Manipulating two-spin coherences and qubit pairs

A. R. P. Rau*
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001
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A compact derivation is given for propagators of a wide class of time-dependent Hamiltonians that describe coupled spin (''qubit'') pairs. As many as eight of the 16 operators in the system, each with its own time-dependent coefficient, can be handled with no more difficulty than a single spin in a magnetic field. A single first-order (in time), quadratically nonlinear differential equation for a classical function is the only nontrivial ingredient in constructing the full quantum propagator for a wide variety of magnetic coherences and qubit interactions.

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Nuclear magnetic resonance (NMR) and other spin resonance spectroscopies have long studied coherences between two or more quantum spins, both their establishment and their measurement with the aid of suitable magnetic field pulses [1,2]. More recently, coupled spins as models for various logic gates have been of much interest for quantum computation [3,4]. NMR itself provides one of the candidate systems as possible ''hardware'' for a realizable quantum computer [5]. All these problems involve the study of the Hamiltonian, often time dependent, for coupled spins. Indeed, such a study has an even broader context because of the well-known mapping of any two-level system into a quantum spin $\frac{1}{2}$, of four-level systems into two coupled spin $\frac{1}{2}$, etc. Pairs of spin $\frac{1}{2}$, in particular, have modeled a wide range of problems in physics, from combined spin and isospin [the groups U(4) and SU(4)] in nuclei and particles [6] to the states of an *f* electron in the crystal field of CeB_6, which are associated with unusual magnetic phases [7]. We present in this paper a general technique for handling such pairs of spins with time-dependent coupling.

Although the general formalism we use [8] applies to arbitrary spin *j*, we will focus primarily on $j=\frac{1}{2}$, which has specific simplifications. For a pair of spin $\frac{1}{2}$ (two qubits in the terminology of quantum computation [3,4]),there are in all 4×4 linearly independent operators that close under mutual commutator brackets. As a result, any Hamiltonian of the system can be solved in terms of these 16 operators. However, most of the NMR coherences and quantum logic gates that are studied involve smaller subsets, typically sets of four or six of the 16 operators [1,3]. These have been well studied and documented. The main aim of this paper is to present simple, compact, closed form solutions of time-dependent Hamiltonians involving as many as eight of the operators and thus eight arbitrary functions of time as coefficients. Further, the complete solution of the time-dependent Schrödinger equation, or the equivalent Liouville-Bloch equation for the density matrix, reduces to the solution of the same classical Riccati (first order in time with quadratic nonlinearity) equation that occurs in a single-spin problem as recently presented [8], together with simple integrations and exponentiations. A key result that underlies our solution may be of interest by itself. To our knowledge, it does not seem to have been noted before that our construction below in Eq. (9) recasts six two-spin operators as a pair of independent pseudospins.

Representing the operators for the two spins by $\frac{1}{2}\vec{\sigma}$ and $\frac{1}{2}\vec{\tau}$, along with their unit operators, where $\vec{\sigma}$ and $\vec{\tau}$ are Pauli spinors and we have set $\hbar=1$, the 16 independent operators of the pair are given in Table I in a standard notation [9].

Any operator describing magnetic couplings between the spins as well as the coupling of each spin to an external field can be cast as a linear combination of the 16 operators O_i with coefficients which may, in general, be functions of time:

$$H(t)=\sum_{i=1}^{16} a_i(t)O_i\,. \tag{1}$$

Various groupings of the 16 O_i have physical significance. Thus, in the literature on NMR coherences, the first row in Table I is a ''diagonal'' set of four, the second and third rows describe ''transverse, single-quantum coherences,'' respectively, of σ and τ spins, and the last row gives ''zero- and double-quantum coherences'' [9]. Further subdivision refers to O_2 and O_3 as ''polarizations'' of σ and τ spins, respectively, and O_4 as ''longitudinal two-spin order,'' whereas in the second and third rows, O_5 is called ''*x* magnetization'' or ''in-phase *x* coherence'' of σ, O_7 as the ''*x* coherence of σ in antiphase with τ,'' etc. [1]. An alternative to the grouping by rows of four is to regard the 4×4 elements as a scalar singlet O_1, two vector triplets $\{O_5,O_6,O_2\}$ and $\{O_9,O_{10},O_3\}$ of σ and τ spins, respectively, and a nonet tensor of rank 2. A ''dipolar coupled'' Hamiltonian is described by [3]

$$H=\omega_1O_2+\omega_2O_3+2kO_4, \tag{2}$$

where ω_1, ω_2, and *k* may be functions of time.

