On the generation of sequential unitary gates from continuous time Schrödinger equations driven by external fields

Claudio Altafini*

SISSA-ISAS
International School for Advanced Studies
via Beirut 2-4, 34014 Trieste, Italy [†]

In most of the proposals for quantum computers, a common feature is that the quantum circuits are expected to be made of cascades of unitary transformations acting on the quantum states. Such unitary gates are normally assumed to belong to a given discrete set of transformations. However, arbitrary superposition of quantum states may be achieved by utilizing a fixed number of transformations, each depending on a parameter. A framework is proposed to dynamically express these parameters directly in terms of the control inputs entering into the continuous time forced Schrödinger equation.

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I. INTRODUCTION

In quantum information, the "computing" with quantum states is accomplished by applying sequences of discrete unitary gates, i.e. predetermined elements of the transformation group that acts on the state of the quantum system and determines its dynamical properties. One could say that what in a different context would be simply a parameterization of a group manifold, like a set of Euler angles, in the context of quantum computing becomes the "hardware" basis for the construction of quantum circuits. This "mimicking" the behavior of classical circuits is motivated by the need to simplify as much as possible the influence of the dynamics in the logic of the circuits, but it is complicated by the continuum of values in which the quantum state can exist, as opposed to its classical counterpart (i.e. the bit).

Such set of unitary transformations is normally specified in terms of the corresponding infinitesimal generators and, in order to guarantee arbitrary manipulation of the quantum states, it should be enough rich to generate the whole transformation group. In quantum computing, this property is called universality of the gates [6] and in [9] it is shown that "almost all gates are universal", see also [22, 24] for a control theoretic reformulation of the same idea. The problem is treated also in [5] by recollecting results on the uniform generation of the rotation groups. The main result is the following: arbitrary state transfer is achievable by means of a number of unitary gates equal to the dimension of the transformation group (henceforth $SU(N)$ of dimension $N^2 - 1$). In order to produce *any* arbitrary superposition state in an N-dimensional Hilbert space, the $N^2 - 1$ gates have to depend on equally many parameters. Such unitary gates do not have to correspond to linearly independent infinitesimal generators: in fact, owing to the semisimple nature of $SU(N)$, almost all pairs of infinitesimal generators in the Lie algebra $\mathfrak{su}(N)$ allows to achieve arbitrary state transfer by cascading $N^2 - 1$ exponentials of the two generators in alternate sequence. For the single qbit, this is the idea behind for example the ZYZ parameterization of rotations of the corresponding group of transformations $SU(2)$. For Nqbit systems, parameterizations aiming at the same scope are proposed for instance in [14, 19]. From a technological viewpoint, this is a great simplification as it means that in practice arbitrary manipulation can be done by sequencing control pulses applied along (almost) any pair of laboratory fixed axes. 2D NMR spectroscopy is one field where such techniques of sequencing pulses from two different directions has reached the level of a very sophisticated science [3, 7, 12]. The cascade of unitary transformations obtained in this way is a product of exponentials, each exponential containing a parameter expressing the time duration of the pulse (scaled by a constant depending on the "strength" of the applied field). As mentioned above, in the sequential model for quantum computing it is normally expected that the

elementary gates that constitute the "quantum circuits" will be made of *discrete* sets of unitary operators corresponding to *fixed* values of the $N^2 - 1$ parameters mentioned above, applied in a fixed order. This is enough for example to map eigenstates to eigenstates, but not to generate arbitrary superpositions. By varying the $N^2 - 1$ parameters of the product of exponentials, every quantum state is reached.

The main scope of this paper is to provide a framework for conciliating the continuous time driven dynamics of the forced Schrödinger equation with the "sequential dynamics" of quantum computers. In practice, it corresponds to rewriting the Schrödinger equation directly in terms of the gates of the quantum circuits. The formalism used is that of the Wei-Norman formula, which relates the Magnus expansion (suitable to represent the continuous time evolution of the Schrödinger equation) with the product of exponentials expansion corresponding to complete sets of parameterized elementary gates. Essentially, both expansions define local coordinate charts on the group of unitary transformations by means of a basis of the corresponding Lie algebra and via the exponential map. That is why these are sometimes referred to as *exponential coordinates* (or, in some cases, canonical coordinates). For compact groups, the two corresponding parameter spaces are different: one is a solid sphere and the other a cube, and the two sets of coordinates are related by nonlinear differential equations. An algorithm for the explicit computation of such differential equations (i.e. of the Wei-Norman formula) in terms of the structure constant of the Lie algebra was recently proposed in [2]. As for all series expansions on semisimple Lie groups, existence is not a global property, see [25]. In fact also the Wei-Norman formula has a singular locus which is an algebraic set of the parameter space.

Another control-theoretically sound way to design inputs that resemble elementary quantum gates is to use piecewise constant controls [18, 20] (or the closely related idea of coherent averaging used in NMR, see Section V for a comment). The methods proposed here could be seen as the differential version of the control design obtained via piecewise constant controls. In fact, also the flow induced by piecewise constant controls looks like a product of exponentials which resembles a cascade of elementary gates.

