Quantum-based solution of time-dependent complex Riccati equations

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Using the Wei-Norman theory, we obtain a time-dependent complex Riccati equation (TDCRE) as the solution of the time evolution operator (TEO) of quantum systems described by time-dependent (TD) Hamiltonians that are linear combinations of the generators of the su(1, 1), su(2), and so(2, 1) Lie algebras. Using a recently developed solution for the time evolution of these quantum systems, we solve the TDCRE recursively as generalized continued fractions, which are optimal for numerical implementations, and establish the necessary and sufficient conditions for the unitarity of the TEO in the factorized representation. The inherited symmetries of quantum systems can be recognized by a simple inspection of the TDCRE, allowing effective quantum Hamiltonians to be associated with it, as we show for the Bloch-Riccati equation whose Hamiltonian corresponds to that of a generic TD system of the Lie algebra su(2). As an application, but also as a consistency test, we compare our solution with the analytic one for the Bloch-Riccati equation considering the Rabi frequency driven by a complex hyperbolic secant pulse generating spin inversion, showing an excellent agreement.

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I. INTRODUCTION

Symmetries have always had an important place in physics, and they became mainstays since Emmy Noether's theorem [1], where they were formally connected with conserved quantities. This theorem arises from the study of a lagrangian under the action of groups of infinitesimal transformations known as Lie groups [2], which are of special interest in physics because they are continuous groups with the structure of a differential manifold [3]. Lie groups can be introduced through their corresponding Lie algebras [4], with the group structures identified from the commutation relations satisfied by the generators of the algebra. A paradigmatic example of algebraic methods, i.e., methods that use the algebraic structure to describe and solve physical systems, can be found in one of the many ways of solving the quantum harmonic oscillator, where ladder operators are introduced to diagonalize the Hamiltonian, allowing a precise and elegant way of finding the corresponding energy levels and energy eigenfunctions [5]. Algebraic methods are important not just in the obtainment of the energy spectrum of physical systems [6], but also in the computation of dynamical properties as the time evolution operator (TEO), Feynman propagators, or Green functions [7,8]. Moreover, these methods can be used in the treatment of physical systems described by time-dependent (TD) Hamiltonians, which are natural scenarios for describing interactions with external agents. As a remarkable example, the so-called *Wei-Norman theory* [9,10] allows to find the exact solution of these systems when their Hamiltonians can be written as a linear combination of time-independent generators of a finite Lie algebra. Using this method, the Schrödinger equation is mapped on a set of coupled nonlinear differential equations from which the TEO can be calculated as a factorized element (that is, as a product of exponentials each containing only one generator of the algebra) of the correspondent Lie group. It is worth emphasizing that in most cases such solutions must be computed numerically, and the same is true for other exact solutions, such as those involving invariant quantities [11,12], for example. A different algebraic approach, based on Baker-Campbell-Haussdorf (BCH)-like relations obtained recently [13], provides a simple recursive way to directly compute the TEO of physical systems described by TD Hamiltonians which are written as linear combinations of the generators of the su(1, 1), su(2), and so(2, 1) Lie algebras. Notably, its numerical implementation is easy and limited only by computational capacity, and such an approach has proven to be efficient in the study of the time evolution of a TD quantum harmonic oscillator [14,15] and a system of two coupled TD qubits [16]. The main purpose of this work is to develop a formalism to recursively solve the differential equations that arise from the use of the Wei-Norman theory and to use the latter theory to directly obtain effective quantum Hamiltonians for the physical systems described by these differential equations.

In Sec. II we present the mathematical scenario and apply the Wei-Norman theory to quantum systems of the su(1, 1), su(2), and so(2, 1) Lie algebras, arriving at the time-dependent complex Riccati equation (TDCRE). Moreover, we obtain the complete unitarity criteria for the TEO in the factorized representation. In Sec. III we use an explicit solution for time-dependent quantum systems to solve the TDCRE recursively as generalized continued fractions. In Sec. IV we apply our results. Initially, we map the so-called Bloch-Riccati equation (BRE) [17,18] into an effective quantum Hamiltonian of the su(2) Lie algebra that can be performed by a TD qubit.

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TABLE I. Relations between the Lie algebras under consideration and parameters ϵ and δ.

Lie algebra	ϵ	δ
su(1, 1)	1	1
su(2)	−1	1
so(2, 1)	$i/2$	i

Subsequently, we solve the BRE numerically considering a complex hyperbolic secant pulse in the Rabi frequency and with a parameter domain where spin inversion phenomenon is generated. Comparison with the analytical results shows excellent agreement. Section V is left for conclusions and final comments.

II. FROM SCHRÖDINGER TO RICCATI

In this section we initially set the mathematical scenario for the simultaneous treatment of quantum systems described by TD hermitian Hamiltonians that are written as linear combinations of the generators of the aforementioned algebras. Let us consider the following Hamiltonian:

$$\hat{H}(t) = \eta_+(t)\hat{T}_+ + \eta_c(t)\hat{T}_c + \eta_-(t)\hat{T}_-, \tag{1}$$

where the η coefficients are in principle arbitrary (at least piecewise constant) scalar functions of time, and the $\hat{T}$'s are time-independent operators satisfying

$$[\hat{T}_-, \hat{T}_+] = 2\epsilon\hat{T}_c \text{ and } [\hat{T}_c, \hat{T}_\pm] = \pm\delta\hat{T}_\pm. \tag{2}$$

The parameters ϵ and δ allow us to identify the operators $\hat{T}$ as the generators of the su(1, 1), su(2), or so(2, 1) Lie algebras, as indicated in Table I.