Subsets of the operators O_i also provide different logic gates in quantum computation. Thus, as examples, we have [3]

$$\text{NOT:}\quad 2O_5,$$

$$\text{XOR:}\quad \tfrac{1}{2}O_1+O_3+O_5-2O_7,$$

*Electronic address: arau@rouge.phys.lsu.edu

TABLE I. Operators and matrices for a pair of spins [9].

$$O_1=I=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix} \qquad O_2=\frac{1}{2}\sigma_z=\frac{1}{2}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}$$

$$O_3=\frac{1}{2}\tau_z=\frac{1}{2}\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix} \qquad O_4=\frac{1}{4}\sigma_z\tau_z=\frac{1}{4}\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}$$

$$O_5=\frac{1}{2}\sigma_x=\frac{1}{2}\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix} \qquad O_6=\frac{1}{2}\sigma_y=\frac{i}{2}\begin{pmatrix}0&0&-1&0\\0&0&0&-1\\1&0&0&0\\0&1&0&0\end{pmatrix}$$

$$O_7=\frac{1}{4}\sigma_x\tau_z=\frac{1}{4}\begin{pmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{pmatrix} \qquad O_8=\frac{1}{4}\sigma_y\tau_z=\frac{i}{4}\begin{pmatrix}0&0&-1&0\\0&0&0&1\\1&0&0&0\\0&-1&0&0\end{pmatrix}$$

$$O_9=\frac{1}{2}\tau_x=\frac{1}{2}\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} \qquad O_{10}=\frac{1}{2}\tau_y=\frac{i}{2}\begin{pmatrix}0&-1&0&0\\1&0&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix}$$

$$O_{11}=\frac{1}{4}\sigma_z\tau_x=\frac{1}{4}\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-1\\0&0&-1&0\end{pmatrix} \qquad O_{12}=\frac{1}{4}\sigma_z\tau_y=\frac{i}{4}\begin{pmatrix}0&-1&0&0\\1&0&0&0\\0&0&0&1\\0&0&-1&0\end{pmatrix}$$

$$O_{13}=\frac{1}{4}\sigma_x\tau_x=\frac{1}{4}\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix} \qquad O_{14}=\frac{1}{4}\sigma_y\tau_y=\frac{1}{4}\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix}$$

$$O_{15}=\frac{1}{4}\sigma_x\tau_y=\frac{i}{4}\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&-1&0&0\\1&0&0&0\end{pmatrix} \qquad O_{16}=\frac{1}{4}\sigma_y\tau_x=\frac{i}{4}\begin{pmatrix}0&0&0&-1\\0&0&-1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}$$

Pound-Overhauser (PO) XOR: $\frac{1}{2}O_1+O_2+i(O_{10}-2O_{12})$,

Square root of XOR: $(c^*+c/2)O_1+c(O_3+O_5-2O_7)$,

$$c=(1-i)/\sqrt{2},$$

Spin coherence XOR: $(1/\sqrt{2})[\frac{1}{2}O_1+O_3+iO_2+iO_5+iO_6+2iO_4-2iO_7-2iO_8]$. (3)

The NMR and quantum computation literatures have considered the effects of such operator combinations on paired spins and the solutions of the corresponding Hamiltonians. All the coefficients in Eq. (3) are constants and, except for the last item, the literature deals only with sets of four or six operators. Thus, more general than Eq. (2), which involves only operators diagonal in the z representation, is the so-called ''scalar coupling Hamiltonian,'' which replaces the last term $\sigma_z\tau_z$ by the scalar product $\vec{\sigma}\cdot\vec{\tau}$ [1,3]. Such Hamiltonians, with all coefficients arbitrary, would be described by

