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2008 J. Phys. A: Math. Theor. 41 312005

(http://iopscience.iop.org/1751-8121/41/31/312005)

IOP Publishing
Journal of Physics A: Mathematical and Theoretical

J. Phys. A: Math. Theor. **41** (2008) 312005 (12pp) doi:10.1088/1751-8113/41/31/312005

FAST TRACK COMMUNICATION

Generalization of short coherent control pulses: extension to arbitrary rotations

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Received 30 May 2008, in final form 24 June 2008
Published 9 July 2008
Online at stacks.iop.org/JPhysA/41/312005

Abstract

We generalize the problem of the coherent control of small quantum systems to the case where the quantum bit (qubit) is subject to a fully general rotation. Following the ideas developed in Pasini *et al* (2008 *Phys. Rev.* A **77** 032315), the systematic expansion in the shortness of the pulse is extended to the case where the pulse acts on the qubit as a general rotation around an axis of rotation varying in time. The leading and the next-leading corrections are computed. For certain pulses we prove that the general rotation does not improve on the simpler rotation with fixed axis.

PACS numbers: 03.67.Lx, 03.67.Pp, 03.65.Yz, 76.60.−k

1. Introduction

The ability to maintain a two-level system, for instance a $S = 1/2$ spin or a quantum bit (qubit) in the language of quantum information, in a coherent state as long as possible has always been of vital importance in nuclear magnetic resonance (NMR). Nowadays, decoherence is considered one of the basic difficulties to overcome [1] for the realization of a quantum information device. The decoherence of a qubit, i.e., its decay from an initial state to a mixture, is attributed to the coupling of the qubit to the macroscopic environment.

Among the numerous techniques developed to cope with decoherence we consider the dynamical decoupling (DD) [2–4]. The central idea of DD is to disentangle the qubit from the bath by means of repetitive, instantaneous rotations in spin space that prevent the qubit from precessing. Put sloppily, the coupling to the environment is averaged to zero. It has been shown that various optimizations of such sequences are possible. We cite here the Carr–Purcell and Meiboom–Gill sequence [5–7], the concatenated sequence proposed by Khodjasteh and Lidar [8, 9], and the fully optimized non-equidistant (UDD) sequence [10, 11].

The necessary rotations for DD are achieved by means of ideal π pulses which are instantaneous and infinitely strong, i.e., δ peaks. During their application the qubit has no time to experience the effect of the bath. Thus the rotation of the qubit can be treated separately from the evolution due to the qubit-plus-bath Hamiltonian. Note that ideal pulses on single qubits correspond to single qubit gates in the framework of quantum information processing.

Given the significant interest in coherent control by short pulses there have already been a number of previous investigations into the effects of the realistically finite pulse lengths $\tau_p > 0$. For instance, their cumulative effect in pulse sequences has been analyzed by Khodjasteh and Lidar [9].

In the context of NMR the tuning of pulses to improve their properties is well known [4], mostly going back to the early work by Tycko [12]. Static effects are compensated, yet no baths with internal dynamic are considered [13–15]. Numerical investigations into how to reduce the influence of classical noise also exist [16]. The possibilities of tailored pulses for specific examples of sets of interacting qubits were investigated numerically in [17]. We will motivate our approach by comparing with the pulses found there, see section 2.

In our previous work [18] we addressed the issue of a general dynamic quantum bath analytically by an expansion in the shortness of the pulse, i.e., in powers of τ_p. The zeroth order of such an expansion is the instantaneous pulse corresponding to a δ function. In the subsequent orders the main difficulty is the non-commutation of the Hamiltonian describing the pulse and of the Hamiltonian describing the coupling to the environment. Our approach separates both contributions up to corrections in τ_p. Then tailoring the pulse is used to make as many perturbative corrections vanish as possible. This improves the quality of the real pulses significantly as has been illustrated by numerical investigations [19].

Note that we do not aim at eliminating the coupling to the bath during the pulse. This is left to the pulse sequence in which the optimized real pulses are intended to replace the ideal pulses.

The real pulses considered in [18, 19] consider rotations of the qubit around a fixed axis. In the present communication we generalize the analytic expansion to the case where the rotation takes place around an axis varying in time. Thereby we aim at two goals. The first one is to be able to describe experimental pulses more realistically where the pulses are never strictly around a fixed axis. The second one is to examine whether certain ideal pulses can be better approximated by real general rotations than by real fixed-axis rotations. This means we attempt to relax the no-go results previously proven for real fixed-axis rotations [18].

We will show, however, that the no-go statements also apply to general rotations. This sends the clear message to the experiment that more complicated rotations do not need to be considered, at least not for the single qubit gates under study.

This communication is organized as follows. First, we give a motivation for our analytical approach by comparison with numerical results in section 2. In section 3 we introduce the model and the ansätze we will implement. Also the relations between the pulse shape, the axis and the angle of rotation are shown. In section 4 the relevant Schrödinger equations are solved formally. In section 5, the expansion in the shortness of the pulse is presented by which we arrive at the final form for the general corrections. They are discussed in section 6 where we prove that the general rotations suffer from the same limitations found for the fixed-axis rotations [18]. The findings are concluded and summarized in section 7.

