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TWO-QUBIT QUANTUM GATES DESIGN VIA UNITARY FACTORIZATION UNDER ANISOTROPIC HEISENBERG-ISING INTERACTION

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Quantum information and quantum computation are emerging research areas based on the properties of quantum resources, such as superposition and entanglement. In the quantum gate array version, the use of convenient and proper gates is essential. While these gates adopt theoretically convenient forms to reproduce computational algorithms, their design and feasibility depend on specific quantum systems and physical resources used in their setup. These gates should be based on systems driven by physical interactions ruled by a quantum Hamiltonian. Then, the gate design is restricted to the properties and the limitations imposed by the interactions and the physical elements involved. This work shows how anisotropic Heisenberg-Ising interactions, written in a non-local basis, allow the reproduction of quantum computer operations based on unitary processes. We show that gates can be generated by a pulse sequence of driven magnetic fields. This fact states alternative techniques in quantum gate design for magnetic systems. A brief final discussion around associated fault tolerant extensions to the current work is included.

Keywords: Gate design; Unitary matrix factorization; Heisenberg-Ising anisotropic model; Quantum algorithms.
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1 Introduction

Quantum information is the utmost contemporary application of quantum mechanics. Entanglement, one of the more disruptive properties of quantum mechanics [1, 2, 3, 4, 5], plays a central role in the improvement of storage capacity and processing speed of quantum information [6, 7, 8] by using alternative methods to those of classical computer science. Useful appliances are being settled up on this property: quantum computation [9, 10, 11], quantum cryptography [12, 13], superdense coding [14] and teleportation [15].

In terms of similarity, quantum gate array computation (QGAC) is the most common and universal approach to classical computer science. This is due to its use of controlled quantum evolution as quantum gates, a replica of classical computer gates. However, quantum gates should be reproduced via physical interactions and resources (ion traps and electromagnetic cavities [16, 17], Josephson junctions [18], nuclear magnetic resonance [19] and spins [20, 21, 22]). These have no direct or immediate setup and require complex control operations, and sometimes require iterative procedures in order to be reached. Thus, QGAC is experimental

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(in terms of noise control and reproduction of theoretical gates [16, 17, 18, 19, 20, 21, 22]), with physical resources adapted to set certain universal gates. For implementations based on matter, quantum dots and electronic gases are developments towards a scalable spin-based quantum computer controlled by electromagnetic interactions to reproduce certain quantum universal operations [23, 24, 25] to meet DiVincenzo criteria [26]: reliability in the state preparation, well identified qubits and accurate quantum gate operations.

It is still useful to understand alternative approaches for efficient and scalable procedures reproducing basic elements in quantum gate array computation for a couple of qubits. There are at least two results to support this fact: a) two-level quantum channel processing is universal in the quantum gate version of quantum computation [27], and b) universal sets of two-level gates can be constructed, as exemplified by the Boykin *et al.* gates [28, 29]. Due to the large array of qubits to be manipulated in quantum applications, gate construction departs from operations by pairs. In this trend, several proposals to construct or introduce more general quantum information processes have been made. As there is no general procedure for translating multipartite processes into bipartite ones using a universal set of gates, alternative trends have been developed. An example is the Cosine-Sine decomposition [30], which allows a multipartite gate decompose in a nesting series of rotations, a kind of evolution easily achievable in all bipartite qubit systems. Other proposals use efficient decomposition based on combinations of single qubit and multiplexor gates [31], the construction of Gray codes basis [32] or $q-$deformed algebras on harmonic oscillators [33]. Recent work has exploited the natural properties of a physical system to reproduce some universal gates naturally, a trend that relates to the topics discussed in this paper. These works tend to connect the number of involved CNOT gates to circuit complexity. However, their main focus is the basis on which the construction was done. Computational bases are common in QGAC, as they chiefly relate to traditional computing rather than entanglement generation (a central and mandatory quantum phenomenon). Thus, while physical systems require entangling operations in their evolution, the computational basis typically departs from this behavior.

In this arena, unitary factorization is an alternative approach to quantum gate design [34, 35, 36, 37, 38]. This approach allows the reproduction of complex or dedicated gates (otherwise rarely constructed when departing from a universal gate set) by means of a finite series of simpler unitary operations $M^{(i,j)^\dagger}$ ($P-$ unitary operations):

$$U = \overrightarrow{\prod_{\substack{1\leq j<n \\ n>i\geq j}}} M^{(i,j)\dagger} \tag{1}$$

where symbol $\rightarrow$ represents the forward product, stacking factors from left to right. In this vein, the paper aims to show how driven anisotropic Heisenberg-Ising (HI) interactions for bipartite systems can be used to reproduce gates based on a natural unitary factorization and a universal grammar for those systems. This construction is an example of how grammar in quantum information systems should be adapted to reproduce physical evolution dynamics, an aspect sometimes lost in theoretical quantum information developments.

Procedure becomes useful in quantum simulations when reproducing controlled simulations for specific computational problems. The present paper is organized as follows: Section

2 summarizes the unitary factorization process, which is useful for further development. Section 3 presents the physical background to set the unitary factorization based on a recent proposal of $SU(2)$ decomposition for the driven HI Hamiltonian on a non-local basis [39]. Section 4 analyzes the feasibility of the factorization presented in terms of a set of prescriptions for general implementation. The analysis includes the implementation based on single and double external magnetic pulses to generate adequate unitary factors. Section 5 presents the analytical solution for matrices with real entries. Section 6 presents a couple of implementations with two concrete gates reported in the literature. Section 7 sets some elements to carry the proposal into quantum error correction theory and the fault tolerant processing domain. This section also presents some information about the generalization of the factorization process. Conclusions are presented at the end of the paper, including some ideas for the possible generalization for bigger systems as a future work. The complex details of feasibility are discussed in the appendices. In this discussion, anisotropy included in the model is referred to a generalization of the models in the contemporary literature, though not all results presented in this paper depend on this generalization.

2 P-unitary matrices factorization

The factorization of unitary matrices has been referred to an approach to develop programmed quantum operations that depart from the natural evolutions under specific Hamiltonians. In quantum processes, local $SU(2)$ operations plus entangling operations ($SU(4)$ or still $SU(2)$ non-local operations, meaning a non-local operation between a pair of entangled states) reproduce more complex operations [28]. This procedure has been used, for example, in optics [27] using a Mach-Zehnder interferometer and for atoms [40] using two-level systems driven by fields properly detuned from resonance. Unitary factorization has been addressed in terms of Householder reflections [41, 37], as well as a suitable adaptation of Gauss-Jordan factorization [42] for unitary quantum evolution operators [38]. In this section, we state a recursive version of this factorization.

2.1 $P-$unitary matrices

A two-level $n-$dimensional $P-$unitary matrix is a unitary matrix that departs from the $n \times n$ identity matrix, $\mathbf{I}_n$, but includes a substitution of some of its elements as follows: if $P = \{j_1, j_2, ..., j_n\}$ is a permutation from $\{1, 2, ..., n\}$, the $P-$unitary matrix $M^n_{j_k,j_{k+1}}$ is said of type $k \in \{1, 2, ..., n-1\}$ if the block defined by the entries $(j_k, j_k), (j_k, j_{k+1}), (j_{k+1}, j_k), (j_{k+1}, j_{k+1})$ is substituted by the entries of an arbitrary 2×2 unitary matrix $s_{j_k,j_{k+1}}$. Then, $M^n_{j_k,j_{k+1}} = s_{j_k,j_{k+1}} \oplus \mathbf{I}_{n-2}$, where $\mathbf{I}_{n-2}$ is the identity matrix located in the remaining rows and columns. For $n = 4$, the $P-$unitary matrices $M^4_{j_k,j_{k+1}} = M^4_{j_{k+1},j_k}$ with $j_k < j_{k+1}$ are:

$$M^4_{1,2} = \begin{pmatrix} * & * & 0 & 0 \\ * & * & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, M^4_{3,4} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{pmatrix} \in \mathrm{S}_1 \tag{2}$$

$$M_{1,4}^4 = \begin{pmatrix} * & 0 & 0 & * \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ * & 0 & 0 & * \end{pmatrix}, M_{2,3}^4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & * & * & 0 \\ 0 & * & * & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \mathrm{S}_2 \tag{3}$$

$$M_{1,3}^4 = \begin{pmatrix} * & 0 & * & 0 \\ 0 & 1 & 0 & 0 \\ * & 0 & * & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, M_{2,4}^4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & * & 0 & * \\ 0 & 0 & 1 & 0 \\ 0 & * & 0 & * \end{pmatrix} \in \mathrm{S}_3 \tag{4}$$

where $*$ represents the elements of a 2×2 unitary matrix embedded in $M_{j_k,j_{k+1}}^4$. $\mathrm{S}_i \subset SU(4), i = 1, 2, 3$ are three subgroups of $P-$unitary matrices. In this work we will focus on $M_{1,2}^4, M_{2,3}^4$ and $M_{3,4}^4$.

2.2 $P-$unitary matrices factorization procedure

$P-$unitary matrices allow the expression of any special unitary matrix U as a product of at most $\frac{n(n-1)}{2}$ factors (6 factors for $n = 4$). The procedure admits $U \in U(n)$ [37, 38]. Despite the discussion in this work will be restricted to $U(4)$ due to the interest in the evolution matrices $U \in SU(4)$ depicting the interactions between a pair of qubits, we will state the factorization matrix procedure for n arbitrary. Departing from the $n \times n$ unitary matrix, $U = \{a_{i,j}\}$, factorization can be settled as the following recursive procedure: transforming U into $\mathbf{I}_n$ by multiplying with a series of $P-$unitary matrices to eliminate the elements $a_{i,j}$ below the diagonal for each column j, with $1 \leq j < n, n \geq i > j$ (in this order). This procedure resembles the Gaussian elimination procedure [42]. If $U^{(i,j)} = \{a_{i,j}\}$ is the step matrix obtained by eliminating the element in the row $i+1$ and column j in the previous step of this process, then a $P-$unitary matrix $M_{i-1,i}^n(j)$ could be properly constructed to eliminate its element $a_{i,j} = u_{i,j}$ and to obtain the matrix $U^{(i-1,j)}$:

$$\begin{aligned} U^{(i-1,j)} &\equiv \begin{pmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & u_{i-1,j} & a_{i-1,j+1}^{(i,j)} & \dots & a_{i-1,n}^{(i,j)} \\ 0 & \dots & 0 & a_{i,j+1}^{(i,j)} & \dots & a_{i,n}^{(i,j)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & a_{n,j+1}^{(n,j)} & \dots & a_{n,n}^{(n,j)} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & * & * & \dots & 0 \\ 0 & \dots & * & * & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & a_{i-1,j}^{(i-1,j-1)} & a_{i-1,j+1}^{(i-1,j-1)} & \dots & a_{i-1,n}^{(i-1,j-1)} \\ 0 & \dots & u_{i,j} & a_{i,j+1}^{(i+1,j)} & \dots & a_{i,n}^{(i+1,j)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & a_{n,j+1}^{(n,j)} & \dots & a_{n,n}^{(n,j)} \end{pmatrix} \\ &\equiv M_{i-1,i}^n(j) \cdot U^{(i,j)} \end{aligned} \tag{5}$$