$$\begin{aligned}H(t)&=E_0O_1+\omega_1O_2+\omega_2O_3+2kO_4+2k_xO_{13}+2k_yO_{14}\\&=E_0I+\tfrac{1}{2}[\omega_1\sigma_z+\omega_2\tau_z+k\sigma_z\tau_z+k_x\sigma_x\tau_x+k_y\sigma_y\tau_y],\end{aligned} \tag{4}$$

where E_0, ω_1, ω_2, k, k_x, and k_y may be distinct functions of time. Reference [3] has constructed propagators in closed form for a slightly less general Hamiltonian with some coefficients equal and all constant in time while Sec. 4.5.3 of Ref. [1] has considered solutions of Eq. (4) for the problem of ''cross polarization'' in liquids.

We will now construct general solutions for an even larger Hamiltonian than in Eq. (4), embracing two additional ''cross terms'' in x and y, namely the operators O_{15} and O_{16} describing ''heteronuclear two-spin coherences,''

$$\begin{aligned}H(t)=E_0I+\tfrac{1}{2}[&\omega_1\sigma_z+\omega_2\tau_z+k\sigma_z\tau_z+k_x\sigma_x\tau_x\\&+k_y\sigma_y\tau_y+k_{xy}\sigma_x\tau_y+k_{yx}\sigma_y\tau_x].\end{aligned} \tag{5}$$

Remarkably, our procedure calls for no more effort than that involved in solving single-spin problems. Before turning to the derivation, we note a physical context for the last two heteronuclear-coherence terms in Eq. (5). Ref. [1] considers two spins initially in thermal equilibrium that are subjected to a pulse sandwich with $\omega_1=\omega_2=\cos\pi Jt$ and $k_{xy}=k_{yx}=\sin\pi Jt$. Such an interaction converts the polarization entirely to double-quantum coherences in time $t=(2J)^{-1}$. Thus, whereas the terms in Eq. (4) are involved in chemical shifts and dipolar couplings in oriented solid and liquid crystal phases [1], the heteronuclear terms in Eq. (5) are of interest when an axially symmetric quadrupole interaction is also present.

Wave functions or density matrices can be obtained once the evolution operator or propagator for the Hamiltonian is constructed [8]. This propagator $U(t)$ obeys the equation,

$$i\dot{U}(t)=H(t)U(t), U(0)=I, \tag{6}$$

where an overdot denotes differentiation with respect to time. For Hermitian $H(t)$, that is, real coefficients in Eqs. (4) and (5), $U(t)$ is unitary. We have recently explored a variety of such problems involving single particles by writing $U(t)$ as a product of exponential factors, involving in the exponents each of the operators occurring in $H(t)$ and all subsequent operators that arise as a result of successive commutations between them [8,10]. For a single spin-$\frac{1}{2}$ problem, there are four such factors, the set $\{I,\vec{\sigma}\}$ closing under commutation. For paired spins, since the 16 operators in Table I similarly afford a closed set, the most general $U(t)$ will involve 16 factors, $\exp[-i\mu_i(t)O_i]$. Our procedure leads to coupled first-order, nonlinear differential equations for the classical functions $\mu_i(t)$. We saw further the advantage of working with the operators $\{\sigma_\pm=\sigma_x\pm i\sigma_y\}$, rather than the Cartesian set because it leads to simpler equations for the μ_i and also, as a result of the relations $\sigma_\pm^2=0$, simpler evaluations when the exponentials in U operate on some initial spin state $\psi(0)$. Even though each exponential factor is not individually unitary when one uses $\sigma_\pm$ rather than σ_x and σ_y, the final $U(t)$ remains unitary [8].

We take this opportunity to note that some of these results of [8] have existed in earlier literature, seemingly having been rediscovered several times. Instead of the Magnus expansion that writes the solution of Eq. (6) as a single exponential, Wei and Norman [11] gave the alternative of a product of exponentials, each involving one of the operators O_i that form a closed Lie algebra. In a series of papers [12], Sanctuary and co-workers used this technique for the Liouville-Bloch equation for a general spin j, writing the solution of Eq. (6) in terms of three exponential factors involving successively J_z, J_y, and J_z, the coefficients identified as Euler parameters. Reference [8] used instead J_z, J_y, and J_x. Siminovitch and Habot [13] had similar results, along with the alternative of using J_z, J_+, and J_-, which leads directly to a Riccati equation as the key one in solving for the Euler parameters. Further, Siminovitch [14] recast the set of three nonlinear equations as four coupled linear ones for the so-called Euler-Rodrigues parameters that have a long history in rigid-body kinematics. And, independently, an early paper [15] had also recorded both the Cartesian and the $\{J_z,J_\pm\}$ set of equations for solving Eq. (6).