2. Motivation

If the total Hamiltonian $H_{\mathrm{tot}}(t)$ comprising the qubits H and the pulse $H_0(t)$ reads $H_{\mathrm{tot}}(t) = H + H_0(t)$ our primary goal is to make the time evolution $U_p(\tau_p, 0)$ during the pulse of length

τ_p as close as possible to

$$U_p(\tau_p, 0) = T\left\{\exp\left[-\mathrm{i}\int_0^{\tau_p} H_{\mathrm{tot}}(t)\,\mathrm{d}t\right]\right\} \tag{1}$$

$$\approx \exp(-\mathrm{i}(\tau_p - \tau_s)H)\hat{P}_\theta \exp(-\mathrm{i}\tau_s H), \tag{2}$$

where T stands for the conventional time ordering and $\hat{P}_\theta$ for the unitary operator of the ideal pulse rotating by the angle θ. It is assumed to occur at the instant $\tau_s \in [0, \tau_p]$, cf [18] for details.

The literature so far [12–15, 17] pursues the goal

$$U_p(\tau_p, 0) \approx \hat{P}_\theta. \tag{3}$$

Both goals coincide if we focus on π pulses ($\theta = \pi$) with $\tau_s = \tau_p/2$ and $H = \sum_j \lambda_j \sigma_z^{(j)}$. Then our goal implies

$$U_p(\tau_p, 0) = \exp(-\mathrm{i}(\tau_p/2)H)\hat{P}_\pi \exp(-\mathrm{i}(\tau_p/2)H) \tag{4a}$$

$$= \hat{P}_\pi \exp(\mathrm{i}(\tau_p/2)H)\exp(-\mathrm{i}(\tau_p/2)H) \tag{4b}$$

$$= \hat{P}_\pi. \tag{4c}$$

The analogous argument holds if every second qubit is flipped and there are Ising couplings between adjacent qubits, see, e.g., [17].

For such systems Sengupta and Pryadko [17] have proposed fine-tuned symmetric pulses labeled S_L and Q_L with $L \in \{1, 2\}$. The S_L pulses make the linear order $\mathcal{O}(\tau_p)$ vanish in $U_p(\tau_p, 0)$, the Q_L pulses also make the quadratic order $\mathcal{O}(\tau_p^2)$ vanish. Additionally, the $2L - 1$ first derivatives of the pulse amplitudes are zero at the beginning ($t = 0$) and at the end ($t = \tau_p$) of the pulse. We verified that all four pulses make the linear corrections vanish, which we have computed analytically in [18]. As far as the second-order corrections are concerned, we must distinguish between terms which involve only the coupling to the environment A (see equation (5) in the following section) and terms where also the bath Hamiltonian H_b appears, namely in the commutator $[A, H_b]$. According to the notation in [18] the former corresponds to the coefficient η_{23} while the latter to the coefficients η_{21} and η_{22}. The Q_L pulses make the former coefficient η_{23} vanish. Note that the other two possible second order terms, η_{21} and η_{22}, do not occur in an Ising model since the coupling A to the qubits commutes with the bath Hamiltonian H_b. So there is no contradiction to our proven result that a π pulse cannot be corrected in second order because this finding relied on the generic model with internal dynamics, i.e., with $[A, H_b] \neq 0$.

From these results we see that all but one Fourier coefficients found numerically, see table II in [17], are determined by the analytic nonlinear equations derived in [18]. The numerics required the variation of the Runge–Kutta solution to a high-dimensional set of differential equations. Thus we conclude that the analytic expansion helps to avoid an important part of tedious numerics. This observation shall serve as an additional motivation for the generalization of our analytic approach to general rotations which we present in what follows.

3. Ansätze

Let us consider the following Hamiltonian of the qubit and its environment,

$$H = H_b + \lambda A \sigma_z, \tag{5}$$

with H_b representing a generic bath and A its coupling operator to the qubit. This Hamiltonian is not the most general one because one spin direction is singled out. But it is applicable to all experimental situations where the time T_1 is much longer than T_2. Generically, this will be the case wherever there is a large energetic splitting between the level $\sigma_z = -1$ and the level $\sigma_z = 1$. Then Hamiltonian (5) is the effective Hamiltonian in the rotating-wave approximation.

The internal energy scale (inverse time scale) of H_b shall be denoted by ω_b. It is a measure for the internal dynamics of the bath. Analogously, λ measures the strength of the coupling between the qubit and the bath.

The Hamiltonian of the control pulse reads

$$H_0(t) = \vec{\sigma} \cdot \vec{v}(t), \tag{6}$$

where $\vec{\sigma}$ is the vector of the Pauli matrices and $\vec{v}(t) = (v_x(t), v_y(t), v_z(t))$ is a vector which defines the shape of the pulse along the three spin directions. The axis of rotation at the instant t is given by $\vec{v}(t)/|\vec{v}(t)|$.