where $U^{(n,1)} = U$, and $a_{k,l}^{(i,j)}$ is the transformed entry k, l in the matrix when element i in column j is being eliminated. The superscript (i, j) is only a reference to set the elimination step in the process. In each step, one entry is eliminated and only two rows modified: the current row of that entry and the immediate above. Block $s_{i-1,i} \in U(2)$ in $M_{i-1,i}^{n}(j) = s_{i-1,i} \oplus \mathbf{I}_{n-2}$ should be:

$$s_{i-1,i} \equiv \begin{pmatrix} \frac{a_{i-1,j}^{(i-1,j-1)*}}{u_{i-1,j}} & \frac{u_{i,j}^{*}}{u_{i-1,j}} \\ -\frac{\mu_{i,j} u_{i,j}}{u_{i-1,j}} & \frac{\mu_{i,j} a_{i-1,j}^{(i-1,j-1)}}{u_{i-1,j}} \end{pmatrix} \tag{6}$$

where $a_{k,l}^{(i,0)} = a_{k,l}$, and $\mu_{i,j}$ is an arbitrary unitary complex number, and:

$$u_{i-1,j} = \begin{cases} a_{n,j}^{(n,j-1)} & , i = n+1 \\ \sqrt{|a_{i-1,j}^{(i-1,j-1)}|^2 + |u_{i,j}|^2} & , i \neq n+1 \end{cases} . \tag{7}$$

With this, we get:

$$U^{(n-1,n-1)} = \left(\prod_{\substack{1 \leq j < n \\ n > i \geq j}}^{\leftarrow} M_{i-1,i}^{n}(j) \right) \quad U \tag{8}$$

where the dependence of $M_{i-1,i}^{n}(j)$ on j appoints to the $P-$unitary matrix used in each column, and the symbol $\leftarrow$ states the backward product stacking factors from right to left according to script order. Each $M_{i-1,i}^{n}(j)$ and $\det(M_{i-1,i}^{n}(j)) = \mu_{i,j}$ are unitary too, so $U^{(j,j)}$ is unitary. In this process, each row and column are unitary; when the first column of entries below the diagonal are set to zero, $u_{1,1}$automatically equals 1. As such, the remaining elements in row 1 become zero [38]. This repeats for each column and row j in $U^{(j,j)}$ in spite of the $u_{j,j}$ definition:

$$u_{j,j} = \sqrt{\sum_{j \leq i \leq n} |a_{i,j}^{(i,j-1)}|^2} \tag{9}$$

Finally, $U^{(n-1,n-1)}$ is a residual diagonal matrix with 1 in all rows except for the unitary $a_{n,n}^{(n,n-1)}$. With this:

$$\det(U^{(n-1,n-1)}) = a_{n,n}^{(n,n-1)} = \left(\prod_{\substack{1 \leq j < n \\ j < i \leq n}} \mu_{i,j} \right) \quad \det(U) \tag{10}$$

noting that $a_{n,n}^{(n,n-1)}$ depends on $\det(U)$ and the selections made for $\mu_{i,j}$. The way to fulfill (10) is open in principle, but it can be used to fit specific requirements in the construction of each $M_{i-1,i}^{n}(j)$. Then, the main result is:

$$U = \left(\prod_{\substack{1 \le j < n \\ n > i \ge j}}^{\rightarrow} M_{i-1,i}^{n}(j)^{\dagger} \right) \quad U^{(n-1,n-1)} \tag{11}$$

This procedure implies that a desired artificial evolution matrix could be reproduced by a series of $P-$unitary matrices $M_{i-1,i}^{n}(j)^{\dagger}$ if natural evolutions can be fitted to them. If $U^{(n-1,n-1)} = \mathbf{I}_n$, then (11) becomes (1) by identifying $M_{i-1,i}^{n}(j)$ with $M^{(i,j)}$. When any original entry in (11) is zero, the process skips it with $M_{i-1,i}^{n}(j) = \mathbf{I}_n$ or equivalently $s_{i-1,i} = \mathbf{I}_2$.

3 Analytic evolution of anisotropic HI model in three dimensions

Magnetic systems are potential environments for quantum applications. They are susceptible matter for quantum memories and quantum processors. HI Hamiltonian is a simple interaction model that brings an easy setup to analyze the manipulation of quantum processing, particularly under adequate magnetic control as shown in Figure 1. Here, two qubits interact via HI model under additional local magnetic fields as driven elements. This model [43, 44, 45, 46] has been used as an approach for the interaction of magnetic quantum objects. Here, entanglement is naturally achievable. Despite the extensive research for this interaction, most developments in multipartite systems are numerical due to the growing number of elements. In this trend, different HI interaction models (XX, XY, XYZ depending on physical systems and arrays being considered) have been used to model bipartite and multipartite systems [47, 48, 49, 50, 51]. In this section, we examine some useful results to explore gate design using unitary factorization.

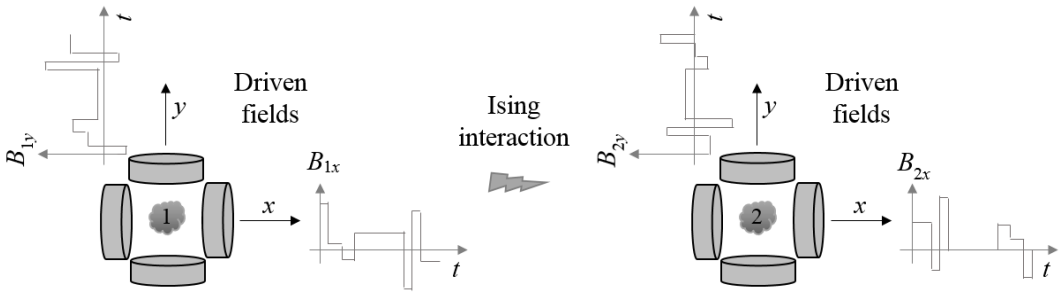

Fig. 1. HI interaction between two qubits including local magnetic fields to drive the information exchange in the system. A non-local description exhibits a block form in the evolution operator, which can be used to reproduce unitary factorization.

A recent analysis for the anisotropic HI model reveals an underlying algebraic structure when it is analyzed in the Bell basis [39] as a natural grammar. Following that work, we focus on the next bipartite Hamiltonian, including an inhomogeneous driven magnetic field in the h-direction ($h = 1, 2, 3$ corresponding to x, y, z):

$$H_h = \sum_{k=1}^{3} J_k \sigma_{1k} \sigma_{2k} - B_{1h}\sigma_{1h} - B_{2h}\sigma_{2h} \tag{12}$$

comprising several models discussed in the literature. [39] has shown that Ising interaction is diagonal in this basis, and H_h has a 2×2 block structure when it is expressed in the Bell basis. This structure is passed on the evolution matrix $U_h(t)$. Denoting the Bell basis as $|\beta_{--}\rangle \equiv |\beta_{00}\rangle, |\beta_{-+}\rangle \equiv |\beta_{01}\rangle, |\beta_{+-}\rangle \equiv |\beta_{10}\rangle, |\beta_{++}\rangle \equiv |\beta_{11}\rangle$, this work obtains the generic block form for the evolution operator $U_h(t) = U_{\alpha,\beta;\gamma,\delta} |\beta_{\alpha\beta}\rangle \langle\beta_{\gamma\delta}|$ (Einstein summation convention assumed):

$$U_h(t) = s_{h_1} \oplus s_{h_2} \in S_h \tag{13}$$

where $s_{h_j} \in U(1) \times SU(2) \subset U(2)$ is a 2×2 block. $S_h \subset SU(4)$ is the corresponding subgroup of unitary block matrices containing each $U_h(t)$ structure (corresponding to $S_{j_k, j_{k+1}}$ given in the previous section). s_{h_j} has the general structure for the time independent case [39, 52]:

$$s_{hj} = e^{i\Delta_{h\alpha}} \begin{pmatrix} e_{h\alpha}^{\beta *} & -qi^h d_{h\alpha} \\ qi^{*h} d_{h\alpha} & e_{h\alpha}^{\beta} \end{pmatrix} \tag{14}$$

The complete reference of each parameter in the last expression is given in [39], and a brief description has been included in Appendix A. The explicit form for $U_h(t)$ will be seminal in this work (note that each row and column is labeled with a pair of scripts $\alpha\beta \in \{--, -+, +-, ++\}$ in this order). $U_h(t)$ has a 2×2 block structure preserved under multiplication in each S_h. As has been shown [39], by fixing the parameters $\{|j_{h_{\mp\alpha}}|\}$ and $\{s_{b_{h_{\mp\alpha}}}\}$, we get a subgroup in S_h. Thus, identity, inverses and product closure properties are fulfilled in each one. The full group structure [39] is essential in the current work because it assures the existence of factorization solutions in terms of finite products of $U_h(t)$. The last structure allows the tentative achievement of the factor matrices' forms in the unitary factorization on $SU(4)$.

4 Unitary factorization based on HI model evolution

The 4×4 evolution matrices $M_{i-1,i}^4 \in \mathrm{S}_{i-1,i}$ (2) have the form of HI evolution matrices written in the Bell basis. In the described process, only $U_1(t)$ and $U_2(t)$ are reducible to the matrices ${M_{i-1,i}^4}^{\dagger}$. This is notable because the process can be managed by two-dimensional systems as anyons. Thus, the challenge is to fit s_{hj} in (14) to ${s_{i-1,i}}^{\dagger}$ in (6) to obtain the adequate prescriptions. We develop this analysis in the following subsections, giving the mathematical details in the appendices.