Recasting Eq. (5) in terms of $\sigma_\pm$ and $\tau_\pm$, which obey the relations

$$[\sigma_z,\sigma_\pm]=\pm 2\sigma_\pm,\ [\sigma_+,\sigma_-]=4\sigma_z, \tag{7a}$$

$$\sigma_z\sigma_\pm=\pm\sigma_\pm=-\sigma_\pm\sigma_z,\quad \sigma_\pm\sigma_\mp=2(I\pm\sigma_z), \tag{7b}$$

and a similar set for τ, we have

$$\begin{aligned}H(t)=&E_0I+\tfrac{1}{2}[\omega_1\sigma_z+\omega_2\tau_z+k\sigma_z\tau_z]\\&+\tfrac{1}{4}[K_+\sigma_+\tau_++K_-\sigma_-\tau_-+k_+\sigma_+\tau_-+k_-\sigma_-\tau_+],\end{aligned} \tag{8}$$

where

$$K_\pm=\tfrac{1}{2}(k_x-k_y\mp ik_{xy}\mp ik_{yx}),\quad k_\pm=\tfrac{1}{2}(k_x+k_y\pm ik_{xy}\mp ik_{yx}).$$

Once again, the coefficients E_0, ω, K, and k may be arbitrary functions of time.

The central result of this paper hinges on the recognition that the eight operators in Eq. (8) divide into two triplets defined by

$$\begin{aligned}S_z=\tfrac{1}{2}(\sigma_z+\tau_z),\quad S_\pm=\tfrac{1}{2}\sigma_\pm\tau_\pm;\\ s_z=\tfrac{1}{2}(\sigma_z-\tau_z),\quad s_\pm=\tfrac{1}{2}\sigma_\pm\tau_\mp.\end{aligned} \tag{9}$$

These obey the commutation relations

$$\begin{aligned}[S_z,S_\pm]=\pm 2S_\pm,\quad [S_+,S_-]=4S_z;\\ [s_z,s_\pm]=\pm 2s_\pm,\quad [s_+,s_-]=4s_z,\end{aligned} \tag{10a}$$

and

$$S_\pm^2=0=s_\pm^2. \tag{10b}$$

Further each member of the triplet $\{S_z,S_\pm\}$ commutes with each of the other triplet $\{s_z,s_\pm\}$ and the two remaining operators in Eq. (8), I and $\sigma_z\tau_z$, commute with all six of them. Thus, upon rewriting $\omega_1\sigma_z+\omega_2\tau_z$ in Eq. (8) as $\omega_+S_z+\omega_-s_z$, with $\omega_\pm=\omega_1\pm\omega_2$, the Hamiltonian splits into that of two decoupled ''pseudospins'' S and s, obeying in Eq. (10) the same commutations as those obtained between σ and τ in Eq. (7a), and two ''diagonal'' objects, $I=O_1$ and $\sigma_z\tau_z=4O_4$. This recognition of $\vec{S}$ and $\vec{s}$ as two independent sets of ''pseudospins'' may be of more general interest to NMR coherences than its use below to write the solution of Eq. (8) with no more input than the solution for a single spin. We use the term independent sets only to mean that the operators of one commute with every member of the other set.