We concentrate on the evolution of the total system $H_{\text{tot}}(t) = H + H_0(t)$ comprising the qubit and the bath during the application of the pulse. The total time evolution is given by the time-ordered exponential in equation (1). In what follows, we follow the same ideas as in [18].

The goal is to expand around the ideal instantaneous pulse which we take to be located at the instant $\tau_s \in [0, \tau_p]$. To this end, we split the time evolution into its part before τ_s, $U_p(\tau_s, 0)$, and its part after τ_s, $U_p(\tau_p, \tau_s)$. For these two evolutions we use the following ansätze

$$U_p(\tau_s, 0) = U_1(\tau_s, 0) T\left\{\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_0^{\tau_s} \vec{v}(t)\,\mathrm{d}t}\right\} \mathrm{e}^{-\mathrm{i}\tau_s H} \tag{7a}$$

$$U_p(\tau_p, \tau_s) = \mathrm{e}^{-\mathrm{i}(\tau_p-\tau_s)H} T\left\{\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau_p} \vec{v}(t)\,\mathrm{d}t}\right\} U_2(\tau_p, \tau_s), \tag{7b}$$

where the time ordering is required because of the non-commutation of $H_0(t)$ with itself at different instants $[H_0(t_1), H_0(t_2)] \neq 0$. This fact marks the major difference to our previous analysis [18].

Both U_1 and U_2 are seen as the corrections which are necessary in order to factorize the two exponentials of the system and pulse even though they do not commute. The corrections U_1 and U_2 are determined from the Schrödinger equation, see section 4.

The time-ordered exponential in (7) can be translated into an overall rotation around an unknown axis $\hat{a}(\tau)$ ($|\hat{a}(\tau)| = 1$) about an angle $\psi(\tau)$,

$$\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\hat{a}(\tau)\psi(\tau)/2} := T_+\left\{\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau} \vec{v}(t)\,\mathrm{d}t}\right\}, \qquad \text{if} \quad \Delta\tau \geqslant 0 \tag{8a}$$

$$:= T_-\left\{\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau} \vec{v}(t)\,\mathrm{d}t}\right\}, \qquad \text{if} \quad \Delta\tau < 0 \tag{8b}$$

$$= T_{\text{sign}(\Delta\tau)}\left\{\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau} \vec{v}(t)\,\mathrm{d}t}\right\}, \quad \forall\tau, \tag{8c}$$

where $\Delta\tau := \tau - \tau_s$ with $\tau \in [0, \tau_p]$ and $T_\pm$ stands for the increasing or decreasing time ordering, respectively. Note that upon inversion the following identity holds:

$$\left(T_-\left(\mathrm{e}^{-\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau} \vec{v}(t)\,\mathrm{d}t}\right)\right)^\dagger = T_+\left\{\mathrm{e}^{\mathrm{i}\vec{\sigma}\cdot\int_{\tau_s}^{\tau} \vec{v}(t)\,\mathrm{d}t}\right\}. \tag{9}$$

For the sake of brevity, we introduce

$$\hat{p}(t) := \vec{\sigma} \cdot \hat{a}(t)\psi(t)/2, \tag{10}$$

which is a scalar operator.

Of course, there is a well-defined relation between $\vec{v}(t)$ on the one hand and $\hat{a}(t)$ and $\psi(t)$ on the other. From definition (8) we know

$$\mathrm{i}\partial_t \, \mathrm{e}^{-\mathrm{i}\hat{p}(t)} = H_0(t) \, \mathrm{e}^{-\mathrm{i}\hat{p}(t)}. \tag{11}$$

The rotation in spin space can explicitly be written as

$$\mathrm{e}^{-\mathrm{i}\hat{p}(t)} = \cos(\psi(t)/2) - \mathrm{i}(\vec{\sigma} \cdot \hat{a}(t)) \sin(\psi(t)/2). \tag{12}$$

Its time derivative simply reads

$$\partial_t \, \mathrm{e}^{-\mathrm{i}\hat{p}} = \frac{\psi'(t)}{2}(-\sin(\psi(t)/2) - \mathrm{i}\vec{\sigma} \cdot \hat{a}(t)\cos(\psi(t)/2)) - \mathrm{i}\vec{\sigma} \cdot \hat{a}'(t)\sin(\psi(t)/2). \tag{13}$$

Inserting (6) in (11), then exploiting (12) and

$$\vec{\sigma}(\vec{\sigma} \cdot \vec{n}) = \vec{n} + \mathrm{i}(\vec{n} \times \vec{\sigma}), \tag{14}$$

which holds for any vector $\vec{n}$, yields an explicit expression for $\partial_t \, \mathrm{e}^{-\mathrm{i}\hat{p}(t)}$ linear in $\vec{v}(t)$. Its comparison with (13) yields

$$2\vec{v}(t) = \psi'(t)\hat{a}(t) + \hat{a}'(t)\sin\psi(t) - (1 - \cos\psi(t))(\hat{a}'(t) \times \hat{a}(t)). \tag{15}$$

Multiplication with $\hat{a}(t)$ yields the derivative of $\psi(t)$

$$\vec{v}(t) \cdot \hat{a}(t) = \psi'(t)/2. \tag{16}$$

Equation (15) clearly determines $\vec{v}(t)$ from given $\hat{a}(t)$ and $\psi(t)$. But it can also be used to find $\psi(t)$ and $\hat{a}(t)$ from $\vec{v}(t)$ by integration which is the way one has to take from an experimentally given pulse to its theoretical description.