For sake of comprehension, a parallel with what happens in the control of robot arms [4] is useful to understand this relation: while at each time instant one can express the position of the end-effector (i.e. the tip of the arm where a robotic tool is placed) of a robot in terms of joint angles and topology of the robot via a *static* map, called forward kinematics, (in quantum control: a map constructed from the Lie group decompositions of the unitary propagator, i.e. from products of exponentials), in order to describe dynamic changes it is convenient to pass to the differential forward kinematics i.e. to the *Jacobian* map obtained by differentiating the static map mentioned above. In Robotics, the use of differential maps is crucial whenever a closed form expression of the inverse of the forward kinematics (giving the values of the joint angles in terms of the end effector position) is not available. The Wei-Norman formula is exactly the Jacobian of the change of coordinates between single exponential and product of exponentials. Furthermore, as we will see, it automatically allows to bypass what is the main problem of the piecewise constant control methods, that is to say finding an explicit value of the $N^2 - 1$ parameters that constitute a decomposition of an element in $SU(N)$ for $N > 2$ (in the robotic case this would correspond to the inversion of the forward kinematic map) by numerically integrating a differential map from a known initial condition. Lastly, while the Lie group decompositions used in piecewise constant control methods [18, 21] are not directly related to the positioning of the laboratory equipment that produces the control fields on the quantum system, this factor is implicitly considered in the product of exponentials we will use here.

II. EXPONENTIAL COORDINATES ON $SU(N)$

Consider a closed finite level quantum system described by a state $|\psi\rangle$ evolving according to the time dependent Schrödinger equation

$$
\begin{aligned}
i\hbar|\dot{\psi}(t)\rangle &= H(t)|\psi\rangle = (H_0 + H_I(t))\,|\psi(t)\rangle \\
|\psi(0)\rangle &= |\psi_0\rangle
\end{aligned}
\tag{1}
$$

where the state of the N-level quantum system $|\psi\rangle$ lives on the sphere in N-dimensional complex Hilbert space $\mathbb{S}^{N-1} = \{|\psi\rangle \in \mathbb{C}^N \text{ s.t. } \langle\psi|\psi\rangle = 1\}$, and the traceless Hermitian matrices H_0 and $H_I(t)$ are respectively the constant internal Hamiltonian and the external time-varying Hamiltonian, this last representing the interaction of the system with the control fields. The solution of (1) is normally written in terms of the unitary propagator $U(t) \in SU(N)$:

$$
|\psi\rangle = U(t)|\psi_0\rangle
$$

with $U(t)$ satisfying an equation similar to (1) but lifted from the sphere $\mathbb{S}^{N-1}$ to the special unitary group $SU(N)$:

$$\begin{aligned} i\hbar\dot{U}(t) = H(t)U(t) = (H_0 + H_I(t))\,U(t) \\ U(0) = I \end{aligned} \tag{2}$$

From now on, we shall use atomic units $\hbar = 1$. Assume $A_1, \ldots, A_n$, $n = N^2 - 1$, are skew-hermitian matrices forming a basis of the Lie algebra $\mathfrak{su}(N)$ and that the semiclassical approximation can be made for the external fields along each of the basis directions. Then the Hamiltonian $H(t)$ can be written in this basis as

$$-iH(t) = -i\,(H_0 + H_I) = \sum_{j=1}^{n} a_j A_j + \sum_{j=1}^{n} u_j A_j$$

where a_j and $u_j = u_j(t)$ are respectively the (constant) components of the free Hamiltonian along the basis directions and the (time-varying) control parameters of the interaction part, some of which might be zero if the control along the corresponding direction is missing.

If T is the Dyson time ordering operator, the solution of (2) is formally written in terms of the exponential map as

$$U(t) = T\exp\left(-i\int_0^t H(\tau)d\tau\right) = T\exp\left(-i\int_0^t \sum_{j=1}^{n}(a_j + u_j(\tau))A_j d\tau\right) \tag{3}$$

normally referred to as Magnus expansion [10]. Alternatively, instead of (3), the solution of (2) locally admits an expression in terms of product of exponentials, first due to Wei-Norman [26]

$$U(t) = \exp(\gamma_1 A_1)\ldots\exp(\gamma_n A_n) \tag{4}$$

with generally time dependent parameters $\gamma_i = \gamma_i(t)$. The relation between the two expansions (3) and (4) is given by the so-called *Wei-Norman formula*, which expresses the functions $\gamma_i(t)$ in terms of the $a_i + u_i(t)$ via a system of differential equations:

$$\Xi(\gamma_1, \ldots, \gamma_n)\begin{bmatrix}\dot{\gamma}_1 \\ \vdots \\ \dot{\gamma}_n\end{bmatrix} = \begin{bmatrix}a_1 + u_1 \\ \vdots \\ a_n + u_n\end{bmatrix} \qquad \gamma_i(0) = 0 \tag{5}$$

with the $n \times n$ matrix Ξ analytic in the variables γ_i. The matrix Ξ of elements $(\Xi)_{ki} = \xi_i^k$ is defined in terms of the γ_i as:

$$\prod_{j=1}^{m} e^{\gamma_j \operatorname{ad}_{A_j}} A_i = \sum_{k=1}^{n} \xi_i^k A_k \qquad m = 1, \ldots, n \tag{6}$$

When the cardinality of the basis ordering is followed in (4), the matrix Ξ assumes also the meaning of map between canonical coordinates of the first kind and canonical coordinates of the second kind, see [23]. In this case, since $\gamma_i(0) = 0$, $\Xi(0) = I$ and thus Ξ is locally invertible. However, any fundamental parameterization of $SU(N)$ could be used: various possible sets of Euler-like angles for $SU(N)$ are discussed in [14, 15, 19]. For example, we will concentrate on the ZYZ parameterization of $SU(2)$ in the example of Section IV. Because of the semisimplicity of $SU(N)$, all parameterizations lead to a Wei-Norman formula that is subject to singularities and as such Ξ^{-1} has only a local validity. Call Σ the singular set of Ξ. By inverting Ξ when possible, equation (5) assumes the more traditional aspect of a system of first order differential equations in the γ_i variables:

$$\begin{bmatrix}\dot{\gamma}_1 \\ \vdots \\ \dot{\gamma}_n\end{bmatrix} = \Xi(\gamma_1, \ldots, \gamma_n)^{-1}\begin{bmatrix}a_1 + u_1 \\ \vdots \\ a_n + u_n\end{bmatrix} \qquad \gamma_i(0) = 0 \tag{7}$$

If the time evolution of one of the two vectors of coordinates $\gamma_i(t)$ or $a_i + u_i(t)$ is known, the formulæ (5) or (7) can be used to obtain the other one. A method for the explicit closed-form calculation of the Wei-Norman formula is proposed in [2] and will not be repeated here.

