Representing multiqubit unitary evolutions via Stokes tensors

Claudio Altafini*
SISSA-ISAS, International School for Advanced Studies, via Beirut 2-4, 34014 Trieste, Italy
(Received 2 April 2004; revised manuscript received 29 April 2004; published 30 September 2004)

For the Stokes tensor parametrization of a multiqubit density operator, we provide an explicit formulation of the corresponding unitary dynamics at the infinitesimal level. The main advantage of this formalism (clearly reminiscent of the ideas of "coherences" and "coupling Hamiltonians" of spin systems) is that the pattern of correlation between qubits and the pattern of infinitesimal correlation are highlighted simultaneously and can be used constructively for qubit manipulation. For example, it allows us to compute explicitly Rodrigues' formula for the one-parameter orbits of nonlocal Hamiltonians. The result is easily generalizable to orbits of Cartan subalgebras and allows us to express the Cartan decomposition of unitary propagators as a linear action directly in terms of the infinitesimal generators.

DOI: 10.1103/PhysRevA.70.032331 PACS number(s): 03.67.Mn, 03.65.Ud

I. INTRODUCTION

The easiest and most promising type of "quantum network," i.e., of a collection of quantum systems to be manipulated individually or jointly for the purposes of quantum information processing, is by far composed of qubits, i.e., of collections of two-level systems. In Ref. [1] we investigated the use of a particular tensorial representation of such systems which generalizes the idea of the (affine) Bloch vector parametrization of a single qubit to two or more qubits, and which is of widespread use (with minor variations) under different names, such as cluster operators [2] or, in the literature on nuclear magnetic resonance (NMR) spectroscopy, product operators [3,4]. In Ref. [1] this tensor was referred to as "tensor of coherences" but, following Refs. [5–8], the less ambiguous name of Stokes tensor will be used thereafter.[1] Our Stokes tensor could be considered an unfolding of the "nonsymmetric real density matrix" of Ref. [9] especially suited to emphasize the Lie algebraic point of view of the equations of motion. It is also closely related to multiparticle spacetime algebra [10].

The scope of the present paper is to discuss how the differential equations describing unitary dynamics can be formulated in the Stokes tensor basis. The idea that the unitary evolution of a qubit density matrix (pure or mixed) given by the Liouville–von Neumann equation becomes a linear vectorial ordinary differential equation for the Bloch vector is generalized to multiqubit densities. Mathematically, this could be thought of as "passing to the adjoint representation," its starting point being a formula for the decomposition of nonlocal commutators in terms of local commutators and anticommutators (see the Appendix); practically it corresponds still to replacing a conjugation action on matrices with a linear action on the vector obtained by stacking the columns of the tensor. In particular, when operations are local, a unitary transformation reduces to a multilinear action, i.e., a linear action on each piece of the Stokes tensor. When instead nonlocal transformations are used, their infinitesimal generators are no longer acting multilinearly and multispin correlations are induced. In this case the notation highlights which qubits are involved in each nonlocal gate. As a matter of fact, the major advantage of the formalism is that both the pattern of correlations of the density tensor and the pattern of the couplings at the infinitesimal level become very transparent, as both are decomposed with respect to the same basis of observables. In particular, they both show the same hierarchy of correlations (that originate from the affine structure of the tensors and of the corresponding Lie algebras of generators) which allows one to keep track of the reduced dynamics and reduced densities in a natural way. The idea of associating coherences to the degrees of freedom of qubits, and of manipulating qubits through the corresponding Hamiltonians, is common for example in the literature on spin systems in magnetic fields [4,11–14]. However, the principles apply to any network of qubits. The price to pay is a larger dimension for the matrices representing the infinitesimal generators: while the size of the Hamiltonians grows as 2^n in the number n of qubits, in the adjoint representation it grows as $4^n = 2^{2n}$.

As an example of the insight gained into the dynamics of the system, we compute explicitly the integral flow of any nonlocal (constant) Hamiltonian by means of Rodrigues' formula [15], which expresses the sum of the exponential series in terms of the first and second power of the infinitesimal generator. Since a Cartan subalgebra [16] contains only commuting vector fields, the multiparameter orbit of a set of generators belonging to a Cartan subalgebra also admits an explicit integration. The Cartan decomposition then becomes a concatenation of local and nonlocal linear actions that can be expressed directly in terms of the infinitesimal generators, rather than of exponentials. Such a decomposition has recently attracted considerable attention as a tool for construct-

*Electronic address: altafini@sissa.it

[1]Often the concept of "coherence" is associated with the off-diagonal elements of a density matrix. More generally, it is also used to identify states that are not eigenstates of a given Hamiltonian, and in this case even a nonrandom diagonal density operator may yield a nontrivial "coherence" contribution. Lendi's "coherence vector" is defined even more generally as the vector of expectation values of a complete orthonormal set of Hermitian matrices; see Ref. [25]. The Stokes tensor is just a tensorial version of the coherence vector parametrization.

1050-2947/2004/70(3)/032331(9)/$22.50

ing universal quantum gates which are optimal in the sense of minimizing time or complexity [11,17].

A couple of other examples are discussed, mainly focused on the manipulation of qubits in the presence of entanglement. In particular, we show how to create entanglement at a distance between qubits that are not directly coupled according to two different schemes, one in which the entanglement is distributed via an entangled ancilla, the other via a (always) separable ancilla as in Ref. [18].

II. LIE BRACKETS AND ADJOINT REPRESENTATION FOR SPIN-$\frac{1}{2}$ SYSTEMS

A. One spin

Consider the rescaled Pauli matrices and identity matrix

$$\lambda_0 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \lambda_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\lambda_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \lambda_3 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

with the commutation relations

$$[\lambda_0,\lambda_k] = 0, \quad [\lambda_1,\lambda_2] = \sqrt{2}i\lambda_3,$$

$$[\lambda_2,\lambda_3] = \sqrt{2}i\lambda_1, \quad [\lambda_3,\lambda_1] = \sqrt{2}i\lambda_2$$

and the anticommutators

$$\{\lambda_j,\lambda_k\} = \sqrt{2}\,\delta_{jk}\lambda_0,$$

$$\{\lambda_j,\lambda_0\} = \{\lambda_0,\lambda_j\} = \sqrt{2}\lambda_j, \tag{1}$$

$j,k \in \{1,2,3\}$. The operator "ad" is defined as follows: $\mathrm{ad}_{\lambda_j}\lambda_k = [\lambda_j,\lambda_k] = \Sigma_{l=0}^{3} c_{jk}^{l}\lambda_l$, where operations involving the 0 index only produce a null result: $c_{0k}^{l} = c_{j0}^{l} = c_{jk}^{0} = 0$. Using the "structure constants" c_{jk}^{l} we obtain an "adjoint basis" associated to the λ_j matrices, given by the four 4×4 matrices $\mathrm{ad}_{\lambda_0},\ldots,\mathrm{ad}_{\lambda_3}$ of purely imaginary entries $(\mathrm{ad}_{\lambda_j})_{kl} = c_{jk}^{l}$,

$$\mathrm{ad}_{\lambda_0} = 0_{4\times 4}, \quad \mathrm{ad}_{\lambda_1} = \sqrt{2}i\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

$$\mathrm{ad}_{\lambda_2} = \sqrt{2}i\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \quad \mathrm{ad}_{\lambda_3} = \sqrt{2}i\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