Although the objects S and s do not behave in all respects like Pauli spinors [results analogous to Eq. (7b) are not obtained, and $S_x^2=S_y^2=S_z^2=\frac{1}{2}(I+\sigma_z\tau_z)$, $s_x^2=s_y^2=s_z^2=\frac{1}{2}(I-\sigma_z\tau_z)$], since their behavior under commutation remains the same and this is all we need for our constructive procedure for the propagator $U(t)$, the solution of Eq. (6) for the Hamiltonian in Eq. (8) follows immediately from our earlier result for single spins [8] to give

$$\begin{aligned}U(t)=&\exp[-i\Omega_0(t)]\exp[-\tfrac{1}{2}i\Omega_z(t)\sigma_z\tau_z]\\&\times\exp[-\tfrac{1}{2}i\nu_+(t)S_+]\exp[-\tfrac{1}{2}i\nu_-(t)S_-]\\&\times\exp[-\tfrac{1}{2}i\nu_3(t)S_z]\exp[-\tfrac{1}{2}i\mu_+(t)s_+]\\&\times\exp[-\tfrac{1}{2}i\mu_-(t)s_-]\exp[-\tfrac{1}{2}i\mu_3(t)s_z],\end{aligned} \tag{11}$$

where the classical functions in the exponents obey

$$\dot{\Omega}_0 = E_0(t), \quad \dot{\Omega}_z = k(t), \tag{12a}$$

$$\dot{\mu}_+ - \mu_+^2 k_-(t) + i\omega_-(t)\mu_+ = k_+(t),$$
$$\dot{\mu}_- - i\mu_-\dot{\mu}_3 = k_-(t), \quad \dot{\mu}_3 - 2ik_-(t)\mu_+ = \omega_-(t), \tag{12b}$$

$$\dot{\nu}_+ - \nu_+^2 K_-(t) + i\omega_+(t)\nu_+ = K_+(t),$$
$$\dot{\nu}_- - i\nu_-\dot{\nu}_3 = K_-(t), \quad \dot{\nu}_3 - 2iK_-(t)\nu_+ = \omega_+(t). \tag{12c}$$

In our procedure [8], in evaluating $i\dot{U}$ from Eq. (11), operators have to be moved to the left through exponentials of noncommuting operators (with the aid of an operator identity for $e^A B e^{-A}$) so as to cast the expression in the form of the right-hand side of Eq. (6). Because I and $\sigma_z\tau_z$ commute with all the other six operators and because S and s behave as independent mutually commuting sets, the maximum any operator has to be moved is through two exponentials, just as in the treatment of a single spin in [8].

The full quantum solution in Eq. (11) for Eqs. (6) and (8) is thereby obtained as soon as the classical equations in Eq. (12) are solved, together with the boundary conditions that all these functions vanish at $t=0$. The only nontrivial equations are the first of Eqs. (12b) and (12c), which are of Riccati form for μ_+ and ν_+, respectively. Once they are obtained, all the rest of the equations yield to simple first-order integrations in time.

As previously observed [8], the Riccati equations may be transformed instead into linear second-order differential equations through

$$\mu_+(t) = -(1/k_-)[\dot{\gamma}(t)/\gamma(t)], \tag{13a}$$

to obtain

$$\ddot{\gamma} + (i\omega_- - \dot{k}_-/k_-)\dot{\gamma} + (k_+k_-)\gamma = 0, \ \gamma(0)=1, \ \dot{\gamma}(0)=0, \tag{13b}$$

and similarly for $\nu_+(t)$. These may be more convenient for handling, particularly for certain time dependences of the coefficients ω, K, and k. In particular, for constant coefficients, Eq. (13b) is trivially solved.

Returning to Table I, our principal result is that interactions involving various sets of eight of these operators can be solved through appropriate choices of S and s that act like decoupled spins. Hamiltonians in which the original spins σ and τ are uncoupled, each individually interacting with an arbitrary external magnetic field can, of course, be immediately solved. The set involved in this case is $\{O_1; O_4; O_5, O_6, O_2; O_9, O_{10}, O_3\}$, corresponding to diagonal plus x and y magnetizations separately of σ and τ spins. When σ and τ are coupled according to the Hamiltonian in Eq. (5), the set involved is $\{O_1; O_2; O_3, O_4, O_{13}; O_{14}, O_{15}, O_{16}\}$, that is, the first and last rows in Table I, comprising both diagonal and double-quantum coherences. The last item in Eq. (3) corresponds to yet another set, comprising the first and second rows of the table, diagonal plus single-quantum coherences of σ. Thus, all these instances that involve nontrivial couplings of σ and τ spins can be solved as easily as the case of uncoupled spins through our recasting in terms of S and s.