4.1 Getting $P-$unitary matrices through one magnetic pulse

The present section analyzes the fitting of the evolution for (12) to the unitary factorization process of section 2. First, sector j is reduced to the identity $s_{h_j} = \mathbf{I}_{h_j} = \mathbf{I}_2$. As reported in [52, 53] for control purposes, the prescriptions to reduce s_{hj} to $\mathbf{I}_{h_j}$ (2×2 identity matrix) at time t are:

$$t = \frac{2m_\alpha + n_\alpha}{\alpha J_h}\pi > 0, \quad {B_h}^2_{-\alpha} = (\frac{J_h n_\alpha}{2m_\alpha + n_\alpha})^2 - {J_{\{h\}}}_\alpha{}^2 \tag{15}$$

with $n_\alpha, m_\alpha \in \mathbf{Z}$. This form will be useful later and should be compatible with the restrictions to construct the required $P-$unitary matrices in the other block to eliminate each entry. A brief review reveals $\mu_{i,j} = e^{-2i\Delta_{h\alpha}^{+}}$ as a necessary condition for the consistency of the equations settled by $s_{h_j} = s^{\dagger}_{i-1,i}$ for the remaining unitary sector. In addition, due to (10), the following global restriction should be fulfilled:

$$\Delta_{x^{+}_{+,(4,1)}} + \Delta_{y^{+}_{-,(3,1)}} + \Delta_{x^{+}_{-,(2,1)}} + \Delta_{x^{+}_{+,(4,2)}} + \Delta_{y^{+}_{-,(3,2)}} + \Delta_{x^{+}_{+,(4,3)}} = N\pi \tag{16}$$

with $N \in \mathbf{Z}$. Here, the subscripts (i, j) relate to the entry being eliminated. The first equation in (15) fits one block to $\mathbf{I}_2$ (changing α by $-\alpha$ in (15), thus using the parameter α to label the remaining unitary non-diagonal sector), then $\Delta_{h^{+}_{\alpha,(i,j)}}$ becomes a multiple integer of π, satisfying (16) automatically. Because $U_h(t) \in SU(4)$, then $\mu_{i,j} = 1$; thus, (16) is fulfilled and reduced to $a^{(n,n-1)}_{n,n} = \det(U)$ (thus, $U^{(n-1,n-1)} = \mathbf{I}_4$ in (1) if $U \in SU(4)$). From (6) and (14), only two equations should be solved for the remaining block (as instance, for the entries $1,1$ and $2,1$):

$$\begin{aligned} 1,1: \quad & e_{h\alpha}^{\beta *} e^{i\Delta_{h\alpha}^{+}} = \frac{a^{(i-1,j-1)}_{i-1,j}}{u_{i-1,j}} \\ 2,1: \quad & q i^{*h} d_{h\alpha} e^{i\Delta_{h\alpha}^{+}} = \frac{u_{i,j}}{u_{i-1,j}}. \end{aligned} \tag{17}$$

Unfortunately, one single magnetic pulse is unable to generate solutions in most cases (concretely for those factors needed for the $h = 1$ case, despite $h = 2$ solutions are easily reached, especially for real entries matrices). The details of this analysis are included in Appendix B. To summarize, one pulse solutions are in most cases unable to generate evolutions to work as factors of a general unitary operation. Thus, more complex schemes should be analyzed to combine at least two magnetic pulses.

4.2 Getting $P-$unitary matrices through two magnetic pulses

Evolution prompted by (13) allows any $U(2)$ element to be obtained for each block by combining two adequate pulses [39] (more precisely, any $U(2)$ element can be generated by two consecutive s_{hj} blocks). As before, one block $(-\alpha)$ should be driven to $\mathbf{I}_2$ while the remaining block (α) reproduces the $P-$unitary matrix as part of the factorization presented previously. When two pulses are combined into $s'_{h_j} s_{hj}$, the generic form of the resulting block [39] should be fitted to $\mathbf{I}_2$ in block $-\alpha$ (see Appendix C). Thus, the process to fit each matrix $M^4_{i-1,i}(j)^{\dagger}$ into the evolution matrix for two pulses is based on equations (C.1) to obtain $t', B_{h\alpha}, B'_{h\alpha}$ in terms of t:

$$t' \quad = \quad -\frac{J_h}{J'_h} t - \frac{\alpha(2m_{-\alpha} + n_{-\alpha})\pi}{J'_h} \tag{18}$$

$$B_{h\alpha} = \pm\sqrt{\left(\frac{n_{-\alpha}\pi}{t+S_\alpha t'}\right)^2 - J_{\{h\}_{-\alpha}}^2}$$
$$\text{where}: \quad S_\alpha = \frac{J'_{\{h\}_{-\alpha}}}{J_{\{h\}_{-\alpha}}} = \frac{B'_{h\alpha}}{B_{h\alpha}}.$$

Note that equation (16) is still required. Due to $\Delta_{h_{-\alpha}}^{+} + \Delta'^{+}_{h_{-\alpha}} = -(\Delta_{h_\alpha}^{+} + \Delta'^{+}_{h_\alpha})$ and the second equation in (17), this condition is again fulfilled automatically. As for the single pulse case, the relevant equations for non-diagonal block α in $U'_h(t')U_h(t)$ are:

$$1,1: \quad (e'^{\beta^*}_{h\alpha} e_{h\alpha}^{\beta^*} - d'_{h\alpha}d_{h\alpha})e^{i(\Delta'^{+}_{h_\alpha}+\Delta_{h_\alpha}^{+})} = \frac{a_{i-1,j}^{(i-1,j-1)}}{u_{i-1,j}} \tag{19}$$
$$2,1: \quad qi^{*h}(e'^{\beta}_{h\alpha}d_{h\alpha} + e_{h\alpha}^{\beta^*}d'_{h\alpha})e^{i(\Delta'^{+}_{h_\alpha}+\Delta_{h_\alpha}^{+})} = \frac{u_{i,j}}{u_{i-1,j}} \tag{20}$$

and as before, it is now required that $\mu_{i,j} = e^{-2i(\Delta'^{+}_{h_\alpha}+\Delta_{h_\alpha}^{+})}$ to automatically fulfill those equations for entries $1,2$ and $2,2$. Despite their complexity (see Appendix C), the solution is warranted due to the connectivity of the block elements s_{hj} in (13) through of finite products as part of the group $U(2) = U(1) \times SU(2)^2$ when those blocks are adequately combined [39]. In some cases, the solutions could correspond to non-physical or experimentally complex situations, such as $|b_{h\pm\alpha}|, |b'_{h\pm\alpha}| = 1$. The development of this analysis has been included in Appendix C. Because there are many direct and indirect parameters involved, the best strategy is to generate a computational procedure to solve this problem. First, the procedure states the form of each P-unitary matrix factor, $M_{i-1,i}^4(j)^\dagger$, then applies a numerical procedure to solve equations (18,C.9-C.12) together. In it, parameters $z_{j_h}, z_{b_h}, c_\alpha, c'_\alpha, N_{-\alpha}$, introduced in Appendix C, should be selected. Because there are multiple roots, a stochastic procedure to find a specific solution through the correspondent graphs (as those in Figure C.1) becomes more practical. This procedure seeks out solutions to the factorization problem for special unitary evolution matrices U with complex entries based on HI interaction pulses.

5 Special case: Factorization of unitary matrices with real entries

A specific, but very common case can be addressed easily: special unitary matrices U with real entries. This case exhibits an analytical solution depicted in this section in terms of the previous results.

5.1 Analytical solution for $P-$unitary matrix factors with $h = 1$

For $M_{3,4}^4(1)^\dagger, M_{1,2}^4(1)^\dagger, M_{3,4}^4(2)^\dagger$ and $M_{3,4}^4(3)^\dagger$, we cannot the single-pulse case described in section 4.1 due to the factors i^{*h}, i^h on the antidiagonal entries limit to obtain real antidiagonal entries. A possible alternative is to view all entries as imaginary rather than real, and select $\Delta_{h_\alpha}^{-} = \frac{2n_\alpha+1}{2}\pi$. Thus, for the non-diagonal block:

$$s_{hj} = -ie^{i\Delta_{h_\alpha}^{+}}(-1)^{n_\alpha}\begin{pmatrix} \beta j_{h-\alpha} & qb_{h-\alpha} \\ qb_{h-\alpha} & -\beta j_{h-\alpha} \end{pmatrix}. \tag{21}$$

Unfortunately, the impossibility remains because factor i cannot be eliminated to register $e^{i\Delta_{h\alpha}^{+}}$ as imaginary, as it must be real to fit the remaining block to $\mathbf{I}_2$. However, a case with two-pulse solutions does not have this restriction. In stating $\mathcal{R}_\varphi = \mathcal{I}_\phi = 0$, we find several analytic solutions. An easier solution can be found by taking two-pulse s_{hj}, s'_{hj} with the form (21) to obtain:

$$\begin{aligned} s_{hj} \quad &= \quad e^{i(\Delta'^{+}_{h\alpha}+\Delta^{+}_{h\alpha})}(-1)^{n'_\alpha+n_\alpha+1}\begin{pmatrix} A_+ & -q\beta A_- \\ q\beta A_- & A_+ \end{pmatrix} \\ &\text{with}: \quad A_+ = j_{h-\alpha}j'_{h-\alpha} + b_{h-\alpha}b'_{h-\alpha} \\ &\qquad\quad A_- = j_{h-\alpha}b'_{h-\alpha} - b_{h-\alpha}j'_{h-\alpha} \\ &\qquad\quad A_+^2 + A_-^2 = 1 \end{aligned} \tag{22}$$

where the uncomfortable factor i has disappeared. Here, $\Delta_{h\alpha}^{-} = \frac{2n_\alpha+1}{2}\pi \equiv \frac{N_\alpha}{2}\pi, \Delta'^{-}_{h\alpha} = \frac{2n'_\alpha+1}{2}\pi \equiv \frac{N'_\alpha}{2}\pi$. Still, the following equations should be solved to get $b_{h-\alpha}, b'_{h-\alpha}$:

$$\begin{aligned} m_{1,1}^{(i,j)} \quad &\equiv \quad \frac{a_{i-1,j}^{(i-1,j-1)}}{u_{i-1,j}} = (-1)^S(j_{h-\alpha}j'_{h-\alpha} + b_{h-\alpha}b'_{h-\alpha}) \\ m_{2,1}^{(i,j)} \quad &\equiv \quad \frac{u_{i,j}}{u_{i-1,j}} = \beta q(-1)^S(j_{h-\alpha}b'_{h-\alpha} - b_{h-\alpha}j'_{h-\alpha}) \end{aligned} \tag{23}$$

where $S \equiv 2m_{-\alpha} + n_{-\alpha} + n_\alpha + n'_\alpha + 1$ retrieves some integer constants appearing in the procedure. Terms $m_{1,1}^{(i,j)}, m_{2,1}^{(i,j)}$, for short, correspond to entries in each matrix $M_{i-1,i}^4(j)^\dagger$. Those equations can be reduced to the first one by noting ${m_{1,1}^{(i,j)}}^2 + {m_{2,1}^{(i,j)}}^2 = 1$. In the end, both equations only require a review about their signs' concordance in adequately selecting the parameters in S. Still, it is required to write t, t' in terms of $\frac{2n_\alpha+1}{2}$, $\frac{2n'_\alpha+1}{2}$ and $R_{h\alpha}, R'_{h\alpha}$. Then, they may be substituted in the first equation in (18):

$$j_{h-\alpha}\frac{N_\alpha}{2c_\alpha} + j'_{h-\alpha}\frac{N'_\alpha}{2c'_\alpha} \quad = \quad -\alpha(2m_{-\alpha} + n_{-\alpha}) \tag{24}$$