Let us assume $\hat{T}_+ = \hat{T}_-^\dagger$. Therefore, from Eqs. (2) $\hat{T}_c$ is antihermitian for the so(2, 1) algebra or hermitian for the other two. Using the above, it can be shown that the hermiticity of the Hamiltonian is guaranteed if $\eta_+(t) = \eta_-^*(t)$, with $*$ denoting complex conjugation, while $\eta_c(t)$ must be either pure imaginary for the so(2, 1) algebra or real for the other two. Accordingly, three independent real-valued functions are needed to define completely the Hamiltonian, namely, two for $\eta_+(t)$ and one for $\eta_c(t)$. The Hamiltonian can be thus written as

$$\hat{H}(t) = \eta_+(t)\hat{T}_+ + \eta_c(t)\hat{T}_c + \eta_+^*(t)\hat{T}_-. \tag{3}$$

The state vector of a quantum system $|\psi(t)\rangle$ obeys the Schrödinger equation $i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$ ($\hbar = 1$) [19], and the corresponding TEO is defined by $|\psi(t)\rangle = \hat{U}(t, 0)|\psi(0)\rangle$, where we set the initial time at $t = 0$. Thereupon, the TEO fulfils the initial condition $\hat{U}(0, 0) = \mathbb{1}$, obeys the differential equation

$$i\frac{\partial}{\partial t}\hat{U}(t, 0) = \hat{H}(t)\hat{U}(t, 0), \tag{4}$$

and satisfies the composition property

$$\hat{U}(t, 0) = \hat{U}(t, t_{N-1})\hat{U}(t_{N-1}, t_{N-2})\dots\hat{U}(t_2, t_1)\hat{U}(t_1, 0). \tag{5}$$

There is no general method to find the TEO in Eq. (4) for an arbitrary TD Hamiltonian. However, when symmetries corresponding to the Lie groups can be identified in it, there is a general way to proceed, as we show below.

A. Wei-Norman theory and the Riccati equation

The Wei-Norman theory [9,10] ensures that when a Hamiltonian can be expressed as a linear combination of time-independent generators of a finite Lie algebra, the TEO can be written as an element of the correspondent Lie group, expressed as a product of exponentials of the algebra generators [20]. Accordingly, for our Hamiltonian in Eq. (3) we are allowed to consider the TEO factorized in the following convenient arrangement:

$$\hat{U}(t) = e^{\alpha(t)\hat{T}_+}e^{\ln(\beta(t))\hat{T}_c}e^{\gamma(t)\hat{T}_-}, \tag{6}$$

where we suppressed the initial time in our notation. Notice that there are six different but equivalent ways of ordering the exponentials of the generators, each arrangement with a different set of coefficients. Substituting the above equation together with Eq. (3) in Eq. (4), and with the aid of ordering techniques [21] (similarly to those found in Appendix B), we obtain the following set of coupled differential equations for the coefficients of the TEO:

$$\begin{aligned}
&\dot{\alpha} - \delta\frac{\dot{\beta}}{\beta}\alpha + \epsilon\delta\frac{\dot{\gamma}}{\beta^\delta}\alpha^2 + i\eta_+ = 0,\\
&\frac{\dot{\beta}}{\beta} - 2\epsilon\frac{\dot{\gamma}}{\beta^\delta}\alpha + i\eta_c = 0,\\
&\frac{\dot{\gamma}}{\beta^\delta} + i\eta_+^* = 0,
\end{aligned} \tag{7}$$

satisfying the initial conditions $\alpha = 0$, $\gamma = 0$, and $\beta = 1$ at $t = 0$, and where the overdot indicates time derivative. Notice that in the latter expressions we have omitted the temporal dependence in the argument of the functions for simplicity of notation. We shall do that along the text whenever there is not risk of confusion. The decoupling of the above equations leads to

$$\dot{\alpha} + \epsilon\delta(i\eta_+^*)\alpha^2 + \delta(i\eta_c)\alpha + i\eta_+ = 0, \tag{8}$$

which is a TDCRE in α. Actually, the above equation represents three families of TDCREs, each associated with one of the Lie algebras presented in Table I. Note that η_+ is the parameter associated with the nonlinearity of Eq. (8), and the solution for $\eta_+ = 0$ with the mentioned initial condition for α is the trivial one, namely, $\alpha(t) = 0$. Once the equation for α is solved, one can find β from Eqs. (7) as

$$\beta(t) = \exp\left\{-2i\epsilon\int_0^t \eta_+^*(t')\alpha(t')dt' - i\int_0^t \eta_c(t')dt'\right\}, \tag{9}$$

and then γ can be calculated as

$$\gamma(t) = -i\int_0^t \eta_+^*(t')\beta^\delta(t')dt'. \tag{10}$$

We can conclude, therefore, that the solution of the TEO corresponding to the TD Hamiltonian in Eq. (3) is equivalent to solve the TDCRE of Eq. (8). Notice that the TDCRE is of great importance, e.g., in mathematics [22], physics [23–26], and optimal control theory [27,28]. More specifically, in quantum physics the Hamiltonian of many prominent systems, such as coupled harmonic oscillators, models for spin and coupled spins, a charged particle moving in a magnetic field, or coupled two-photon lasers, can be put in the form of Eq. (3) (the above and other examples can be found in Ref. [12] and the references therein). Recall that the TDCRE has some known analytical solutions but, in general, it must be solved numerically [29].

One important nontrivial example of a TDCRE with a known analytical solution is the BRE [17], which we shall use in Sec. IV to do a consistency test of our results. Hence, it is appropriate to look at the problem from a reverse perspective and ask: When can we use our results if we start with a generic TDCRE as

$$\dot{\alpha} + b_0\alpha^2 + b_1\alpha + b_2 = 0, \tag{11}$$

with b_0, b_1, and b_2 arbitrary complex functions of time? A comparison between the above equation and Eq. (8) allows us to conclude that, to apply our solution, b_1 must be a pure imaginary function of time, b_2 arbitrary, and b_0 depending on the algebra as $b_0 = \frac{b_2^*}{2}$ so(2, 1), $b_0 = -b_2^*$ su(1, 1), or $b_0 = b_2^*$ su(2). Importantly, using the above prescription it is possible to relate TDCREs directly with quantum Hamiltonians of the mentioned algebras, as we shall show in Sec. IV.