4. General equations

First, we consider $U_p(\tau_p, \tau_s)$. From the Schrödinger equation

$$\mathrm{i}\partial_\tau U_p(\tau, \tau_s) = (H + H_0(\tau))U_p(\tau, \tau_s), \tag{17}$$

and the ansatz (7*b*) we obtain

$$H_0(\tau)U_p(\tau, \tau_s) = \mathrm{e}^{-\mathrm{i}H\Delta\tau} H_0(t) \, \mathrm{e}^{-\mathrm{i}\hat{p}(\tau)} U_2(\tau, \tau_s) + \mathrm{i}\mathrm{e}^{-\mathrm{i}H\Delta\tau} \, \mathrm{e}^{-\mathrm{i}\hat{p}(\tau)} \partial_\tau U_2(\tau, \tau_s). \tag{18}$$

For the time derivative of U_2 this equation implies

$$\mathrm{i}\partial_\tau U_2(\tau, \tau_s) = F(\tau)U_2(\tau, \tau_s) \tag{19}$$

where

$$F(\tau) := \mathrm{e}^{\mathrm{i}\hat{p}(\tau)}[\tilde{H}_0(\tau) - H_0(\tau)] \, \mathrm{e}^{-\mathrm{i}\hat{p}(\tau)} \tag{20}$$

and $\tilde{H}_0(\tau) = \mathrm{e}^{\mathrm{i}H\Delta\tau} H_0(\tau) \, \mathrm{e}^{-\mathrm{i}H\Delta\tau}$. The formal solution to this Schrödinger equation reads

$$U_2(\tau_p, \tau_s) = T_+ \left\{ \exp\left(-\mathrm{i} \int_{\tau_s}^{\tau_p} F(t) \, \mathrm{d}t \right) \right\}, \tag{21}$$

where $\Delta t := t - \tau_s$.

The analogous procedure is used to obtain U_1 starting from

$$-\mathrm{i}\partial_\tau U_p(\tau_s, \tau) = U_p(\tau_s, \tau)(H + H_0(\tau)), \tag{22}$$

where $\tau \in [0, \tau_s]$. Finally, one finds

$$U_1(\tau_s, 0) = T_+ \left\{ \exp\left(-\mathrm{i} \int_0^{\tau_s} F(t) \, \mathrm{d}t \right) \right\}. \tag{23}$$

The time-dependent operator $F(t)$ is the same as that appearing in equation (20). Note that $F(t) = 0$ if there is no coupling between the qubit and the bath ($\lambda = 0$) because $\tilde{H}_0(t) = H_0$ holds in this case. Hence we have

$$F(t) = \mathcal{O}(t\lambda). \tag{24}$$

Finally, we combine both corrections U_1 and U_2 to one correction $U_F(\tau_p, 0)$,

$$U_p(\tau_p, 0) = U_p(\tau_p, \tau_s)U_p(\tau_s, 0) \tag{25a}$$

$$= \mathrm{e}^{-\mathrm{i}\Delta\tau_p H}\, \mathrm{e}^{-\mathrm{i}\hat{p}(\tau_p)} U_F(\tau_p, 0)\, \mathrm{e}^{\mathrm{i}\hat{p}(0)}\, \mathrm{e}^{-\mathrm{i}\tau_s H} \tag{25b}$$

where $\Delta\tau_p = \tau_p - \tau_s$ and

$$U_F(\tau_p, 0) := U_2(\tau_p, \tau_s)U_1(\tau_s, 0) \tag{26a}$$

$$= T_+\left\{\mathrm{e}^{-\mathrm{i}\int_{\tau_s}^{\tau_p} F(t)\,\mathrm{d}t}\right\} T_+\left\{\mathrm{e}^{-\mathrm{i}\int_0^{\tau_s} F(t)\,\mathrm{d}t}\right\} \tag{26b}$$

$$= T_+\left\{\mathrm{e}^{-\mathrm{i}\int_0^{\tau_p} F(t)\,\mathrm{d}t}\right\}. \tag{26c}$$

Note that the intervals for the integration variable t in (26b) are such that the global time ordering in (26c) does not introduce any change compared to (26b).

If the total correction $U_F(\tau_p, 0)$ equals the identity then the operator $\mathrm{e}^{-\mathrm{i}\hat{p}(\tau_p)}\, \mathrm{e}^{\mathrm{i}\hat{p}(0)}$ occurs in the middle of the right-hand side of (25b). We require this factor to be equal to the desired ideal pulse $\hat{P}_\theta$,

$$\mathrm{e}^{-\mathrm{i}\hat{p}(\tau_p)}\, \mathrm{e}^{\mathrm{i}\hat{p}(0)} = \hat{P}_\theta, \tag{27}$$

for instance $\Theta = \pi$ for a π pulse. The choice of the global axis of rotation is arbitrary in the xy plane of spin directions in view of the rotation symmetry around σ_z. Hence we may assume $\hat{P}_\theta = \mathrm{e}^{\mathrm{i}\sigma_y\Theta/2}$.