in terms of $j_{h-\alpha}, j'_{h-\alpha}$. As before, while we do not focus explicitly on time here, the definitions introduced in (C.12) for non-dimensional time $\tau = j_{h-\alpha}\frac{N_\alpha}{2}\pi, \tau' = j'_{h-\alpha}\frac{N'_\alpha}{2}\pi$ are useful for reporting specific results regarding the parameters $j_{h\pm\alpha}, j'_{h\pm\alpha}, b_{h\pm\alpha}, b'_{h\pm\alpha}, \tau, \tau'$, without involving the physical parameters $J_{\{h\}_{\pm\alpha}}, J'_{\{h\}_{\pm\alpha}}, J_h, J'_h$. For the identity block, second and third equation in (12), this becomes:

$$\begin{aligned} |j_{h\alpha}| \quad &= \quad |j'_{h\alpha}| = \frac{1}{n_{-\alpha}\pi}(\tau\frac{c_{-\alpha}}{c_\alpha} + \tau'\frac{c'_{-\alpha}}{c'_\alpha}) \\ |b_{h\alpha}| \quad &= \quad |b'_{h\alpha}| \end{aligned} \tag{25}$$

where similarly to c_α, c'_α, we define $c_{-\alpha} = \frac{J_{\{h\}-\alpha}}{J_h}, c'_{-\alpha} = \frac{J'_{\{h\}-\alpha}}{J'_h}$. Signs in $j_{h\alpha}, j'_{h\alpha}$ are physical prescriptions, but not restrictions in the signs of $b_{h\alpha}, b'_{h\alpha}$. For further applications, we assume

these formulas to obtain the diagonal block prescriptions for the two pulses case, which will not be reported explicitly as it requires $c_{\pm\alpha}, c'_{\pm\alpha}$.

Equations (23) and (24) must be solved simultaneously for $j_{h\alpha}$ and $j'_{h\alpha}$. This problem is reduced to quadratic equations, whose solutions can be expressed as:

$$\begin{aligned} j_{h-\alpha} &= \frac{C(A+D) \pm |B|\sqrt{B^2 - C^2 + (A+D)^2}}{B^2 + (A+D)^2} \\ j'_{h-\alpha} &= \frac{E(A+F) \pm |B|\sqrt{B^2 - E^2 + (A+F)^2}}{B^2 + (A+F)^2} \\ \text{with}: \quad & A = (-1)^S m^{(i,j)}_{1,1}, B = m^{(i,j)}_{2,1} \\ & C = \frac{2N_{-\alpha}c'_\alpha}{N'_\alpha}, E = \frac{2N_{-\alpha}c_\alpha}{N_\alpha} \\ & D = F^{-1} = \frac{N_\alpha c'_\alpha}{N'_\alpha c_\alpha} \end{aligned} \tag{26}$$

where solutions still should be selected by reviewing the correct signs in both equations (23), together with the election of signs in $b_{h-\alpha}, b'_{h-\alpha}$. There is no mandatory correspondence between signs in both formulas (26). Ultimately, it is possible to find all parameters involved to generate $M^4_{i-1,i}(j)^\dagger$ with $U_2(t)$. Formula (25) should be analyzed more carefully, due to $|j_{h\alpha}|, |j'_{h\alpha}| \leq 1$. A detailed view shows that the existence of solutions in (26) depends on greater values for N_α, N'_α, while $|j_{h\alpha}|, |j'_{h\alpha}|$ values simultaneously increase. Thus, there are restrictions achieving lower $c_{-\alpha}, c'_{-\alpha}$ and $B_{h_{-\alpha}}$ values.

5.2 Analytical solution for $P-$unitary matrix factors with $h = 2$

This case offers an easy solution for single-pulse selection of $j_{h-\alpha} = 0, |b_{h-\alpha}| = 1$ for the non-diagonal block (requiring strict control on $J_{\{h\}_\alpha}$ value):

$$s_{hj} = (-1)^{n-\alpha} \begin{pmatrix} \cos B_{h-\alpha}t & q\text{sign}(b_{h-\alpha}) \sin B_{h-\alpha}t \\ -q\text{sign}(b_{h-\alpha}) \sin B_{h-\alpha}t & \cos B_{h-\alpha}t \end{pmatrix} \tag{27}$$

This involves the acquisition of t and $B_{h\alpha}$ from (15), to obtain $\mathbf{I}_2$ for the remaining diagonal block, at which point we solve:

$$\begin{aligned} B_{h-\alpha} &= \frac{1}{t}\cos^{-1}\frac{(-1)^{n-\alpha}a^{(i-1,j-1)}_{i-1,j}}{u_{i-1,j}} \\ &\text{with}: \\ & \text{sign}(B_{h-\alpha}) = (-1)^{n-\alpha+1} q\text{sign}(\frac{u_{i,j}}{u_{i-1,j}} \sin B_{h-\alpha}t) \end{aligned} \tag{28}$$

to obtain $B_{h-\alpha}$. This equation is equivalent to (B.5). This procedure works to obtain $M^4_{2,3}(1)^\dagger, M^4_{2,3}(2)^\dagger$. Two-pulse practical solutions are not possible because they require the same condition $j_{h-\alpha} = 0$ to have the form (6). Because $j_{h-\alpha} = 0$, variables as τ are not appropriate. Instead, we introduce the variables $\tau_0 \equiv J_h t$ and $b_0 \equiv \frac{B_{h-\alpha}}{J_h}$ (the equivalent

expression for (28) in these terms is immediate) to report results for non-diagonal block α. For the identity block, $-\alpha$, the use of $j_{h\alpha}$ is still appropriate and can be written as $j_{h\alpha} = \frac{N_{-\alpha}c_{-\alpha}}{n_{-\alpha}}$, where, as for the two-pulse case: $N_{-\alpha} = -\alpha(2m_{-\alpha} + n_{-\alpha}), c_{-\alpha} = \frac{J_{\{h\}-\alpha}}{J_h}$. As usual, $|b_{h\alpha}| = \sqrt{1 - j_{h\alpha}^2}$ with the sign selected arbitrarily. We will assume these formulas to report the diagonal block prescriptions for the single-pulse case (with the exception of $b_{h\alpha}$).

5.3 Existence of solutions for U with real entries

Formulas for $h = 2$ are simple; their only issue is the restriction of $j_{h-\alpha} = 0$, which implies some control of the interaction strength in (12). In addition, the correct election of signs depicted in formula (28) is a trivial aspect in spite of trigonometric function properties. For $h = 1$, several parameters appear, but analytical solutions are possible. As for the values of c_α, c'_α, the signs of $j_{h-\alpha}, j'_{h-\alpha}$ are not eligible because they are physical constants from the system. Still, by example, if $|B| > |C|, C > 0, A + D > 0$ then $j_{h-\alpha} > 0$; here, however, if $|B| > |C|, C > 0, A + D < 0$ then $j_{h-\alpha} < 0$. Conditions are similar for $j'_{h-\alpha}$. A brief analysis shows these expressions acquire both signs for $j_{h-\alpha}, j'_{h-\alpha}$ with an adequate selection of $N_{-\alpha} \in \mathbf{Z}$ and N_α, N'_α (both odd). Typically, a change of signs in N_α, N'_α implies a change of signs in $j_{h-\alpha}, j'_{h-\alpha}$ solutions. In addition, solutions are physically meaningful ($|j_{h-\alpha}|, |j'_{h-\alpha}| \leq 1$) if we select higher values for $|N_\alpha|, |N'_\alpha|$ because they reduce C, E values. By this reason, typically large values in $N_{-\alpha}$ do not give physical solutions; this election could give $|j_{h-\alpha}|, |j'_{h-\alpha}| > 1$ because D and F values increase. This can be avoided only if c_α, c'_α can be manipulated.

6 Application to dedicated gates

As stated previously, quantum gate design can be approached as a product of successive gates selected from a universal set [28]. Such is the case for the Shor basis $\{H, \sigma_z^{1/2}, C^aNOT_b\}$ and the Boykin basis $\{H, \sigma_z^{1/4}, C^aNOT_b\}$, which have been shown to be fault tolerant [54, 55, 29]. The main limitation with this approach is the difficulty in constructing arbitrary gates in such terms. A factorization approach, despite having complex prescriptions, avoids this limitation and could be useful to dedicated gates (as opposed to gates for universal-purpose quantum computers). This is the main reason to not discuss how to construct the first kind of basic universal sets in terms of HI interaction, despite they can be obtained under unitary factorization. These aspects have been reviewed for equivalent gates to C^aNOT_b and others (evolution loops and exchange operations) [39, 52, 56]. Similarly, it is easy to realize that $\sigma_z^{1/2}$ and $\sigma_z^{1/4}$ can be generated (based on the Bell basis grammar) from the block (14) for a single pulse by choosing $b_{h-\alpha} = 0, |j_{h-\alpha}| = 1$, at least if interaction strengths can be controlled. The following cases demonstrate applications for the factorization procedure for some standard or dedicated gates under specific processing tasks.

The next special unitary matrices in $SU(4)$ are not achievable for exclusive interactions in only one S_h, but are so through a combination of elements from at least two groups showing the factorization approach. The use of the non-local basis of Bell states as a common grammar for the three Hamiltonians (12) is seminal [39], and current results establish that an operation $U \in SU(4)$ can be reproduced by a finite product of elements in $\mathrm{S}_1, \mathrm{S}_2$ via unitary factorization. In the following analysis, we assume that factorization is being developed by a system with some physical properties as: a) interaction strength constants positive (or zero

if it is required), $j_{h\pm\alpha}, j'_{h\pm\alpha}$, and b) relative strength ratios settled as $c_\alpha, c'_\alpha = 1, c_\alpha, c'_\alpha = 0.5$. Note that these settings are selected only to report concrete results, they are not real restrictions. Because of the multiplicity of solutions in terms of the parameters involved $m_{-\alpha}, n_{-\alpha}, n_\alpha, n'_\alpha$ (or some of their associated values as $N_{\pm\alpha}, N'_\alpha$), we will select the lowest ones possible. Due to τ, τ' definitions, they can become negative (but not in the actual case with $j_{h\pm\alpha}, j'_{h\pm\alpha}$ positive), remembering that they are non-physical times (positiveness of t, t' is always recovered). In the following section, a couple of applications will be developed to show how the factorization procedure is carried out for unitary matrices with real entries.