The Pauli matrices are such that $-i\lambda_1$, $-i\lambda_2$, and $-i\lambda_3$ form a basis of su(2), while the $-i\mathrm{ad}_{\lambda_j}$, $j=1,2,3$, form a basis of $\mathfrak{so}(3) = \mathrm{ad}_{\mathfrak{su}(2)}$, the adjoint representation of $\mathfrak{su}(2)$. The "anti-adjoint" operators aad_{λ_j}, $j=0,1,2,3$, can also be defined in the same fashion as the ad_{λ_j}, i.e., by means of 4×4 matrices obtained from $\mathrm{aad}_{\lambda_j}\lambda_k = \{\lambda_j,\lambda_k\} = \Sigma_{l=0}^{3} s_{jk}^{l}\lambda_l$, $j,k,l \in \{0,1,2,3\}$, so that a linear representation of aad_{λ_j} is given by $(\mathrm{aad}_{\lambda_j})_{kl} = s_{jk}^{l}$ with the 4×4 matrices aad_{λ_j} easily computed from Eq. (1):

$$\mathrm{aad}_{\lambda_0} = \sqrt{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathrm{aad}_{\lambda_1} = \sqrt{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathrm{aad}_{\lambda_2} = \sqrt{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathrm{aad}_{\lambda_3} = \sqrt{2}\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

B. Two spins

Call $\Lambda_{jk} = \lambda_j \otimes \lambda_k$, $j,k \in \{0,1,2,3\}$. Up to a constant, the Λ_{jk} form the so-called *product operators basis* [3], and are subdivided into zero-spin operators (Λ_{00}), one-spin operators (Λ_{01}, Λ_{02}, Λ_{03}, Λ_{10}, Λ_{20}, Λ_{30}), and two-spin operators (Λ_{11}, Λ_{12}, Λ_{13}, Λ_{21}, Λ_{22}, Λ_{23}, Λ_{31}, Λ_{32}, Λ_{33}). The set of $-i\Lambda_{jk}$ $j,k \in \{0,1,2,3\}$ contains a basis of the nine-dimensional tensor product Lie algebra $\mathfrak{su}(2)\otimes\mathfrak{su}(2)$ plus a basis of the six-dimensional "tensor sum" Lie algebras $\mathfrak{su}(2)\oplus\mathfrak{su}(2)$ arising from the one-spin operators. As $i\lambda_0 \notin \mathfrak{su}(2)$, so $-i\Lambda_{00} \notin \mathfrak{su}(2)\otimes\mathfrak{su}(2)$ and $-i\Lambda_{00} \notin \mathfrak{su}(2)\oplus\mathfrak{su}(2)$. From Eq. (A3)

$$\begin{aligned}[\Lambda_{jk},\Lambda_{lm}] &= [\lambda_j \otimes \lambda_k, \lambda_l \otimes \lambda_m] = \mathrm{ad}_{\Lambda_{jk}}\Lambda_{lm} = \mathrm{ad}_{\lambda_j\otimes\lambda_k}\lambda_l \otimes \lambda_m \\ &= \tfrac{1}{2}([\lambda_j,\lambda_l]\otimes\{\lambda_k,\lambda_m\} + \{\lambda_j,\lambda_l\}\otimes[\lambda_k,\lambda_m]) \\ &= \tfrac{1}{2}(\mathrm{ad}_{\lambda_j}\lambda_l \otimes \mathrm{aad}_{\lambda_k}\lambda_m + \mathrm{aad}_{\lambda_j}\lambda_l \otimes \mathrm{ad}_{\lambda_k}\lambda_m). \end{aligned} \tag{2}$$

In terms of the adjoint representation, Eq. (2) can be expressed as a 4-tensor, which in turn is a function of the two 2-tensors c_{jk}^{l} and s_{jk}^{l} because

$$\mathrm{ad}_{\Lambda_{jk}} = \mathrm{ad}_{\lambda_j\otimes\lambda_k} = \tfrac{1}{2}(\mathrm{ad}_{\lambda_j}\otimes\mathrm{aad}_{\lambda_k} + \mathrm{aad}_{\lambda_j}\otimes\mathrm{ad}_{\lambda_k}) \tag{3}$$

consists of elements

$$(\mathrm{ad}_{\Lambda_{jk}})_{lm}^{pq} = \tfrac{1}{2}(c_{jl}^{p}\otimes s_{km}^{q} + s_{jl}^{p}\otimes c_{km}^{q}), \tag{4}$$

so that Eq. (2) becomes

$$[\Lambda_{jk},\Lambda_{lm}] = (\mathrm{ad}_{\lambda_j\otimes\lambda_k})_{lm}^{pq}\Lambda_{pq} = \tfrac{1}{2}(c_{jl}^{p}\otimes s_{km}^{q} + s_{jl}^{p}\otimes c_{km}^{q})\Lambda_{pq}, \tag{5}$$

where we have used the summation convention over repeated indexes (in the range $0-3$). For $j\neq 0$ and $k\neq 0$, the $-i\mathrm{ad}_{\Lambda_{jk}}$ of Eq. (3) form a basis of the adjoint representation of $\mathfrak{su}(2)\otimes\mathfrak{su}(2)$, $\mathrm{ad}_{\mathfrak{su}(2)\otimes\mathfrak{su}(2)} = \mathfrak{so}(3)\otimes\mathfrak{so}(3)$. The remaining elements account for the affine structure i.e., for $\mathrm{ad}_{\mathfrak{su}(2)\oplus\mathfrak{su}(2)} = \mathfrak{so}(3)\oplus\mathfrak{so}(3)$. As c_{jl}^{p} and s_{km}^{q} are 4×4 matrices, the resulting Kronecker product $\mathrm{ad}_{\Lambda_{jk}}$ is a 16×16 matrix. However, it has a row and a column entirely composed of zeros in correspondence of Λ_{00} and, given Λ_{jk} with $jk\neq 00$, $\nexists\ \Lambda_{lm}$ with $(lm)\neq(00)$ such that $\mathrm{ad}_{\Lambda_{jk}}\Lambda_{lm} = \Lambda_{00}$. Furthermore,

$\mathrm{ad}_{\Lambda_{00}}$ being the trivial matrix of all zeros, it is not a basis element in the adjoint representation. Also in the adjoint representation the index 0 in a slot corresponds to trivial dynamics in the corresponding site. For example,

$$\mathrm{ad}_{\Lambda_{j0}} = \frac{1}{2}(\mathrm{ad}_{\lambda_j} \otimes \mathrm{aad}_{\lambda_0} + \mathrm{aad}_{\lambda_j} \otimes 0) = \frac{1}{\sqrt{2}}\mathrm{ad}_{\lambda_j} \otimes I_4. \quad (6)$$

C. *n* spins

In the n-spin case, $\Lambda_{j_1\cdots j_n}=\lambda_{j_1}\otimes\cdots\otimes\lambda_{j_n}$, $j_k\in\{0,1,2,3\}$, $k\in\{1,\ldots,n\}$, are the basis elements. The Lie bracket $[\Lambda_{j_1\cdots j_n},\Lambda_{k_1\cdots k_n}]$ can be computed according to the rule (A1). For example, for $n=3$ from Eq. (A4),