A. Analysis of the parameter space of the two expansions

While (5) is global, (7) is valid only as long as $\det(\Xi) \neq 0$, and thus the nonsingularity of Ξ needs to be checked at the point of application. In general the exponential map does not posses any good property globally: for example for semisimple Lie groups it is surjective but not injective. The Lie algebra $\mathfrak{su}(N)$ being "compact" implies that the parameter space $\Gamma \subset \mathbb{R}^n$ of the coordinates corresponding to the exponential map, i.e. the set of values of the real coefficients needed to cover the whole Lie group under the exponential map, is a bounded domain, corresponding to the principal values of the logarithm map. For the single exponential representation and the basis A_i chosen above, the parameter space is a solid sphere of radius 2π. 2π is a conventional choice, see [8], p. 127, which originates from the standard choice of a factor $\frac{1}{2}$ in the exponentiation of the Pauli matrices, convention that we also follow in the example of Section IV. The radius could obviously be rescaled by any real normalization factor. In fact, given any vector $A \in \mathfrak{su}(N)$, the straight line through the origin γA, $\gamma \in \mathbb{R}$, is mapped to a one-parameter subgroup (a geodesic curve if the metric is obtained from the Killing form) of $SU(N)$. Because of compactness, exp is periodic and for such straight line it holds that $e^{(\gamma + 4\pi r)A} = e^{\gamma A}$ for some real constant r depending on the norm of A. Since this is true for all $A = \sum_{j=1}^n \alpha_j A_j$, the principal values of the logarithm map will correspond to a solid ellipsoid in general, and to a solid sphere in $\mathbb{R}^n$ of radius 2π when the A_j are suitably normalized and the α_j are such that $\sum_{j=1}^n \alpha_j^2 = 1$.

The lack of global properties of the exponential map is amplified in the products of exponentials such as (4). Call pexp the homomorphism

$$
\begin{aligned}
\text{pexp} \ : \ \Gamma &\to SU(N) \\
\gamma &\mapsto \prod_{k=1}^n e^{\gamma_k A_{\rho(k)}}
\end{aligned}
\tag{8}
$$

where $\rho(k)$ represents the ordering of the basis elements corresponding to the parameterization chosen for $SU(N)$ (in (4) $\rho(k) = k$, in the ZYZ parameterization of $SU(2)$ used below $\rho(1, 2, 3) = 3, 2, 3$). Although we have $\gamma_k \in \mathbb{R}$, also in this case the parameter space, i.e. the subset of $\mathbb{R}^n$ containing the principal values of pexp^{-1}, is a bounded domain in $\mathbb{R}$. However, since each γ_k enters into pexp(γ) independently from γ_j, $k \neq j$, this time the parameter space $\Gamma_\text{p} \subset \mathbb{R}^n$ corresponds to a cube in $\mathbb{R}^n$ centered in the origin and with sides of length 4π for the same basis A_j for which the logarithm has domain of principal values equal to the sphere of radius 2π.

III. ELEMENTARY QUANTUM GATES AS OUTPUT OF A SYSTEM OF DIFFERENTIAL EQUATIONS

Calling $\gamma = [\gamma_1 \ldots \gamma_n]^T$, $a = [a_1 \ldots a_n]^T$ and $u = [u_1 \ldots u_n]^T$, from (7) and (4) the state of the quantum system can be thought of as the output of the following system of first order nonlinear differential equations:

$$
\begin{cases}
\dot{\gamma} &= \Xi^{-1}(\gamma)\,(a + u) \qquad \gamma(0) = 0 \qquad \gamma \in \Gamma_\text{p} \setminus \Sigma \\
|\psi\rangle &= \text{pexp}(\gamma)|\psi_0\rangle
\end{cases}
\tag{9}
$$

While the differential equation (2) was linear in $U(t)$ and affine in the controls, the differential equation (9) is still affine in control but it is highly nonlinear in the variables γ.

The study of systems of nonlinear differential equations like (9) is quite common in systems theory, provided we call γ the "state vector" and $|\psi\rangle$ the "output". As they are quite confusing in the present context, these systems theory notations will not be used in the paper.

Essentially (9) transforms the problem of solving the driven Schrödinger equation (1) into a set of $N^2 - 1$ nonlinear differential equations defined on a subset $\Gamma_\text{p} \setminus \Sigma$ of $\mathbb{R}^{N^2-1}$. The only advantage over (1) is that the (numeric) solution of (9) is already in a form suitable for quantum computation as the γ have the interpretation of gates of a "quantum circuit".

A. Coherent states and γ-coherent states

In the whole paper we will always neglect global phase factors $e^{i\phi}$ as they are irrelevant for our purposes: $|\psi\rangle = e^{i\phi}|\psi\rangle$.