In view of the above, the essential issue is the deviation of $U_F(\tau_p, 0)$ from the identity. Thus we study $F(t)$ and rewrite (20)

$$F(t) = \mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{v}(t) \cdot \Delta\vec{\sigma}(\Delta t)\, \mathrm{e}^{\mathrm{i}\hat{p}(t)}, \tag{28}$$

where (with $\Delta t := t - \tau_s$)

$$\Delta\vec{\sigma}(\Delta t) := \mathrm{e}^{\mathrm{i}H\Delta t}\vec{\sigma}\, \mathrm{e}^{-\mathrm{i}H\Delta t} - \vec{\sigma}. \tag{29}$$

From (28) we see that transforms of $\vec{\sigma}$ play an important role. Hence we define for later use

$$\vec{S}(t) := \mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{\sigma}\, \mathrm{e}^{-\mathrm{i}\hat{p}(t)}. \tag{30}$$

This vector operator is a rotation of $\vec{\sigma}$ about the axis $\hat{a}$ by the angle ψ. Hence it can be also be written as

$$\vec{S}(t) = D_{\hat{a}}(\psi)\vec{\sigma}, \tag{31}$$

where $D_{\hat{a}}(\psi)$ is the 3×3 dimensional matrix describing the rotation about the axis $\hat{a}$ by the angle ψ. The time dependences of $\hat{a}(t)$ and $\psi(t)$ are omitted to lighten the notation. For completeness, we also give the explicit form

$$\vec{S}(t) = \vec{\sigma}\cos\psi + \hat{a}(\vec{\sigma}\cdot\hat{a})(1 - \cos\psi) + (\vec{\sigma}\times\hat{a})\sin\psi, \tag{32}$$

which can be found using relations (12) and (14).

We will see shortly that the z-component $S_z(t)$ is what we need to know. Hence we calculate

$$S_z(t) = \hat{z} \cdot D_{\hat{a}}(\psi)\vec{\sigma} \tag{33a}$$

$$= (D_{\hat{a}}(-\psi)\hat{z}) \cdot \vec{\sigma} \tag{33b}$$

$$= \hat{n}(t) \cdot \vec{\sigma} \tag{33c}$$

where $\hat{z}$ is the unit vector in the z-direction. We put all the time dependence in the conventional unit vector $\hat{n}(t) := D_{\hat{a}}(-\psi)\hat{z}$ in $\mathbb{R}^3$. It will enable us to give a geometrical interpretation to the final equations.

Finally, we state which effect a pulse of angle θ exerts on $\vec{S}(t)$. We start from (27) and (30) which imply

$$\vec{S}(0) = \mathrm{e}^{\mathrm{i}\hat{p}(\tau_p)}\,\hat{P}_\theta \vec{\sigma}\,\hat{P}_\theta^\dagger\,\mathrm{e}^{-\mathrm{i}\hat{p}(\tau_p)} \tag{34a}$$

$$= \mathrm{e}^{\mathrm{i}\hat{p}(\tau_p)}(D_{\hat{y}}(\theta)\vec{\sigma})\,\mathrm{e}^{-\mathrm{i}\hat{p}(\tau_p)} \tag{34b}$$

$$= D_{\hat{y}}(\theta)\vec{S}(\tau_p). \tag{34c}$$

Hence, a θ pulse rotates $\vec{S}(\tau_p)$ about $\hat{y}$ by the angle θ. For $\theta = \pi$ this implies

$$S_z(0) = -S_z(\tau_p) \quad \Leftrightarrow \quad \hat{n}(0) = -\hat{n}(\tau_p). \tag{35}$$

Note that for other angles the implications on the vector $\hat{n}(t)$ can be much less trivial in general.

5. Expansion in $\tau_p H$

We consider the case where the duration τ_p of the pulse is short. This means that our expansion parameters are $\tau_p\lambda$ and $\tau_p\omega_b$, or in shorthand we expand in $\tau_p H$.

The vector operator $\Delta\vec{\sigma}(\Delta t)$ is expanded in a power series of Δt, cf [18], $\Delta\vec{\sigma}(\Delta t) = \sum_{n=1}^{\infty}\frac{\mathrm{i}^n}{n!}(\Delta t)^n[[H,\vec{\sigma}]]_n$, with the notation $[[H,\vec{\sigma}]]_1 = [H,\vec{\sigma}]$, $[[H,\vec{\sigma}]]_2 = [H,[H,\vec{\sigma}]]$ and so on. For our Hamiltonian (5) the first and second orders are

$$\Delta\vec{\sigma}(\Delta t) = -2\Delta t(\vec{\sigma}\times\hat{z})\lambda A - (\Delta t)^2(\lambda[H_b, A]\vec{\sigma}\times\hat{z} + 2\lambda^2A^2\vec{\sigma}_\perp) + \mathcal{O}(\Delta t^3), \tag{36}$$

where $\vec{\sigma}_\perp := (\sigma_x, \sigma_y, 0)$.