$$\begin{aligned}
[\Lambda_{jkl},\Lambda_{mpq}] &= \tfrac{1}{4}(\mathrm{ad}_{\lambda_j}\lambda_m \otimes \mathrm{aad}_{\lambda_k}\lambda_p \otimes \mathrm{aad}_{\lambda_l}\lambda_q \\
&\quad + \mathrm{aad}_{\lambda_j}\lambda_m \otimes \mathrm{ad}_{\lambda_k}\lambda_p \otimes \mathrm{aad}_{\lambda_l}\lambda_q \\
&\quad + \mathrm{aad}_{\lambda_j}\lambda_m \otimes \mathrm{aad}_{\lambda_k}\lambda_p \otimes \mathrm{ad}_{\lambda_l}\lambda_q \\
&\quad + \mathrm{ad}_{\lambda_j}\lambda_m \otimes \mathrm{ad}_{\lambda_k}\lambda_p \otimes \mathrm{ad}_{\lambda_l}\lambda_q) \\
&= \tfrac{1}{4}(\mathrm{ad}_{\lambda_j} \otimes \mathrm{aad}_{\lambda_k} \otimes \mathrm{aad}_{\lambda_l} + \mathrm{aad}_{\lambda_j} \otimes \mathrm{ad}_{\lambda_k} \otimes \mathrm{aad}_{\lambda_l} \\
&\quad + \mathrm{aad}_{\lambda_j} \otimes \mathrm{aad}_{\lambda_k} \otimes \mathrm{ad}_{\lambda_l} \\
&\quad + \mathrm{ad}_{\lambda_j} \otimes \mathrm{ad}_{\lambda_k} \otimes \mathrm{ad}_{\lambda_l})_{mpq}^{rst}\Lambda_{rst} \\
&= \tfrac{1}{4}(c_{jm}^r \otimes s_{kp}^s \otimes s_{lq}^t + s_{jm}^r \otimes c_{kp}^s \otimes s_{lq}^t \\
&\quad + s_{jm}^r \otimes s_{kp}^s \otimes c_{lq}^t + c_{jm}^r \otimes c_{kp}^s \otimes c_{lq}^t)_{mpq}^{rst}\Lambda_{rst} \\
&= (\mathrm{ad}_{\Lambda_{jkl}})_{mpq}^{rst}\Lambda_{rst}. \qquad (7)
\end{aligned}$$

Remarkably, the building blocks needed for the n-qubit case are just the structure constants c_{jk}^l and s_{jk}^l computed above. For n spins, the affine structure propagates itself throughout and determines a hierarchy of subalgebras of tensor product and tensor sum type. The $-i\Lambda_{j_1\cdots j_n}$, $(j_1\cdots j_n)\neq(0\cdots 0)$, form a joint basis of the Lie algebras $\mathfrak{su}(2)^{\otimes n}$, $\mathfrak{su}(2)\oplus\mathfrak{su}(2)^{\otimes(n-1)},\ldots,\mathfrak{su}(2)\oplus\cdots\oplus\mathfrak{su}(2)$ (plus all factor permutations) and $-i\mathrm{ad}_{\Lambda_{j_1\cdots j_n}}$, $(j_1\cdots j_n)\neq(0\cdots 0)$, a joint basis of $\mathrm{ad}_{\mathfrak{su}(2)^{\otimes n}}, \mathrm{ad}_{\mathfrak{su}(2)\oplus\mathfrak{su}(2)^{\otimes(n-1)}},\ldots,\mathrm{ad}_{\mathfrak{su}(2)\oplus\cdots\oplus\mathfrak{su}(2)}$ (plus, again, all factor permutations). In both notations, the number and position of the indexes "0" uniquely determine which spins are involved in the $-i\mathrm{ad}_{\Lambda_{j_1\cdots j_n}}$.

III. UNITARY EVOLUTION IN TERMS OF THE STOKES TENSOR

For qubits, the same basis elements $\Lambda_{j_1\cdots j_n}$ that describe the infinitesimal generators can also be used for the density operators. This is well known in the literature on spin systems [3], and can be formalized in terms of $4\times 4\times\cdots\times 4$ tensors which we call Stokes tensors. See Refs. [1,2,6,19–21] for an overview. The purpose of this section is to show how Stokes tensors and adjoint representations fit together in the description of the unitary dynamics of multiqubit densities.

A. Density operators and Stokes tensors

This section follows Ref. [1]. The $\Lambda_{j_1\cdots j_n}$ form a complete orthonormal set of Hermitian matrices and can be used to obtain an affine tensorial representation of the density operator of n qubits: $\rho=\varrho^{j_1\cdots j_n}\Lambda_{j_1\cdots j_n}$, $j_k\in\{0,1,2,3\}$, $k\in\{1,\ldots,n\}$, with $\varrho^{j_1\cdots j_n}=\mathrm{tr}(\rho\Lambda_{j_1\cdots j_n})$ the expectation value for the observable $\Lambda_{j_1\cdots j_n}$. This representation has several advantages which are briefly recalled below.

(i) It captures all degrees of freedom of a density operator.

(ii) Each term $\varrho^{j_1\cdots j_n}$ in the tensor depends on a certain number of qubits: this is uniquely determined by the number of nonzero indexes in the sequence $j_1\cdots j_n$. The pattern of nonzero indexes also identifies which qubits are involved.

(iii) All correlations of all orders and all reduced densities are already contained in the tensor: tracing out a qubit means collapsing the corresponding index to 0 and rescaling everything by $\sqrt{2}$. For example, if $\rho_{A_2\cdots A_n}=\mathrm{tr}_{A_1}(\rho)=\varrho^{j_2\cdots j_n}\Lambda_{j_2\cdots j_n}$, then $\varrho^{j_2\cdots j_n}=\sqrt{2}\varrho^{0j_2\cdots j_n}$;

(iv) Since

$$\mathrm{tr}(\Lambda_{jk}\Lambda_{lm}) = \delta_{jl}\delta_{km}, \quad (8)$$

$j,k,l,m\in\{0,1,2,3\}$, the degree of mixing becomes the Euclidean norm of $\varrho^{j_1\cdots j_n}$,

$$\mathrm{tr}(\rho) = \sum_{j_1,\ldots,j_n=0}^{3}(\varrho^{j_1\cdots j_n})^2 \quad (9)$$

and hence, since $\varrho^{0\cdots 0}=(1/\sqrt{2})^n$, for $(j_1\cdots j_n)\neq(0\cdots 0)$ the tensor $\varrho^{j_1\cdots j_n}\in\mathbb{S}_r^{4^n-2}\subset\mathbb{R}^{4^n-1}$ with $0\leqslant r\leqslant\sqrt{1-(\varrho^{0\cdots 0})^2}=\sqrt{1-(1/2)^n}$.

(v) Complete mixing corresponds to $r=0$ (i.e., to the null tensor except for the affine constant $\varrho^{0\cdots 0}$).

(vi) Pure states correspond to $r=\sqrt{1-(1/2)^n}$.

(vii) Factorizability corresponds to $\varrho^{j_1\cdots j_n}=\varrho_{A_1}^{j_1}\varrho_{A_2}^{j_2}\cdots\varrho_{A_n}^{j_n}$, where $\varrho_{A_1}^{j_1}=(\sqrt{2})^{n-1}\varrho^{j_1 0\cdots 0}$ is the four-vector of the reduced density $\rho_{A_1}=\mathrm{tr}_{A_2\cdots A_n}(\rho)$ and so on.[2]

(viii) Partial transposition of a qubit becomes a change of sign in the terms having index 2 in the corresponding slot, for example

$$\begin{aligned}
\rho^{T_{A_1}} &= \varrho^{0j_2\cdots j_n}\Lambda_{0j_2\cdots j_n} + \varrho^{1j_2\cdots j_n}\Lambda_{1j_2\cdots j_n} - \varrho^{2j_2\cdots j_n}\Lambda_{2j_2\cdots j_n} \\
&\quad + \varrho^{3j_2\cdots j_n}\Lambda_{3j_2\cdots j_n} \qquad (10)
\end{aligned}$$

and so on.

(ix) Checking bipartite entanglement can be done by the simple test (10).

B. Liouville–von Neumann equation

The Liouville–von Neumann equation for the n-qubits density ρ is

[2] In the context of our parametrization, the term "tensor" is not equivalent to the notion of "density which is a tensor product" and should not be confused with it. Every density admits a Stokes tensor, even if it is nonfactorizable or nonseparable. In these cases, the corresponding Stokes tensors will be nonfactorizable or nonseparable.

$$\dot{\rho} = -i[H,\rho] = -i\,\mathrm{ad}_H(\rho), \tag{11}$$

where $H=H^\dagger$ is the Hamiltonian of the system. From Sec. II, we have that $H=h^{j_1\cdots j_n}\Lambda_{j_1\cdots j_n}$, $j_k \in \{0,1,2,3\}$, $k\in\{1,\ldots,n\}$.