In general, an action of a Lie group on a manifold is said transitive if each pair of elements of the manifold can be joined by an element of the Lie group. On $\mathbb{S}^{N-1}$, the Lie group $SU(N)$ acts transitively: $\forall\, |\psi\rangle,\, |\psi_0\rangle \in \mathbb{S}^{N-1}$ there exists a unitary transformation $U \in SU(N)$ such that $|\psi\rangle = U|\psi_0\rangle$. The manifold in this case is a homogeneous space of the Lie group. The following definitions are standard for a quantum mechanical system (see [17, 27]). The *maximal isotropy subgroup* of $|\psi_0\rangle$ is given by

$$H_{|\psi_0\rangle} = \{h \in SU(N) \;\text{s.t.}\; h|\psi_0\rangle = |\psi_0\rangle\}$$

Since the action is transitive, $H_{|\psi_0\rangle}$ is a subgroup. In fact, if $h_1,\, h_2 \in H_{|\psi_0\rangle}$, then $h_2 h_1|\psi_0\rangle = h_2|\psi_0\rangle = |\psi_0\rangle$ and $h_1^{-1}|\psi_0\rangle = |\psi_0\rangle$. States that differ by an element $H_{|\psi_0\rangle}$ are *indistinguishable* from $|\psi_0\rangle$: if $U \in H_{|\psi_0\rangle}$ then $|\psi\rangle = U|\psi_0\rangle = |\psi_0\rangle$, again (and always) up to an irrelevant global phase factor. Calling $C_{|\psi_0\rangle}$ the *coset space* of $|\psi_0\rangle$ in $SU(N)$, i.e. the space of equivalence classes determined by the isotropy subgroup,

$$C_{|\psi_0\rangle} = SU(N)/H_{|\psi_0\rangle} \tag{10}$$

each $U \in SU(N)$ can be decomposed into $U = \Omega\, h$ with $\Omega \in C_{|\psi_0\rangle}$ and $h \in H_{|\psi_0\rangle}$. The "effective" change in $|\psi_0\rangle$ given by a unitary transformation $U = \Omega\, h$ corresponds to the coset component alone:

$$|\psi\rangle = U|\psi_0\rangle = \Omega\, h|\psi_0\rangle = \Omega|\psi_0\rangle$$

The set

$$\big\{\Omega|\psi_0\rangle \;\text{s.t.}\; \Omega \in C_{|\psi_0\rangle}\big\} = C_{|\psi_0\rangle}|\psi_0\rangle \tag{11}$$

is called the set of *coherent states* of $|\psi_0\rangle$. As can be seen from (11), the coherent states of $|\psi_0\rangle$ are obviously in 1-1 correspondence with the elements of the coset space $C_{|\psi_0\rangle}$.

For the product of exponentials map (8), the preimage $\mathrm{pexp}^{-1}(U)$ may vary from point to point. In particular, $\mathrm{pexp}^{-1}(I)$ varies according to the order $\rho(k)$ selected. For example, in the canonical coordinates of the second kind $(\rho(k) = k)$ $\mathrm{pexp}^{-1}(I) = \{0\}$, but in general it might be a nontrivial set. Call such set $H_\gamma(U)$, the γ-isotropy subgroup at U of the map pexp at $U \in SU(N)$

$$H_\gamma(U) = \{\gamma \in \Gamma_{\mathrm{p}} \;\text{s.t.}\; \mathrm{pexp}(\gamma) = U\} = \mathrm{pexp}^{-1}(U)$$

For example, $H_\gamma(I)$ is the set of all coordinates $\gamma \in \Gamma_{\mathrm{p}}$ that certainly do not produce any effect on $|\psi\rangle$ because their corresponding unitary operator is the identity. More generally, all γ such that $\mathrm{pexp}(\gamma) \in H_{|\psi_0\rangle}$ will produce no effect on an initial quantum state $|\psi_0\rangle$. We indicate the composition of the two types of isotropy subgroups as

$$H_\gamma(|\psi_0\rangle) = \text{``}H_\gamma \circ H_{|\psi_0\rangle}\text{``} = \big\{\gamma \in \Gamma_{\mathrm{p}} \;\text{s.t.}\; \mathrm{pexp}(\gamma) = h,\; \text{with}\; h \in H_{|\psi_0\rangle}\big\} \tag{12}$$

and call $H_\gamma(|\psi_0\rangle)$ the *γ-isotropy subgroup at $|\psi_0\rangle$*.

Thus $H_\gamma(|\psi_0\rangle)$ contains all the values $\gamma \in H_\gamma(|\psi_0\rangle)$ that are indistinguishable when looked from $|\psi\rangle$.

Similarly to (10), one can define the *γ-coset space $C_\gamma(|\psi_0\rangle)$* as

$$C_\gamma(|\psi_0\rangle) = \Gamma_{\mathrm{p}}/H_\gamma(|\psi_0\rangle)$$

and call the *γ-coherent states* the values assumed by $|\psi\rangle$ for γ varying in $C_\gamma(|\psi_0\rangle)$.

B. Universality of the gates for products of exponentials coordinates

The universality of the gates property mentioned in the introduction corresponds to $C_\gamma(|\psi_0\rangle)$ being all of $\mathbb{S}^{N-1}$. The corresponding concept for the Schrödinger equation (1) is the notion of controllablity [22, 24] i.e.

arbitrary manipulation of $|\psi\rangle$ by means of the control fields $u_j(t)$. It holds almost everywhere and depends on the free Hamiltonian (i.e. on the parameters a_i) being nondegenerate, see [1].

