathcal{L}}$ (Theorem 2).

For the cases $n = 2$ and $n = 3$ spins:

2. We explicitly describe the dynamical Lie algebra $\mathcal{P}$ which is the direct sum of $u(1)$ with $u(3)$ inside $su(2^2)$ for the case $n = 2$. It is the direct sum of two copies of $u(2)$ plus $u(4)$ inside $su(2^3)$ for the case $n = 3$. From this, a parametrization of the Lie group of the available evolutions is obtained and controllability between any two permutation invariant pure states is proved. Results are summarized in Theorem 3 and 4 for the cases $n = 2$ and $n = 3$, respectively.

3. We use the above parametrization of the Lie group of available evolutions and Lie group decomposition techniques to provide explicit control algorithms to transfer between any two permutation invariant states (Section IV).

A. Definitions and elementary properties

The Pauli matrices $\sigma_{x,y,z}$ are defined as

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4}$$

Let $\mathbf{1}$ be the two dimensional identity matrix, the Pauli matrices satisfy

$$\begin{array}{ccc} \sigma_x\sigma_x = \sigma_y\sigma_y = \sigma_z\sigma_z = \mathbf{1}, & & \\ \sigma_x\sigma_y = i\sigma_z, & \sigma_y\sigma_z = i\sigma_x, & \sigma_z\sigma_x = i\sigma_y \\ \sigma_y\sigma_x = i\sigma_z, & \sigma_z\sigma_y = i\sigma_x, & \sigma_x\sigma_z = i\sigma_y \end{array} \tag{5}$$

The quantum system we study in this paper is the *symmetric Ising spin network* under the control of a common electromagnetic field which was also considered in [1]. The corresponding, time varying controlled Hamiltonian, for $n \to 2$ spin $\frac{1}{2}$ particles is defined as:

$$H(t) = H_{zz} + H_x u_x(t) + H_y u_y(t), \tag{6}$$

where

$$\begin{aligned} H_{zz} &= \textstyle\prod_{1\le k<m\le n} \mathbf{1} \bullet \cdots \bullet \underbrace{\sigma_z}_{k^{th}} \bullet \mathbf{1} \bullet \cdots \bullet \underbrace{\sigma_z}_{m^{th}} \bullet \mathbf{1} \bullet \cdots \bullet \mathbf{1}, \\ H_x &= \textstyle\prod_{k=1}^{n} \mathbf{1} \bullet \cdots \bullet \underbrace{\sigma_x}_{k^{th}} \bullet \mathbf{1} \bullet \cdots \bullet \mathbf{1}, \\ H_y &= \textstyle\prod_{k=1}^{n} \mathbf{1} \bullet \cdots \bullet \underbrace{\sigma_y}_{k^{th}} \bullet \mathbf{1} \bullet \cdots \bullet \mathbf{1}. \end{aligned} \tag{7}$$

Here u_x and u_y represent the x and y components of a control electromagnetic field. H_{zz} is the *interaction Hamiltonian* which is the sum of $\binom{n}{2}$ Ising interactions between all pairs of spins. The Hamiltonians H_x, H_y model the interaction of the spins with the external control field.

It is clear that the given Hamiltonian is invariant under a permutation of the spins. We next define the Lie subalgebra of $u(2^n)$ of matrices which are permutation invariant. The $4 \oplus 4$ matrix

$$\Pi := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{8}$$

is such that for any two, $2 \oplus 2$ matrices, σ_1 and σ_2

$$\Pi\, \sigma_1 \bullet \sigma_2\, \Pi = \sigma_2 \bullet \sigma_1. \tag{9}$$

The n 1 matrices $\Pi_{j,j+1}$, $j = 1, ..., n$ 1, defined as

$$\Pi_{j,j+1} := \mathbf{1}^{\otimes j-1} \bullet \Pi \bullet \mathbf{1}^{\otimes n-j-1}, \tag{10}$$

generate the whole group of permutations in the sense that every permutation of the n factors in a tensor product can be obtained by multiplications of such matrices. Therefore the Lie subalgebra of $u(2^n)$ of matrices which are permutation invariant can be described as

$$\mathcal{P}^{PI} := \}A \ / \ u(2^n) \ \sqrt{\Pi_{j,j+1} A \Pi_{j,j+1}, \ j = 1, \dots n \quad 1\rangle}. \tag{11}$$

Since $\Pi^2 = \mathbf{1} \bullet \mathbf{1}$, we have that $\Pi^2_{j,j+1} = \mathbf{1}^{\otimes n}$, for every $j = 1, 1, ..., n$ 1. From this it follows that if general $2^n \oplus 2^n$ skew-Hermitian matrices A and B are such $\Pi_{j,j+1} A \Pi_{j,j+1} = A$ and $\Pi_{j,j+1} B \Pi_{j,j+1} = B$, AB is also such that $\Pi_{j,j+1} AB \Pi_{j,j+1} = \Pi_{j,j+1} A \Pi^2_{j,j+1} B \Pi_{j,j+1} = AB$. This confirms that $\mathcal{P}^{PI}$ is a Lie subalgebra of $u(2^n)$, since it is closed under commutation (it is, in fact, closed under matrix product).

II. CONTROLLABILITY

Applying general results on the controllability of systems on Lie groups [11] and quantum systems (see, e.g., [2], [10], [15]) the study of the controllability of system (6) will be carried out by evaluating the dynamical Lie algebra $\mathcal{P}$ in $u(2^n)$ generated by the matrices $\}iH_{zz}, iH_x, iH_y\rangle$ in (6). It is known that the set of reachable evolutions is dense in the Lie group, $e^{\mathcal{L}}$, associated with the dynamical Lie algebra $\mathcal{P}$ and coincides with such a Lie group if this Lie group is compact. The following result characterizes the dynamical Lie algebra for system (6). It shows that, except for the fact that the matrices corresponding to H_{zz}, H_x and H_y in (7) have zero trace, the dynamical Lie algebra is the full Lie algebra of permutation invariant skew-Hermitian matrices in $u(2^n)$.

Theorem 1. *(Dynamical Lie Algebra) The dynamical Lie algebra $\mathcal{P}$ associated with system (6) coincides with the space of all permutation invariant matrices in $su(2^n)$, i.e., with $\mathcal{P}^{PI}$ in (11),*

$$\mathcal{P} = \mathcal{P}^{PI} \ \lfloor \ su(2^n). \tag{12}$$

The set of possible evolutions for the system (6) (7) is described in the following theorem.

Theorem 2. *(Controllability) The set of possible evolutions for the system characterized by the Hamiltonian (6) is the connected Lie group corresponding to the Lie algebra $\mathcal{P}^{PI} \ \lfloor \ su(2^n)$.*

Proof. From the above recalled general results on the controllability of right invariant systems on Lie groups [11] and quantum mechanical systems [2], [10], [15], the reachable set is the connected Lie group (containing the identity) associated with the dynamical Lie algebra, under the assumption that such a Lie group is compact. In our case, $e^{\mathcal{L}^{PI}}$ is compact (which is proved in Remark III.3 below) and $SU(2^n)$ is also compact, so that

$$e^{\mathcal{L}^{PI} \cap su(2^n)} = e^{\mathcal{L}^{PI}} \ \lfloor \ SU(2^n),$$

is also compact. Therefore, applying such known results, the set of available evolutions is exactly equal to the Lie group, $e^{\mathcal{L}^{PI} \cap su(2^n)}$, i.e., the connected Lie group associated with $\mathcal{P}^{PI} \ \lfloor \ su(2^n)$. □

We now calculate the **dimension** of the Lie algebra $\mathcal{P}$ in (12). To do this we first introduce some notations. Let $\sigma_0 := \mathbf{1}$. For an n ple $\underline{l} := (l_1, l_2, ..., l_n)$ of elements in the set $\}0, x, y, z\rangle$, we denote by

$$\sigma_{\underline{l}} := \sigma_{l_1} \bullet \times\times\bullet \ \sigma_{l_n}. \tag{13}$$