If we have two qubits, then, in terms of the Stokes tensor, Eq. (11) corresponds to

$$\dot{\varrho}^{pq} = -ih^{jk}(\mathrm{ad}_{\Lambda_{jk}})^{pq}_{lm}\varrho^{lm} = -\frac{ih^{jk}}{2}(c^p_{jl}\otimes s^q_{km} + s^p_{jl}\otimes c^q_{km})\varrho^{lm}. \tag{12}$$

In order to show Eq. (12), derive $\varrho^{pq}=\mathrm{tr}(\rho\Lambda_{pq})$ and use Eqs. (4) and (8):

$$\begin{aligned}\dot{\varrho}^{pq} &= \mathrm{tr}(\dot{\rho}\Lambda_{pq}) = \mathrm{tr}(-i[H,\rho]\Lambda_{pq}) = \mathrm{tr}(-ih^{jk}[\Lambda_{jk},\Lambda_{lm}]\varrho^{lm}\Lambda_{pq})\\ &= \mathrm{tr}\left(-\frac{i}{2}h^{jk}(c^r_{jl}\otimes s^s_{km}+s^r_{jl}\otimes c^s_{km})\Lambda_{rs}\varrho^{lm}\Lambda_{pq}\right)\\ &= -\frac{i}{2}h^{jk}(c^r_{jl}\otimes s^s_{km}+s^r_{jl}\otimes c^s_{km})\varrho^{lm}\mathrm{tr}(\Lambda_{rs}\Lambda_{pq})\\ &= -\frac{i}{2}h^{jk}(c^r_{jl}\otimes s^s_{km}+s^r_{jl}\otimes c^s_{km})\varrho^{lm}\delta_{rp}\delta_{sq}\\ &= -\frac{i}{2}h^{jk}(c^p_{jl}\otimes s^q_{km}+s^p_{jl}\otimes c^q_{km})\varrho^{lm}.\end{aligned}$$

The component of the Hamiltonian along Λ_{00} is irrelevant: even if $h^{00}\neq 0$ it has no effect, since $-ih^{00}\mathrm{ad}_{\Lambda_{00}}=0$. The meaning is similar to the single-spin case: global phases are neglected in Eqs. (11) and (12).

Since Eq. (12) is a linear system, if the coefficients h^{jk} are constant the integration can be carried out explicitly,

$$\varrho^{pq}(t) = (e^{-ith^{jk}\mathrm{ad}_{\Lambda_{jk}}})^{pq}_{lm}\varrho^{lm}(0). \tag{13}$$

Notice that when two-spin generators are lacking, $h^{jk}=0$ $\forall j\neq 0$ and $k\neq 0$, i.e., when only local operations and classical communication (LOCC) are performed, the exponential in Eq. (13) splits. In fact, $[\Lambda_{j0},\Lambda_{0k}]=0$ and therefore the infinitesimal generators Λ_{j0} and Λ_{0k} can be "reduced" as well. Using Eq. (6), the unitary propagator in Eq. (13) becomes

$$\begin{aligned}&e^{-it(h^{j0}\mathrm{ad}_{\Lambda_{j0}}+h^{0k}\mathrm{ad}_{\Lambda_{0k}})}\\ &\quad= (e^{-ith^{j0}\mathrm{ad}_{\Lambda_{j0}}})(e^{-ith^{0k}\mathrm{ad}_{\Lambda_{0k}}})\\ &\quad= ((e^{-it(h^{j0}/\sqrt{2})\mathrm{ad}_{\lambda_j}})\otimes I_4)(I_4\otimes(e^{-it(h^{0k}/\sqrt{2})\mathrm{ad}_{\lambda_k}})),\end{aligned}$$

where the factor $1/\sqrt{2}$ comes from Eq. (6). Therefore,

$$\begin{aligned}&(e^{-it(h^{j0}/\sqrt{2})\mathrm{ad}_{\lambda_j}})\otimes(e^{-it(h^{0k}/\sqrt{2})\mathrm{ad}_{\lambda_k}})\\ &\quad\in \begin{bmatrix}1 & 0\\ 0 & \mathrm{SO}(3)\end{bmatrix}\otimes\begin{bmatrix}1 & 0\\ 0 & \mathrm{SO}(3)\end{bmatrix},\end{aligned} \tag{14}$$

which allows the state to evolve on at most a six-parameter orbit sitting inside the 15-dimensional affine sphere $\mathbb{S}^{15}_r$, with r defined as in Eq. (9). If $\rho(0)$ is separable, then so is the result $\rho(t)$ of evolving it under Eq. (14) for all t, and hence the six-dimensional manifold contains all the separable states. When instead the Hamiltonian has $h^{jk}\neq 0$ for $j\neq 0$ and $k\neq 0$, the evolution of the two qubits becomes coupled.

Similarly to the two-qubit case, if we have n qubits we obtain

$$\dot{\varrho}^{p_1\cdots p_n} = -ih^{j_1\cdots j_n}(\mathrm{ad}_{\Lambda_{j_1\cdots j_n}})^{p_1\cdots p_n}_{k_1\cdots k_n}\varrho^{k_1\cdots k_n},$$

where $\mathrm{ad}_{\Lambda_{j_1\cdots j_n}}$ is computed as in Sec. II C.

IV. INTEGRAL FLOW OF NONLOCAL HAMILTONIANS

We first restrict to two qubits, although all arguments generalize to n qubits. To begin with, we give an explicit formula for the integral of each "elementary" generator Λ_{jk}. From Sec. II A, we have that $\mathrm{ad}_{\lambda_j}\mathrm{aad}_{\lambda_j}=\mathrm{aad}_{\lambda_j}\mathrm{ad}_{\lambda_j}=0$. This implies that the series expansion $\exp(-it\mathrm{ad}_{\Lambda_{jk}}) = \Sigma_{p=0}^{\infty}((-it)^p/p!)\mathrm{ad}^p_{\Lambda_{jk}}$ has a particularly simple expression, since for all p

$$\mathrm{ad}^p_{\Lambda_{jk}} = \frac{1}{2^p}(\mathrm{ad}^p_{\lambda_j}\otimes\mathrm{aad}^p_{\lambda_k}+\mathrm{aad}^p_{\lambda_j}\otimes\mathrm{ad}^p_{\lambda_k}).$$

The powers of ad_{λ_j} and aad_{λ_j} are easily computed since $\mathrm{ad}^2_{\lambda_j}$ and $\mathrm{aad}^2_{\lambda_j}$ are diagonal and "complementary":

(i) if $j=1$, $\mathrm{ad}^2_{\lambda_1}=2(\delta_{33}+\delta_{44})$, $\mathrm{aad}^2_{\lambda_1}=2(\delta_{11}+\delta_{22})$;

(ii) if $j=2$, $\mathrm{ad}^2_{\lambda_2}=2(\delta_{22}+\delta_{44})$, $\mathrm{aad}^2_{\lambda_2}=2(\delta_{11}+\delta_{33})$;