B. Unitarity criteria

As previously mentioned, three independent real-valued functions are needed to fully define the Hamiltonian, and thus the same is true to fully describe the TEO [3]. However, although these functions should be identified directly from the constraints derived from the unitarity criteria for the TEO, we note that the latter is not easily found in the literature for the elements in the representation of Eq. (6). Therefore, due to the importance of unitarity in physical systems, and also as a per se relevant mathematical result, in Appendix A we take advantage of the algebraic methods developed in Ref. [13] to demonstrate the complete unitarity criteria that we list next. For an arbitrary element of the Lie groups under consideration, written as $\hat{G} = e^{|\alpha|e^{i\theta}\hat{T}_+}e^{\ln(|\beta|e^{i\xi})\hat{T}_c}e^{|\gamma|e^{i\phi}\hat{T}_-}$, the first constraint is

$$|\alpha| = |\gamma|, \tag{12}$$

independently of the group. For the SO(2, 1) Lie group the remaining two constraints are

$$e^{-\xi} = 1 + \frac{|\alpha|^2}{2} \quad \text{and} \quad \ln|\beta| = \theta + \phi \pm n\pi, \tag{13}$$

with $n = 1, 2, \ldots$. On the other hand, for the su(1, 1) and su(2) Lie groups the remaining two constraints are

$$|\beta| + \epsilon|\alpha|^2 = 1 \quad \text{and} \quad \xi = \theta + \phi \pm n\pi, \tag{14}$$

with $n = 1, 2, \ldots$. While he did not formally calculate the above relations for the groups under consideration, in an important paper of Truax [30] he showed that, starting with an unfactorized representation for an unitary element of the su(1, 1) and su(2) Lie groups, the factorized representation remains unitary.

III. TIME EVOLUTION OF QUANTUM SYSTEMS

We now follow a simple recursive solution recently developed in Ref. [13] to calculate the TEO corresponding to the Hamiltonian in Eq. (1). There, the authors considered a time splitting in N intervals of equally small enough size $\tau = t/N$ such that the Hamiltonian coefficients, and therefore the Hamiltonian itself, can be regarded as constant in each jth time interval ($j = 1, 2, \ldots, N$). Formally, this implies that the present solution will coincide with the exact one only in the limit $N \to \infty$ (and $\tau \to 0$). Nevertheless, for numerical implementation of this method, it is enough to choose τ to be much smaller than the typical timescale of the Hamiltonian coefficients. For our Hamiltonian in Eq. (3) let us write these functions compactly, henceforth, as $\boldsymbol{\eta} = (\eta_+, \eta_c, \eta_+^*)$. Without loss of generality we define their jth value as $\boldsymbol{\eta}_j \equiv \boldsymbol{\eta}(t = j\tau)$, where $\boldsymbol{\eta}_j = (\eta_{j+}, \eta_{jc}, \eta_{j+}^*)$, and the correspondent jth TEO can be thus written as a Lie group element in the *unfactorized* representation $\hat{U}_j = \exp(\lambda_{j+}\hat{T}_+ + \lambda_{jc}\hat{T}_c + \lambda_{j-}\hat{T}_-)$, where $\boldsymbol{\lambda}_j \equiv (\lambda_{j+}, \lambda_{jc}, \lambda_{j-}) = -i\tau\boldsymbol{\eta}_j$. Using BCH-like relations (see Appendix B for details) each $\hat{U}_j$ can be reexpressed in the factorized representation $\hat{U}_j = e^{\Lambda_{j+}\hat{T}_+}e^{\ln(\Lambda_{jc})\hat{T}_c}e^{\Lambda_{j-}\hat{T}_-}$, with the coefficients given by

$$\Lambda_{jc} = \left(\cosh(\nu_j) - \frac{\delta\lambda_{jc}}{2\nu_j}\sinh(\nu_j)\right)^{-\frac{2}{\delta}}, \tag{15}$$

$$\Lambda_{j\pm} = \frac{2\lambda_{j\pm}\sinh(\nu_j)}{2\nu_j\cosh(\nu_j) - \delta\lambda_{jc}\sinh(\nu_j)}, \tag{16}$$

and

$$\nu_j^2 = \left(\frac{\delta\lambda_{jc}}{2}\right)^2 - \delta\epsilon\lambda_{j+}\lambda_{j-}. \tag{17}$$

Since each $\hat{U}_j$ is a Lie group element and the TEO is given by the composition of them, then the total TEO must also be an element of the Lie group, so that it can be written in the form

$$\hat{U}(t) = e^{\alpha_N\hat{T}_+}e^{\ln(\beta_N)\hat{T}_c}e^{\gamma_N\hat{T}_-}, \tag{18}$$

where the choice of the coefficients in the previous expression is not coincidental. Indeed, comparing it with Eq. (6), it is clear that the solution for α, β, and γ is the same. Using the composition rule shown in Appendix A, the coefficients in the above equation can be written recursively as [13]

$$\alpha_j = \Lambda_{j+} + \frac{\alpha_{(j-1)}(\Lambda_{jc})^\delta}{1 - \epsilon\delta\alpha_{(j-1)}\Lambda_{j-}}, \tag{19}$$

$$\beta_j = \frac{\beta_{(j-1)}\Lambda_{jc}}{(1 - \epsilon\delta\alpha_{(j-1)}\Lambda_{j-})^{\frac{2}{\delta}}}, \text{ and} \tag{20}$$

$$\gamma_j = \gamma_{(j-1)} + \frac{\Lambda_{j-}(\beta_{(j-1)})^\delta}{1 - \epsilon\delta\alpha_{(j-1)}\Lambda_{j-}}, \tag{21}$$

with $\alpha_1 = \Lambda_{1+}$, $\beta_1 = \Lambda_{1c}$, $\gamma_1 = \Lambda_{1-}$, and $j = 1, 2, \ldots, N$. Notice that the α parameter is an independent term of β and γ, since the latter two need the former to be calculated.