Consider a matrix X of the type $X = i \prod_{\underline{l}} \alpha_{\underline{l}} \sigma_{\underline{l}} \ / \ su(2^n)$, where the sum is taken among the 4^n possible n ples in $\}0, x, y, z\rangle$, with coefficients $\alpha_{\underline{l}}$. For any permutation π we let $X^\pi = i \prod_{\underline{l}} \alpha_{\underline{l}} \sigma_{\pi(\underline{l})}$. Thus X is permutation invariant, i.e. $X \ / \ \mathcal{P}^{PI}$ (see equation (11)), if and only if $X = X^\pi$ for all permutations $\pi \ / \ S_n$, where S_n denotes the symmetric group of degree n. For a triple (k_x, k_y, k_z) indicating the numbers of $\}x, y, z\rangle$ symbols, we denote by $\Phi(k_x, k_y, k_z)$ the set of n-ples with k_x, $x's$, k_y, $y's$, and k_z, $z's$. We let, with definition (13),

$$X^n_{(k_x,k_y,k_z)} = i \prod_{\underline{l} \in \Phi(k_x,k_y,k_z)} \sigma_{\underline{l}}.$$

Then $X^n_{(k_x,k_y,k_z)}$ is a permutation invariant matrix, and any permutation invariant matrix can be written as a linear combination of matrices of the type $X^n_{(k_x,k_y,k_z)}$. With these notations, in particular we have:

$$iH_{zz} = X^n_{(0,0,2)}, \quad iH_x = X^n_{(1,0,0)}, \quad iH_y = X^n_{(0,1,0)}. \tag{14}$$

We first calculate the dimension of the Lie algebra $\mathcal{P}^{PI}$ in (11). Elements forming a basis for the Lie algebra $\mathcal{P}^{PI}$ in (11) are in one to one correspondence with triple (k_x, k_y, k_z). Therefore, the dimension of $\mathcal{P}^{PI}$ is given by all the ways to choose the triples (k_x, k_y, k_z), with $0 \geq k_x + k_y + k_z \geq n$.

Now, given $0 \geq k \geq n$, we have $\frac{(k+1)(k+2)}{2}$ ways of choosing (k_x, k_y, k_z), with $k = k_x + k_y + k_z$. In fact, k_x can be chosen in $k+1$ ways, then k_y can be chosen in $k+1 \quad k_x$ ways, while $k_z = k \quad (k_x + k_y)$ is now fixed. Thus by varying k_x, from 0 to k, we have that the total ways are:

$$\prod_{k_x=0}^{k} (k+1 \quad k_x) = \prod_{l=1}^{k+1} l = \frac{(k+1)(k+2)}{2}.$$

The dimension of the Lie algebra $\mathcal{P}^{PI}$ in (11) is obtained by summing the above numbers as $k = 0, 1, ..., n$. We have

$$\dim \mathcal{P}^{PI} = \prod_{k=0}^{n} \frac{(k+1)(k+2)}{2} = \frac{1}{2}\prod_{k=0}^{n} (k+1)(k+2) = \frac{1}{2}\frac{(n+3)(n+2)(n+1)}{3} := \binom{n+3}{n}. \tag{15}$$

where the third equality is proved by induction on n.

Therefore, the dimension of the Lie algebra $\mathcal{P}$ in (12) is $\binom{n+3}{n} - 1$.

A. Proof of Theorem 1

The dynamical Lie algebra $\mathcal{P}$ is generated by iH_{zz}, iH_x, and iH_y and since iH_{zz}, iH_x, and iH_y belong to $\mathcal{P}^{PI} \lfloor su(2^n)$, $\mathcal{P} \leq \mathcal{P}^{PI} \lfloor su(2^n)$. To prove Theorem 1 we need to establish also the converse inclusion, i.e. $\mathcal{P}^{PI} \lfloor su(2^n) \leq \mathcal{P}$. To get this inclusion, we will prove that,

$$\mathcal{A}(k_x, k_y, k_z) \text{ such that } 1 \geq k_k + k_y + k_z \geq n,\ X^n_{(k_x,k_y,k_z)} \ / \mathcal{P}. \tag{16}$$

We will prove equation (16) by induction on $\bar{k} = k_x + k_y + k_z$ $(1 \geq \bar{k} \geq n)$. We will derive equation (16) for $\bar{k} = 1$, 2 first and then will prove the inductive step.

$\subseteq \bar{k} = 1$.

For $\bar{k} = 1$ there are only three possible triples (k_x, k_y, k_z), with $k_x + k_y + k_z = \bar{k}$. $X^n_{(1,0,0)}$ and $X^n_{(0,1,0)}$ are already in $\mathcal{P}$ because of (14). Moreover a direct calculation gives

$$[X^n_{(1,0,0)}, X^n_{(0,1,0)}] = 2X^n_{(0,0,1)}.$$

In fact

$$[X^n_{(1,0,0)}, X^n_{(0,1,0)}] = \prod_{i,j=1}^{n} [\mathbf{1} \bullet \cdots \mathbf{1} \bullet \underbrace{\sigma_x}_{i^{th}} \bullet \mathbf{1} \bullet \cdots \mathbf{1}, \mathbf{1} \bullet \cdots \mathbf{1} \bullet \underbrace{\sigma_y}_{j^{th}} \bullet \mathbf{1} \bullet \cdots \mathbf{1}] =$$

$$= 2i \prod_{i}^{n} \mathbf{1} \bullet \cdots \mathbf{1} \bullet \underbrace{\sigma_z}_{i^{th}} \bullet \mathbf{1} \bullet \cdots \mathbf{1},$$

since we have that, if $i \neq j$ then the two matrices commute, and if $i = j$ then $[\sigma_x, \sigma_y] = \quad 2i\sigma_z$.

$\subseteq \bar{k} = 2$.

For $\bar{k} = 2$ there are only 6 possible triples (k_x, k_y, k_z) with $k_x + k_y + k_z = \bar{k}$. $X^n_{(0,0,2)}$ is already in $\mathcal{P}$ because of (14). Moreover, we calculate

$$\begin{array}{rcl} [X^n_{(1,0,0)}, X^n_{(0,0,2)}] & = & 2X^n_{(0,1,1)} \\ [X^n_{(0,1,0)}, X^n_{(0,0,2)}] & = & 2X^n_{(1,0,1)} \end{array} \tag{17}$$

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Let us give details on the first equation. The second one is similar. First we notice that:

$$[\mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_x}_{i^{th}}\bullet\mathbf{1}\bullet\cdots\mathbf{1},\ \mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_z}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_z}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1}]=$$

$$=\begin{cases}0 & \text{if } i\neq j \text{ and } i\neq l\\ 2i\ \mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_y}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_z}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1} & \text{if } i=j\\ 2i\ \mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_z}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_y}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1} & \text{if } i=l\end{cases} \tag{18}$$

Thus:

$$[X^n_{(1,0,0)},X^n_{(0,0,2)}]=\prod_{\substack{i,j,l=1\\ j<l}}^{n}[\mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_x}_{i^{th}}\bullet\mathbf{1}\bullet\cdots\mathbf{1},\ \mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_z}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_z}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1}]=$$

$$=\left(\prod_{\substack{j,l=1\\ j<l}}^{n}2i\right)\mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_y}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_z}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1}+\mathbf{1}\bullet\cdots\mathbf{1}\bullet\underbrace{\sigma_z}_{j^{th}}\bullet\cdots\bullet\underbrace{\sigma_y}_{l^{th}}\bullet\cdots\mathbf{1}\bullet\cdots\mathbf{1}\Big]=$$

$$=2X^n_{(0,1,1)}.$$

This shows that $X^n_{(0,1,1)}$ and $X^n_{(1,0,1)}$ are in $\mathcal{P}$. Moreover we have, with similar calculations (cf. Appendix A),

$$\begin{aligned}[X^n_{(0,1,1)},X^n_{(1,0,0)}] &= 4X^n_{(0,2,0)}\quad 4X^n_{(0,0,2)}\\ [X^n_{(1,0,1)},X^n_{(0,1,0)}] &= 4X^n_{(2,0,0)}+4X^n_{(0,0,2)},\end{aligned} \tag{19}$$

and therefore $X^n_{(0,2,0)}$, and $X^n_{(2,0,0)}$ are also in $\mathcal{P}$. Finally, using a similar argument as the one used to prove (17), we have,

$$[X^n_{(0,0,1)},X^n_{(2,0,0)}]=2\,X^n_{(1,1,0)}. \tag{20}$$

Therefore all the basis matrices corresponding to $\bar{k}=2$ are in $\mathcal{P}$.