The aim here is to provide the same result on universality of the gates as [5, 6, 9] when the gates themselves are subordinated to the dynamics (9). Notice that whenever $\Sigma \subseteq H_\gamma(|\psi_0\rangle)$, the singular points of the representation (9) are ininfluent in the quantum state manipulation, i.e. they are not seen from $|\psi\rangle$ of (9). Thus we have the following:

Proposition 1 *Assume that the system* (1) *is controllable and that a fixed order of infinitesimal generators is chosen in* (8). *For a quantum state* $|\psi_0\rangle$,

  i) *if* $\Sigma \subseteq H_\gamma(|\psi_0\rangle)$, *then the gates in* (8) *are universal;*

  ii) *if* $\Sigma \nsubseteq H_\gamma(|\psi_0\rangle)$, *then the gates in* (8) *may not be universal. In this case the analysis of the singular locus Σ is required in order to establish universality of the gates.*

While the value of Σ depends only on the order chosen in (8), $H_\gamma(|\psi_0\rangle)$ varies also with the initial condition $|\psi_0\rangle$. Thus the previous sufficient condition for universality of the gates may hold only for some values of $|\psi_0\rangle$. Notice that, provided that (1) is controllable, the sufficient conditions above does not depend on the control authority available (i.e. on how many u_j, $j = 1, \ldots, n$ are different from 0). However, when $\Sigma \nsubseteq H_\gamma(|\psi_0\rangle)$ and the singular points of Σ are investigated, universality depends essentially on which control fields are available.

All the constructions and characterizations discussed so far are easily clarified by means of a concrete example.

IV. APPLICATION TO A SINGLE QBIT

The most elementary quantum state of interest here is the single qbit, defined on the sphere $\mathbb{S}^1$. In the computational basis $|0\rangle$, $|1\rangle$, the state is $|\psi\rangle \simeq \begin{bmatrix} y_1 & y_2 \end{bmatrix}^T$ with $|y_1|^2 + |y_2|^2 = 1$, thus the complex sphere in $\mathbb{C}^2$ is expressed in the computational basis coordinates as

$$\mathbb{S}^1 = \left\{ \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \in \mathbb{C}^2 \ \text{ s.t. } \ |y_1|^2 + |y_2|^2 = 1 \right\}$$

$SU(2)$ acts transitively on $\mathbb{S}^1$ and we shall concentrate on $SU(2)$ unitary transformations as elementary gates for $|\psi\rangle$. A skew-symmetric basis for $\mathfrak{su}(2)$ is obtained from the Pauli matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

for example by taking $A_j = \frac{i}{2}\sigma_j$, $j = 1, 2, 3$, i.e.

$$A_1 = \frac{1}{2} \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} \quad A_2 = \frac{1}{2} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad A_3 = \frac{1}{2} \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \tag{13}$$

and it corresponds to all real structure constants $c_{12}^3 = c_{23}^1 = c_{31}^2 = 1$. The corresponding adjoint matrices are

$$\text{ad}_{A_1} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \quad \text{ad}_{A_2} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad \text{ad}_{A_3} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

A. Magnus expansion

1. Constant controls case

For *fixed* and *constant* controls u_j, the Hamiltonian H in (1) becomes fully linear time-invariant and its exponential solution can be written down explicitly in terms of A_1, A_2, A_3 and I, see [8], p. 123. Call κ the

normalization factor

$$\kappa = \sqrt{(a_1 + u_1)^2 + (a_2 + u_2)^2 + (a_3 + u_3)^2} \tag{14}$$

Then

$$e^{t\left(\sum_{j=1}^3 (a_j + u_j)A_j\right)} = \cos\left(t\frac{\kappa}{2}\right)I + \frac{2}{\kappa}\left(\sum_{j=1}^3 (a_j + u_j)A_j\right)\sin\left(t\frac{\kappa}{2}\right) \tag{15}$$

It is now straightforward to verify that the time periodicity is 4π. If we assume the modulus $\kappa = 1$ by properly choosing the controls u_j, then [28]

$$\cos\left(\frac{t+4\pi}{2}\right)I + 2\left(\sum_{j=1}^3 (a_j + u_j)A_j\right)\sin\left(\frac{t+4\pi}{2}\right) = \cos\left(\frac{t}{2}\right)I + 2\left(\sum_{j=1}^3 (a_j + u_j)A_j\right)\sin\left(\frac{t}{2}\right)$$

The parameter space Γ, i.e. the portion of the Lie algebra that is needed to parameterize the group under the single exponential, is a solid sphere of radius 2π and with all the points on the surface identified (they all correspond to $-I$).

The Magnus expansion (3), and thus also (15), is well known to be only locally convergent, as can be seen by looking at the differential of the exponential map [23]. The singularities, i.e. the points where the exponential map fails to be a diffeomorphism, correspond to the operator

$$\mathrm{ad}_{\sum_{j=1}^3 (a_j+u_j)A_j} = \begin{bmatrix} 0 & -(a_3 + u_3) & a_2 + u_2 \\ a_3 + u_3 & 0 & -(a_1 + u_1) \\ -(a_2 + u_2) & a_1 + u_1 & 0 \end{bmatrix} \tag{16}$$

having eigenvalues equal to $2\pi m i$, $m \in \mathbb{Z} \setminus 0$ [25]. Since $\det\left(sI - \mathrm{ad}_{\sum_{j=1}^3 (a_j+u_j)A_j}\right) = s\left(s^2 + (a_1 + u_1)^2 + (a_2 + u_2)^2 + (a_3 + u_3)^2\right)$, from (14) and (16), the singular points of (15) are in:

$$\kappa = 2\pi m, \qquad m \in \mathbb{Z} \setminus 0$$

2. Time-varying controls

When the controls are piecewise constant, then the procedure of exponentiation has to be iterated, each time checking the nonsingularity condition. For general time varying controls instead, nothing can be said in general about convergence of the Magnus series except when the matrix norm $\| \cdot \|$ of $H(t)$ is such that

$$\int_0^t \|H(s)\|ds \leq \int_0^{2\pi} \frac{ds}{4 + s\left(1 - \cot\left(\frac{s}{2}\right)\right)} \simeq 1.086868702$$

see [13] and references therein.