Furthermore, it can be written as

$$\alpha_j = \Lambda_{j+} - \cfrac{(\Lambda_{jc})^\delta}{\epsilon\delta\Lambda_{j-} - \cfrac{1}{\Lambda_{(j-1)+} - \cfrac{(\Lambda_{(j-1)c})^\delta}{\epsilon\delta\Lambda_{(j-1)-} - \cfrac{1}{\dots - \cfrac{1}{\Lambda_{1+}}}}}}, \tag{22}$$

i.e., as a generalized continued fraction (GCF). This kind of mathematical object is important in the realm of complex analysis and is specially useful to study analyticity of functions as well as number theory, among other fields (see Ref. [31] and references therein). More importantly, its numerical implementation is straightforward and limited only by computational capacity, as demonstrated in Refs. [14–16].

Note that, although α is written recursively, the analytical calculation of its derivatives can be done by finding the differential equation that it satisfies, which we have demonstrated in Sec. II to be the TDCRE. Furthermore, there is a way to demonstrate this last result directly from the recursive solution for α given in Eq. (19). To do this, let us consider the limit of small time intervals satisfying $|\eta_j|\tau \ll 1$, so that $\nu_j \ll 1$. Up to first order in τ, we have $\sinh(\nu_j) \approx \nu_j$ and $\cosh(\nu_j) \approx 1$. In this case, one trivially finds $(\Lambda_{jc})^\delta \approx 1 - i\delta\,\eta_{jc}\tau$, $\Lambda_{j+} \approx -i\eta_{j+}\tau$, and $\Lambda_{j-} \approx -i\eta^*_{j+}\tau$. Therefore, $(1 - \epsilon\delta\Lambda_{j-}\alpha_{j-1})^{-1} \approx 1 - i\epsilon\delta\,\eta^*_{j+}\,\alpha_{j-1}\,\tau$, and up to first order in τ the recurrence relation for α becomes

$$\alpha_j \approx \alpha_{j-1} - \tau\left(i\epsilon\delta\,\eta^*_{j+}\,\alpha^2_{j-1} + i\delta\eta_{jc}\alpha_{j-1} + i\eta_{j+}\right). \tag{23}$$

When $\tau \to 0$, the finite difference ratio in α approaches a derivative resulting in the Riccati equation (8). In this way, the connection between the generalized continued fraction and the complex Riccati equation for α is straightforward.

As a particular case, we can realize that $j = 1$ corresponds to the exact analytic solution for a sudden change (also called a jump or a quench) in the Hamiltonian coefficients at $t = 0$. Moreover, Eqs. (19)–(21) represent the exact analytic solution for a sequence of N jumps equally spaced in time of the Hamiltonian coefficients. For one jump at $t = 0$, they can be written as $\boldsymbol{\eta}(t) = \boldsymbol{\eta}^o + (\boldsymbol{\eta}^f - \boldsymbol{\eta}^o)\Theta(t)$, where $\boldsymbol{\eta}^o \equiv \boldsymbol{\eta}(t < 0)$, $\boldsymbol{\eta}^f \equiv \boldsymbol{\eta}(t \geqslant 0)$, and Θ is the usual Heaviside step function. The corresponding TEO is therefore given by $\hat{U}_1(t,0) = e^{\Lambda_{1+}\hat{T}_+}e^{\ln(\Lambda_{1c})\hat{T}_c}e^{\Lambda_{1-}\hat{T}_-}$, with the Λ functions given by Eqs. (15) and (16) evaluated for $\boldsymbol{\lambda}_1 = -it(\eta^f_+, \eta^f_c, \eta^{*f}_+)$. Notice that, as we are using essentially the composition rule for the elements of the groups corresponding to the algebras under consideration, our solution also contemplates the calculation of the TEO for systems with a finite number of jumps in their parameters that are not necessarily equally spaced in time, e.g., the case of a quantum harmonic oscillator with frequency jumps [32–35], being useful in the construction of squeezed states of atomic motion in optical lattices [36]. Moreover, they can also be used to calculate the arbitrary composition of squeeze operators, rotation operators, and many other interesting unitary operators of the Lie algebras under consideration (see, for instance, Refs. [37,38]).

To end this section, it is important to note that the constraints obtained from the unitarity in Eqs. (12)–(14) can be used as a fundamental test for the numerical implementations of our results, once the Λ functions in Eqs. (15) and (16) must satisfy them at any time (for any j), and the same is true for Eqs. (19)–(21).

IV. EFFECTIVE HAMILTONIAN AND SOLUTION OF THE BLOCH EQUATIONS

Since its publication in 1946 [39], the Bloch equations became of fundamental importance in the realm of NMR. They provide a quantitative description of any NMR experiment that involves radio frequency pulses, which are at the heart of all modern NMR experiments [18]. In this section we shall use our results to identify the effective quantum Hamiltonian for the Bloch-Riccati equation and numerically recover the remarkable results of Silver *et al.* [17] as an application of our results. Following this reference, the Bloch equations in the rotating frame, neglecting relaxation terms, can be written as

$$\begin{aligned} &\dot{M} + i\Delta\omega M + M_z\Omega(t) = 0,\\ &\dot{M}_z - \frac{i}{2}(M\Omega^*(t) - M^*\Omega(t)) = 0, \end{aligned} \tag{24}$$

where M is the complex magnetization in the x–y plane, M_z is the longitudinal magnetization, and $\Omega(t) = -g(B_{1x} + iB_{1y})$ is the complex TD driving function. Using the definition

$$f = \frac{M}{M_o + M_z}, \tag{25}$$

where M_o is the equilibrium magnetization, Eqs. (24) can be transformed into the BRE [17], namely,

$$\dot{f} - \frac{i}{2}\Omega^*(t)f^2 + i\Delta\omega f + \frac{i}{2}\Omega(t) = 0. \tag{26}$$

Notice that the above equation is identical to Eq. (8) for the particular case of the Lie algebra su(2) ($\delta = 1$ and $\epsilon = -1$), with the identifications $\eta_+ = \Omega(t)/2$ and $\eta_c = \Delta\omega$. Therefore, using our results of Sec. II A, the corresponding effective Hamiltonian is simply given by

$$\hat{H}(t) = \tfrac{1}{2}\Omega(t)\hat{T}_+ + \Delta\omega\hat{T}_c + \tfrac{1}{2}\Omega^*(t)\hat{T}_-. \tag{27}$$

Furthermore, if we consider a realization of this algebra for the Pauli operators σ_+, σ_-, and σ_z, with $\sigma_\pm = \sigma_x \pm i\sigma_y$, we note that the above Hamiltonian will be exactly the same as a TD qubit [40], with $\Omega(t)$ the Rabi frequency and $\Delta\omega$ an effective detuning. We conclude, therefore, that the time evolution of a TD qubit is, among several other possible TD systems of the su(2) Lie algebra, a setup equivalent to NMR described by the Bloch equations in the rotation frame and with relaxation terms neglected, a result that is in agreement with the well-known connection between quantum optics and NMR [18]. Note that, although there are some exact solutions for a TD qubit with certain driving terms (see, e.g., Ref. [41]), our general approach allows us to consider arbitrary complex TD functions for the Rabi frequency as well as arbitrary real-valued functions for the detuning.