⊆ By exchanging the roles of x, y and z, we can see the following:

Fact: Assume that $X^n_{(k_x,k_y,k_z)}\ /\ \mathcal{P}$ for all triples (k_x,k_y,k_z), with $k_x+k_y+k_z\geq\hat{k}$ and that $X^n_{(\tilde{k}_x,\tilde{k}_y,\tilde{k}_z)}$, with $\tilde{k}_x+\tilde{k}_x+\tilde{k}_x>\hat{k}$ is obtained as a Lie bracket of elements $X^n_{(k_x,k_y,k_z)}$ with $k_x+k_y+k_z\geq\hat{k}$, and therefore is in $\mathcal{P}$. Then, every $X^n_{(\hat{k}_x,\hat{k}_y,\hat{k}_z)}$ is also in $\mathcal{P}$, where $(\hat{k}_x,\hat{k}_y,\hat{k}_z)$ is any permutation of $(\tilde{k}_x,\tilde{k}_y,\tilde{k}_z)$.

⊆ Inductive step: Let $2\geq\bar{k}\quad 1<n$ and assume that all possible $X^n_{(k_x,k_y,k_z)}\ /\ \mathcal{P}$ for $1\geq k_x+k_y+k_z\geq\bar{k}\quad 1$. Then also all $X^n_{(k_x,k_y,k_z)}\ /\ \mathcal{P}$ with $k_x+k_y+k_z=\bar{k}$.

Proof. By the symmetry property of the above **Fact**, it is enough to prove that, using Lie bracket of elements $X^n_{(k_x,k_y,k_z)}\ /\ \mathcal{P}$ with $1\geq k_x+k_y+k_z\geq\bar{k}\quad 1$, we can obtain all $X^n_{(k_x,k_y,k_z)}$ for $k_x+k_y+k_z=\bar{k}$ *with the restriction that* $k_z\geq k_y\geq k_x$. Such a restriction does not imply a loss of generality.

We set $k_x=\bar{k}\quad j$ and will prove this fact by induction on j. The possible range of values for j is $0\geq j\geq\lfloor\frac{2\bar{k}}{3}\{$ (here, for any $x\ /\ \mathbf{R}$, $\lfloor x\{$ denotes its integer part). In fact, if $j=\lfloor\frac{2\bar{k}}{3}\{+1$, then in particular $j>\frac{2\bar{k}}{3}$, thus $k_x=\bar{k}\quad j<\bar{k}\quad\frac{2\bar{k}}{3}=\frac{\bar{k}}{3}$, so also $k_x+k_y+k_z\geq 3k_x<\bar{k}$. On the other hand if $j=\lfloor\frac{2\bar{k}}{3}\{$, then $k_x=\bar{k}\quad j\rightarrow\frac{\bar{k}}{3}$, thus $3k_x\rightarrow\bar{k}$, so there exists a triple $(\bar{k}\quad j,k_y,k_z)$, with $\bar{k}\quad j+k_y+k_z=\bar{k}$ and $k_z\geq k_y\geq\bar{k}\quad j$

Base step: $j = 0$ ($k_x = \bar{k}$).

To get this base step, $j = 0$, we will prove also the cases $j = 1$ and $j = 2$. It holds that:

$$[X^n_{(\bar{k}-1,0,0)}, X^n_{(1,1,0)}] = 2X^n_{(\bar{k}-1,0,1)} + 2X^n_{(\bar{k}-2,0,1)}. \tag{21}$$

To see this, assume we have an n ple $\underline{i}$ which has $\bar{k}$ 1 elements equal to x and all the other equal to 0 and an n ple $\underline{j}$ with one element $j_x = x$ one $j_y = y$ and all the other equal to 0. Denote by A the set of indexes such that $i_l = x$. We have:

$$[\sigma_{\underline{i}}, \sigma_{\underline{j}}] = \begin{cases} 0 & \text{if } j_y \forall A \\ 2i\sigma_{l_1} \bullet \cdots \bullet \sigma_{l_n} & \text{if } j_x \not\in A \text{ and } j_y \not\in A \\ 2i\sigma_{s_1} \bullet \cdots \bullet \sigma_{s_n} & \text{if } j_x \forall A \text{ and } j_y \not\in A \end{cases}, \tag{22}$$

where the n ple $\underline{l} = (l_1, \ldots, l_n)$ has $\bar{k}$ 2 indexes equal to x and one equal to z, while the n ple $\underline{s} = (s_1, \ldots, s_n)$ has $\bar{k}$ 1 indexes equal to x and one equal to z. Since $[X^n_{(\bar{k}-1,0,0)}, X^n_{(1,1,0)}]$ is a permutation invariant matrix, and $X^n_{(\bar{k}-1,0,0)}$ is a sum of all elements of the type $\sigma_{\underline{i}}$, while $X^n_{(1,1,0)}$ is a sum of all elements of the type $\sigma_{\underline{j}}$, from (22), equation (21) follows.

From equation (21) since $X^n_{(\bar{k}-2,0,1)}$ is in $\mathcal{P}$, we have that $X^n_{(\bar{k}-1,0,1)} \not\in \mathcal{P}$. By the symmetry property of the above **Fact** we also have $X^n_{(\bar{k}-1,1,0)} \not\in \mathcal{P}$. The next two equations can be proved by direct calculation:

$$[X^n_{(\bar{k}-1,1,0)}, X^n_{(0,0,1)}] = 2X^n_{(\bar{k}-2,2,0)} + 2X^n_{(\bar{k},0,0)}. \tag{23}$$

$$[X^n_{(\bar{k}-1,0,1)}, X^n_{(0,1,0)}] = 2X^n_{(\bar{k}-2,0,2)} \quad 2X^n_{(\bar{k},0,0)}. \tag{24}$$

We now compute $[X^n_{(\bar{k}-2,1,0)}, X^n_{(1,0,1)}]$ with an argument similar to the one used to derive equation (21). Assume we have an n ple $\underline{i}$ which has $\bar{k}$ 2 elements equal to x, one element $i_y = y$, and all the others equal to 0, and an n ple $\underline{j}$ with one element $j_x = x$ one $j_z = z$ and all the others equal to 0. Denote by A the set of indexes such that $i_l = x$. We have:

$$[\sigma_{\underline{i}}, \sigma_{\underline{j}}] = \begin{cases} 0 & \begin{array}{l} j_x \forall A \cap \{i_y\rangle \text{ and } j_z \not\forall A \cap \{i_y\rangle \text{ or} \\ \text{if } j_x \not\in A \text{ and } j_z \forall A \cap \{i_y\rangle \text{ or} \\ j_x = i_y \text{ and } j_z \not\in A \end{array} \\ 2i\sigma_{l_1} \bullet \cdots \bullet \sigma_{l_n} & \text{if } j_x \forall A \cap \{i_y\rangle \text{ and } j_z = i_y \\ 2i\sigma_{s_1} \bullet \cdots \bullet \sigma_{s_n} & \text{if } j_x \forall A \cap \{i_y\rangle \text{ and } j_z \not\in A \\ 2i\sigma_{m_1} \bullet \cdots \bullet \sigma_{m_n} & \text{if } j_x \not\in A \text{ and } j_z \not\in A \\ 2i\sigma_{q_1} \bullet \cdots \bullet \sigma_{q_n} & \text{if } j_x \not\in A \text{ and } j_z = i_y \\ 2i\sigma_{r_1} \bullet \cdots \bullet \sigma_{r_n} & \text{if } j_x = i_y \text{ and } j_z \forall A \cap \{i_y\rangle. \end{cases} \tag{25}$$