(iii) if $j=3$, $\mathrm{ad}^2_{\lambda_3}=2(\delta_{22}+\delta_{33})$, $\mathrm{aad}^2_{\lambda_3}=2(\delta_{11}+\delta_{44})$;

so that $\mathrm{ad}^2_{\lambda_j}+\mathrm{aad}^2_{\lambda_j}=2I_4$. Cubic powers instead are $\mathrm{ad}^3_{\lambda_j}=2\mathrm{ad}_{\lambda_j}$ and $\mathrm{aad}^3_{\lambda_j}=2\mathrm{aad}_{\lambda_j}$, hence $\mathrm{ad}^3_{\Lambda_{jk}}=\mathrm{ad}_{\Lambda_{jk}}$. We can therefore explicitly write down the sum of the series as

$$\begin{aligned}\exp(-it\mathrm{ad}_{\Lambda_{jk}}) &= I_4\otimes I_4 - i\left(t-\frac{t^3}{3!}+\frac{t^5}{5!}-\cdots\right)\mathrm{ad}_{\Lambda_{jk}}\\ &\quad+\left(-\frac{t^2}{2!}+\frac{t^4}{4!}-\cdots\right)\mathrm{ad}^2_{\Lambda_{jk}}\end{aligned}$$

or, adding and subtracting $\mathrm{ad}^2_{\Lambda_{jk}}$,

$$\exp(-it\mathrm{ad}_{\Lambda_{jk}}) = I_4\otimes I_4 - i\sin(t)\mathrm{ad}_{\Lambda_{jk}} - (1-\cos(t))\mathrm{ad}^2_{\Lambda_{jk}}, \tag{15}$$

where the extra terms added are needed because the zero-order terms do not match: $I_4\otimes I_4\neq\mathrm{ad}^2_{\Lambda_{jk}}$. Notice that a formula equivalent to Eq. (15) was used for the same purposes as ours in Ref. [9]. Both are tensorial versions of Rodrigues' formula for rotations; see Ref. [22], p. 291 or [23], p. 28. The splitting is into skew-symmetric $(-i\mathrm{ad}_{\Lambda_{jk}})$ and symmetric parts ($I_4\otimes I_4$ and $\mathrm{ad}^2_{\Lambda_{jk}}$) of the flow.[3] Notice that both $-i\mathrm{ad}_{\Lambda_{jk}}$ and $\mathrm{ad}^2_{\Lambda_{jk}}$ are sums of tensor products of matrices. The nonlocality of the Hamiltonian of Eq. (15) is reflected in the fact that we do not obtain a

[3]The sign difference with respect to the standard SO(3) formula is due to the fact that here the skew-symmetric generator is $-i\mathrm{ad}_{\Lambda_{jk}}$.

"single" tensor product but rather a sum.[4] Clearly the overall evolution of Eq. (15) is orthogonal. However, the single pieces do not describe rotations, either locally nor globally.

The same argument can be repeated for any number of qubits. For example, for three qubits we have $\exp(-it\mathrm{ad}_{\Lambda_{jkl}})=\Sigma_{p=0}^{\infty}((-it)^p/p!)\mathrm{ad}^p_{\Lambda_{jkl}}$, with

$$\mathrm{ad}^p_{\Lambda_{jkl}}=\frac{1}{4^p}(\mathrm{ad}^p_{\lambda_j}\otimes \mathrm{aad}^p_{\lambda_k}\otimes \mathrm{aad}^p_{\lambda_l}+\mathrm{aad}^p_{\lambda_j}\otimes \mathrm{ad}^p_{\lambda_k}\otimes \mathrm{aad}^p_{\lambda_l}+\mathrm{aad}^p_{\lambda_j}\otimes \mathrm{aad}^p_{\lambda_k}\otimes \mathrm{ad}^p_{\lambda_l}+\mathrm{ad}^p_{\lambda_j}\otimes \mathrm{ad}^p_{\lambda_k}\otimes \mathrm{ad}^p_{\lambda_l}), \quad (16)$$

where now $\mathrm{ad}^3_{\Lambda_{jkl}}=\frac{1}{2}\mathrm{ad}_{\Lambda_{jkl}}$. The sum of the series is then

$$\exp(-it\mathrm{ad}_{\Lambda_{jkl}})=I_4^{\otimes 3}-i\sqrt{2}\sin\left(\frac{t}{\sqrt{2}}\right)\mathrm{ad}_{\Lambda_{jkl}}-2\left(1-\cos\left(\frac{t}{\sqrt{2}}\right)\right)\mathrm{ad}^2_{\Lambda_{jkl}}. \quad (17)$$

So far we have only considered a single "coordinate direction" (Λ_{jk} for the two-qubit case). The formulas, however, extend in a straightforward manner to linear combinations of commuting generators, even depending on more than one parameter. A maximal orbit of integrable flow is obtained obviously in correspondence to a Cartan subalgebra [16,17], i.e., a maximal commuting subalgebra in the Lie algebra of nonlocal operations of the system. For the two-qubit case, let us concentrate on the "nonlocal subalgebra" $\mathrm{ad}_{\mathfrak{su}(2)\otimes\mathfrak{su}(2)}=\mathfrak{so}(3)\otimes\mathfrak{so}(3)$. A Cartan subalgebra is, for example, given by $\mathrm{ad}_{\mathfrak{h}}=\mathrm{span}\{-i\mathrm{ad}_{\Lambda_{11}},-i\mathrm{ad}_{\Lambda_{22}},-i\mathrm{ad}_{\Lambda_{33}}\}$ (or by $\mathrm{span}\{-i\mathrm{ad}_{\Lambda_{12}},-i\mathrm{ad}_{\Lambda_{21}},-i\mathrm{ad}_{\Lambda_{33}}\}$, etc.) where $\mathfrak{h}$ is a Cartan subalgebra in $\mathfrak{su}(2)\otimes\mathfrak{su}(2)$: $\mathfrak{h}=\mathrm{span}\{-i\Lambda_{11},-i\Lambda_{22},-i\Lambda_{33}\}$. The three-parameter orbits of such subalgebra are integrable, as can be seen by the splitting of the exponential,

$$\exp(-i(\beta^{11}\mathrm{ad}_{\Lambda_{11}}+\beta^{22}\mathrm{ad}_{\Lambda_{22}}+\beta^{33}\mathrm{ad}_{\Lambda_{33}}))=\exp(-i\beta^{11}\mathrm{ad}_{\Lambda_{11}})\exp(-i\beta^{22}\mathrm{ad}_{\Lambda_{22}})\exp(-i\beta^{33}\mathrm{ad}_{\Lambda_{33}}) \quad (18)$$

for real β^{jj}. The "marginal" subalgebra of local operations $\mathfrak{so}(3)\oplus\mathfrak{so}(3)$ does not commute with the Cartan subalgebra. It is known [16] that $[\mathfrak{so}(3)\oplus\mathfrak{so}(3),\mathrm{ad}_{\mathfrak{h}}]$ generates the entire 15-dimensional Lie algebra $\mathfrak{so}(3)\oplus\mathfrak{so}(3)\cup\mathfrak{so}(3)\otimes\mathfrak{so}(3)$ and that "exponentiating" this splitting gives the Cartan decomposition of the corresponding Lie group. When an arbitrary two-qubit gate, call it U_c, is constructed by means of the Cartan decomposition of SU(4), then

$$U_c=U_{1\alpha}\otimes U_{2\alpha}\exp(-i(\beta^{11}\Lambda_{11}+\beta^{22}\Lambda_{22}+\beta^{33}\Lambda_{33}))\times U_{1\gamma}\otimes U_{2\gamma}$$

with $U_{j\alpha},U_{j\gamma}\in SU(2)$, $j=1,2$, and its action on a density operator is by conjugation. With our formalism, such a conjugation action becomes a linear action, obtained by the concatenation of bilocal exponentials of the form shown in Eq. (14) and of the nonlocal exponential of Eq. (18). In other words, any unitary operation acting on the Stokes tensor of a two-qubit density can be written as a product of the following form:

$$(e^{-i(\alpha^{j0}/\sqrt{2})\mathrm{ad}_{\lambda_j}})\otimes(e^{-i(\alpha^{0k}/\sqrt{2})\mathrm{ad}_{\lambda_k}})\times\exp(-i\beta^{11}\mathrm{ad}_{\Lambda_{11}})\exp(-i\beta^{22}\mathrm{ad}_{\Lambda_{22}})\exp(-i\beta^{33}\mathrm{ad}_{\Lambda_{33}})\times(e^{-i(\gamma^{j0}/\sqrt{2})\mathrm{ad}_{\lambda_j}})\otimes(e^{-i(\gamma^{0k}/\sqrt{2})\mathrm{ad}_{\lambda_k}})$$

for real α^{jk}, β^{jj}, and γ^{jk}. Each exponential can be replaced by the corresponding sum of tensors [given by Eq. (15) for the nonlocal pieces and by $\exp(-it\mathrm{ad}_{\lambda_j})=I_4-(i/\sqrt{2})\sin(\sqrt{2}t)\mathrm{ad}_{\lambda_j}-(1/2)(1-\cos(\sqrt{2}t))\mathrm{ad}^2_{\lambda_j}$ for the one-parameter orbit of a single qubit].