B. ZYZ quantum logic gates

Probably the most common set of gates for the single qbit is given by the ZYZ Euler angles. Choosing such a parameterization for $SU(2)$, the ZYZ-operations on $|\psi_0\rangle$ are described by the following product of exponentials

$$|\psi\rangle = U(\gamma_1, \gamma_2, \gamma_3)|\psi_0\rangle = e^{i\gamma_1\frac{\sigma_3}{2}}e^{i\gamma_2\frac{\sigma_2}{2}}e^{i\gamma_3\frac{\sigma_3}{2}}|\psi_0\rangle = e^{\gamma_1 A_3}e^{\gamma_2 A_2}e^{\gamma_3 A_3}|\psi_0\rangle \tag{17}$$

where $\gamma = \begin{bmatrix} \gamma_1 & \gamma_2 & \gamma_3 \end{bmatrix}^T$ is defined in $\Gamma_{\mathrm{p}} = (-2\pi, 2\pi]^3$ and $\gamma_i = \gamma_i(t)$.

From the expressions for the exponentials of the Pauli matrices:

$$
e^{\gamma_1 A_1} = \cos\frac{\gamma_1}{2} I + i\sin\frac{\gamma_1}{2}\sigma_1 = \begin{bmatrix} \cos\frac{\gamma_1}{2} & i\sin\frac{\gamma_1}{2} \\ i\sin\frac{\gamma_1}{2} & \cos\frac{\gamma_1}{2} \end{bmatrix}
$$

$$
e^{\gamma_2 A_2} = \cos\frac{\gamma_2}{2} I + i\sin\frac{\gamma_2}{2}\sigma_2 = \begin{bmatrix} \cos\frac{\gamma_2}{2} & \sin\frac{\gamma_2}{2} \\ -\sin\frac{\gamma_2}{2} & \cos\frac{\gamma_2}{2} \end{bmatrix}
$$

$$
e^{\gamma_3 A_3} = \cos\frac{\gamma_3}{2} I + i\sin\frac{\gamma_3}{2}\sigma_3 = \begin{bmatrix} e^{i\frac{\gamma_3}{2}} & 0 \\ 0 & e^{-i\frac{\gamma_3}{2}} \end{bmatrix}
$$

the ZYZ product of exponentials is

$$
U(\gamma_1,\,\gamma_2,\,\gamma_3) = \begin{bmatrix} e^{i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\cos\frac{\gamma_2}{2} & e^{i(\frac{\gamma_1}{2}-\frac{\gamma_3}{2})}\sin\frac{\gamma_2}{2} \\ -e^{i(-\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\sin\frac{\gamma_2}{2} & e^{-i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\cos\frac{\gamma_2}{2} \end{bmatrix} \tag{18}
$$

C. Wei-Norman formula for the ZYZ Euler angles

The Wei-Norman formula corresponding to the ZYZ ordered product (17) is (see [2]):

$$
\Xi = \begin{bmatrix} 0 & -\sin\gamma_1 & \cos\gamma_1\sin\gamma_2 \\ 0 & \cos\gamma_1 & \sin\gamma_1\sin\gamma_2 \\ 1 & 0 & \cos\gamma_2 \end{bmatrix} \tag{19}
$$

and its inverse

$$
\Xi^{-1} = \begin{bmatrix} -\cos\gamma_1\cot\gamma_2 & -\sin\gamma_1\cot\gamma_2 & 1 \\ -\sin\gamma_1 & \cos\gamma_1 & 0 \\ \cos\gamma_1\csc\gamma_2 & \sin\gamma_1\csc\gamma_2 & 0 \end{bmatrix} \tag{20}
$$

Since $\det(\Xi) = \sin\gamma_2$, the singular points correspond to $\gamma_2 = k\pi$, $k \in \mathbb{Z}$, as is well-known for such a parameterization. Thus, in Γ_{p}, Ξ^{-1} can be used everywhere except in $\Sigma = \{\gamma \in \Gamma_{\mathrm{p}} \text{ s.t. } \gamma_2 = -\pi,\, 0,\, \pi,\, 2\pi\}$.

It is worth emphasizing that it is a fundamental topological fact that singularities cannot be avoided in a minimal parameterization of a semisimple Lie group. One possible way to get around the problem is obviously to use "redundant" parameterizations like unit quaternions, another to choose two different local charts i.e. two sets of of exponential coordinates corresponding for example to a different ordering in (17).