Here the n ple $\underline{l} = (l_1, \ldots, l_n)$ has $\bar{k}$ indexes equal to x, the n-ple $\underline{s} = (s_1, \ldots, s_n)$ has $\bar{k}$ 2 indexes equal to x and two equal to y, the n ple $\underline{m} = (m_1, \ldots, m_n)$ has $\bar{k}$ 3 indexes equal to x and two equal to y, the n-ple $\underline{q} = (q_1, \ldots, q_n)$ has $\bar{k}$ 2 indexes equal to x, and the n-ple $\underline{r} = (r_1, \ldots, r_n)$ has $\bar{k}$ 2 indexes equal to x and two equal to z. Since $X^n_{(\bar{k}-2,1,0)}$ is a sum of all elements of the type $\sigma_{\underline{i}}$, while $X^n_{(1,0,1)}$ is a sum of all elements of the type $\sigma_{\underline{j}}$, from (25), we have:

$$[X^n_{(\bar{k}-2,1,0)}, X^n_{(1,0,1)}] = 2X^n_{(\bar{k}-3,2,0)} + 2X^n_{(\bar{k}-2,0,0)} \quad 2X^n_{(\bar{k}-2,2,0)} \quad 2X^n_{(\bar{k}-2,0,2)} + 2X^n_{(\bar{k},0,0)}. \tag{26}$$

Since $X^n_{(\bar{k}-3,2,0)}$ and $X^n_{(\bar{k}-2,0,0)}$ are in $\mathcal{P}$, putting together equations (23), (24), and (26), we get that

$$X^n_{(\bar{k},0,0)}, X^n_{(\bar{k}-2,2,0)}, X^n_{(\bar{k}-2,0,2)} \not\in \mathcal{P}^n.$$

So, in particular, we have proven that $\mathcal{P}$ contains all $X^n_{(\bar{k},0,0)}$, which is the base step, $j = 0$.

Induction step: Assume we have in $\mathcal{P}$ all $X^n_{(k_x,k_y,k_z)}$ with $k_x + k_y + k_z = \bar{k}$ and $k_x = \bar{k}$ (j 1), we want to show that we also have all $X^n_{(k_x,k_y,k_z)}$ with $k_x = \bar{k}$ j.

Fix a triple $k_x + k_y + k_z = \bar{k}$, with $k_x = \bar{k}$ j. Certainly k_y or k_z is different from 0.

Assume $k_z \neq 0$, consider the triple $(\bar{k}-(j-1), k_y, k_z-1)$. We have that the sum of the three elements is $\bar{k}$, and also $\bar{k}-(j-1)+k_y+k_z-1$, thus, by the inductive assumption $X^n_{(\bar{k}-(j-1),k_y,k_z-1)} \in \mathcal{P}$. We have:

$$[X^n_{(\bar{k}-(j-1),k_y,k_z-1)}, X^n_{(0,1,0)}] = 2X^n_{(\bar{k}-j,k_y,k_z)} - 2X^n_{(\bar{k}-j+2,k_y,k_z-2)}.$$

Since the second element is in $\mathcal{P}$ by the inductive assumption, we have that $X^n_{(\bar{k}-j,k_y,k_z)} \in \mathcal{P}$.

If $k_z = 0$, the triple is $(\bar{k}-j, j, 0)$. We compute:

$$[X^n_{(\bar{k}-(j-1),j-1,0)}, X^n_{(0,0,1)}] = -2X^n_{(\bar{k}-j,j,0)} - 2X^n_{(\bar{k}-j+2,j-2,0)}.$$

Again we can conclude, since the second element on the right hand side is in $\mathcal{P}$. □

III. DYNAMICAL LIE ALGEBRA ANALYSIS FOR $n = 2$ AND $n = 3$

A. Case $n = 2$ and generalizations

The symmetric (permutation invariant) vectors $|\phi_0\rangle$, $|\phi_1\rangle$, and $|\phi_2\rangle$, defined in (3) are an orthonormal basis of the $+1$ eigenspace of Π in (8) while the unit (antisymmetric) vector

$$|\psi_0\rangle := \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle), \tag{27}$$

span the, 1-dimensional, -1 eigenspace of Π. Writing the corresponding change of basis matrix in the computational basis, we obtain, with $a := \frac{1}{\sqrt{2}}$,

$$T^\dagger := [|\psi_0\rangle, |\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle] := \begin{pmatrix} 0 & 1 & 0 & 0 \\ a & 0 & a & 0 \\ a & 0 & -a & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{28}$$

We shall use the notation $\mathbf{1}_{j,k}$ for $diag(\underbrace{-1, \ldots, -1}_{j}, \underbrace{1, 1, \ldots, 1}_{k})$ with j '-1's and k '1's. We have, with Π in (8), $T\Pi T^\dagger = diag(-1, -1, 1, 1) = \mathbf{1}_{1,3}$. Therefore a matrix $A \in u(4)$ is in $\mathcal{P}^{PI}$ defined in (11) if and only if

$$T\Pi T^\dagger (TAT^\dagger) T\Pi T^\dagger = \mathbf{1}_{1,3}(TAT^\dagger)\mathbf{1}_{1,3} = TAT^\dagger,$$

that is, if and only if $\tilde{A} := TAT^\dagger$ commutes with $\mathbf{1}_{1,3}$. This happens if and only if $\tilde{A}$ has a block diagonal form with blocks of dimension 1 and 3. This proves that $\mathcal{P}^{PI}$ is included in $u(1) \otimes u(3)$ in this case, where the sum is a direct sum of Lie algebras (the two addenda commute). Using the dimension formula (15) for $n = 2$ we see that we must have equality. The corresponding Lie group is the direct product of $U(1)$ and $U(3)$, a compact Lie group.

Remark III.1. A different way to arrive at the change of coordinates T in (28), which will then be generalized to the case $n = 3$ is to notice that $|\phi_0\rangle$, $|\phi_1\rangle$ and $|\phi_2\rangle$ span an invariant subspace for the generators H_{zz}, H_x and H_y of the Lie algebra $\mathcal{P}^{PI}$ and therefore for the whole Lie algebra. The same thing is true for the subspace spanned by $|\psi_0\rangle$. Therefore, in the basis given by the matrix T in (28), the elements of $\mathcal{P}^{PI}$ are in the $1 + 3$ block diagonal form.

Remark III.2. The result on the structure of $\mathcal{P}^{PI}$ can be generalized in at least two ways to the case of any number $n > 2$ of spins. In particular, assume we have n spins and we are interested in the superalgebra of $\mathcal{P}^{PI}$ of matrices invariant under permutation of two of the spins, which we can assume without loss of generality to be the first two. That is, we are interested in the superalgebra of $\mathcal{P}^{PI}$

$$\mathcal{P}^{PI12} := \{A \in u(2^n) \mid \Pi_{1,2} A \Pi_{1,2}\}. \tag{29}$$

Using the change of coordinates $T \bullet \mathbf{1}_{2^{n-2}}$, we have that $T \bullet \mathbf{1}_{2^{n-2}} \Pi_{1,2} T^\dagger \bullet \mathbf{1}_{2^{n-2}} = \mathbf{1}_{2^{n-2},3\times 2^{n-2}}$ so that, analogously to above, modulo a change of coordinates, the matrices in $\mathcal{P}^{PI12}$ are all the matrices in $u(2^n)$ which are block diagonal with blocks of dimension 2^{n-2} and $3 \oplus 2^{n-2}$. Therefore $\mathcal{P}^{PI12} = u(2^{n-2}) \otimes u(3 \oplus 2^{n-2})$ and the corresponding Lie group is the direct product of $U(2^{n-2})$ and $U(3 \oplus 2^{n-2})$, again a compact Lie group.