A nontrivial emblematic example with an analytical solution for the BRE and with relevant experimental applications in NMR comes from the use of a complex hyperbolic secant pulse as the driving function for the Rabi frequency [17]. Moreover, choosing appropriately the domain of the involved functions, spin inversion phenomenon can be achieved. As a consistency test, we now shall recover the results for such driving. Let us consider the following family of functions for the Rabi frequency:

$$\Omega(t) = \Omega_o(\text{sech}\,\chi(t - t_o))^{1+i\mu}, \tag{28}$$

where μ is a real constant and Ω_o is the pulse amplitude. Using the above driving, the BRE (26) can be transformed in a hypergeometric equation with known solutions. After taking into account the initial conditions, the authors in Ref. [17] found for the stationary solution of the magnitude of $f(t)$ the following simple expression:

$$|f|^2_{t\to\infty} = \frac{\cosh^2(\pi\mu/2) - \cos^2(\pi y)}{\cosh^2(\pi\Delta\omega/2\chi) - \sin^2(\pi y)}, \tag{29}$$

with

$$y = \left\{\left(\frac{\Omega_o}{2\chi}\right)^2 - \left(\frac{\mu}{2}\right)^2\right\}^{1/2}, \tag{30}$$

and where they considered solutions for y real and $2y \neq 1, 2, 3, \ldots$. The quantity that serves to predict the spin inversion is given by $\frac{M_z}{M_o} = \frac{1-|f|^2_{t\to\infty}}{1+|f|^2_{t\to\infty}}$. Using Eq. (29), it can be shown that

$$\frac{M_z}{M_o} = \tanh\varphi_1 \tanh\varphi_2 + \text{sech}\varphi_1 \text{sech}\varphi_2 \cos\varphi_3, \tag{31}$$

where

$$\varphi_1 = \pi\left\{\frac{\Delta\omega}{2\chi} + \frac{\mu}{2}\right\}, \quad \varphi_2 = \pi\left\{\frac{\Delta\omega}{2\chi} - \frac{\mu}{2}\right\},$$

$$\text{and} \quad \varphi_3 = \pi\left\{\left(\frac{\Omega_o}{\chi}\right)^2 - \mu^2\right\}^{1/2}. \tag{32}$$

Spin inversion is achieved if the above quantity changes from $\frac{M_z}{M_o} = 1$ to $\frac{M_z}{M_o} = -1$ (and vice versa). Moreover, notice from Eq. (31) that without phase modulation ($\mu = 0$) and whenever $\Omega_o = 2n\chi$ with $n = 1, 2, \ldots$, there is an excursion of the magnetization ($M_z = M_o$). On the other hand, in the limit of $\mu \to \infty$, $\chi \to 0$, with $\mu\chi \to C$ a constant, and $\Omega_o \geqslant C$, the magnetization is inverted over all frequencies ($M_z = -M_o$). To capture this phenomenon and taking into account the considered analytical solutions, we chose for the numerical calculations the following values of the parameters in arbitrary units: $\Omega_o = 10$, $\chi = \Omega_o/2\mu$, and $\mu = \{7/5, 2, 4\}$ for the phase modulation parameter, with fixed values of $\Delta\omega$ sweeping the interval $-15 \leqslant \Delta\omega \leqslant 15$. We also chose a time interval for the analysis of $t \in [0, 40]$. In Fig. 1, we plot in solid lines the analytic solution of Eq. (31) for the chosen values of the parameters. Recall that the intermediary numerical calculations of Eqs. (15)–(17) allow for the testing of the code using the unitary relations given in Eqs. (12) and (14) ($\epsilon = -1$). Now, considering the time splitting in $N = 8 \times 10^3$ intervals for each value (point) of $\Delta\omega$, we numerically calculate a total of 300 points within the effective detuning interval to evaluate the same quantity with our formalism. The calculations took less than 20 min on a laptop machine

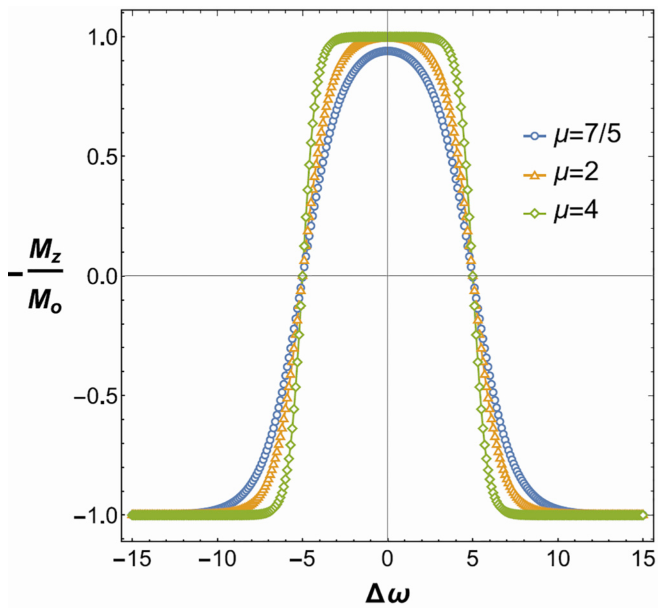

FIG. 1. Spin inversion as a function of the detuning using the driving in Eq. (28) for different values of the real parameter μ. Solid lines are calculated with the analytic expression of Eq. (31), while the points are numerically calculated with our general approach.

and are plotted as the dot patterns in Fig. 1. As it can be noted, the matching is excellent, allowing us to validate our results. Recall that our formalism allows one to fully calculate the TEO corresponding to the NMR effective Hamiltonian obtained in Eq. (27), i.e., the β and γ functions in addition to α, and, consequently, to evolve any initial state. Nevertheless, the only necessary parameter to describe spin inversion in this case is α. This is because the Bloch equations (24) consider intrinsically the initial state of the system as the ground state, where α is the protagonist of the dynamics. Therefore, we can expect that in NMR analysis using arbitrary drivings and initial states, our results will be useful.