V. EXAMPLES

In Sec. V A it is shown how the discrete unitary propagator corresponding to a standard two-qubit gate, the controlled NOT (CNOT) gate, is expressed in terms of the Stokes tensor. In the three-qubit example of Sec. V B, entanglement between two "distant" qubits is achieved by indirect coupling through an entangled ancilla. In Sec. V C, the scheme of Ref. [18] is used for the same purposes, but in this scheme the ancilla remains separable for all times.

A. CNOT gate

It is well known that since the elementary gates of a quantum computer are discrete unitary operations, they can be written in terms of the corresponding infinitesimal Hamiltonians. In particular, in the literature on quantum information processing by means of NMR spectroscopy [4] this was done in terms of the product operators basis, of which our formalism is just a variation. For example, in the computational basis of two qubits $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$, the Hamiltonian of the CNOT gate

$$U_{\mathrm{CNOT}}=\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{bmatrix}$$

is given by

$$H_{\mathrm{CNOT}}=\frac{\pi}{2}\begin{bmatrix}0&0&0&0\\0&1&0&-1\\0&0&0&0\\0&-1&0&1\end{bmatrix}.$$

In terms of the Λ_{jk}, this is $H_{\mathrm{CNOT}}=\pi/2(\Lambda_{00}-\Lambda_{03}-\Lambda_{10}+\Lambda_{13})$, and therefore for ϱ^{jk} we have the orthogonal matrix

$$R_{\mathrm{CNOT}}=e^{-i(\pi/2)(\mathrm{ad}_{\Lambda_{00}}-\mathrm{ad}_{\Lambda_{03}}-\mathrm{ad}_{\Lambda_{10}}+\mathrm{ad}_{\Lambda_{13}})},$$

which computed by means of Eq. (3) yields

[4] This does not mean that we have separable superoperators [26], however, since unitary operators yield "pure" quantum operations [27].

$$
R_{\mathrm{CNOT}} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{bmatrix}.
$$

If we are given the four computational basis states

$$|00\rangle \leftrightarrow \varrho^{jk} = \left\{ \begin{matrix} 1/2,0,0,1/2,0,0,0,0, \\ 0,0,0,0,1/2,0,0,1/2 \end{matrix} \right\},$$

$$|01\rangle \leftrightarrow \varrho^{jk} = \left\{ \begin{matrix} 1/2,0,0,-1/2,0,0,0,0, \\ 0,0,0,0,1/2,0,0,-1/2 \end{matrix} \right\},$$

$$|01\rangle \leftrightarrow \varrho^{jk} = \left\{ \begin{matrix} 1/2,0,0,1/2,0,0,0,0, \\ 0,0,0,0,-1/2,0,0,-1/2 \end{matrix} \right\},$$

$$|11\rangle \leftrightarrow \varrho^{jk} = \left\{ \begin{matrix} 1/2,0,0,-1/2,0,0,0,0, \\ 0,0,0,0,-1/2,0,0,1/2 \end{matrix} \right\},$$

it is straightforward to check that R_{CNOT} behaves as a CNOT gate with the second qubit acting as control qubit. Notice that H_{CNOT} is not traceless, hence we have a Hamiltonian with $h^{00} \neq 0$. As mentioned above, this is irrelevant because $\mathrm{ad}_{\Lambda_{00}}=0$, i.e., in the adjoint representation one always obtains the corresponding traceless Hamiltonian.

The structure of the basis used indicates that H_{CNOT} is a nonlocal operation since it contains Λ_{13} (and the splitting into basis elements is obviously unique). While it leaves unentangled the computational basis elements, the same is not true in general for any state.

Comparing U_{CNOT} and R_{CNOT}, the price to pay in order to use the Stokes tensor parametrization is a larger dimension of the operator involved. On the other hand, the matrices are normally sparse and the formalism allows us to perform the same operation also on mixed states.

B. Three-qubit: Entangling at distance (I)

Assume we have available coupling Hamiltonians between A and B and between B and C. The qubit B can be thought of as an ancilla being first entangled with A and then sent to interact with C. Given a state in which A is maximally entangled with B while C is separable from the two (and known), we want to transfer the entanglement from the pair (AB) to the pair (AC) leaving B unentangled at the end of the evolution, without making use of a coupling Hamiltonian between A and C. Assume $\rho_{AB}(0)$ is the pure maximally entangled state

$$\varrho^{\{00,11,23,32\}}(0) = \tfrac{1}{2},$$

$$\varrho^{jk}(0) = 0 \quad \text{otherwise}.$$

and $\rho_C=(1/\sqrt{2})(\lambda_0+\lambda_1)$. The desired task is accomplished in half of the period $\tau_p=2\sqrt{2}\pi$, for example, by the following piecewise constant Hamiltonian:

$$-i\mathrm{ad}_H(t) = \begin{cases} -i\mathrm{ad}_{\Lambda_{033}}, & t \in \left[0, \dfrac{\tau_p}{4}\right) \\ -i\mathrm{ad}_{\Lambda_{220}}, & t \in \left[\dfrac{\tau_p}{4}, \dfrac{\tau_p}{2}\right] \end{cases}.$$

We obtain also that $\rho_{AB}(0)=\rho_{AC}(\pi/2)$ and $\rho_B(\pi/2)=\rho_C(0)$. As can be seen from Fig. 1, at $\tau_p/4$ the entanglement swaps from the pair AB to the pair AC. The scheme can be iterated to n qubits.

C. Three-qubit: Entangling at distance (II)

While the previous example is rather straightforward, in the literature there exist more sophisticated and surprising

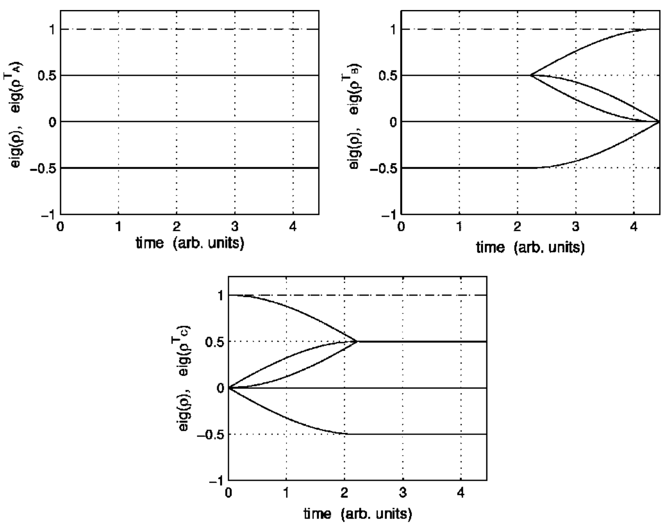

FIG. 1. The eigenvalues of ρ (dashed lines) and of its three partial transposes (solid lines): ρ^{T_A} (upper left plot), ρ^{T_B} (upper right), and ρ^{T_C} (lower left).