The perturbative computation of U_F requires us to solve equation (26c). This can be done by average Hamiltonian theory [7, 20] which requires integrations over $F(t)$ defined in (28). We show that the occurring integrals can be simplified by integration by parts. To this end, we write terms containing $\vec{v}(t)$ as time derivatives.

Inserting the expansion (36) into (28) the terms $\mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{v}\cdot(\vec{\sigma}\times\hat{z})\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)} = \mathrm{e}^{\mathrm{i}\hat{p}(t)}\hat{z}\cdot(\vec{v}\times\vec{\sigma})\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)}$ and $\mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{v}\cdot\vec{\sigma}_\perp\mathrm{e}^{-\mathrm{i}\hat{p}(t)}$ occur. The combination of (11) with its Hermitian conjugate and (14) provides us with

$$\partial_t\vec{S}(t) = 2\mathrm{e}^{\mathrm{i}\hat{p}(t)}(\vec{v}(t)\times\vec{\sigma})\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)}, \tag{37}$$

which expresses the first of the above terms concisely as

$$\partial_t S_z(t) = 2\mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{v}\cdot(\vec{\sigma}\times\hat{z})\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)}. \tag{38}$$

Note that the given value of the total angle of rotation θ implies that $\partial_t S_z(t) \propto 1/|\vec{v}| \propto 1/\tau_p$.

The second term is found from the combination of (11) with its Hermitean conjugate *without* using (14) implying

$$\partial_t S_z(t) = \mathrm{i}\mathrm{e}^{\mathrm{i}\hat{p}(t)}[\vec{v}\cdot\vec{\sigma}, \sigma_z]\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)} \tag{39}$$

whence

$$S_z(t)\partial_t S_z(t) = \mathrm{i}\mathrm{e}^{\mathrm{i}\hat{p}(t)}\sigma_z[\vec{v}\cdot\vec{\sigma},\sigma_z]\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)}. \tag{40}$$

Exploiting the identity

$$2\vec{\sigma}_\perp = \vec{\sigma} - \sigma_z\vec{\sigma}\sigma_z \tag{41a}$$

$$= \sigma_z[\sigma_z,\vec{\sigma}] \tag{41b}$$

we finally arrive at

$$-\mathrm{i}S_z(t)\partial_t S_z(t) = 2\mathrm{e}^{\mathrm{i}\hat{p}(t)}\vec{v}\cdot\vec{\sigma}_\perp\,\mathrm{e}^{-\mathrm{i}\hat{p}(t)}. \tag{42}$$

With the help of (40) and (42) the expansion of $F(t)$ reads

$$F(t) = -\lambda A\Delta t\partial_t S_z(t) - \mathrm{i}(\Delta t)^2\lambda[H_b, A]\partial_t S_z(t) - \mathrm{i}\lambda^2A^2(\Delta t)^2 S_z(t)\partial_t S_z(t) + \mathcal{O}(\Delta t^3). \tag{43}$$

Only the z-component of $\vec{S}$ is important. This a direct consequence of the coupling between the qubit and the bath in the Hamiltonian (5). In this context, it is noteworthy that higher terms in the expansion of $\Delta\sigma(\Delta t)$ (36) depend also only on the two terms $\vec{\sigma}\times\hat{z}$ and $\vec{\sigma}_\perp$. This implies that all orders of $F(t)$ are functions of $S_z(t)$ and $\partial_t S_z(t)$.

To reach an expansion of U_F in terms of $\tau_p H$ we first express it by means of the Magnus expansion [7, 20]

$$U_F(\tau_p, 0) = \exp[-\mathrm{i}\tau_p(F^{(1)} + F^{(2)} + F^{(3)} + \cdots)], \tag{44}$$

where each term $\tau_p F^{(j)}$ is of the order of $(\tau_p F)^j$. The leading term is the time average $\tau_p F^{(1)} = \int_0^{\tau_p} F(t)\,\mathrm{d}t$ while the next-leading term comprises the commutator of $F(t)$ with itself at different instants $\tau_p F^{(2)} = \frac{-\mathrm{i}}{2\tau_p}\int_0^{\tau_p}\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2[F(t_1), F(t_2)]$.

Because $F(t)$ itself is given by a series in Δt, see equation (43), the expansion (44) is not yet the desired expansion in τ_p,

$$U_F(\tau_p, 0) = \exp[-\mathrm{i}(\eta^{(1)} + \eta^{(2)} + \cdots)], \tag{45}$$

where $\eta^{(j)}$ represents the contribution of the power of $(\tau_p H)^j$. Inserting (43) into (44) and expanding again in τ_p yields the linear term

$$\eta^{(1)} = -\lambda A\int_0^{\tau_p}\Delta t\partial_t S_z(t)\,\mathrm{d}t \tag{46}$$

and the quadratic term

$$\eta^{(2)} = -\mathrm{i}\lambda^2A^2\left[\int_0^{\tau_p}(\Delta t)^2 S_z(t)\partial_t S_z(t)\,\mathrm{d}t + \frac{1}{2}\int_0^{\tau_p}\mathrm{d}t_1\Delta t_1\int_0^{t_1}\mathrm{d}t_2\Delta t_2[\partial_{t_1}S_z(t_1), \partial_{t_2}S_z(t_2)]\right] - \mathrm{i}\lambda[H_b, A]\int_0^{\tau_p}(\Delta t)^2\partial_t S_z(t)\,\mathrm{d}t. \tag{47}$$