Assume now n even, and consider the superalgebra of $\mathcal{P}^{PI}$

$$\mathcal{P}^e := \{A \in u(2^n) \mid \Pi \bullet \Pi \bullet \cdots \bullet \Pi A \Pi \bullet \Pi \bullet \cdots \bullet \Pi = A\}. \tag{30}$$

Using the change of coordinates $A \in T \bullet T \bullet \times\times\times \bullet TAT^\dagger \bullet T^\dagger \bullet \times\times\times \bullet T^\dagger$, we see that, in the new coordinates, the matrices in $\mathcal{P}^e$ are tensor products of block diagonal $4 \oplus 4$ matrices with one block of dimension 1 and one block of dimension 3. Thus, the Lie algebra $\mathcal{P}^e$ is spanned by all the matrices in $i\left[iu(1) \otimes iu(3)\right]^{\otimes \frac{n}{2}}$. Using the fact that $iu(j) \bullet iu(k) = iu(jk)$, we see that

$$\mathcal{P}^e = \otimes_{j=0}^{\frac{n}{2}} \left(\begin{matrix} \frac{n}{2} \\ j \end{matrix} \right) iu(3^j), \tag{31}$$

where for a positive integer k, we have denoted by $ku(\times)$ the direct sum of k copies of $u(\times)$.

Remark III.3. The Lie algebra $\mathcal{P}^{PI}$ is the intersection of all the Lie algebras $\mathcal{P}^{PIjk}$ defined analogously to $\mathcal{P}^{PI12}$ in (29). All these Lie algebras are conjugate (and therefore isomorphic) to $\mathcal{P}^{PI12}$. Therefore the corresponding Lie group $e^{\mathcal{L}^{PI}}$ is the intersection of the compact Lie groups $e^{\mathcal{L}^{PIjk}}$ and therefore compact.

Applying the change of coordinates T in (28) to the basis $\{ \phi_0|, \phi_1|, \phi_2| \rangle$, we obtain the basis

$$\tilde{\phi}_0| := T \phi_0| = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \tilde{\phi}_1| := T \phi_1| = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \tilde{\phi}_2| := T \phi_2| = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{32}$$

Since the Lie group of block diagonal matrices, direct product of $U(1)$ and $U(3)$, is transitive on the manifold of linear combinations of $\tilde{\phi}_0|, \tilde{\phi}_1|, \tilde{\phi}_2|$ with unit norm, pure state controllability, within the set of permutation invariant states, follows. We summarize in the following Theorem:

Theorem 3. *In the coordinates given by the matrix T in (28) the Lie algebra of permutation invariant matrices $\mathcal{P}^{PI}$ is made of block diagonal matrices with skew-Hermitian blocks of dimensions 1 and 3. The set of reachable evolutions is the Lie group of block diagonal matrices $diag(U_1, U_3)$ with U_1 (U_3) unitary of dimension 1 (3) and $\det(U_1)\det(U_3) = 1$. System (6) is pure state controllable on the space of permutation invariant states.*

B. Case $n = 3$

For $n = 3$, the dynamical Lie algebra $\mathcal{P}$ is the intersection of $\mathcal{P}^{PI12}$ and $\mathcal{P}^{PI23}$ defined in Remark III.2 inside $su(8)$. In order to find a system of coordinates where $\mathcal{P}^{PI}$ has a form which displays its Lie algebra structure we follow the idea of Remark III.1 and find orthonormal subspaces which are invariant for the generators of $\mathcal{P}^{PI}$ and therefore for all of $\mathcal{P}^{PI}$. One such subspace is given by

$$\cup_\phi := \mathtt{span}\{ \phi_0|, \phi_1|, \phi_2|, \phi_3| \rangle,$$

with $\phi_j|$ defined in (3). Let

$$\psi_0| := \frac{1}{\sqrt{2}} 010| + \frac{1}{\sqrt{2}} 100|$$

and

$$\psi_1| := \frac{1}{\sqrt{2}} 011| + \frac{1}{\sqrt{2}} 101|.$$

It is a straightforward calculation to show that the subspace

$$\cup_\psi := \mathtt{span}\{ \psi_0|, \psi_1| \rangle,$$

is invariant under H_{zz}, H_x and H_y defined in (6) and (7) (cf. Appendix B) and therefore for the whole Lie algebra $\mathcal{P}^{PI}$. Moreover consider the orthonormal vectors

$$\chi_0| := \frac{\sqrt{2}}{\sqrt{3}} 001| \quad \frac{1}{\sqrt{6}} 010| \quad \frac{1}{\sqrt{6}} 100|,$$

$$\chi_1| := \frac{1}{\sqrt{6}} 011| + \frac{1}{\sqrt{6}} 101| \quad \frac{\sqrt{2}}{\sqrt{3}} 110|.$$

Again, a straightforward calculation (Appendix B) shows that the subspace

$$\cup_\chi := \mathtt{span}\{ \sqrt{\chi_0}|,\ \sqrt{\chi_1}|\rangle,$$

is invariant under H_{zz}, H_x and H_y defined in (6) and (7) and therefore for the whole Lie algebra $\mathcal{P}^{PI}$. Moreover it is orthogonal to both $\cup_\phi$ and $\cup_\psi$. Therefore, the matrix

$$M^\dagger := [\sqrt{\psi_0}|,\ \sqrt{\psi_1}|,\ \sqrt{\chi_0}|,\ \sqrt{\chi_1}|,\ \sqrt{\phi_0}|,\ \sqrt{\phi_1}|,\ \sqrt{\phi_2}|,\ \sqrt{\phi_3}|] := \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{33}$$

is such that the matrices in $M\mathcal{P}^{PI}M^\dagger$ have the form

$$MAM^\dagger := \begin{pmatrix} W_1 & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & W_3 \end{pmatrix}, \tag{34}$$

with $W_1 \ / \ u(2)$, $W_2 \ / \ u(2)$, $W_3 \ / \ u(4)$. Furthermore using the fact that $\Pi_{23}A\Pi_{23} = A$, for $A \ / \ \mathcal{P}^{PI}$ and (34), we obtain

$$M\Pi_{23}M^\dagger \begin{pmatrix} W_1 & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & W_3 \end{pmatrix} M\Pi_{23}M^\dagger = \begin{pmatrix} W_1 & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & W_3 \end{pmatrix}. \tag{35}$$

Using $M^\dagger$ in (33) and the (easily verifiable) relations[16]

$$\Pi_{23}\sqrt{\psi_0}| = \frac{1}{2}\sqrt{\psi_0}| \quad \frac{\overline{3}}{2}\sqrt{\chi_0}|, \qquad \Pi_{23}\sqrt{\psi_1}| = \frac{1}{2}\sqrt{\psi_1}| \quad \frac{\overline{3}}{2}\sqrt{\chi_1}|, \tag{36}$$

$$\Pi_{23}\sqrt{\chi_0}| = \frac{1}{2}\sqrt{\chi_0}| \quad \frac{\overline{3}}{2}\sqrt{\psi_0}|, \qquad \Pi_{23}\sqrt{\chi_1}| = \frac{1}{2}\sqrt{\chi_1}| \quad \frac{\overline{3}}{2}\sqrt{\psi_1}|,$$

we calculate

$$M\Pi_{23}M^\dagger := \begin{pmatrix} \frac{1}{2}\mathbf{1}_2 & \frac{\sqrt{3}}{2}\mathbf{1}_2 & 0 & 0 \\ \frac{\sqrt{3}}{2}\mathbf{1}_2 & \frac{1}{2}\mathbf{1}_2 & 0 & 0 \\ 0 & 0 & \mathbf{1}_2 & 0 \\ 0 & 0 & 0 & \mathbf{1}_2 \end{pmatrix}. \tag{37}$$