Rearranging the entries in Table I as a direct product of the operators of the two spins

$$\begin{pmatrix} O_1 & O_5 & O_6 & O_2 \\ O_9 & O_{13} & O_{16} & O_{11} \\ O_{10} & O_{15} & O_{14} & O_{12} \\ O_3 & O_7 & O_8 & O_4 \end{pmatrix} = \begin{pmatrix} I & \frac{\sigma_x}{2} & \frac{\sigma_y}{2} & \frac{\sigma_z}{2} \\ \frac{\tau_x}{2} & \frac{\sigma_x\tau_x}{4} & \frac{\sigma_y\tau_x}{4} & \frac{\sigma_z\tau_x}{4} \\ \frac{\tau_y}{2} & \frac{\sigma_x\tau_y}{4} & \frac{\sigma_y\tau_y}{4} & \frac{\sigma_z\tau_y}{4} \\ \frac{\tau_z}{2} & \frac{\sigma_x\tau_z}{4} & \frac{\sigma_y\tau_z}{4} & \frac{\sigma_z\tau_z}{4} \end{pmatrix}, \tag{14}$$

the alternative sets of eight mentioned above correspond to choosing the four corner elements together with one of the quartets $\{O_5, O_6, O_7, O_8\}$ (remaining entries in first and last rows), $\{O_9, O_{10}, O_{11}, O_{12}\}$ (remaining entries in first and last columns), $\{O_5, O_6, O_9, O_{10}\}$, and a similar $\{O_7, O_8, O_{11}, O_{12}\}$, and $\{O_{13}, O_{14}, O_{15}, O_{16}\}$ (four ''interior'' elements). An interesting and instructive analogy can be drawn to similar alternative choices in other 4×4 contexts such as the electromagnetic field's tensor $F_{\mu\nu}$,

$$\begin{pmatrix} 0 & iE_x & iE_y & iE_z \\ -iE_x & 0 & B_z & -B_y \\ -iE_y & -B_z & 0 & B_x \\ -iE_z & B_y & -B_x & 0 \end{pmatrix},$$

with $\vec{E}$ and $\vec{B}$ the electric and magnetic fields [16], and the $O(4)$ symmetry operators of the hydrogen atom

$$\begin{pmatrix} 0 & -A_x & -A_y & -A_z \\ A_x & 0 & L_z & -L_y \\ A_y & -L_z & 0 & L_x \\ A_z & L_y & -L_x & 0 \end{pmatrix},$$

where $\vec{L}$ is the orbital angular momentum and $\vec{A}$ the Laplace-Runge-Lenz vector [17]. In both these examples, as well as in the Euler-Rodrigues parameters of [14], the 4×4 matrix is antisymmetric, the only nonzero elements being $\vec{E}$ and $\vec{B}$ fields [16], or the orbital angular momentum $\vec{L}$ and the Laplace-Runge-Lenz vector $\vec{A}$ [17]. The decomposition scalar+two triplets+nonet corresponds to the basic vectors $(\vec{E},\vec{B})$ and $(\vec{A},\vec{L})$, both triplets reducing to the same polar vector ($\vec{E}$ or $\vec{A}$) apart from a minus sign, and the antisymmetric nonet becoming an axial vector ($\vec{B}$ or $\vec{L}$). Alternative divisions into sets of eight as discussed for Eq. (14) correspond to the choice appropriate to an electromagnetic wave or that involved in the parabolic separation of the hydrogen Hamiltonian [17].

The operator combinations in the quantum gates (3) involve different subsets of O_i than in Eqs. (5) or (8). Here again, our solution of Eq. (5) in the form of Eq. (11) applies. First, since the only input we need is the commutators in Eq. (7), our procedure is not tied to any specific representation. This feature can be exploited to relabel the *x*, *y*, and *z* in the Pauli spinors as most convenient, choosing which ever one to be diagonal that makes the Hamiltonian easiest to handle. In the most general case, again involving eight operators but somewhat different from Eq. (5), all such gates are special cases of

