Use of Wei-Norman formulæ and parameter differentiation in quantum computing

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Abstract

For the unitary operator, solution of the Schrödinger equation corresponding to a time-varying Hamiltonian, the relation between the Magnus and the product of exponentials expansions can be expressed in terms of a system of first order differential equations in the parameters of the two expansions, often referred to as Wei-Norman formula. It is shown how to use Wei-Norman formulæ for the purposes of quantum computing.

1 Introduction

For time-varying finite dimensional closed quantum systems, the time evolution of the quantum state $|\psi\rangle$ can be written as $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, with the unitary propagator $U(t) \in SU(n)$ expressed locally as a formal exponential of the Hamiltonian $H(t)$. Alternatively, if $A_1, \ldots, A_n$, $n = N^2 - 1$, is a basis of $\mathfrak{su}(N)$, it is possible to write $U(t)$ in terms of some Euler-like parameterization of $SU(N)$. These parameterizations are essentially ordered products of exponentials on $SU(N)$ and for a Lie group there are as many such products as there are Lie group decompositions. See [8, 13, 9] for a few examples of explicit choices on $SU(N)$. Such decompositions are very useful for example in the generation of elementary gates in quantum computing or more generally in the control of driven dynamics [12, 15], but also in quantum state disentanglement [11], in the study of coherent states [7, 9], in the solution of the Liouville-von Neumann equation and in the design of schemes for the numerical integration of differential equations on Lie groups [5]. The two expressions for the $U(t)$ go under the names of Magnus expansion [6] and product of exponentials expansion [17]. We are interested here in studying how the two expansions relate, in particular how the parameters of the one series can be expressed as functions of the parameters of the other one. *In nuce*, such a transformation is already in the original papers of Wei-Norman, but its importance is made clear in [18]. In practice, it consists in studying a system of nonlinear differential equations having as variables the two sets of parameters contained in the two expansions. Such a system of differential equations is called the *Wei-Norman formula* and it corresponds to the *Jacobian* of the change of coordinates i.e. of the transformation from single exponential to product of exponentials.

The Wei-Norman formula appears in several different contexts in the literature, see [2, 3, 4, 14] just to mention a few. In [1] we propose a method to compute it explicitly and systematically for any dimension, based only on the structure constants of the Lie algebra. Such method seems to be new. The *rationale* behind it is a technique to compute in closed form one parameter groups of automorphisms i.e. exponentials of the matrices of the adjoint representation of any linear Lie algebra. As an example, here we compute two Wei-Norman formulæ for $\mathfrak{su}(2)$ for the same basis obtained from the Pauli matrices but for different ordering of the basis elements (i.e. different choices of Euler angles), and then propose a potential application in the context of quantum computing.

2 Magnus expansion versus product of exponentials expansion

Assume the Hamiltonian $H(t)$ is skew-Hermitian and belongs for all t to the finite dimensional Lie algebra $\mathfrak{su}(N)$. If we choose a basis of skew-symmetric matrices $A_1, \dots A_n$ for $\mathfrak{su}(N)$, then $[A_i,\, A_j] = \sum_{\mu=1}^{n} c_{ij}^{\mu} A_\mu$ where c_{ij}^{k} are the structure constants of $\mathfrak{su}(N)$. Since $A_1, \dots, A_n$ are time independent operators in $\mathfrak{su}(N)$, $H(t) = \sum_{\mu=1}^{n} u^{\mu}(t) A_\mu$ with $u^i(t)$ analytic functions of time. For the Schrödinger equation:

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \qquad |\psi(0)\rangle = |\psi_0\rangle.$$

Then $|\psi(t)\rangle = U(t)|\psi_0\rangle$, where $U(t)$ in the Magnus expansion is given by the formal expression

$$U(t) = T\exp\left(\int_0^t u^{\mu}(\tau) A_\mu d\tau\right) \tag{2.1}$$

where T is the Dyson operator and exp, the exponential map for $SU(N)$, is the ordinary matrix exponential. The *Wei-Norman formula* relates (2.1) with the expansion as a product of exponentials, i.e. it affirms that (2.1) can be written locally around the identity of $SU(N)$ as

$$U(t) = \exp\left(\gamma^1(t) A_1\right) \dots \exp\left(\gamma^n(t) A_n\right) \tag{2.2}$$