These relations can be integrated by parts yielding

$$\eta^{(1)} = -\lambda A\big[[\Delta t S_z(t)]_0^{\tau_p} - \Sigma\big], \tag{48}$$

where we use the shorthand $\Sigma := \int_0^{\tau_p} S_z(t)\,\mathrm{d}t$. The quadratic order reads

$$\eta^{(2)} = -\mathrm{i}\lambda[H_b, A]\eta^{(2a)} - (\mathrm{i}/2)\lambda^2A^2\eta^{(2b)}, \tag{49}$$

where

$$\eta^{(2a)} = [(\Delta t)^2 S_z(t)]_0^{\tau_p} - 2\int_0^{\tau_p} \Delta t\, S_z(t)\,\mathrm{d}t \tag{50a}$$

$$\eta^{(2b)} = \tau_s(\tau_p - \tau_s)[S_z(\tau_p), S_z(0)] - [(\tau_p - \tau_s)S_z(\tau_p) - \tau_s S_z(0), \Sigma] + \int_0^{\tau_p} \mathrm{d}t_1 \int_0^{t1} \mathrm{d}t_2 [S_z(t_1), S_z(t_2)]. \tag{50b}$$

In the simple case where the pulse acts only as a rotation in the xz plane, i.e., $v_x = v_z = 0 \forall t$, one has $\hat{a} = \hat{y}$ and thus $S_z(t) = \sigma_z \cos\psi(t) + \sigma_x \sin\psi(t)$ according to (32). With (16) one sees that (48) and (50) reproduce the previous results obtained for fixed-axis rotations [18].

6. Discussion of the corrections

In order to have pulses which well approximate ideal instantaneous pulses at $\tau = \tau_s$ we want to shape the real pulse such that $\eta^{(1)} = \eta^{(2)} = 0$. The pulse shape is given in terms of the time dependences of $\hat{a}$ and ψ. They in turn determine the amplitude vector $\vec{v}$ uniquely via equation (15).

The conditions $\eta^{(1)} = \eta^{(2)} = 0$ represent operator equations as they stand. But they can be simplified using $\hat{n}(t)$ defined in (33c). Any equation linear in $S_z(t) = \hat{n}(t)\cdot\vec{\sigma}$ must hold for each vector component due to the linear independence of the Pauli matrices. Hence $\eta^{(1)} = 0$ is equivalent to

$$(\tau_p - \tau_s)\hat{n}(\tau_p) + \tau_s \hat{n}(0) = \int_0^{\tau_p} \hat{n}(t)\,\mathrm{d}t. \tag{51}$$

Equally, the vanishing of $\eta^{(2a)}$ is equivalent to

$$(\tau_p - \tau_s)^2 \hat{n}(\tau_p) - \tau_s^2 \hat{n}(0) = 2\int_0^{\tau_p} \Delta t \hat{n}(t)\,\mathrm{d}t. \tag{52}$$

In case that $S_z(t)$ occurs quadratically (or in even higher powers) the relation (14) helps reduce the expression under study to terms at most linear in $\vec{\sigma}$. Again, each component has to vanish separately and we can thus transform $\eta^{(2b)}$ in (50b) to a function of $\hat{n}(t)$ only. Assuming that (51) holds the resulting expression equals

$$\tau_s(\tau_p - \tau_s)\hat{n}(\tau_p) \times \hat{n}(0) = \int_0^{\tau_p} \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\, \hat{n}(t_1) \times \hat{n}(t_2). \tag{53}$$

It is very convenient that the complex condition on operators $\eta^{(1)} = \eta^{(2)} = 0$ is simplified to three three-dimensional vector equations (51), (52) and (53). These three equations allow us to visualize the effect of the generally rotating pulse. All one has to know about the pulse is the orbit of $\hat{n}(t)$ on the unit sphere. This is the geometrical interpretation of the corrections.

6.1. No-go result for $\tau_s = \tau_p$

We pose the question of whether a pulse can be tailored such that $\tau_s = \tau_p$ holds. This would mean that a cleverly designed pulse of a finite duration corresponds to an ideal instantaneous pulse at the very end of the real pulse. Experimentally, this would be very advantageous because one could start with measurements of the effects of such a pulse without any delay, right after the end of the tailored pulse.