This, used in (35) gives $W_1 = W_2$. In conclusion in the new coordinates, matrices in $\mathcal{P}^{PI}$ must be of the form

$$\hat{B} := \begin{pmatrix} W & 0 & 0 \\ 0 & W & 0 \\ 0 & 0 & Q \end{pmatrix}, \tag{38}$$

with W and Q skew-Hermitian matrices of dimensions 2 and 4, respectively. Since the number of degrees of freedom in (38) is equal to the dimension of $\mathcal{P}^{PI}$ calculated in (15) (which for $n = 3$ is 20) the Lie algebra of matrices in (38) with trace equal to 0 gives exactly $\mathcal{P}$. The Lie group corresponding to the dynamical Lie algebra $\mathcal{P} = \mathcal{P}^{PI} \lfloor su(8)$, which is the space of available evolutions for the system (6) is, in the given coordinates, the Lie group of matrices of the form

$$\begin{pmatrix} U_2 & 0 & 0 \\ 0 & U_2 & 0 \\ 0 & 0 & U_4 \end{pmatrix}, \tag{39}$$

with U_2 and U_4 arbitrary unitary matrices of dimensions 2 and 4, respectively, and $[\det(U_2)]^2\det(U_4)=1$. In the new coordinates $\phi_0|$, $\phi_1|$, $\phi_2|$ and $\phi_4|$ are the elements of the standard basis $\vec{e}_5$, $\vec{e}_6$, $\vec{e}_7$, $\vec{e}_8$. From this, and the fact that $U(4)$ is transitive on the complex sphere of dimension 4, pure state controllability of system (6), in the space of permutation invariant states, follows. Summarizing we have the following Theorem which is the corresponding of Theorem 3 for the case $n=3$.

Theorem 4. *In the coordinates given by the matrix M in (33), the Lie algebra of permutation invariant matrices $\mathcal{P}^{PI}$ is made of block diagonal matrices with skew-Hermitian blocks of dimensions 2, 2 and 4, where the blocks of dimension 2 are equal. The set of reachable evolutions is the Lie group of block diagonal matrices $diag(U_2,U_2,U_4)$ with U_2 (U_4) unitary of dimension 2 (4) and $\det(U_2)^2\det(U_4)=1$. System (6) is pure state controllable on the space of permutation invariant states.*

IV. ALGORITHMS FOR CONTROL

We now give algorithms for control to perform an arbitrary unitary operation on the space of permutation invariant states. The change of coordinates displayed in the previous section shows that we have a problem of control on $U(3)$ and $U(4)$ respectively. In fact the upper blocks of the matrices in $\mathcal{P}$ (in the new coordinates) can be neglected since they do not affect the space of permutation invariant states. We shall assume that in (6) we can use arbitrarily large controls possibly in very short time (hard pulses). This will allow us to use methods of Cartan decompositions of Lie groups for control.

A. Case $n=2$

Consider the matrices iH_x, iH_y and iH_{zz} defined in (7) for the case $n=2$. In the new coordinates defined by the matrix T in (28), iH_x, iH_y and iH_{zz} transform respectively into

$$A_x := T(iH_x)T^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \quad A_y := T(iH_y)T^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

$$A_{zz} := T(iH_{zz})T^\dagger = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}.$$

One extra change of coordinates $A \in \hat{T}A\hat{T}^\dagger$ with

$$\hat{T} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{-i}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \end{pmatrix}, \tag{40}$$

gives

$$\hat{A}_x := \hat{T}(A_x)\hat{T}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{A}_y := \hat{T}(A_y)\hat{T}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix},$$

$$\hat{A}_{zz} := \hat{T}(A_{zz})\hat{T}^\dagger = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}.$$

In these coordinates the system (6) becomes the right invariant system on a Lie group

$$\dot{X} = \hat{A}_{zz} X + \hat{A}_x X u_x + \hat{A}_y X u_y. \tag{41}$$

Neglecting the upper $1 \oplus 1$ block of the matrix X (which does not affect the permutation invariant states), and neglecting matrices which are multiples of the identity which only add a phase factor to the solution, this system has a $P \quad K$ structure, i.e., there exists a Cartan decomposition of $su(3) = \mathcal{L} \otimes \mathcal{S}$, with

$$[\mathcal{L}, \mathcal{L}] \leq \mathcal{L}, \qquad [\mathcal{L}, \mathcal{S}] \leq \mathcal{S}, \qquad [\mathcal{S}, \mathcal{S}] \leq \mathcal{L},$$

such that the matrices multiplying the control (in this case $\hat{A}_x$ and $\hat{A}_y$) generate the Lie subalgebra $\mathcal{L}$ and the drift matrix (in this case $\hat{A}_z$) belongs to $\mathcal{S}$. In our case, the decomposition is obtained with $\mathcal{L} = so(3)$ while $\mathcal{S}$ is the space of purely imaginary matrices. The method of control in this case is as follows:

First write the desired final condition $X_f \ / \ SU(3)$ according to the Cartan decomposition as $X_f := K_1 A K_2$ where K_1 and K_2 which are in the Lie group corresponding to $\mathcal{L}$ (in this case $SO(3)$). The matrix A is an element of the Lie group associated to a Cartan subalgebra (i.e., a maximal Abelian subalgebra contained in $\mathcal{S}$). Then the problem is to obtain evolutions which implement K_2, A and K_1 in that order. K_1 and K_2 are obtained with hard pulses, i.e., high amplitude short time controls, which essentially allow us to neglect the drift term. The element A is implemented by alternating hard pulses with free evolutions (setting the controls equal to zero).

Details of the approach to control based on decompositions of Lie groups are described in [2] which also gives computational methods to find the factors $K_{1,2}$ and A in the decomposition. The paper [12] shows that this method of control is, in fact, time optimal.

B. Case $n = 3$

Analogously to the case $n = 2$, we first transform iH_x, iH_y and iH_{zz} in new coordinates using the transformation M in (33). A direct calculation (using Appendix B) shows:

$$M(iH_x)M^\dagger := i \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \overline{3} & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & \overline{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{3} & 0 \end{pmatrix} \tag{42}$$

$$M(iH_y)M^\dagger := \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \overline{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \overline{3} & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & \overline{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & \overline{3} & 0 \end{pmatrix} \tag{43}$$

$$M(iH_{zz})M^\dagger := i \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix} \tag{44}$$

From now on we shall only focus on the last four rows and columns which represent the evolution of the dynamics on the subspace of permutation invariant states spanned by $\phi_0|$, $\phi_1|$, $\phi_2|$, and $\phi_3|$. The problem of control is solved

if we are able to factorize the desired final evolution $X_f \;/\; U(4)$ in exponentials of matrices proportional to (cf. (42), (43), (44))

$$B_x := \begin{pmatrix} 0 & \overline{3}i & 0 & 0 \\ \overline{3}i & 0 & 2i & 0 \\ 0 & 2i & 0 & \overline{3}i \\ 0 & 0 & \overline{3}i & 0 \end{pmatrix}, \qquad B_y := \begin{pmatrix} 0 & \overline{3} & 0 & 0 \\ \overline{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \overline{3} \\ 0 & 0 & \overline{3} & 0 \end{pmatrix}, \qquad \tilde{B}_{zz} := \begin{pmatrix} 3i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 3i \end{pmatrix}, \tag{45}$$

that is as exponentials of the form $e^{B_x t}$, $e^{B_y t}$ and $e^{\tilde{B}_{zz} t}$ for real t. The exponentials of the form $e^{B_x t}$ and $e^{B_y t}$ can be obtained using hard pulses in the Hamiltonian (6), the elements $e^{\tilde{B}_{zz} t}$ are obtained by setting the controls equal to zero and allowing the system free evolution. Notice that the orbit $\{e^{\tilde{B}_{zz} t} \;/\; t \in \mathbf{R}\}$ is periodic and so we can obtain all the values in it even if we restrict ourselves to positive values of the time t as it is required in physical applications. Furthermore, by neglecting an overall phase factor which does not have a physical meaning, and rescaling the time t, we can consider instead of the matrix $\tilde{B}_{zz}$ in (45), the matrix

$$B_{zz} := \frac{1}{2}\tilde{B}_{zz} + i\mathbf{1} = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}, \tag{46}$$

and restrict to matrices $X_f \;/\; SU(4)$.