6.1 Equivalent gate to C^1NOT_2 gate in Bell basis

C^1NOT_2 gate in the computational basis is a very common and useful gate in quantum computation. An equivalent gate with a determinant equal to one is the controlled gate $C^1(iY_2)$. This gate can be reproduced in the factorization scheme, noting that in the Bell basis it is:

$$\begin{aligned} U &= \frac{1}{2}\begin{pmatrix} 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 \end{pmatrix} \\ &= (\mathcal{H}_1 \otimes \mathbf{I}_2) C^1NOT_2 (C^1(iY_2)) C^1NOT_2 (\mathcal{H}_1 \otimes \mathbf{I}_2). \end{aligned} \tag{29}$$

This gate can be generated using the current procedure through magnetic pulses. Quantum algorithms using C^1NOT_2 gates could be translated in terms of $C^1(iY_2)$. The Bell basis version of this gate was used to design control gates to mimic the traditional teleportation quantum algorithm using HI interaction [39, 53] (there, the treatment is a little different because $C^1(iY_2)$ operates on a grammar based on Bell states instead of the typical computational basis). It suggests that specialized gates can be constructed via factorization in magnetic systems through HI interaction.

We can decompose the process described in the previous sections in several $P-$unitary factors achievable by physical interactions. They and their respective design parameters are reported in Table 1 in the terms presented previously and in the order in which they should be applied.

6.2 Characterization process

The preparation of quantum states requires the ability to change their properties. A characterization process [57] is a unitary operation by which to change the superposition ratios and entanglement amount in an initial state. The importance of this operation lies in the DiVincenzo criteria for the reliability of quantum states preparation. The current example shows that for a real characterization matrix ($\alpha^2 + \beta^2 + \gamma^2 + \delta^2 = 1$):

$$U = \begin{pmatrix} \alpha & \beta & \gamma & -\delta \\ \beta & -\alpha & \delta & \gamma \\ \gamma & -\delta & -\alpha & -\beta \\ \delta & \gamma & -\beta & \alpha \end{pmatrix} \tag{30}$$

Table 1. Factorization in $P-$unitary matrices for $C^1(iY_2)$ and design parameters for the non-diagonal block.

$P-$unitary factors	Design parameters
$M^4_{3,4}(1)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.681$ $N_\alpha = 3, N'_\alpha = -3$ $j_{-\alpha} = 0.120, b_{-\alpha} = 0.993$ $j'_{-\alpha} = 0.787, b'_{-\alpha} = 0.617$ $\tau = 0.568, \tau' = 3.709$
$M^4_{2,3}(1)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$m_{-\alpha} = -2, n_{-\alpha} = 3$ $j_\alpha = 0.167$ $b_0 = 0.696$ $\tau_0 = 3.142$
$M^4_{1,2}(1)^\dagger$ $\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.968$ $N_\alpha = 3, N'_\alpha = -3$ $j_{-\alpha} = 0.312, b_{-\alpha} = 0.950$ $j'_{-\alpha} = 0.978, b'_{-\alpha} = 0.205$ $\tau = 1.471, \tau' = 4.613$
$M^4_{3,4}(2)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.692$ $N_\alpha = 3, N'_\alpha = -3$ $j_{-\alpha} = 0.128, b_{-\alpha} = -0.992$ $j'_{-\alpha} = 0.795, b'_{-\alpha} = 0.607$ $\tau = 0.603, \tau' = 3.745$
$M^4_{2,3}(2)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$m_{-\alpha} = -2, n_{-\alpha} = 3$ $j_\alpha = 0.167$ $b_0 = 0.696$ $\tau_0 = 3.142$
$M^4_{3,4}(3)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.681$ $N_\alpha = 3, N'_\alpha = -3$ $j_{-\alpha} = 0.120, b_{-\alpha} = 0.993$ $j'_{-\alpha} = 0.787, b'_{-\alpha} = 0.617$ $\tau = 0.568, \tau' = 3.709$

there exist a process of quantum modeling based on factorization. A rich research field for the powers for these unitary characterization matrices is still open in terms of their convergence. The following matrix represents one of these operations (numbers are casual to illustrate the factorization process depicted here):

$$U = \frac{1}{10}\begin{pmatrix} 7 & 1 & 7 & -1 \\ 1 & -7 & 1 & 7 \\ 7 & -1 & -7 & -1 \\ 1 & 7 & -1 & 7 \end{pmatrix} \tag{31}$$

This operation based on the Bell basis allows some initial Bell states (or a superposition of them) to be transformed into other states on demand. Following the process to find the design parameters for their $P-$unitary factors, we can reproduce this operation by factorization. For

Table 2. Factorization in $P-$unitary matrices for a characterization matrix U and design parameters for the non-diagonal block.

$P-$unitary factors	Design parameters
$M^4_{3,4}(1)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{7}{5\sqrt{2}} & -\frac{1}{5\sqrt{2}} \\ 0 & 0 & \frac{1}{5\sqrt{2}} & \frac{7}{5\sqrt{2}} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.500$ $N_\alpha = -3, N'_\alpha = -3$ $j_{-\alpha} = 0.400, b_{-\alpha} = 0.916$ $j'_{-\alpha} = 0.267, b'_{-\alpha} = 0.964$ $\tau = 1.886, \tau' = 1.256$
$M^4_{2,3}(1)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{51}} & -5\sqrt{\frac{2}{51}} & 0 \\ 0 & 5\sqrt{\frac{2}{51}} & \frac{1}{\sqrt{51}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$m_{-\alpha} = -2, n_{-\alpha} = 3$ $j_\alpha = 0.167$ $b_0 = 0.548$ $\tau_0 = 3.142$
$M^4_{1,2}(1)^\dagger$ $\begin{pmatrix} \frac{7}{10} & -\frac{\sqrt{51}}{10} & 0 & 0 \\ \frac{\sqrt{51}}{10} & \frac{7}{10} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.968$ $N_\alpha = -3, N'_\alpha = 3$ $j_{-\alpha} = 0.978, b_{-\alpha} = 0.205$ $j'_{-\alpha} = 0.312, b'_{-\alpha} = 0.950$ $\tau = 4.612, \tau' = 1.471$
$M^4_{3,4}(2)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{7}{10} & -\frac{\sqrt{51}}{10} \\ 0 & 0 & \frac{\sqrt{51}}{10} & \frac{7}{10} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.704$ $N_\alpha = -3, N'_\alpha = 3$ $j_{-\alpha} = 0.802, b_{-\alpha} = 0.596$ $j'_{-\alpha} = 0.136, b'_{-\alpha} = 0.991$ $\tau = 3.783, \tau' = 0.641$
$M^4_{2,3}(2)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{51}} & -5\sqrt{\frac{2}{51}} & 0 \\ 0 & 5\sqrt{\frac{2}{51}} & -\frac{1}{\sqrt{51}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$m_{-\alpha} = -2, n_{-\alpha} = 3$ $j_\alpha = 0.167$ $b_0 = 0.455$ $\tau_0 = 3.142$
$M^4_{3,4}(3)^\dagger$ $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{7}{5\sqrt{2}} & -\frac{1}{5\sqrt{2}} \\ 0 & 0 & \frac{1}{5\sqrt{2}} & \frac{7}{5\sqrt{2}} \end{pmatrix}$	$N_{-\alpha} = -1$ $j_\alpha = j'_\alpha = 0.500$ $N_\alpha = -3, N'_\alpha = -3$ $j_{-\alpha} = 0.400, b_{-\alpha} = 0.916$ $j'_{-\alpha} = 0.267, b'_{-\alpha} = 0.964$ $\tau = 1.886, \tau' = 1.256$

the specific case (31), these factors and parameters are reported in Table 2.

7 Remarks around fault-tolerant implementation and generalization for $N-$qubits

7.1 Natural structure for fault-tolerant implementation and quantum error correction

An additional treatment associated with quantum error correction is recommended for the factorization presented, so we drafted some ideas for further development in that direction. Quantum gate design based on physical interactions should consider more than the possible quantum state errors in the form of flips generated from environmental noise, as has been analyzed under quantum error correction theory based on codification [54, 11, 58]. Fault-tolerant operations are still useful where environmental noise does not generate errors in the exact gate

prescriptions. Thus, in order for quantum error correction schemes to work, we must conduct a more delicate analysis of malfunctioning for the gate factors in the factorization process. Malfunctioning is understood here as the effect of a tiny variation or error δp_i in at least one of the several prescribed parameters $\mathbf{p} = (p_1, ..., p_m)$ ($t, B_{h\pm\alpha}, J_h, J_{\{h\}_{\pm\alpha}}$ in the present context) to blocks of the form (14). Due to the $SU(4)$ decomposition in $U(1) \times SU(2)^2$:

$$U_h = \bigoplus_{j=1}^{2} s_{hj}, |\psi_0\rangle = \bigoplus_{j=1}^{2} \alpha_j \left|\psi_{0j}\right\rangle \Rightarrow |\psi\rangle = U_h \left|\psi_0\right\rangle = \bigoplus_{j=1}^{2} \alpha_j s_{hj} \left|\psi_{0j}\right\rangle \tag{32}$$

emphasizing the direct sum form of matrix evolution, with j appointing to each block in the whole matrix. Thus, each $\left|\psi_{0j}\right\rangle$ is a linear combination of different pairs of Bell states depending on h. Thus, we can focus just on each $s_{hj} \equiv e^{i\phi}u$ ($\phi \in \mathbf{R}, u \in SU(2)$) for the current analysis. If we define the operator (linear in the parameters errors):

$$\mathcal{D} \equiv \delta\mathbf{p} \cdot \nabla = \sum_{i=1}^{m} \delta p_i \frac{\partial}{\partial p_i} \tag{33}$$

then, developing until the first non-trivial order in $\delta\mathbf{p}$:

$$\begin{aligned}
s_{hj} &= {s_{hj}}^0 + \mathcal{D}{s_{hj}}^0 + \frac{1}{2}\mathcal{D}^2{s_{hj}}^0 + ... && (34)\\
\left|\phi_{fj}\right\rangle &= (1 + (\mathcal{D}{s_{hj}}^0){s_{hj}}^{0\dagger}) \left|\psi_{fj}\right\rangle = (1 + i\mathcal{D}\phi + (\mathcal{D}u)u^\dagger) \left|\psi_{fj}\right\rangle && (35)\\
\mathcal{F}_j^2 &= \left|\left\langle \phi_{fj} | \psi_{fj} \right\rangle\right|^2 && (36)\\
&= 1 + \left|\left\langle \psi_{fj}\right| \mathcal{D}{s_{hj}}^0 {s_{hj}}^{0\dagger} \left|\psi_{fj}\right\rangle\right|^2 - \left\langle \psi_{fj}\right| {s_{hj}}^0 \mathcal{D}{s_{hj}}^{0\dagger} \mathcal{D}{s_{hj}}^0 {s_{hj}}^{0\dagger} \left|\psi_{fj}\right\rangle
\end{aligned}$$

where ${s_{hj}}^0$ corresponds to the evolution with the correct parameters in the gate design; $\left|\psi_{0j}\right\rangle, \left|\psi_{fj}\right\rangle = {s_{hj}}^0 \left|\psi_{0j}\right\rangle, \left|\phi_{fj}\right\rangle$ are the initial, the final desired and the final obtained states; and $\mathcal{F}_j$ is the fidelity in the subspace j for the final state. Additionally, in spite of simplicity, $\mathcal{D}{s_{hj}}^0 \equiv \mathcal{D}s_{hj}\Big|_{{s_{hj}}^0}$. The unitary properties of ${s_{hj}}^0$ have been used to simplify (35) to $\mathcal{D}({s_{hj}}^{0\dagger}{s_{hj}}^0) = 0$. One notable aspect is the quadratic dependence on errors for the fidelity and the probability, suggesting a controllable impact on them.