V. CONCLUSIONS

In the first part of this work we derived a TDCRE from the application of the Wei-Norman theory in TD systems of the su(1, 1), su(2), and so(2, 1) Lie algebras, and so we obtained all the necessary and sufficient conditions for the unitarity of the elements of the correspondent given Lie groups in the factorized representation. This result is important as unitarity guarantees probability conservation. Then, in the second part of this work we used a solution for time-dependent quantum systems to solve the TDCRE recursively as GCFs, which are optimal for numerical implementations. The formalism we developed also allows us to associate effective Hamiltonians directly to TDCREs, as we showed in the third part of this work for the BRE, mapping it in an effective quantum Hamiltonian of the su(2) Lie algebra. Then, as an application, but also as a consistency test, we numerically calculated the solution of the BRE for a complex hyperbolic secant pulse generating spin inversion and compared it to analytical results, showing excellent agreement. Our results are quite general and can be used not just to solve the TEO of any

TD system of the algebras at issue and its related TDCRE, but also TDCREs that do not need to be related to quantum systems. For instance, Newton's laws can be put in the form of Riccati equations under certain conditions [42], and therefore it should be possible to apply the methods discussed in this work.

Our results can be straightforwardly extended to other nonlinear differential equations that can be derived from the TDCRE, e.g., the (dissipative) Ermakov equation [43–45] with its respective invariant, paving the way for new possibilities in the quantum-classical connection [25]. Furthermore, our results can also be extended for other algebras with a higher number of generators [46], arriving at different sets of differential equations that could be solved in terms of GCFs, also amplifying the possibilities of investigating more complex systems as coupled TD-quantum harmonic oscillators [47–50] or coupled TD qubits [16,51]. Our results related to GCFs could also be useful in the analysis of quantum systems using differential Galois theory [52], in extensions for nonhermitian time-dependent systems [53], in the search for special symmetries leading to analytical solutions [54], as well as in the analysis of the Lie-Scheffers theorem [55,56]. Finally, we can expect applications of our results in several branches of physics, as they encompasses the solution of the TEO of important fundamental systems as TD qubits and TD-quantum harmonic oscillators, being useful in the control of quantum systems [57,58], in the design of shortcuts to adiabaticity [59], in the harnessing of nonadiabatic excitations promoted by quantum critical points [60], in the description of ion traps dynamics [61], in quantum thermodynamics [62–65], in the study of (cavity) optomechanical systems [66–69], or in quantum interference of levitated nanorotors [37], among many others.

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APPENDIX A: BCH-LIKE RELATIONS AND UNITARY CRITERIA

The BCH-like relations developed in Ref. [13] are essentially the composition rule for the elements of the groups corresponding to the algebras under consideration, once they are written in the factorized representation of Eq. (6). More specifically, given two arbitrary elements $\hat{G}_1 = e^{\tilde{\alpha}\hat{T}_+}e^{\ln(\tilde{\beta})\hat{T}_c}e^{\tilde{\gamma}\hat{T}_-}$ and $\hat{G}_2 = e^{\alpha\hat{T}_+}e^{\ln(\beta)\hat{T}_c}e^{\gamma\hat{T}_-}$, their product is another element of the group, namely,

$$\hat{G} = \hat{G}_2\hat{G}_1 = e^{\zeta_+\hat{T}_+}e^{\ln(\zeta_c)\hat{T}_c}e^{\zeta_-\hat{T}_-}, \tag{A1}$$

where

$$\zeta_+ = \alpha + \frac{\tilde{\alpha}\beta^\delta}{1-\epsilon\delta\tilde{\alpha}\gamma}, \quad \zeta_c = \frac{\tilde{\beta}\beta}{(1-\epsilon\delta\tilde{\alpha}\gamma)^{\frac{2}{\delta}}},$$
$$\text{and} \quad \zeta_- = \tilde{\gamma} + \frac{\gamma(\tilde{\beta})^\delta}{1-\epsilon\delta\tilde{\alpha}\gamma}. \tag{A2}$$

Notice that the inverse product, i.e., $\hat{G}_1\hat{G}_2$, leads to identical relations as in Eqs. (A2) but interchanging the letters having tildes with those that do not. Suppose that we know $\hat{G}_2$ and we desire to obtain its inverse, namely, $\hat{G}_1$. Accordingly, their product must equal the identity, i.e., $\hat{G}_2\hat{G}_1 = \hat{G}_1\hat{G}_2 = \mathbb{1}$. In Eq. (A2) this implies $\zeta_+ = 0$, $\zeta_c = 1$, and $\zeta_- = 0$, from which we obtain $\tilde{\alpha} = -\frac{\alpha}{l}$, $\tilde{\beta} = \frac{\beta}{l^{\frac{2}{\delta}}}$, and $\tilde{\gamma} = -\frac{\gamma}{l}$, where we define $l \equiv \beta^\delta - \epsilon\delta\,\alpha\,\gamma$. It can also be proven that for the inverse product the above relations holds true, and therefore $\hat{G}_2$ is the inverse of $\hat{G}_1$. Let us now define

$$\alpha = |\alpha|e^{i\theta}, \quad \beta = |\beta|e^{i\xi}, \quad \text{and} \quad \gamma = |\gamma|e^{i\phi}. \tag{A3}$$