We shall again use an appropriate Cartan decomposition along with the method for generating 'new directions' described in [4]. In particular, we use the **AIII** KAK Cartan decomposition [9] of $SU(4)$: every element $X_f \;/\; SU(4)$ can be factorized as

$$X_f := K_1 A K_2, \tag{47}$$

where K_1 and K_2 are matrices with elements at the intersection of rows and columns 1-4 and 2-3 occupied by $2 \oplus 2$ unitary matrices U_1 and U_2 (by permuting row and column indexes these would be block diagonal matrices with $2 \oplus 2$ blocks) and $\det(U_1)\det(U_2) = 1$. The matrix A is the product of two commuting matrices belonging to the associated Cartan subalgebra which we can take equal to $\mathtt{span}\{A_3, C_3\}$ with

$$A_3 := \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad C_3 := \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{48}$$

which are commuting. Methods to compute the factors in (47) are described in [2]. Our task is therefore to show how to express matrices of the form K_1 K_2 and A in (47) as products of exponentials of the matrices B_x, B_y and B_{zz} in (45).

Our treatment is split into two steps: First we introduce two auxiliary Lie algebras and corresponding Lie groups and show that we can obtain the elements K_1, K_2 and A in (47) if we have arbitrary elements in these Lie groups. Then we will show how to use the exponentials of the matrices B_x, B_y and B_{zz} in (45) to obtain the elements of the auxiliary Lie groups.

We consider two auxiliary Lie subalgebras of $su(4)$ which are isomorphic to each other. In particular the Lie algebra $\mathcal{B}$ is given by

$$\mathcal{B} := \mathtt{span}\{A_1, A_2, A_3, E\},$$

with A_3 given in (48) and

$$A_1 := \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad A_2 := \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, E := \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{49}$$

We have the commutation relations

$$[A_1, A_2] = A_3, \qquad [A_2, A_3] = A_1, \quad [A_3, A_1] = A_2, \quad [\mathcal{B}, E] = 0, \tag{50}$$

which show that $\mathcal{B}$ is the direct sum of a Lie subalgebra isomorphic to $su(2)$ with its centralizer spanned by E (this isomorphism will be further confirmed later by performing a change of coordinates).

The second auxiliary Lie algebra we consider is the Lie algebra $\mathcal{K}$, with $\mathcal{K} := \mathtt{span}\{B_1, B_2, B_3, F\rangle$ where $B_1 := A_1$ in (49) and

$$B_2 := \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad B_3 := \frac{1}{2}\begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad F := \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}. \tag{51}$$

We have the commutation relations

$$[B_1, B_2] = B_3, \qquad [B_2, B_3] = B_1, \quad [B_3, B_1] = B_2, \quad [\mathcal{K}, F] = 0, \tag{52}$$

which, compared to (50), show that $\mathcal{K}$ is isomorphic to $\mathcal{B}$.

We shall assume now that we are able to obtain all matrices in the connected Lie groups corresponding to $\mathcal{B}$ and $\mathcal{K}$, that we denote by $e^{\mathcal{A}}$ and $e^{\mathcal{B}}$, respectively. We will show that with these we can construct the decomposition (47).

The matrices of the form $e^{(A_2-E)t} \,/\, e^{\mathcal{A}}$ ($e^{(A_2+E)t} \,/\, e^{\mathcal{A}}$) are equal to the identity except for the rows and columns 2 and 3 (1 and 4) which contain an arbitrary (depending on t) Y rotation. Analogously, the matrices of the form $e^{(B_2-F)t} \,/\, e^{\mathcal{B}}$ ($e^{(B_2-F)t} \,/\, e^{\mathcal{B}}$) are equal to the identity except for the rows and columns 2 and 3 (1 and 4) which contain an arbitrary (depending on t) X rotation. Using these matrices and Euler decompositions we obtain matrices such that the elements corresponding to indexes 1 and 4 give an arbitrary matrix in $SU(2)$, and the elements corresponding to indexes 2 and 3 give an arbitrary matrix in $SU(2)$. Multiplying the overall $4 \oplus 4$ matrix by a matrix of the form $e^{B_{zz}t}$ we obtain matrices of the form K_1 and K_2 in (47). The element A in (47) is obtained as the commuting product of an element of the form $e^{A_3 t}$ and an element of the form $e^{C_3 t}$ (cf. (48)), and we have $e^{A_3 t} \,/\, e^{\mathcal{A}}$ already, while, it is immediate to verify that $e^{-B_{zz}\frac{\pi}{4}} B_3 e^{B_{zz}\frac{\pi}{4}} = C_3$, so that

$$e^{C_3 t} = e^{-B_{zz}\frac{\pi}{4}} e^{B_3 t} e^{B_{zz}\frac{\pi}{4}}.$$

Our last step is to show how to obtain elements in $e^{\mathcal{A}}$ and $e^{\mathcal{B}}$ using exponentials of the matrices B_x, B_y and B_{zz} in (45). We start with $e^{\mathcal{A}}$ ($e^{\mathcal{B}}$ is similar). We are allowed to take exponentials $e^{B_y t}$ for B_y in (45) but also exponentials of

$$\hat{B}_y := e^{B_{zz}\frac{\pi}{2}} B_y e^{-B_{zz}\frac{\pi}{2}} = \begin{pmatrix} 0 & \overline{3} & 0 & 0 \\ \overline{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \overline{3} \\ 0 & 0 & \overline{3} & 0 \end{pmatrix}. \tag{53}$$

In a basis (H) given by eigenvectors of B_y, we write B_y as

$$HB_yH^\dagger := \begin{pmatrix} 2i & 0 & 0 & 0 \\ 0 & 2i & 0 & 0 \\ 0 & 0 & 2i & 0 \\ 0 & 0 & 0 & 2i \end{pmatrix} + \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}. \tag{54}$$

In the same coordinates, $\hat{B}_y$ becomes

$$H\hat{B}_yH^\dagger := \begin{pmatrix} i & \overline{3} & 0 & 0 \\ \overline{3} & i & 0 & 0 \\ 0 & 0 & i & \overline{3} \\ 0 & 0 & \overline{3} & i \end{pmatrix} + \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}. \tag{55}$$

The second matrix in (54) and (55) commutes with both matrices and therefore spans the centralizer of the Lie algebra generated by the two matrices which is conjugate to $\mathcal{B}$. In these coordinates, it is also clear that such a Lie algebra is isomorphic to the direct sum of $su(2)$ and a one dimensional centralizer. The $2 \oplus 2$ blocks of the first matrices on the right hand sides in (54) and (55) are equal to each other. The problem of factorization is therefore a problem on $SU(2)$ with an additional phase factor which we would like to fix arbitrarily. Let us first neglect the second term in (54) and (55) and consider the problem of factorization of elements in $SU(2)$ with matrices $e^{Z_1 t}$ and $e^{Z_2 t}$, with

$$Z_1 := \begin{pmatrix} 2i & 0 \\ 0 & 2i \end{pmatrix}, \qquad Z_2 := \begin{pmatrix} i & \overline{3} \\ \overline{3} & i \end{pmatrix}. \tag{56}$$