methods to distribute entanglement. In Ref. [18] it is shown that for the three-qubit separable state $\rho_{\text{in}} = \frac{1}{6}(\Sigma_{k=0}^{3} |\psi_k, \psi_{-k}, 0\rangle\langle\psi_k, \psi_{-k}, 0| + \Sigma_{j=0}^{1}|j,j,1\rangle\langle j,j,1|)$ with $|\psi_k\rangle = (|0\rangle + e^{ik\pi/2}|1\rangle)/\sqrt{2}$, it is possible to find a cascade of two CNOT gates, one with C as control qubit and acting on A and the other with B as control qubit and acting on C, such that at the end of the operation A and C are both entangled but for the whole process B remains unentangled. In terms of the Hamiltonian of the CNOT computed in Sec. V A, this is equivalent to the following piecewise constant three-qubit infinitesimal generator, obtained by permuting the indexes of H_{CNOT} and adding a "0" in the correct slot,[5]

$$-i\,\mathrm{ad}_H(t) = \begin{cases} -i(-\mathrm{ad}_{\Lambda_{300}} - \mathrm{ad}_{\Lambda_{001}} + \mathrm{ad}_{\Lambda_{301}}), & t \in \left[0, \frac{\pi}{\sqrt{2}}\right) \\ -i(-\mathrm{ad}_{\Lambda_{003}} - \mathrm{ad}_{\Lambda_{010}} + \mathrm{ad}_{\Lambda_{013}}), & t \in \left[\frac{\pi}{\sqrt{2}}, \frac{2\pi}{\sqrt{2}}\right] \end{cases}.$$

If $x = 1/(6\sqrt{2})$, then

$$\rho_{\text{in}} = \frac{1}{2\sqrt{2}}\Lambda_{000} + x\Lambda_{003} + x\Lambda_{110} + x\Lambda_{113} - x\Lambda_{220} - x\Lambda_{223} + x\Lambda_{330} - x\Lambda_{333},$$

$$\rho_{\text{int}} = \frac{1}{2\sqrt{2}}\Lambda_{000} - x\Lambda_{033} + x\Lambda_{111} - x\Lambda_{122} - x\Lambda_{212} - x\Lambda_{221} + x\Lambda_{303} + x\Lambda_{330},$$

[5]Notice that the time interval is rescaled with respect to the two-qubit case of Sec. V A because of the effect of the third qubit; see Eq. (6).

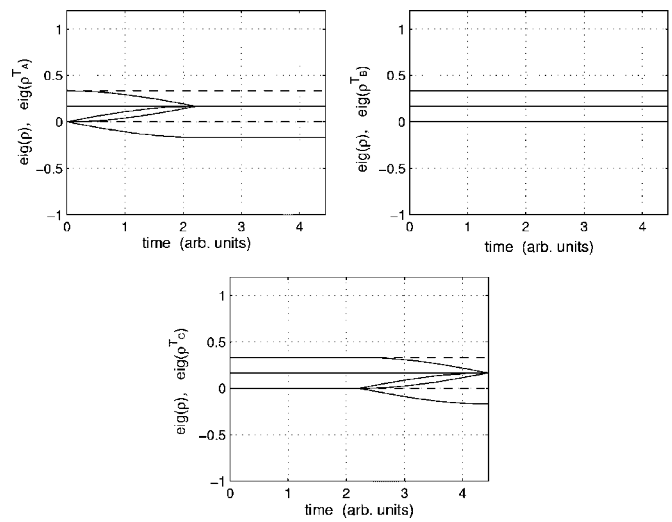

FIG. 2. The eigenvalues of ρ (dashed lines) and of its three partial transposes (solid lines): ρ^{T_A} (upper left plot), ρ^{T_B} (upper right), and ρ^{T_C} (lower left).

$$\rho_{\text{fin}} = \frac{1}{2\sqrt{2}}\Lambda_{000} - x\Lambda_{030} + x\Lambda_{101} + x\Lambda_{131} - x\Lambda_{202} - x\Lambda_{232} + x\Lambda_{303} + x\Lambda_{333},$$

where ρ_{int} is the density after the first CNOT gate and ρ_{fin} is the final state. Simulating the evolution of the system, we get that indeed B maintains a positive partial transpose (PPT) for the whole interval, as can be seen in Fig. 2, while A acquires a negative partial transpose (NPT) in the first half and keeps its through the second half. In this second part also C shows NPT. The behavior can be explained in terms of bipartite entanglement of different cuts of the three qubits. Look at Fig. 2. Since $(\rho^{T_{BC}})^T = \rho^{T_A}$, in the first half of the interval, A is entangling itself with the two-qubit reduced density ρ_{BC}. Such entanglement is bipartite and is not "visible" at the level of one-qubit reduced densities of B and C. The same thing happens between C and (AB) in the second half of the operation. The example is a well-cooked one as for all times there is no entanglement showing between B and (AC) (not just "at the end" of the gate). The doubt that remains is whether the final result is truly creation of entanglement between A and C, or rather a state in which two different types of one-qubit/two-qubit bipartite entanglement coexist without interacting with each other. Notice that a third CNOT operation on A and C (with either of the two as control qubit) leaves all three qubits with PPT.

APPENDIX A: FORMULAS FOR LIE BRACKETS OF TENSOR PRODUCT MATRICES

Proposition 1. Given $A_1, \cdots, A_n, B_1, \cdots, B_n \in M_m$, the commutator of $A_1 \otimes \ldots \otimes A_n$ and $B_1 \otimes \ldots \otimes B_n$ is given by

$$[A_1 \otimes \cdots \otimes A_n, B_1 \otimes \cdots \otimes B_n] = \sum \frac{1}{2^{n-1}}((A_1, B_1) \otimes (A_2, B_2) \otimes \cdots \otimes (A_n, B_n)), \tag{A1}$$

where in each summand the bracket $(\cdot, \cdot)$ is

$$[\cdot,\cdot] \quad k \text{ times, } k \text{ odd,}$$

$$\{\cdot,\cdot\} \quad n-k \text{ times,}$$

and the sum is over all possible (nonrepeated) combinations of $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ and over all odd $k\in[1,n]$.

The anticommutator of $A_1\otimes\cdots\otimes A_n$ and $B_1\otimes\cdots\otimes B_n$ is given by

$$\{A_1\otimes\cdots\otimes A_n, B_1\otimes\cdots\otimes B_n\} = \sum\frac{1}{2^{n-1}}((A_1,B_1)\otimes(A_2,B_2)\otimes\cdots\otimes(A_n,B_n)), \tag{A2}$$

where in each summand the bracket $(\cdot,\cdot)$ is

$$[\cdot,\cdot] \quad k \text{ times, } k \text{ even,}$$

$$\{\cdot,\cdot\} \quad n-k \text{ times,}$$

and the sum is over all possible (nonrepeatd) combinations of $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ and over all even $k\in[1,n]$.

Proof. We will prove the Proposition by induction. The formula (A1) is obviously true for $n=1$ (for $n=2$, 3, and 4 it is explicitly given below). Assume it is true for $n-1$ and write $\alpha=A_1\otimes\cdots\otimes A_{n-1}$, $\beta=B_1\otimes\cdots\otimes B_{n-1}$. Then for n we have

$$\begin{aligned}[\alpha\otimes A_n,\beta\otimes B_n] &= \alpha\beta\otimes A_nB_n-\beta\alpha\otimes B_nA_n\\ &\quad+\tfrac{1}{2}(\alpha\beta\otimes B_nA_n+\beta\alpha\otimes A_nB_n)\\ &\quad-\tfrac{1}{2}(\alpha\beta\otimes B_nA_n+\beta\alpha\otimes A_nB_n)\\ &=\tfrac{1}{2}([\alpha,\beta]\otimes\{A_n,B_n\}+\{\alpha,\beta\}\otimes[A_n,B_n]).\end{aligned}$$