$$\begin{aligned} H(t) &= E_0 I + \tfrac{1}{2}[\omega_1\sigma_z + \omega_2\tau_z + k\sigma_z\tau_z + k_x\sigma_x + k_y\sigma_y \\ &\quad + k_{xz}\sigma_x\tau_z + k_{yz}\sigma_y\tau_z] \\ &= E_0 I + \tfrac{1}{2}[\omega_1\sigma_z + \omega_2\tau_z + k\sigma_z\tau_z + k_-\sigma_+ \\ &\quad + k_+\sigma_- + K_-\sigma_+\tau_z + K_+\sigma_-\tau_z], \end{aligned} \tag{15}$$

with E_0, ω_1, ω_2, k, $k_\pm \equiv \frac{1}{2}(k_x \pm ik_y)$ and $K_\pm \equiv \frac{1}{2}(k_{xz} \pm ik_{yz})$ arbitrary functions of time.

In writing the solution for $U(t)$, the order of the noncommuting exponential factors may also be chosen for convenience, the simplest equations for the classical functions in the exponents resulting when all σ_z terms are kept to the right of $\sigma_\pm$,

$$\begin{aligned} U(t) &= \exp[-i\Omega_0(t)]\exp[-\tfrac{1}{2}i\Omega_z(t)\tau_z] \\ &\quad \times \exp[-\tfrac{1}{2}i\nu_+(t)\sigma_+\tau_z]\exp[-\tfrac{1}{2}i\mu_+(t)\sigma_+] \\ &\quad \times \exp[-\tfrac{1}{2}i\nu_-(t)\sigma_-\tau_z]\exp[-\tfrac{1}{2}i\mu_-(t)\sigma_-] \\ &\quad \times \exp[-\tfrac{1}{2}i\nu_3(t)\sigma_z\tau_z]\exp[-\tfrac{1}{2}i\mu_3(t)\sigma_z]. \end{aligned} \tag{16}$$

This leads to a pair of coupled nonlinear equations,

$$\begin{aligned} &\dot{\mu}_+ - \mu_+^2 k_+ + i\omega_1\mu_+ + ik\nu_+ - 2K_+\mu_+\nu_+ - \nu_+^2 k_+ = k_-, \\ &\dot{\nu}_+ - \nu_+^2 k_+ + i\omega_1\nu_+ + ik\mu_+ - 2K_+\mu_+\nu_+ - \mu_+^2 K_+ = K_-, \end{aligned} \tag{17}$$

an obvious counterpart of the first equations in Eqs. (12b) and (12c). Once solved for μ_+ and ν_+, the other four classical functions can be obtained in turn through simple integrations (Ω_0 and Ω_z are again trivially integrals of E_0 and ω_2, respectively)

$$\begin{aligned} &\dot{\mu}_3 - 2ik_+\mu_+ - 2iK_+\nu_+ = \omega_1, \quad \dot{\mu}_- - i\mu_-\dot{\mu}_3 - i\nu_-\dot{\nu}_3 = k_+ \\ &\dot{\nu}_3 - 2ik_+\mu_+ - 2iK_+\nu_+ = k, \quad \dot{\nu}_- - i\nu_-\dot{\mu}_3 - i\mu_-\dot{\nu}_3 = K_+. \end{aligned} \tag{18}$$

Most quantum gates as in Eq. (3) are simpler subsets of this general case, involving fewer coefficients, some of which are further time independent. In these cases, particularly when $K_\pm/k_\pm$ is constant, Eqs. (17) further simplify with μ and ν decoupling and being essentially equal.

We conclude with remarks on extension to a larger number of spins. Thus, with three spins, $\frac{1}{2}\vec{\sigma}^{(i)}$, $i=1,2,3$, out of the full set of 64 operators involved, 20 provide a closed set under commutation I, $\sigma_z^{(i)}$, $\sigma_+^{(i)}\sigma_-^{(j)}$, $\sigma_z^{(i)}\sigma_z^{(j)}$, $\sigma_-^{(i)}\sigma_+^{(j)}\sigma_z^{(k)}$ and $\sigma_z^{(i)}\sigma_z^{(j)}\sigma_z^{(k)}$. Such a Hamiltonian involving linear combinations of these operators conserves the total *z* projection of spin, and its propagator $U(t)$ may be written as a product of 20 exponential factors.

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