This problem can be solved (with minimum number of switches) with the method described in [5] (see also [13]). The extra phase factor can be introduced by adding an extra identity matrix factor which can be obtained in arbitrary time. More in detail, assume we want to obtain the matrix with $e^{-i\mu}X_f$ in the upper block and $e^{i\mu}X_f$ in the lower block, for $X_f \ / \ SU(2)$. Let $\sum_{j=1} e^{Z_1 t_{j1}} e^{Z_2 t_{j2}}$ the sequence which gives X_f according to the method of [5]. Moreover let $\sum_{j=1} e^{Z_1 a_{j1}} e^{Z_2 a_{j2}}$ the sequence which gives $R_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sum_{j=1} e^{Z_1 b_{j1}} e^{Z_2 b_{j2}}$ the sequence which gives $R_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Notice that $R_1 e^{Z_1\alpha} R_1^\dagger e^{Z_1\alpha} = \mathbf{1}$, independently of α. We use

$$\left[\sum_{j=1} e^{HB_yH^\dagger t_{j1}} e^{H\hat{B}_yH^\dagger t_{j2}}\right] \oplus \left[\sum_{j=1} e^{HB_yH^\dagger a_{j1}} e^{H\hat{B}_yH^\dagger a_{j2}}\right] \oplus e^{HB_yH^\dagger\alpha} \left[\sum_{j=1} e^{HB_yH^\dagger b_{j1}} e^{H\hat{B}_yH^\dagger b_{j2}}\right] \oplus e^{HB_yH^\dagger\alpha}. \quad (57)$$

Set $t_{tot} := \prod_j (t_{j1} + t_{j2}) + \prod_j (a_{j1} + a_{j2}) + \prod_j (b_{j1} + b_{j2})$. In the upper (lower) block, the sequence (57) gives $X_f e^{-it_{tot}} e^{-2i\alpha}$ ($X_f e^{it_{tot}} e^{2i\alpha}$) and choosing $2\alpha + t_{tot} = \mu$ we obtain the desired final condition.

The treatment of $e^{\mathcal{B}}$ is perfectly analogous starting with B_x in (45) rather than B_y and obtaining the extra 'direction' (cf. (53))

$$\hat{B}_x := e^{B_{zz}\frac{\pi}{2}} B_x e^{-B_{zz}\frac{\pi}{2}} = \begin{pmatrix} 0 & \overline{3}i & 0 & 0 \\ \overline{3}i & 0 & 2i & 0 \\ 0 & 2i & 0 & \overline{3}i \\ 0 & 0 & \overline{3}i & 0 \end{pmatrix}. \quad (58)$$

We express the matrices B_x and $\hat{B}_x$ in the coordinates given by the eigenvectors of B_x, that is, for an appropriate matrix U, we have (cf. (54) and (55))

$$UB_xU^\dagger = \begin{pmatrix} 2i & 0 & 0 & 0 \\ 0 & 2i & 0 & 0 \\ 0 & 0 & 2i & 0 \\ 0 & 0 & 0 & 2i \end{pmatrix} + \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix},$$

$$U\hat{B}_xU^\dagger = \begin{pmatrix} i & \overline{3} & 0 & 0 \\ \overline{3}i & i & 0 & 0 \\ 0 & 0 & i & \overline{3}i \\ 0 & 0 & \overline{3}i & i \end{pmatrix} + \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}.$$

Then the treatment follows, as for the case of $e^{\mathcal{A}}$ from the results on factorizations of $SU(2)$ in [5].

Remark IV.1. Similar ideas can very likely be applied to the cases $n > 3$. In fact, computations for the case $n = 4$ suggest the conjecture that the Lie algebra generated by the restrictions of iH_{zz}, iH_x and iH_y in (7) to the space spanned by the symmetric states ϕ_j, $j = 0, 1, ..., n$ in (3) is always $u(n+1)$. Given therefore such a full operator controllability property on this subspace, one can in principle apply general constructive techniques such as those in [4] to obtain control algorithms. Lie groups decompositions, like Cartan decompositions, applied on a case by case basis, can be combined with such techniques to give more efficient and simple controls.

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[16] Notice also the relations which will not be used $\Pi_{12}|\psi_0\rangle = -|\psi_0\rangle$, $\Pi_{12}|\psi_1\rangle = -|\psi_1\rangle$, $\Pi_{12}|\chi_0\rangle = |\chi_0\rangle$, $\Pi_{12}|\chi_1\rangle = |\chi_1\rangle$ which together with (36) show the invariance of the subspaces $\mathtt{span}\{|\psi_0\rangle, |\chi_0\rangle\}$ and $\mathtt{span}\{|\psi_1\rangle, |\chi_1\rangle\}$ under both Π_{12} and Π_{23}.

Appendix A: Proof of formula (19)

To prove the first one, let first observe that:

$$[\mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_y}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_z}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1},\ \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_x}_{i^{th}}\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}] =$$

$$= \begin{cases} 0 & \text{if } i \neq j \text{ and } i \neq l \\ 2i\ \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_z}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_z}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1} & \text{if } i = j \\ 2i\ \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_y}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_y}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1} & \text{if } i = l \end{cases} \tag{59}$$

Using the previous equation we have:

$$[X^n_{(0,1,1)}, X^n_{(1,0,0)}] = \prod_{\substack{i,j,l=1 \\ j\neq l}}^{n} [\mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_y}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_z}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1},\ \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_x}_{i^{th}}\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}]$$

$$= \left(\prod_{\substack{j,l=1 \\ j\neq l}}^{n} 2i\right) \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_z}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_z}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}\quad \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{\sigma_y}_{j^{th}}\otimes\cdots\otimes\underbrace{\sigma_y}_{l^{th}}\otimes\cdots\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1}\Big] \sum_{4}$$

$$4\,X^n_{(0,0,2)} + 4\,X^n_{(0,2,0)}.$$

The second equality can be proved in a similar way.

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Appendix B: Calculation of the action of H_x, H_y and H_{zz} on the basis $\{|\psi_0\rangle, |\psi_1\rangle, |\chi_0\rangle, |\chi_1\rangle, |\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle\}$

$$
\begin{array}{lll}
H_x\,|\psi_0\rangle = |\psi_1\rangle & H_y\,|\psi_0\rangle = i\,|\psi_1\rangle & H_{zz}\,|\psi_0\rangle = |\psi_0\rangle \\
H_x\,|\psi_1\rangle = |\psi_0\rangle & H_y\,|\psi_1\rangle = i\,|\psi_0\rangle & H_{zz}\,|\psi_1\rangle = |\psi_1\rangle \\
H_x\,|\chi_0\rangle = |\chi_1\rangle & H_y\,|\chi_0\rangle = i\,|\chi_1\rangle & H_{zz}\,|\chi_0\rangle = |\chi_0\rangle \\
H_x\,|\chi_1\rangle = |\chi_0\rangle & H_y\,|\chi_1\rangle = i\,|\chi_0\rangle & H_{zz}\,|\chi_1\rangle = |\chi_1\rangle \\
H_x\,|\phi_0\rangle = \sqrt{3}\,|\phi_1\rangle & H_y\,|\phi_0\rangle = i\sqrt{3}\,|\phi_1\rangle & H_{zz}\,|\phi_0\rangle = 3\,|\phi_0\rangle \\
H_x\,|\phi_1\rangle = \sqrt{3}\,|\phi_0\rangle + 2\,|\phi_2\rangle & H_y\,|\phi_1\rangle = i\sqrt{3}\,|\phi_0\rangle - 2i\,|\phi_2\rangle & H_{zz}\,|\phi_1\rangle = |\phi_1\rangle \\
H_x\,|\phi_2\rangle = \sqrt{3}\,|\phi_3\rangle + 2\,|\phi_1\rangle & H_y\,|\phi_2\rangle = i\sqrt{3}\,|\phi_3\rangle + 2i\,|\phi_1\rangle & H_{zz}\,|\phi_2\rangle = |\phi_2\rangle \\
H_x\,|\phi_3\rangle = \sqrt{3}\,|\phi_2\rangle & H_y\,|\phi_3\rangle = i\sqrt{3}\,|\phi_2\rangle & H_{zz}\,|\phi_3\rangle = 3\,|\phi_3\rangle
\end{array}
$$