D. Example: nuclear spin qbit

In (9), some of the a_j and/or u_j might be zero. If for example the free Hamiltonian H_0 is diagonal then $a_1 = a_2 = 0$. In this case, most likely $u_3 = 0$ if we consider the dipole approximation for the coupling with the control fields. Consider a simple model for a spin $\frac{1}{2}$ in a static magnetic field along the Z axis and assume that independent tunable fields along both X and Y directions are available. The driven Schrödinger equation in this case has the familiar form

$$
|\dot\psi\rangle = -i\left(\frac{\omega_0}{2}\sigma_3 + \omega_1(t)\sigma_1 + \omega_2(t)\sigma_2\right)|\psi\rangle
$$

with $-i\frac{\omega_0}{2}\sigma_3$ the Zeeman Hamiltonian. In terms of the components of the skew-Hermitian basis (13), it can be written as ($\omega_0 = -a_3$, $u_j = -\frac{\omega_j}{2}$, $j = 1, 2$)

$$
|\dot\psi\rangle = (a_3 A_3 + u_1(t)A_1 + u_2(t)A_2)|\psi\rangle.
$$

Then, for the constant control case, formula (15) becomes:

$$
e^{t(a_3 A_3 + u_1 A_1 + u_2 A_2)} = \begin{bmatrix} \cos\left(t\frac{\kappa}{2}\right) + \frac{ia_3}{\kappa}\sin\left(t\frac{\kappa}{2}\right) & \frac{u_2+iu_1}{\kappa}\sin\left(t\frac{\kappa}{2}\right) \\ \frac{-u_2+iu_1}{\kappa}\sin\left(t\frac{\kappa}{2}\right) & \cos\left(t\frac{\kappa}{2}\right) - \frac{ia_3}{\kappa}\sin\left(t\frac{\kappa}{2}\right) \end{bmatrix}
$$

while, for time varying controls, using (20), (9) reads as

$$
\begin{cases}
\begin{bmatrix} \dot{\gamma}_1 \\ \dot{\gamma}_2 \\ \dot{\gamma}_3 \end{bmatrix} = \begin{bmatrix} a_3 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} -\cos\gamma_1 \cot\gamma_2 & -\sin\gamma_1 \cot\gamma_2 \\ -\sin\gamma_1 & \cos\gamma_1 \\ \cos\gamma_1 \csc\gamma_2 & \sin\gamma_1 \csc\gamma_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\[20pt]
|\psi\rangle \simeq \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} e^{i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\cos\frac{\gamma_2}{2} & e^{i(\frac{\gamma_1}{2}-\frac{\gamma_3}{2})}\sin\frac{\gamma_2}{2} \\ -e^{i(-\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\sin\frac{\gamma_2}{2} & e^{-i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}\cos\frac{\gamma_2}{2} \end{bmatrix} \begin{bmatrix} y_{1_0} \\ y_{2_0} \end{bmatrix}
\end{cases}
\tag{21}
$$

E.   Coherent states for $SU(2)$

The isotropy subgroup of a generic state $|\psi\rangle$ can be obtained by solving the algebraic equation

$$
|\psi\rangle = U(\gamma_1,\,\gamma_2,\,\gamma_3)|\psi\rangle \tag{22}
$$

The ZYZ representation is convenient is this respect since it is easy to notice that (22) is solved for all $|\psi_0\rangle$ at least by the submanifold $\gamma_2 = 0$ and $\gamma_3 = -\gamma_1$. In fact $U(\gamma_1, 0, -\gamma_1) = I$ and therefore $H_\gamma(|\psi_0\rangle) \supseteq H_\gamma(I) = \{\gamma \in \Gamma_{\mathrm{p}} \text{ s.t. } \gamma_2 = 0,\, \gamma_3 = -\gamma_1\}$. A complete computation of the $H_\gamma(|\psi_0\rangle)$ depends on the value of $|\psi_0\rangle$. For example, for $|0\rangle \simeq [1\ 0]^T$ (22) is solved by all γ such that $\gamma_2 = 0$ or $\gamma_2 = 2\pi$, since in this case $e^{i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}$ becomes an ininfluent global phase factor: $|0\rangle = \pm e^{i(\frac{\gamma_1}{2}+\frac{\gamma_3}{2})}|0\rangle$. Thus $H_\gamma(|0\rangle) = \{\gamma \in \Gamma_{\mathrm{p}} \text{ s.t. } \gamma_2 = 0,\, 2\pi\}$. In fact $|0\rangle$ is a highest weight state in $\mathbb{S}^1$, for which the computation of coherent states is easier [27]. If instead $|\psi_0\rangle$ is a superposition ($y_{1_0} \neq 0$ and $y_{2_0} \neq 0$), then the γ-isotropy subgroup contains $H_\gamma(I)$ but may also contain other points, according to the value of $|\psi_0\rangle$. We are in the case ii) of Proposition 1: $\Sigma \nsubseteq H_\gamma(|\psi_0\rangle)$ for some $|\psi_0\rangle$ (other than $|0\rangle$ and $|1\rangle$).

F.   Analysis of the singularity of the Wei-Norman formula

Let us look in detail to what happens on the singular set Σ to the product of exponentials (18):

<u>Case 1</u>

$$
\gamma_2 = -\pi \quad \Rightarrow \quad U(\gamma_1, -\pi, \gamma_3) = \begin{bmatrix} 0 & -e^{i(\frac{\gamma_1-\gamma_3}{2})} \\ e^{-i(\frac{\gamma_1-\gamma_3}{2})} & 0 \end{bmatrix}
$$

<u>Case 2</u>

$$
\gamma_2 = 0 \quad \Rightarrow \quad U(\gamma_1, 0, \gamma_3) = \begin{bmatrix} e^{i\frac{\gamma_1+\gamma_3}{2}} & 0 \\ 0 & e^{-i(\frac{\gamma_1+\gamma_3}{2})} \end{bmatrix}
$$

<u>Case 3</u>

$$
\gamma_2 = \pi \quad \Rightarrow \quad U(\gamma_1, \pi, \gamma_3) = \begin{bmatrix} 0 & e^{i(\frac{\gamma_1-\gamma_3}{2})} \\ -e^{-i(\frac{\gamma_1-\gamma_3}{2})} & 0 \end{bmatrix}
$$

<u>Case 4</u>

$$
\gamma_2 = 2\pi \quad \Rightarrow \quad U(\gamma_1, 2\pi, \gamma_3) = \begin{bmatrix} -e^{i\frac{\gamma_1+\gamma_3}{2}} & 0 \\ 0 & -e^{-i(\frac{\gamma_1+\gamma_3}{2})} \end{bmatrix}
$$

Thus an advantage of the product of exponentials formalism over the Magnus series is that the effect of the singular locus on $|\psi\rangle$ can be computed a priori, while the same type of problem is not easily treatable for the Magnus expansion with time varying control inputs.