The Wei-Norman formula consists in expressing the functions $\gamma^i(t)$ in terms of the $u^i(t)$ via a system of differential equations:

$$\Xi(\gamma^1, \dots, \gamma^n) \begin{bmatrix} \dot{\gamma}^1 \\ \vdots \\ \dot{\gamma}^n \end{bmatrix} = \begin{bmatrix} u^1 \\ \vdots \\ u^n \end{bmatrix} \qquad \gamma^i(0) = 0 \tag{2.3}$$

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 and of the structure constants as:

$$\prod_{j=1}^{m} e^{\gamma^j \mathrm{ad}_{A_j}} A_i = \sum_{\mu=1}^{n} \xi_i^{\mu} A_\mu \qquad m = 1, \dots, n \tag{2.4}$$

When the A_i form a basis of $\mathfrak{su}(N)$, the matrix Ξ assumes also the meaning of map between canonical coordinates of the first kind (2.1) and canonical coordinates of the second kind (2.2), see [16]. In this case, since $\gamma^i(0) = 0$, $\Xi(0) = I$ and thus Ξ is locally invertible. However, 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. By inverting Ξ, equation (2.3) assumes the more traditional aspect of a system of first order differential equations in the γ^i variables:

$$\begin{bmatrix} \dot{\gamma}^1 \\ \vdots \\ \dot{\gamma}^n \end{bmatrix} = \Xi(\gamma^1, \ldots, \gamma^n)^{-1} \begin{bmatrix} u^1 \\ \vdots \\ u^n \end{bmatrix} \qquad \gamma^i(0) = 0 \tag{2.5}$$

If the time evolution of one of the two vectors of coordinates γ^i or u^i is known, the formulæ (2.3) or (2.5) can be used to obtain the other one. While (2.3) is global, (2.5) 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. Another weak point of the Wei-Norman formula is that the system of differential equations is nonlinear in the γ^i.

3 Example: $\mathfrak{su}(2)$

A skew-symmetric basis for $\mathfrak{su}(2)$ is obtained from the Pauli matrices

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

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

$$A_1 = \frac{1}{2}\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} \qquad A_2 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \qquad A_3 = \frac{1}{2}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \tag{3.6}$$

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

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

whose exponentials are:

$$e^{\gamma^1 \mathrm{ad}_{A_1}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma^1 & -\sin\gamma^1 \\ 0 & \sin\gamma^1 & \cos\gamma^1 \end{bmatrix} \qquad e^{\gamma^2 \mathrm{ad}_{A_2}} = \begin{bmatrix} \cos\gamma^2 & 0 & \sin\gamma^2 \\ 0 & 1 & 0 \\ -\sin\gamma^2 & 0 & \cos\gamma^2 \end{bmatrix} \qquad e^{\gamma^3 \mathrm{ad}_{A_3}} = \begin{bmatrix} \cos\gamma^3 & -\sin\gamma^3 & 0 \\ \sin\gamma^3 & \cos\gamma^3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The Magnus expansion (2.1) is given by $U(t) = T\int_0^t e^{u^1 A_1 + u^2 A_2 + u^3 A_3} d\tau$ (with $u^i = u^i(t)$).