But in [18] we proved that such a pulse does not exist in the framework of fixed-axis rotations. Hence we pose the question here again for a general rotation. Unfortunately, the generalization of the pulse does not help and we are able to prove even in the extended framework that $\tau_s = \tau_p$ is not possible. For $\tau_p = \tau_s$ equation (51) becomes

$$\tau_p \hat{n}(0) - \int_0^{\tau_p} \hat{n}(t)\,\mathrm{d}t = 0. \tag{54}$$

We multiply this equation by $\hat{n}(0)$ to reach

$$\tau_p = \int_0^{\tau_p} \mathrm{d}t \cos\alpha(t) \leqslant \int_0^{\tau_p} \mathrm{d}t = \tau_p, \tag{55}$$

where

$$\cos\alpha(t) := \hat{n}(t) \cdot \hat{n}(0). \tag{56}$$

The equality in (55) holds if and only if $\alpha(t)$ is a multiple of 2π almost everywhere in the interval of integration. Hence only abrupt jumps of multiples of 2π comply with the condition (55). But such jumps correspond to instantaneous pulses. Thus we conclude that $\tau_p = \tau_s$ is impossible for real pulses in linear order and so to all orders.

This finding, independent of the total angle θ, generalizes our previous no-go result from fixed-axis rotations to pulses with varying axis of rotation.

6.2. No-go result for second-order corrections of π pulses

The ideal pulses with $\theta = \pi$ are the most important ones for dynamical decoupling. We showed previously that they can be approximated by real pulses with vanishing linear corrections [18, 19]. But we proved for fixed-axis rotations that it is impossible to tailor the π pulse such that the second order vanishes [18]. The proof holds if the decoherence bath possesses an internal dynamics, i.e., $[A, H_b] \neq 0$, so that the prefactor of this term has to vanish. Note that this is the decisive difference to the Q_L pulses [17] considered in section 2.

Here we again pose the question of whether π pulses can be corrected in second order if one uses general rotations. Unfortunately, our finding is negative. The proof runs as follows.

For a π pulse we know from (35) that $\hat{n}(0) = -\hat{n}(\tau_p)$ holds. Next we multiply (52) by $-\hat{n}(0)$ yielding

$$(\tau_p - \tau_s)^2 + \tau_s^2 = -2\int_0^{\tau_p} \mathrm{d}t\, \Delta t \cos\alpha(t) \tag{57a}$$

$$\leqslant 2\int_0^{\tau_p} \mathrm{d}t |\Delta t| \tag{57b}$$

$$= (\tau_p - \tau_s)^2 + \tau_s^2. \tag{57c}$$

The equality holds if and only if $\alpha(t) = \pi$ modulo 2π for $t > \tau_s$ and $\alpha(t) = 0$ modulo 2π for $t < \tau_s$. So there must be at least one abrupt jump at $t = \tau_s$. Hence only an instantaneous pulse satisfies the second-order condition for a dynamical decoherence bath.

This finding generalizes our previous no-go result for π pulses from fixed-axis rotations to pulses with varying axis of rotation.

7. Conclusions

In this work we have presented an analytical perturbative approach to general short coherent control pulses for a two-level system, which may be given by a $S = 1/2$ spin or by a qubit. The spin is coupled (coupling strength λ) to a quantum bath with internal dynamics (characteristic frequency ω_b). The small expansion parameter is the duration τ_p of the pulse, i.e., $\tau_p\lambda$ and $\tau_p\omega_b$ are taken to be small. The starting point of the expansion is the ideal instantaneous pulse which represents the zeroth order of the expansion with $\tau_p = 0$.

We generalized the previous investigation of pulses which rely on rotations about a fixed axis [18] to general rotation about axes varying in time. The objective was twofold.

First, the general rotation eases the comparison with experiment because it is only approximately possible to realize rotations about a fixed given axis. The generalized formalism allows one to check the quality of complex rotations by equations (51), (52) and (53). Moreover, these formulae render a geometric interpretation possible which facilitates visualization. The general pulse is characterized by a path $\hat{n}(t)$ on a unit sphere.

Second, the generalized rotations allowed us to investigate whether the previous no-go findings for fixed-axis rotations [18] can be circumvented by general rotation about axes varying in time. But unfortunately, we proved that the general rotations comply with the same limitations as the fixed-axis rotations: (i) there is no real pulse which approximates an ideal instantaneous pulse at the end of its time interval of finite duration. (ii) π pulses cannot be corrected in second order in τ_p. Though negative at first glance, the positive message of this finding to the experiment is that there is no need for investigating complicated general rotations, at least as far as the above limitations are concerned.

In which directions can the present results be extended? Certainly, the equations (51), (52), and (53) provide the basis for searching for improved approximations for single quantum gates. For instance, we could not find $\pi/2$ pulses, which realize the so-called Hadamard gate [4], with vanishing second-order correction among the fixed-axis rotations [18]. We were not able to prove the non-existence of such pulses. Thus we cannot exclude the existence of a fixed-axis rotation approximating an ideal $\pi/2$ pulse in the second-order correction. But the present generalized approach definitely widens the range of pulses among which one can look for such a well-approximating pulse.

Another direction of extension is to pass from the two-level system to higher dimensional quantum systems coupled to a bath as they occur in quantum optical manipulations. The basic idea of our analytic approach is to disentangle the control pulse from the time evolution of the system without external pulse. This idea will carry over to more complex situations as well.

Acknowledgment

We are grateful to D Lidar for bringing [17] to our attention.

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