The unitary condition demands $\hat{G}^{-1} = \hat{G}^\dagger$, where $\hat{G}^\dagger = e^{\gamma^*\hat{T}_+}e^{\ln(\beta^*)\hat{T}_c^\dagger}e^{\alpha^*\hat{T}_-}$, leading to

$$\gamma^* = -\frac{\alpha}{l}, \quad \ln(\beta^*)\hat{T}_c^\dagger = \ln\left(\frac{\beta}{l^{\frac{2}{\delta}}}\right)\hat{T}_c, \quad \text{and} \quad \alpha^* = -\frac{\gamma}{l}. \tag{A4}$$

From the left- and right-hand-side equations above and Eqs. (A3) we obtain the following results valid for all the algebras at issue: First, the constraint

$$|\alpha| = |\gamma|. \tag{A5}$$

Second, that l is just a phase once $|l| = 1$. And third, that $l^2 = e^{2i(\theta+\phi)}$. Recall that, by construction, $\hat{T}_c$ is antihermitian for the so(2, 1) algebra and hermitian for the other two. Accordingly, for the so(2, 1) algebra, the middle equation in Eqs. (A4) implies that $|\beta|^{2i} = l^2$, with $l = \beta^i + \frac{\alpha\gamma}{2}$ (see Table I). Using the above results together with Eqs. (A3) and (A4), it is straightforward to show that

$$e^{-\xi} = 1 + \frac{|\alpha|^2}{2} \quad \text{and} \quad \ln|\beta| = \theta + \phi \pm n\pi, \tag{A6}$$

with $n = 1, 2, \ldots$. On the other hand, for the su(1, 1) and su(2) algebras the middle equation in Eqs. (A4) implies that $\frac{\beta}{\beta^*} = l^2$ with $l = \beta - \epsilon\alpha\gamma$, leading to

$$|\beta| + \epsilon|\alpha|^2 = 1 \quad \text{and} \quad \xi = \theta + \phi \pm n\pi, \tag{A7}$$

with $n = 1, 2, \ldots$. Using the above results, it can be shown that, for all the algebras under consideration, $l = -e^{i(\theta+\phi)}$. Finally, notice that the arbitrary composition of squeeze operators, rotation operators, and other interesting unitary operators of the groups under consideration can be calculated using these BCH-like relations.

APPENDIX B: FACTORIZING GROUP ELEMENTS

In this Appendix we show that an arbitrary element of the Lie groups at issue and given in the unfactorized representation, namely,

$$\hat{G}(\boldsymbol{\lambda}) = \exp(\lambda_+\hat{T}_+ + \lambda_c\hat{T}_c + \lambda_-\hat{T}_-), \tag{B1}$$

can be factorized in the usual order, as indicated in Eqs. (15)–(17), or as

$$\hat{G}(\boldsymbol{\Sigma}) = e^{\Sigma_- \hat{T}_-} e^{\ln(\Sigma_c)\hat{T}_c} e^{\Sigma_+ \hat{T}_+}, \tag{B2}$$

where

$$\Sigma_c = \left(\cosh(\nu) + \frac{\delta\lambda_c}{2\nu}\sinh(\nu)\right)^{\frac{2}{\delta}}, \tag{B3}$$

$$\Sigma_\pm = \frac{2\lambda_\pm \sinh(\nu)}{2\nu\cosh(\nu) + \delta\lambda_c \sinh(\nu)}, \tag{B4}$$

with

$$\nu^2 = \left(\frac{\delta\lambda_c}{2}\right)^2 - \epsilon\delta\lambda_+\lambda_-. \tag{B5}$$

Firstly, let us redefine Eq. (B1) as the special case $\rho = 1$ of the operator

$$\hat{F}_1(\rho) = e^{\rho(\lambda_+\hat{T}_+ + \lambda_c\hat{T}_c + \lambda_-\hat{T}_-)}. \tag{B6}$$

The basic idea is to find an equivalent expression in the form

$$\hat{F}_1(\rho) = e^{\Sigma_-(\rho)\hat{T}_-} e^{\ln(\Sigma_c(\rho))\hat{T}_c} e^{\Sigma_+(\rho)\hat{T}_+}, \tag{B7}$$

and therefore, to write the functions Σ_+, Σ_-, and Σ_c in terms of the small lambdas so that the last two equations are equal. The relations between these two set of functions ($\boldsymbol{\Sigma}$ and $\boldsymbol{\lambda}$) are known as BCH-like relations [21]. Accordingly, we derive both expressions with respect to ρ and impose the derivatives to be equal. The derivative of Eq. (B6) is direct, and given by

$$\hat{F}_1' = (\lambda_+\hat{T}_+ + \lambda_c\hat{T}_c + \lambda_-\hat{T}_-)\hat{F}_1, \tag{B8}$$

where the prime indicates derivative with respect to ρ. On the other hand, the derivative of Eq. (B7) can be written as

$$\hat{F}_1' = \left(\Sigma_-\hat{T}_- + \frac{\Sigma_c'}{\Sigma_c}\hat{I}_1 + \Sigma_+\hat{I}_2\right)\hat{F}_1, \tag{B9}$$

with

$$\begin{aligned}\hat{I}_1 &= e^{\Sigma_-\hat{T}_-}\hat{T}_c\, e^{-\Sigma_-\hat{T}_-}\\ \hat{I}_2 &= e^{\Sigma_-\hat{T}_-}\, e^{\ln(\Sigma_c)\hat{T}_c}\hat{T}_+\, e^{-\ln(\Sigma_c)\hat{T}_c}\, e^{-\Sigma_-\hat{T}_-}.\end{aligned} \tag{B10}$$