As in (14), each block operator s_{hj} can be expressed on a proper Pauli basis for $SU(2)$ subspace [39]: $\mathbf{I}_{hj}, \mathbf{X}_{hj}, \mathbf{Y}_{hj}, \mathbf{Z}_{hj}$. As for the computational basis, they require a language for discrete quantum operations in each block, with natural syndromes present (for $h = 2, j = 1$, subspace is generated by $|\beta_{--}\rangle, |\beta_{++}\rangle$, then $\mathbf{X}_{21}$ is a bit flip in the second qubit followed by a phase flip in the first one; $\mathbf{Y}_{21}$ is a phase flip followed by a bit flip in the second qubit; while, $\mathbf{Z}_{21}$ is a phase flip or a bit flip in both qubits). This identification conducts to the possible quantum errors and their associated probabilities. These errors can be solved by traditional quantum error correction methods with the adequate codification.

7.2 Generalization of unitary factorization for $N-$qubits

The generalization of unitary factorization for N qubits under the conditions stated here requires the fulfillment of several restrictions. We discuss briefly the central aspects appearing there in subsections to follow. Nevertheless, note that the procedures presented in this work for two qubits will work properly, still considering quantum systems with more than two qubits because the universality of bipartite processing. The interest in such generalization is useful for designing more complex gates that can to process more than two qubits simultaneously.

7.2.1 Hamiltonian restrictions in the generalization for the 2×2 block decomposition

The 2×2 block structure will not be easy to present in the general case for $N-$qubits in the nearest-neighbour HI chains (reduction to 2×2 block structure is always possible, but it is not evident how to select a realistic basis departing from the Bethe Ansatz approach to get the eigenstates). Despite, still some alternative architectures could be addressed to recover that structure in the Hamiltonian and consequently in the evolution for some achievable basis. For $N = 2d, d \in \mathbf{Z}$, a kind of weakly interactive chains via entanglement, could be realized (those where HI interaction is only allowed at the time between each one of the d pairs of the chain), recovering then the 2×2 structure in the Hamiltonian [63]. Still, a convenient basis should be allocated to reveal it. In this case, the basis becomes the generalized Bell basis [64], making this configuration the best generalization for the scheme presented in [39]. Hamiltonian is diagonal in this basis, and the block structure is recovered through some local or non-local additional interactions; one of them is the local control in just one pair of the qubits interacting already via the HI model. In other cases, further discussion will be applicable in general if an adequate basis can be found.

7.2.2 General structure underlying quantum information dynamics

Because the previous structure is typically expressed on a non-local basis, local interactions can generate multiple transformations in each term of a general quantum state (except in those where the pair possessing HI and local interactions can separate from the remaining system). In this sense, the formalism actually operates on the quantum information grammar settled on the system more than in its physical parts. As such, the structure of the evolution matrix is no longer reduced to $P-$unitary matrices because only two kinds of blocks can be achieved through the entire matrix evolution, each one operating on one half of the overall generalized Bell basis states. Here, a more complex structure appears and factorization should be addressed in different terms. Depending on the direction of the local interactions and the selection of the pair where it is applied, the position of the 2×2 blocks in the evolution matrix can be selected. The options for these selections grow as $3d$ while the number of generalized Bell basis states grows exponentially as 4^d. Although other interactions could be used under this scheme [63], particularly those non-local and able to generate extended entanglement, if this set of interactions can combine to form arbitrary quantum states in the chain, represents an ongoing problem.

8 Conclusions

Quantum storage and quantum information processing allow the fulfillment of computational tasks impossible to achieve using conventional information technologies or with quantum

optical systems exclusively. In this arena, magnetic systems based on trapped ions, nuclear magnetic resonance, doped silicon and quantum dots have exhibited the potential to make stable and efficient developments for spin-based quantum processing [59]. All of them exploit HI interactions in several approaches together with quantum states control and, in particular, with entanglement control [60].

QGAC was the first approach developed for quantum computation, but quantum annealing [61] and measurement-based quantum computation [62], in which magnetic systems modeled by HI interactions can manage a controlled manipulation, now offer alternatives. In addition to traditional quantum algorithms based on classical-like computing gates, several applied problems have been addressed as goals (pattern matching, folding proteins and other particular NP-complete problems [60]). These specific problems require complex dedicated quantum algorithms not always easy to decode in terms of a universal gates set. Here, unitary factorization brings general procedures to construct complex processing rules.

In this work, solutions (25-28) set a concrete theoretical method to generate gates with real entries based on HI interaction for two qubits. More generally, procedure (C.9-C.12) states a numerical strategy to solve the same problem for complex entry gates. An important extension of $SU(2)$ decomposition for $SU(2^n)$ could be achievable for multiqubit systems [63]. Then it would be possible to draw the evolution in terms of manipulation blocks on a grammar of natural states (as Bell states were in this work) extending the current unitary factorization to systems [38] based on two-level interactions or a higher number of qubits to be processed simultaneously. This generalization could be achieved by stating specific rotations in pairs of eigenstates to set the $SU(2)$ blocks. The challenge would be to adapt those rotations to well-known and reproducible states.

As has been demonstrated, $SU(2)$ block decomposition allows the easy recovery of traditional quantum error correction for the unitary factorization procedure, possibly with more complex error syndromes than in $SU(2)$ for single qubits while remaining controllable and discrete. Clearly, error correction is tightly linked to the control of physical parameters (magnetic field, time measurement, precise knowledge of interaction strengths, etc.). In this line of research the inclusion of processing at a finite temperature is an extension by which to consider decoherence effects in the procedures. Despite the theoretical and experimental claim that rectangular magnetic pulses are easily managed when under tight control, an improved analysis using alternative continuous pulses is in order to generate equivalent effects and then effects and factorization procedures equivalent to those developed here. $SU(2)$ decomposition is not exclusive from constant magnetic fields. The use of continuous fields, such as $B_i(t) = B_{i0} + B_i \sin \omega_i t)$ [52] for each magnetic field in (12), suggests that we apply directed waves on matter to generate controlled quantum operations based on unitary factorization.

The presented procedure assumes coherence and stability. For experimental applications to be set up using the current proposal regarding these technologies, a defined position and strict strength interaction controls should be developed. Currently, the capacity to induce and control gate processing on matter is still far-off, but it is emerging with the fast development of quantum technologies.

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Appendix A: 3D anisotropic Ising model and notation

As in [39]: Greek scripts for $-,+$ (or $-1,+1$, as better they adapt to the mathematical expressions), associated with the components of states and operators in the Bell basis as they were settled before; Latin scripts for $h,i,j,k,...$ and for spatial directions x,y,z or $1,2,3$. We use $\cdot$ to emphasize some products to avoid misconceptions in script expressions. If $\{\mathbf{I}_{h_j},\mathbf{X}_{h_j},\mathbf{Y}_{h_j},\mathbf{Z}_{h_j}\}$ is the local Pauli basis for each corresponding $SU(2)$ block j, then the 2×2 block structure in H_h and $U_h(t)$ arises:

$$\begin{aligned} s_{hj} &= e^{i\Delta_{h\alpha}^{+}} e^{-i\Delta_{h\alpha}^{-}\mathbf{n}_{j(\alpha)}\cdot\mathbf{S}_{h_j}} \\ &= e^{i\Delta_{h\alpha}^{+}}(\cos\Delta_{h\alpha}^{-}\mathbf{I}_{h_j} - i\sin\Delta_{h\alpha}^{-}\mathbf{n}_{j(\alpha)}\cdot\mathbf{S}_{h_j}) \\ \text{where}: \quad & \mathbf{n}_{j(\alpha)} = (qb_{h_{-\alpha}}\sin\frac{h\pi}{2}, qb_{h_{-\alpha}}\cos\frac{h\pi}{2}, \beta j_{h_{-\alpha}}) \\ & \mathbf{S}_{h_j} = (\mathbf{X}_{h_j},\mathbf{Y}_{h_j},\mathbf{Z}_{h_j}) \end{aligned} \tag{A.1}$$

explicitly revealing the $U(2)=U(1)\times SU(2)$ nature. This corresponds to the expression for the mixing matrix given in (14), where h is the magnetic field direction; $j=1,2$ is an ordering label for the blocks as they appear consecutively in the rows of the evolution matrix; k_j,l_j are the labels for its rows in $U_h(t)$ (in s_{21}, $k_2=2,l_2=3$ are the labels for the rows of the second block, $j=2$, in $U_{h=2}(t)$). Note that $\det(s_{hj})=e^{2i\Delta_{h\alpha}^{+}}$ is unitary. In addition, $\alpha=(-1)^{h+j+1},\beta=(-1)^{j(h+l_j-k_j+1)}$ and $q=\beta(-1)^{h+1}$. The reduced parameters are [39]:

$$\begin{gathered} b_{h\pm}=\frac{B_{h\pm}}{R_{h\pm}},\quad j_{h\pm}=\frac{J_{\{h\}\mp}}{R_{h\pm}}\in[-1,1],\quad \Delta_{h\mu}^{\nu}=\frac{t}{2}(E_{h\mu+}+\nu E_{h\mu-}) \\ e_{h\alpha}^{\beta}=\cos\Delta_{h\alpha}^{-}+i\beta j_{h-\alpha}\sin\Delta_{h\alpha}^{-},\quad d_{h\alpha}=b_{h-\alpha}\sin\Delta_{h\alpha}^{-} \end{gathered} \tag{A.2}$$

depending on the energy eigenvalues $E_{h\mu\nu}=\mu J_h+\nu R_{h-\mu}$ ($E_{h\pm\pm}$,$E_{h\pm\mp}$) and the physical parameters in H_h:

$$R_{h\pm} = \equiv\sqrt{B_{h\pm}^2+J_{\{h\}\mp}^2},\quad J_{\{h\}\pm}\equiv J_i\pm J_j,\quad B_{h\pm}=B_{1_h}\pm B_{2_h} \tag{A.3}$$

where h,i,j are a cyclic permutation of $1,2,3$; then, $\{h\}$ is said equivalent to the pair i,j. In this terms, as was stated in [39]:

$$U_h(t)=\bigoplus_{j=1}^{2}s_{hj}=\bigoplus_{\alpha\in\{-,+\}}e^{i\Delta_{h\alpha}^{+}}e^{-i\Delta_{h\alpha}^{-}\mathbf{n}_{j(\alpha)}\cdot\mathbf{S}_{h_{j(\alpha)}}} \tag{A.4}$$

This expression states the block structure of U_h, which, due to the independence of the blocks (in terms of the physical parameters involved) lets to set the desired $P-$unitary forms.