3.1 Wei-Norman formula for canonical coordinates of the second kind

In the product of exponentials, choosing the order given by the cardinality of the index gives the canonical coordinates of the second kind on $SU(2)$: $U(t) = e^{\gamma^1 A_1} e^{\gamma^2 A_2} e^{\gamma^3 A_3}$ (again with $\gamma^i = \gamma^i(t)$). For this choice, the Wei-Norman formula reads as:

$$\Xi = \begin{bmatrix} 1 & 0 & \sin\gamma^2 \\ 0 & \cos\gamma^1 & -\cos\gamma^2 \sin\gamma^1 \\ 0 & \sin\gamma^1 & \cos\gamma^1 \cos\gamma^2 \end{bmatrix} \tag{3.7}$$

whose inverse can be computed explicitly:

$$\Xi^{-1} = \begin{bmatrix} 1 & \sin\gamma^1 \tan\gamma^2 & -\cos\gamma^1 \tan\gamma^2 \\ 0 & \cos\gamma^1 & \sin\gamma^1 \\ 0 & -\sec\gamma^2 \sin\gamma^1 & \cos\gamma^1 \sec\gamma^2 \end{bmatrix} \tag{3.8}$$

From (3.7), the determinant of Ξ is simply

$$\det \Xi = \cos\gamma^2$$

and thus the singularities of the representation are $\gamma^2 = \pi/2 + k\pi$, $k \in \mathbb{Z}$. While (2.3) (and (3.7)) is valid everywhere, in the singular points the formula (2.5) cannot be applied (i.e. (3.8) is not defined).

3.2 Wei-Norman formula for the ZYZ Euler angles

When expressed in the basis (3.6), the ZYZ Euler angles correspond to the product of exponentials $U(t) = e^{\gamma^1 A_3} e^{\gamma^2 A_2} e^{\gamma^3 A_3}$ (compare with the expression of Section 3.1). The Wei-Norman formula corresponds in this case to

$$\Xi = \begin{bmatrix} 0 & -\sin\gamma^1 & \cos\gamma^1 \sin\gamma^2 \\ 0 & \cos\gamma^1 & \sin\gamma^1 \sin\gamma^2 \\ 1 & 0 & \cos\gamma^2 \end{bmatrix}$$

and its inverse

$$\Xi^{-1} = \begin{bmatrix} -\cos\gamma^1 \cot\gamma^2 & -\sin\gamma^1 \cot\gamma^2 & 1 \\ -\sin\gamma^1 & \cos\gamma^1 & 0 \\ \cos\gamma^1 \csc\gamma^2 & \sin\gamma^1 \csc\gamma^2 & 0 \end{bmatrix}$$

Since

$$\det(\Xi) = \sin\gamma^2$$

the singularity has now moved to $\gamma^2 = k\pi$, $k \in \mathbb{Z}$, as is well-known for such a parameterization. Thus Ξ^{-1} can be used everywhere except in the identity $U(0) = I$. 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 quaternions.

4 Application to quantum computing

In quantum information [10], state manipulation is achieved via some set of elementary gates, by performing sequences of unitary transformations. This cascades of unitary matrices corresponds to products of exponentials. For $\mathfrak{su}(2)$, both the product of exponentials of Section 3.1 and Section 3.2 can provide a complete set of such unitary gates, i.e. can steer $|\psi_0\rangle$ arbitrarily to any $|\psi\rangle$ in the Hilbert space $\mathcal{H}^2$ respectively via

$$|\psi\rangle = e^{\gamma^1 A_1} e^{\gamma^2 A_2} e^{\gamma^3 A_3} |\psi_0\rangle \qquad \text{and} \qquad |\psi\rangle = e^{\gamma^1 A_3} e^{\gamma^2 A_2} e^{\gamma^3 A_3} |\psi_0\rangle$$

with γ_i computed as above. The method can be straightforwardly generalized to N-level systems.

5 Conclusion

To be able to describe a time varying dynamics in terms of simple unitary operations is an important issue in quantum mechanics and it is foreseen that it will be a crucial one in quantum computation. The method we propose here relates the one parameter flow of the Schrödinger equation with an arbitrary decomposition of $SU(N)$ by computing the Jacobian of the coordinate transformation. It is worth emphasizing that if the symbolic expression of the Wei-Norman formula rapidly explodes with the dimension of the system, its numerical integration can be easily and efficiently handled.

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