Using the BCH relation [21]

$$\begin{aligned}e^{\hat{A}}\hat{B}\,e^{-\hat{A}} =& \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]]\\ &+ \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \cdots\end{aligned} \tag{B11}$$

together with the commutation relations given in Eq. (2) we can solve Eqs. (B10), and then equalize Eqs. (B8) and (B9) to obtain the following set of coupled differential equations:

$$\Sigma_-' + \delta\Sigma_-\frac{\Sigma_c'}{\Sigma_c} + \epsilon\delta(\Sigma_-)^2(\Sigma_c)^\delta\Sigma_+' = \lambda_-, \tag{B12}$$

$$\frac{\Sigma_c'}{\Sigma_c} + 2\epsilon\Sigma_-(\Sigma_c)^\delta\Sigma_+' = \lambda_c, \tag{B13}$$

$$(\Sigma_c)^\delta\Sigma_+' = \lambda_+\,. \tag{B14}$$

Substitution of Eq. (B14) in Eq. (B13) leads to

$$\frac{\Sigma_c'}{\Sigma_c} = \lambda_c - 2\epsilon\lambda_+\Sigma_-, \tag{B15}$$

and we obtain the differential equation for Σ_- by substituting the above equation together with Eq. (B14) into Eq. (B12):

$$\Sigma_-' - \epsilon\delta\lambda_+(\Sigma_-)^2 + \delta\lambda_c\Sigma_- - \lambda_- = 0. \tag{B16}$$

This is a first-order, quadratic, and nonhomogeneous ordinary differential equation known as the (time-independent) complex Riccati equation. It has a unique solution, and can be transformed into an ordinary, homogeneous, and second-order differential equation with the aid of the well-known transformation

$$\Sigma_- = -\frac{1}{\epsilon\delta\lambda_+}\frac{u'}{u}, \tag{B17}$$

leading to

$$u'' + \Gamma u' + \varsigma^2 u = 0, \tag{B18}$$

where we defined $\varsigma^2 = \epsilon\delta\lambda_-\lambda_+$ and $\Gamma = \delta\lambda_c$ in order to identify it as the classical equation of a damped harmonic oscillator with natural frequency ς and damped coefficient Γ. Its general solution is given by

$$u(\rho) = e^{-\frac{\Gamma}{2}\rho}(Ae^{\nu\rho} + Be^{-\nu\rho}), \tag{B19}$$

where ν is given by Eq. (B5) and constants A and B are determined from the initial condition $\Sigma_-(\rho = 0) = 0$. Using the above results in Eq. (B17), we obtain

$$\Sigma_-(\rho) = \frac{2\lambda_-\sinh(\nu\rho)}{2\nu\cosh(\nu\rho) + \delta\lambda_c\sinh(\nu\rho)},$$

which leads to the desired expression written in Eq. (B4) if we take $\rho = 1$. Now, using Eq. (B15) and the above result together with the initial condition $\Sigma_c(\rho = 0) = 1$, we can calculate

$$\Sigma_c = \left(\cosh(\nu\rho) + \frac{\delta\lambda_c}{2\nu}\sinh(\nu\rho)\right)^{\frac{2}{\delta}},$$

which after taking $\rho = 1$ leads to the desired result of Eq. (B3). To find $\Sigma_+(\rho)$ we replace the above equation in Eq. (B14) and take into account the initial condition $\Sigma_+(\rho = 0) = 0$, obtaining

$$\Sigma_+ = \frac{2\lambda_+\sinh(\nu\rho)}{2\nu\cosh(\nu\rho) + \delta\lambda_c\sinh(\nu\rho)},$$

which leads to the desired result in Eq. (B4) with $\rho = 1$. To finish this section we shall factorize expression (B1) in the usual order:

$$\hat{G}(\boldsymbol{\Lambda}) = e^{\Lambda_+\hat{T}_+} e^{\ln(\Lambda_c)\hat{T}_c} e^{\Lambda_-\hat{T}_-}. \tag{B20}$$

Following a similar process, the correspondent set of coupled differential equations is given by

$$\Lambda_+' - \delta\Lambda_+\frac{\Lambda_c'}{\Lambda_c} + \epsilon\delta(\Lambda_+)^2(\Lambda_c)^{-\delta}\Lambda_-' = \lambda_+, \tag{B21}$$

$$\frac{\Lambda_c'}{\Lambda_c} - 2\epsilon\Lambda_+(\Lambda_c)^{-\delta}\Lambda_-' = \lambda_c, \tag{B22}$$

$$(\Lambda_c)^{-\delta}\Lambda_-' = \lambda_-\,. \tag{B23}$$

Then, solving the above system, it is straightforward to show that

$$\Lambda_c = \left(\cosh(\nu) - \frac{\delta\lambda_c}{2\nu}\sinh(\nu)\right)^{-\frac{2}{\delta}}, \tag{B24}$$

$$\Lambda_\pm = \frac{2\lambda_\pm \sinh(\nu)}{2\nu\cosh(\nu) - \delta\lambda_c \sinh(\nu)}, \quad \text{(B25)}$$

which are equivalent to Eqs. (15) and (16) [13]. It must be noted that our expressions in Eqs. (B3) and (B4) differ by one sign from those found in Ref. [21] for the special cases of the su(1, 1) and su(2) Lie algebras. However, we can use Eqs. (B24) and (B25) to check our results as follows. First, notice that the inverse of Eq. (B1) can be easily calculated as $\hat{G}^{-1} = \exp(-\lambda_+\hat{T}_+ - \lambda_c\hat{T}_c - \lambda_-\hat{T}_-)$, i.e., is equivalent to the change $\boldsymbol{\lambda} \to -\boldsymbol{\lambda}$. Using this condition in Eqs. (B3) and (B4), it is straightforward to show that $\Sigma_c \to (\Lambda_c)^{-1}$ and $\Sigma_\pm \to -\Lambda_\pm$. Therefore, from Eq. (B2) it follows that $\hat{G}^{-1} = e^{-\Lambda_-\hat{T}_-}e^{-\ln(\Lambda_c)\hat{T}_c}e^{-\Lambda_+\hat{T}_+}$, which is consistent with Eq. (B20), since $\hat{G}\hat{G}^{-1} = \hat{G}^{-1}\hat{G} = \mathbb{1}$. Notice that the above factorizations do not depend on the unitarity of $\hat{U}_j$, but just on the commutation relations of the generators of the algebra.

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