Appendix B: Solutions for unitary factorization with one magnetic pulse

If $a_{i-1,j}^{(i-1,j-1)}\equiv|a_{i-1,j}^{(i-1,j-1)}|e^{i\phi_{i-1,j}^{(i-1,j-1)}}$ and $u_{i,j}\equiv|u_{i,j}|e^{i\varphi_{i,j}}$ (note that a non-zero phase applies only for $u_{n,j}$, the first element to be eliminated in the bottom of each column), then by

splitting the restrictions for phases and magnitudes, we find the next equivalent conditions to (17), where $\chi \equiv b_{h-\alpha} \sin \Delta_{h\alpha}^{-}$:

$$|\chi| = \frac{|u_{i,j}|}{u_{i-1,j}} = |b_{h-\alpha} \sin \Delta_{h\alpha}^{-}| \tag{B.1}$$

$$\phi_{i-1,j}^{(i-1,j-1)} = \Delta_{h\alpha}^{+} - \tan^{-1}(j_{h-\alpha}\beta \tan \Delta_{h\alpha}^{-}) \tag{B.2}$$

$$\varphi_{i,j} = \Delta_{h\alpha}^{+} - \frac{\pi}{2}(h - 1 + \text{sign}(q\chi)) \tag{B.3}$$

This procedure purports to solve these equations for the non-diagonal block in each $P-$unitary matrix of (1) in combination with the identity block requirements (15) (changing α by $-\alpha$). It fits $U_h(t)$ to the forms (2). Thus, each matrix becomes an evolution boost through a magnetic field pulse with specific strength and duration. Unfortunately, this procedure sometimes fails to give solutions in spite of (B.3), which cannot always be fulfilled $\Delta_{h-\alpha}^{+} = -\Delta_{h\alpha}^{+} = (2m_{-\alpha} + n_{-\alpha})\pi$ [52] and $\Delta_{h-\alpha}^{-} = n_{-\alpha}\pi$ with $m_{-\alpha}, n_{-\alpha} \in \mathbf{Z}$. Then, for $h = 1$, $\varphi_{i,j} = 0$ or the specific value $\varphi_{n,j}$ is usually impossible. For $h = 2$, (B.3) is easily fulfilled for $U^{(i,j)}$ with real entries selecting sign$(q\chi)$ adequately: $\varphi_{i,j} = -((2m_\alpha - n_\alpha) + \frac{1}{2}(1 + \text{sign}(q\chi))\pi$. By defining $\theta \equiv J_{\{h\}_\alpha} t$ and due to $|\chi| \equiv |u_{i,j}|/u_{i-1,j} \in [0, 1]$, (B.1) can be written as:

$$\chi = \text{sign}(b_{h-\alpha}) \sqrt{1 - \frac{\theta^2}{\Delta_{h\alpha}^{2-}}} \sin \Delta_{h\alpha}^{-}. \tag{B.4}$$

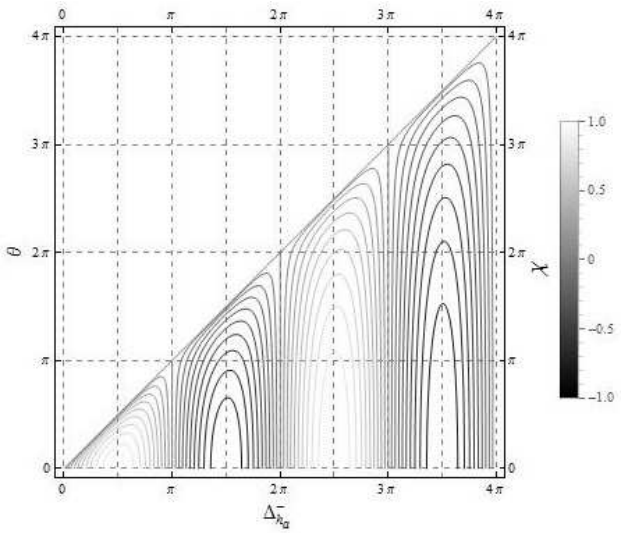

Fig. B.1. Solutions of (B.1) for different values of $\chi \in [-1, 1]$, shown with gray levels in the χ-scale on the right. They are limited to the lower diagonal half in the first quadrant.

Some solutions are shown in Figure B.1 for values $\chi \in [-1, 1]$ (note $0 \leq \chi \leq 1$ because $|u_{i,j}| \leq u_{i-1,j}$). They are reported as a gray scale in the graphs. The range for $\Delta_{h\alpha}^{-}$ becomes

limited while $|\chi|$ increases. Due to (B.4), $\Delta_{h\alpha}^{-}$ values when $\theta = 0$ determines the range of $\Delta_{h\alpha}^{-}$ by continuous sections. These ranges are fixed for each value of χ and are located in the intervals $[(n-1)\pi, n\pi], n \in \mathbf{Z}^{+}$. When $|\chi|$ increases, (B.2) and (B.3) can be fulfilled hardly because the range of $\Delta_{h\alpha}^{-}$ shrinks. In addition, for the real entries case, the equation (B.2) requires $\tan \Delta_{h\alpha}^{-} = 0$ or $j_{h-\alpha} = 0$ (then $|b_{h-\alpha}| = 1$). The first restriction is impossible except for $|\chi| = 0$ (which is seldom useful), and second is only applicable in partially anisotropic or isotropic interactions ($J_{\{y\}_{\alpha}} = J_z - J_x = 0$). In the last case, $|\chi| = |\sin \Delta_{h\alpha}^{-}|$, so $M_{2,3}^{4}(1)$ and $M_{2,3}^{4}(2)$ can be constructed with driven magnetic fields in the $y-$direction in only one pulse. Additional prescriptions are given by (15) by changing α by $-\alpha = +1$, in agreement with (13) for the diagonal block in $U_2(t)$ to fit it to $M_{2,3}^{4}$. For the non-diagonal block (with $\alpha = -1$), it is required that $\mathrm{sign}(a_{i-1,j}^{(i-1,j-1)}) = (-1)^{n_{-\alpha}} \mathrm{sign}(\cos \Delta_{h\alpha}^{-})$, $\mathrm{sign}(u_{i,j}) = (-1)^{n_{-\alpha} - \frac{1}{2}(1+\mathrm{sign}(q\chi))} = (-1)^{n_{-\alpha} - \frac{1}{2}(1-\mathrm{sign}(\chi))}$ (which could be a strong restriction due to $\varphi_{i,j}$) and:

$$B_{h-} = \frac{1}{t} \sin^{-1} \frac{u_{i,j}}{u_{i-1,j}} \tag{B.5}$$

where the election of the inverse for sine function should be selected to fulfill the previous relations for the signs of $a_{i-1,j}^{(i-1,j-1)}, u_{i,j}$.

Appendix C: Solutions for unitary factorization with two magnetic pulses

Prescriptions to obtain $\mathbf{I}_2$ in the block $-\alpha$ using two pulses are [52]:

$$\begin{gathered} \Delta_{h-\alpha}^{-} + \mathrm{sign}(J_{\{h\}_{-\alpha}} J'_{\{h\}_{-\alpha}}) \Delta'^{-}_{h-\alpha} = n_{-\alpha}\pi \\ \Delta_{h-\alpha}^{+} + \Delta'^{+}_{h-\alpha} = (2m_{-\alpha} + n_{-\alpha})\pi \\ \frac{B'_{h\alpha}}{J'_{\{h\}_{-\alpha}}} = \frac{B_{h\alpha}}{J_{\{h\}_{-\alpha}}} \end{gathered} \tag{C.1}$$

with $m_{-\alpha}, n_{-\alpha} \in \mathbf{Z}$ giving (18). For the non-diagonal block, we can divide equations (19-20) into four equations: two for the magnitudes and two for the phases. Because each block is unitary, equations for magnitudes become equivalent. For example, taking the $2,1$ entry:

$$|\chi_h| \equiv \frac{|u_{i,j}|}{u_{i-1,j}} = |e'^{\beta}_{h\alpha} d_{h\alpha} + e_{h\alpha}^{\beta^*} d'_{h\alpha}| \tag{C.2}$$

$$\varphi_{i,j} = \varphi'_{i,j} + (\Delta'^{+}_{h\alpha} + \Delta_{h\alpha}^{+}) - \frac{\pi}{2}(h - 1 + \mathrm{sign}(q)) \tag{C.3}$$

$$\phi_{i-1,j}^{(i-1,j-1)} = \phi'^{(i-1,j-1)}_{i-1,j} + (\Delta'^{+}_{h\alpha} + \Delta_{h\alpha}^{+}) \tag{C.4}$$

for the non-diagonal block α. Here, $\phi'^{(i-1,j-1)}_{i-1,j} = \arg(e'^{\beta^*}_{h\alpha} e_{h\alpha}^{\beta^*} - d'_{h\alpha} d_{h\alpha})$ and $\varphi'_{i,j} = \arg(e'^{\beta}_{h\alpha} d_{h\alpha} + e_{h\alpha}^{\beta^*} d'_{h\alpha})$. Note that phase (C.3) makes a difference with respect to the impossibility in the one-pulse case ($s_{hj} \in U(2)$ by itself cannot generate completely $U(2)$). Meanwhile, $a_{n,n}^{(n,n-1)} = (-1)^P \det(U)$, where P is the global parity for the sum of the $n_{-\alpha}$ values used in each $M_{i-1,i}^{n}(j)^{\dagger}$ in (1) (thus, $U^{(n-1,n-1)} = \mathbf{I}_4$ in (1) if $U \in SU(4)$ and $P = 0$).