In Σ, the Wei-Norman formula (20) is not valid anymore. However, in this case (19) becomes:

$$\Xi(\gamma_1,\, 0,\, \gamma_3) = \begin{bmatrix} 0 & -\sin\gamma_1 & 0 \\ 0 & \cos\gamma_1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{23}$$

Since in Σ, $\operatorname{rank}\Xi(\gamma_1,\, \gamma_2,\, \gamma_3) = 2$, varying u at most two of the $\dot{\gamma}_i$ can be varied independently. From (23) and (9) we get

$$\dot{\gamma}_1 + \dot{\gamma}_3 \;=\; a_3 + u_3 \tag{24}$$
$$\dot{\gamma}_2 \;=\; -(a_1 + u_1)\sin\gamma_1 + (a_2 + u_2)\cos\gamma_1 \tag{25}$$

i.e. it is still possible to obtain a well-defined expression for the dynamics at which γ_2 obeys.

In particular, in the example of (21), the system in Σ reduces to

$$\begin{cases} \begin{bmatrix} \dot{\gamma}_1 + \dot{\gamma}_3 \\ \dot{\gamma}_2 \end{bmatrix} \;=\; \begin{bmatrix} a_3 \\ -u_1\sin\gamma_1 + u_2\cos\gamma_1 \end{bmatrix} \\[2em] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \;=\; \begin{bmatrix} e^{i\left(\frac{\gamma_1+\gamma_3}{2}\right)}y_{1_0} \\ e^{-i\left(\frac{\gamma_1+\gamma_3}{2}\right)}y_{2_0} \end{bmatrix} \end{cases}$$

from which it is easy to observe that the free Hamiltonian only induces a relative phase transformation on a superposition state $|\psi_0\rangle$ (as expected, H_0 being diagonal), while the controlled system can always be steered out of $H_\gamma(|\psi_0\rangle)$ (and also of Σ) by means of the available control authority u_1 and u_2.

In summary: almost all the singular points of Ξ are indistinguishable for $|\psi\rangle$, i.e. they produce no influence on the quantum state. Some care is required in the algebraic set Σ because the exponential coordinates are not defined. The problem is analogous to the lack of global coordinates on a manifold. Even if Ξ^{-1} is not defined in Σ, the implicit equation (5) still governs the dynamics and can be used to pull γ out of Σ.

V.   CONCLUSION AND OUTLOOK

The aim of this work is to build the differential equations of a driven quantum dynamics in a formalism better suited for quantum computation, where a predefined set of quantum gates can be expressed directly in terms of the physical control parameters via exponential coordinates on the group of transformation. Beside the general remark that choosing coordinates on a manifold is always necessary when one wants to do computations, in the present context it is worth stressing that coordinates (here exponential coordinates) have the appealing interpretation of "gains" in the logic gates of the quantum hardware.

We would like to emphasize that the method presented here is by no means the only way to relate the continuous and sequential dynamics. Indeed each implementation proposal for quantum computers has its own method to generate gates, relying on the already existing techniques for state manipulation. See [16] for a survey of the different methods. The practice on NMR spectroscopy for example, bypasses the synthesis of the control fields in continuous time by applying pulses of predetermined time width and by checking the overall effect on the Hamiltonian via coherent averaging and synchronous stroboscopic measurements [3]. In that setting, the Hamiltonian $H(t)$ is computed in an interaction representation (referred to as the "toggling frame" in [7]) and it is averaged over the period T of the rotating magnetic field (the control). Normally then, this procedure is used as a way to solve explicitly the time-dependent Schrödinger equations and in fact as a limit case the Magnus series (3) is recovered. Working on the coarser time scale given by T, averaging gives a Magnus expansion which resembles a product of exponentials or, in control terms, the solution of (1) driven by piecewise constant control inputs. By differentiating such product of exponentials with respect to a set of parameters representing the amplitude of the control on each interval, one can recover (9).

The method we are proposing here not only enables to describe the unitary transformations in terms of the available control inputs, but it also gives the possibility of monitoring their variations due to dynamical

perturbations or uncertainties in the external fields. Furthermore, it has the advantage of keeping the singularities of the series expansion "under control" i.e., once the sequence of exponentials is chosen, also the effect of the singular locus of the Wei-Norman formula on $|\psi\rangle$ is precomputable, while the same is not true for time-dependent Magnus expansions. An obvious drawback is the computational burden related to the Wei-Norman formula, and especially its inversion, when N increases.

Since we choose to work with exponential coordinates for the unitary group $SU(N)$ of the Nqbit, non unitary disturbances like decoherence phenomena cannot be represented. We plan to extend the method to open quantum systems in the future.

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62:867–927, 1990.

[28] Notice that when $\kappa = 1$ the exponential (15) gives elements of $SU(2)$ in the form normally considered for unit quaternions, see [11], p. 304.