If $[\alpha,\beta]$ contains an odd number of commutators, so does $[\alpha,\beta]\otimes\{A_n,B_n\}$. Likewise, if $\{\alpha,\beta\}$ has an even number of commutators, $\{\alpha,\beta\}\otimes[A_n,B_n]$ has to have an odd one. If $[\alpha,\beta]$ and $\{\alpha,\beta\}$ contain all possible nonrepeated combinations of commutators and anticommutators, so does the expression $[\alpha\otimes A_n,\beta\otimes B_n]$, and the induction is thus completed. Concerning the anticommutator (A2), the same induction arguments can be repeated for the following expression:

$$\begin{aligned}\{\alpha\otimes A_n,\beta\otimes B_n\} &= \alpha\beta\otimes A_nB_n+\beta\alpha\otimes B_nA_n\\ &\quad+\tfrac{1}{2}(\alpha\beta\otimes B_nA_n+\beta\alpha\otimes A_nB_n)\\ &\quad-\tfrac{1}{2}(\alpha\beta\otimes B_nA_n+\beta\alpha\otimes A_nB_n)\\ &=\tfrac{1}{2}([\alpha,\beta]\otimes[A_n,B_n]+\{\alpha,\beta\}\otimes\{A_n,B_n\}).\end{aligned}$$

While we are not certain of the complete novelty of the formulas (A1) and (A2), we are sure that various equivalent variants of them are well known[6] for low-dimensional tensors. Restricting to recent related literature, check, for example, [10,16,24]. The commutators for the first cases used in the paper are given explicitly below,

[6]And trivial, since it is enough to replace $AB=\frac{1}{2}([A,B]+\{A,B\})$ in the brute force calculation of the commutator/anticommutator and regroup appropriately.

$$[A_1\otimes A_2,B_1\otimes B_2]=A_1B_1\otimes A_2B_2-B_1A_1\otimes B_2A_2=\tfrac{1}{2}([A_1,B_1]\otimes\{A_2,B_2\}+\{A_1,B_1\}\otimes[A_2,B_2]), \tag{A3}$$

$$\begin{aligned}[A_1\otimes A_2\otimes A_3,B_1\otimes B_2\otimes B_3] &= A_1B_1\otimes A_2B_2\otimes A_3B_3-B_1A_1\otimes B_2A_2\otimes B_3A_3\\ &=\tfrac{1}{4}([A_1,B_1]\otimes\{A_2,B_2\}\otimes\{A_3,B_3\}+\{A_1,B_1\}\otimes[A_2,B_2]\otimes\{A_3,B_3\}+\{A_1,B_1\}\otimes\{A_2,B_2\}\otimes[A_3,B_3]\\ &\quad+[A_1,B_1]\otimes[A_2,B_2]\otimes[A_3,B_3]),\end{aligned} \tag{A4}$$

$$\begin{aligned}[A_1\otimes A_2\otimes A_3\otimes A_4,B_1\otimes B_2\otimes B_3\otimes B_4] &= A_1B_1\otimes A_2B_2\otimes A_3B_3\otimes A_4B_4-B_1A_1\otimes B_2A_2\otimes B_3A_3\otimes B_4A_4\\ &=\tfrac{1}{8}([A_1,B_1]\otimes\{A_2,B_2\}\otimes\{A_3,B_3\}\otimes\{A_4,B_4\}+\{A_1,B_1\}\otimes[A_2,B_2]\otimes\{A_3,B_3\}\otimes\{A_4,B_4\}\\ &\quad+\{A_1,B_1\}\otimes\{A_2,B_2\}\otimes[A_3,B_3]\otimes\{A_4,B_4\}+\{A_1,B_1\}\otimes\{A_2,B_2\}\otimes\{A_3,B_3\}\otimes[A_4,B_4]\\ &\quad+[A_1,B_1]\otimes[A_2,B_2]\otimes[A_3,B_3]\otimes\{A_4,B_4\}+[A_1,B_1]\otimes[A_2,B_2]\otimes\{A_3,B_3\}\otimes[A_4,B_4]\\ &\quad+[A_1,B_1]\otimes\{A_2,B_2\}\otimes[A_3,B_3]\otimes[A_4,B_4]\\ &\quad+\{A_1,B_1\}\otimes[A_2,B_2]\otimes[A_3,B_3]\otimes[A_4,B_4]).\end{aligned} \tag{A5}$$

[1] C. Altafini, Phys. Rev. A **69**, 012311 (2004).
[2] G. Mahler and V. A. Weberruß, *Quantum Networks* (Springer, Berlin, 1998).
[3] R. R. Ernst, G. Bodenhausen, and A. Wokaun, *Principles of*

Magnetic Resonance in One and Two Dimensions (Clarendon Press, Oxford, UK, 1987).
[4] T. F. Havel, D. G. Cory, S. Lloyd, N. Boulant, E. M. Fortunato, M. A. Pravia, G. Teklemariam, Y. S. Weinstein, A. Bhattacharyya, and J. Hou, Am. J. Phys. **70**, 345 (2002).
[5] G. Jaeger, M. Teodorescu-Frumosu, A. Sergienko, B. E. A. Saleh, and M. C. Teich, Phys. Rev. A **67**, 032307 (2003).
[6] G. Jaeger, A. V. Sergienko, B. E. A. Saleh, and M. C. Teich, Phys. Rev. A **68**, 022318 (2003).
[7] D. F. V. James, P. G. Kwiat, W. J. Munro, and A. G. White, Phys. Rev. A **64**, 052312 (2001).
[8] M. Teodorescu-Frumosu and G. Jaeger, Phys. Rev. A **67**, 052305 (2003).
[9] T. F. Havel, Quantum Inf. Proc. **1**, 511 (2002).
[10] T. F. Havel and C. J. L. Doran, in *Applications of Geometric Algebra in Computer Science and Engineering*, edited by L. Dorst, C. J. L. Doran, and J. Lasenby (Birkhäuser, Boston, 2002).
[11] N. Khaneja, R. Brockett, and S. J. Glaser, Phys. Rev. A **63**, 032308 (2001).
[12] A. R. P. Rau, Phys. Rev. A **61**, 032301 (2000).
[13] V. Subrahmanyam, e-print quant-ph/0307135.
[14] M. H. Yung, D. W. Leung, and S. Bose, e-print quant-ph/0312105.
[15] J. Marsden, *Lectures on Mechanics* (Cambridge University Press, Cambridge, 1992).
[16] N. Khaneja and S. J. Glaser, Chem. Phys. **267**, 11 (2001).
[17] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, Phys. Rev. A **67**, 042313 (2003).
[18] T. S. Cubitt, F. Verstraete, W. Dur, and J. I. Cirac, Phys. Rev. Lett. **91**, 037902 (2003).
[19] U. Fano, Rev. Mod. Phys. **55**, 855 (1983).
[20] L. Jakobczyk and M. Siennicki, Phys. Lett. A **286**, 383 (2001).
[21] F. Verstraete, J. Dehaene, and B. DeMoor, Phys. Rev. A **64**, 010101 (2001).
[22] J. Marsden and T. Ratiu, *Introduction to Mechanics and Symmetry*, Texts in Applied Mathematics, Vol. 17, 2nd ed. (Springer-Verlag, New York, 1999).
[23] R. Murray, Z. Li, and S. Sastry, *A Mathematical Introduction to Robotic Manipulation* (CRC Press, Boca Raton, FL, 1994).
[24] D. D'Alessandro, Math. Control, Signals, Syst. **16**, 1 (2003).
[25] R. Alicki and K. Lendi, *Quantum Dynamical Semigroups and Applications*, Lecture Notes in Physics, Vol. 286 (Springer-Verlag, Berlin, 1987).
[26] C. H. Bennett, D. P. DiVincenzo, C. A. Fuchs, T. Mor, E. Rains, P. W. Shor, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **59**, 1070 (1999).
[27] M. A. Nielsen, C. M. Caves, and B. Schumacher, Proc. R. Soc. London, Ser. A **454**, 277 (1998).