Next, (19-20) or (C.2-C.4) should be solved together with (18) to obtain $t, B_{h-\alpha}, B'_{h-\alpha}$. These are more easily solved if they are expressed in terms of the parameters $j_{h-\alpha}, j'_{h-\alpha}, b_{h-\alpha}, b'_{h-\alpha}$, $\Delta_{h\alpha}^{-}, \Delta'^{-}_{h\alpha}$. Separating the real and the imaginary parts in $e'^{\beta}_{h\alpha} d_{h\alpha} + e^{\beta^*}_{h\alpha} d'_{h\alpha}$, we define:

$$\begin{aligned} \mathcal{R}_\varphi &\equiv b_{h-\alpha} \sin\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha} + b'_{h-\alpha} \cos\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha} \\ \mathcal{I}_\varphi &\equiv \beta \sin\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha} (j'_{h-\alpha} b_{h-\alpha} - j_{h-\alpha} b'_{h-\alpha}) \end{aligned} \tag{C.5}$$

and for $e'^{\beta^*}_{h\alpha} e^{\beta^*}_{h\alpha} - d'_{h\alpha} d_{h\alpha}$:

$$\begin{aligned} \mathcal{R}_\phi &\equiv \cos\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha} - \\ &\qquad (j'_{h-\alpha} j_{h-\alpha} + b'_{h-\alpha} b_{h-\alpha}) \sin\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha} \\ \mathcal{I}_\phi &\equiv -\beta (j'_{h-\alpha} \sin\Delta'^{-}_{h\alpha} \cos\Delta_{h\alpha}^{-} + j_{h-\alpha} \sin\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha}) \end{aligned} \tag{C.6}$$

noting $\mathcal{R}_\varphi^2 + \mathcal{I}_\varphi^2 + \mathcal{R}_\phi^2 + \mathcal{I}_\phi^2 = 1$. The procedure will require to solve (C.2) as:

$$\chi_h{}^2 = \mathcal{R}_\varphi{}^2 + \mathcal{I}_\varphi{}^2 = \frac{|u_{i,j}|^2}{u_{i-1,j}^2} \tag{C.7}$$

together with equations (C.3-C.4), but rewritten as:

$$\begin{aligned} \arctan\xi_\varphi &= \varphi_{i,j} - \frac{\pi}{2}(h - \mathrm{sign}(\mathcal{R}_\varphi) + \mathrm{sign}(q)) + (2m_{-\alpha} + n_{-\alpha})\pi \\ \arctan\xi_\phi &= \phi_{i-1,j}^{(i-1,j-1)} - \frac{\pi}{2}(1 - \mathrm{sign}(\mathcal{R}_\phi)) + (2m_{-\alpha} + n_{-\alpha})\pi \\ &\text{with :} \quad \xi_\varphi \equiv \frac{\mathcal{I}_\varphi}{\mathcal{R}_\varphi}, \xi_\phi \equiv \frac{\mathcal{I}_\phi}{\mathcal{R}_\phi} \end{aligned} \tag{C.8}$$

The previous equations show that if $\chi_h{}^2$ covers $[0,1]$ independently of ξ_φ, ξ_ϕ values, then (14) can be adapted to (6) in two pulses. Note particularly the sign in $\mathcal{R}_\varphi, \mathcal{R}_\phi$, which can be easily adapted (if $\cos\Delta_{h\alpha}^{-}, \sin\Delta_{h\alpha}^{-}$ change their signs but not $\cos\Delta'^{-}_{h\alpha}, \sin\Delta'^{-}_{h\alpha}$, or vice versa, then it is easily achievable with selective displacements in $\Delta_{h\alpha}^{-}, \Delta'^{-}_{h\alpha}$). Thus, the last requirements are based on the free ranges for ξ_φ, ξ_ϕ in $\mathbf{R}$ independently from χ_h. Additionally, these equations depend on the relative signs among $j_{h-\alpha}, j'_{h-\alpha}, b_{h-\alpha}, b'_{h-\alpha}$: $z_{j_h} \equiv \mathrm{sign}(j_{h-\alpha} j'_{h-\alpha}), z_{b_h} \equiv \mathrm{sign}(b_{h-\alpha} b'_{h-\alpha})$. The resulting equations are:

$$\xi_\varphi = \frac{\beta \sin\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha} (j'_{h-\alpha} b_{h-\alpha} - j_{h-\alpha} b'_{h-\alpha})}{b_{h-\alpha} \sin\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha} + b'_{h-\alpha} \cos\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha}} \tag{C.9}$$

$$\xi_\phi = \frac{-\beta (j'_{h-\alpha} \sin\Delta'^{-}_{h\alpha} \cos\Delta_{h\alpha}^{-} + j_{h-\alpha} \sin\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha})}{\cos\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha} - (j'_{h-\alpha} j_{h-\alpha} + b'_{h-\alpha} b_{h-\alpha}) \sin\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha}} \tag{C.10}$$

$$\chi_h{}^2 = (1 + \xi_\varphi^2)(b_{h-\alpha} \sin\Delta_{h\alpha}^{-} \cos\Delta'^{-}_{h\alpha} + b'_{h-\alpha} \cos\Delta_{h\alpha}^{-} \sin\Delta'^{-}_{h\alpha})^2 \tag{C.11}$$

involving several parameters, but stating the general procedure for obtain matrix factors. This suggests that these equations can be fulfilled by any $\chi_h, \varphi_{i,j}$ and $\phi_{i-1,j}^{(i-1,j-1)}$, together with (C.1,18) by setting the concrete values for $b_{h\pm\alpha}, b'_{h\pm\alpha}, \Delta_{h\alpha}^{-}, \Delta'^{-}_{h\alpha}$ (or their equivalent parameters $B_{h\pm\alpha}, B'_{h\pm\alpha}, t, t'$).

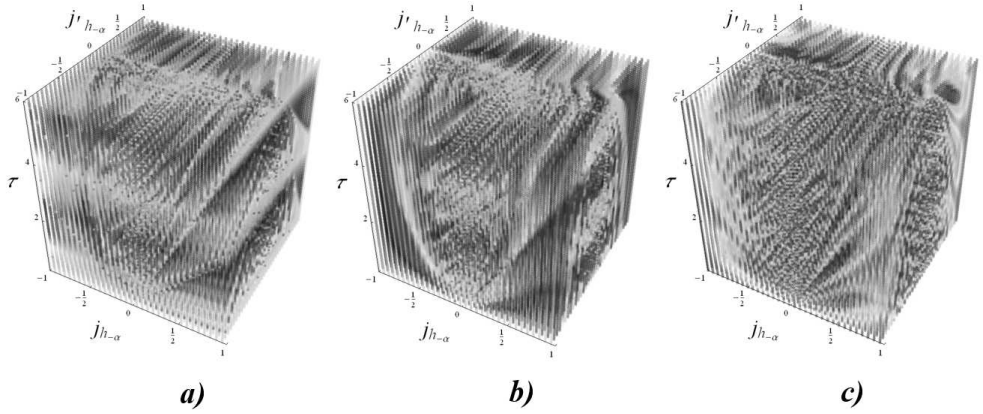

Fig. C.1. Colored maps of a) $\arctan(\xi_\varphi) \in (-\pi/2, \pi/2)$, b) $\arctan(\xi_\phi) \in (-\pi/2, \pi/2)$ and c) $\chi_h^2 \in [0,1]$. All graphs are represented in $(j_{h-\alpha}, j'_{h-\alpha}, \tau) \in [-1,1]\times[-1,1]\times[0,6]$ for $z_{j_h} = z_{b_h} = 1, c_\alpha = c'_\alpha = 1, N_{-\alpha} = 2$ as an example. Dark colors correspond to lower values in their respective range and brighter to higher ones.

The previous equations are a non-linear equation system because $\Delta_{h\alpha}^{-}, \Delta'^{-}_{h\alpha}$ contain $B_{h-\alpha}, B'_{h-\alpha}$. Parameters should be uncoupled regardless of (C.1,18) because there are only three remaining free parameters to solve them (C.7-C.8): $t, B_{h-\alpha}, B'_{h-\alpha}$. Thus, the equation for t' (C.4) should be used explicitly in (C.7-C.8). $\Delta_{h\alpha}^{-}, \Delta'^{-}_{h\alpha}$ should be written conveniently:

$$\begin{aligned}
\Delta_{h\alpha}^{-} &= \frac{R_{h-\alpha}}{J_{\{h\}_\alpha}} J_{\{h\}_\alpha} t \equiv \frac{\tau}{j_{h-\alpha}} \\
\Delta'^{-}_{h\alpha} &= \frac{R'_{h-\alpha}}{J'_{\{h\}_\alpha}} J'_{\{h\}_\alpha} t' \equiv \frac{\tau'}{j'_{h-\alpha}} \\
\tau' &= -\tau \frac{J'_{\{h\}_\alpha}}{J'_h} \frac{J_h}{J_{\{h\}_\alpha}} - \alpha(2m_{-\alpha} + n_{-\alpha})\pi \frac{J'_{\{h\}_\alpha}}{J'_h} \equiv -\tau \frac{c'_\alpha}{c_\alpha} + c'_\alpha N_\alpha \pi
\end{aligned} \tag{C.12}$$

where c_α denotes the ratio between the transverse strengths $J_{h\{\alpha\}}$ and the parallel strength J_h. $N_{-\alpha} = -\alpha(2m_{-\alpha} + n_{-\alpha}) \in \mathbf{Z}$. Parameters $j_{h-\alpha} \in [-1,1], j'_{h-\alpha} \in [-1,1], \tau \in \mathbf{R}$ appear together with $z_{j_h}, z_{b_h}, c_\alpha, c'_\alpha, N_{-\alpha}$ in the equations. The signs in $j_{h-\alpha}, j'_{h-\alpha}$ cannot be selected because they depend on the quantum system's nature; nevertheless, it is not an obstacle because the properties of trigonometric functions warrant multiple solutions with signs changed in ξ_φ, ξ_ϕ. The non-linear nature of equations requires a numerical treatment to find general solutions. Still, each set of required values is expected to have multiple solutions ($\chi_h, \xi_\varphi, \xi_\phi$ reproduce a specific $P-$unitary factor matrix for $U \in SU(4)$).

The numerator and the denominator in the expressions (C.9-C.10), in terms of (C.12), have many opportunities to nullify independently and not simultaneously. Due to continuity, ξ_φ, ξ_ϕ

runs over $\mathbf{R}$. In addition, χ_h^2 lies on $[0,1]$. Here, we take care about the apparent correlation between a null denominator in ξ_φ and a null numerator in χ_h, only due to the written form for χ_h^2 in (C.11). Unfortunately, equations (C.9-C.11) conform families depending on physical parameters $z_{j_h}, z_{b_h}, c_\alpha, c'_\alpha, N_{-\alpha}$ considering (C.12), which cannot be integrated easily in a unique non-dimensional parameter. To illustrate, Figure C.1 shows colored maps representing $\arctan(\xi_\varphi)$, $\arctan(\xi_\phi)$ and χ_h^2 in terms of $j_{h-\alpha}, j'_{h-\alpha}, \tau$ for the particular case of $z_{j_h} = z_{b_h} = 1, c_\alpha = c'_\alpha = 1, N_{-\alpha} = 2$. Dark colors represent lower values and bright colors higher values in their respective ranges ($(-\pi/2, \pi/2)$ for $\arctan(\xi_\varphi), \arctan(\xi_\phi)$ and $[0,1]$ for χ_h^2). These maps show the non-linear complexity of the equations.