

Optimization of short coherent control pulses

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The coherent control of a small quantum system is considered. For a two-level system coupled to an arbitrary bath we consider a pulse of finite duration. We derive the leading and the next-leading order corrections to the evolution operator due to the noncommutation of the pulse and the bath Hamiltonian. The conditions are computed that make the leading corrections vanish. The pulse shapes optimized in this way are given for π and $\frac{\pi}{2}$ pulses.

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I. INTRODUCTION

For a long time, the coherent control of quantum systems has been an important issue. For instance, nuclear magnetic resonance (NMR) is a widely used technique for the analysis of chemical compounds and for imaging techniques. Another broad field of application is the coherent control of the state of quantum dots, both in the charge and in the spin degrees of freedom. In recent years, however, coherent control has gained an even more vivid interest because it is the indispensable prerequisite in quantum information processing.

In its most basic form, the quantum state of a single quantum bit (qubit) is to be changed in a given way. This is called a single qubit gate. A qubit is a two-level system which can be conveniently seen as the $S=1/2$ system. So we use this spin language to describe the qubit gates. The two most common gates are the π pulse, which flips the spin from up to down and vice versa, and the $\pi/2$ pulse or Hadamard gate, which rotates the spin by 90° away from the S_z direction.

The π pulse is particularly interesting for dynamic decoupling [1–8]. In a nutshell, this technique aims at decoupling the single qubit from its environment as well as possible by switching the qubit state by single qubit gates. Mostly, the π pulse is considered. The idea comes from the spin-echo technique in NMR where a π pulse is used to refocus the precessing magnetization. In NMR, the use of sophisticated protocols of π and $\pi/2$ pulses is common to suppress unwanted couplings between nuclear spins [9,10].

Experiments using π pulses have obtained many encouraging results in prolonging the coherence time of a qubit [11–14]. More complex pulse sequences based on $\pi/2$ pulses have also proved useful by diminishing the rate of decoherence in quantum registers considerably [15].

In the theoretical treatments the generic ingredient to dynamic decoupling is an idealized pulse, mostly a π pulse, which is considered to be instantaneous. This means that its amplitude is infinite in the sense of a δ function. This assumption is convenient because the Hamiltonian H_0 of the pulse and the Hamiltonian H of the system at rest do not commute in general. The Hamiltonian H comprises the Hamiltonian of the qubit itself, the Hamiltonian of the environment (henceforth called “bath”), and the coupling between the qubit and the bath which is responsible for its decoherence. But during the pulse, H_0 dominates and H is negligible, and for the rest of the time only H is present. Hence it is relatively straightforward to deal with the time evolution.

Experimentally, however, this idealized situation is not realistic. The real pulses are always of finite amplitude and of finite length. So the question must be addressed which effect a finite pulse duration τ_p has. We want to elucidate this issue in the present work theoretically in a fully quantum mechanical framework.

The issue of pulses of finite duration and finite amplitude has been considered in other papers. Viola and Knill generalized their previous approach of averaging over a symmetry group [16] by instantaneous changes of the effective Hamiltonian to continuous changes requiring only finite, bounded control amplitudes [17]. But the presence of the coupling to the bath during the pulses has not been considered.

Khodjasteh and Lidar considered the effect of finite pulse duration in a comprehensive comparison of various schemes for π pulse sequences [18]. They did not consider to make the detrimental effects of the finite pulse duration vanish on the level of the individual pulse, but they discussed possible cancellations on the higher hierarchical level of the pulse sequence. In the present work, we will choose another route and aim at reducing the decoherence due to finite pulse duration already on the level of the single pulse. As a side remark, we note that the statement in Ref. [18] on optimized pulse sequences [8] that they hold only for bosonic bath operators is very likely not to be correct. It has been conjectured very recently by Lee *et al.* [19] that the optimized sequences apply to the most general phase decoherence model.

Very recently, the effect of classical random telegraph noise during pulses of finite length has been discussed numerically [20]. It was shown that shaping the pulse amplitude in a particular way can be used to improve its performance. This means that one can optimize the pulse such that its effect is closer to the desired one, e.g., a π pulse.

Tuning pulses by shaping them is a possibility of optimization which has been discussed intensively in the vast literature on NMR. But the objectives were mostly different from the consideration of the effects of a bath. For instance, Geen and Freeman aimed at frequency selectivity [21], i.e., the pulse should act only on spins on or close to resonance, but leave others unchanged. Closest to our scope are the investigations by Tycko [22], Cummins *et al.* [23,24], and Brown *et al.* [25] where composite pulses are optimized to be robust against off-resonance effects and pulse length inaccuracies. Again, no dynamic but only static effects are considered. Interestingly, we will see that some of the pulse shapes fulfilling the conditions in first order derived here for

fully dynamical baths coincide with pulse shapes previously derived to compensate static effects.

In this work, we present a systematic expansion in the pulse duration τ_p considering a qubit coupled to a fully quantum mechanical and dynamical bath. This means that the related energy scale $\omega_p := 1/\tau_p$ (\hbar is set to unity for simplicity) is considered to be very large so that all other energy scales, namely the coupling λ between qubit and bath and the internal energy scale of the bath ω_b , are small relative to ω_p . We expand in $\lambda/\omega_p = \tau_p\lambda$ and $\omega_b/\omega_p = \tau_p\omega_b$. The zeroth order is the instantaneous pulse. We compute the first and the second order and discuss the conditions for which they vanish. These conditions allow us to predict pulse shapes which approximate instantaneous pulses in spite of their finite pulse duration.

We emphasize that it is not our primary aim to eliminate the coupling between qubit and bath. On the contrary, it turns out that the expansion around the instantaneous pulse keeps this coupling. But the coupling to the bath is disentangled from the actual pulse. They are expressed by separate, subsequent time evolution operators. Given the thus optimized pulse shapes, the coupling to the bath can be compensated on the higher hierarchical level of an appropriate pulse sequence, i.e., by dynamic decoupling [1–8].

The paper is organized as follows. After introducing the model (Sec. II), we start describing the method we used to derive our general equations for the first and second order (Sec. III). Then we discuss the results and provide various examples for pulses that satisfy our conditions (Sec. IV). At last we discuss our results and compare them with other proposals for shaped pulses in the literature (Sec. V).

II. MODEL

We consider the time evolution operator from $t=0$ to $t = \tau_p$,

$$U_p(\tau_p, 0) = T \left[\exp \left(-i \int_0^{\tau_p} H_0(t) dt - iH\tau_p \right) \right]. \quad (1)$$

For simplicity the pulse is chosen to start at $t=0$; T stands for the usual time ordering. The control Hamiltonian of the pulse shall be given by

$$H_0 = v(t)\sigma_y, \quad (2)$$

where $v(t)$ stands for the pulse shape as a function of time, see Fig. 1. The time-independent Hamiltonian of the bath and the coupling to the qubit reads

$$H = H_b + \lambda A \sigma_z, \quad (3)$$

with H_b representing a generic bath and A its coupling operator to the qubit. The internal energy scale of H_b shall be denoted by ω_b . Note that H_0 and H do not commute so that the evolution operator (1) is a nontrivial expression.

The model (3) does not include spin flips; hence it implies an infinite lifetime T_1 . But the decoherence of a precessing spin in the xy plane is described in full generality because we do not specify for which operator A stands or the bath dynamics described by H_b . Such a model is experimentally

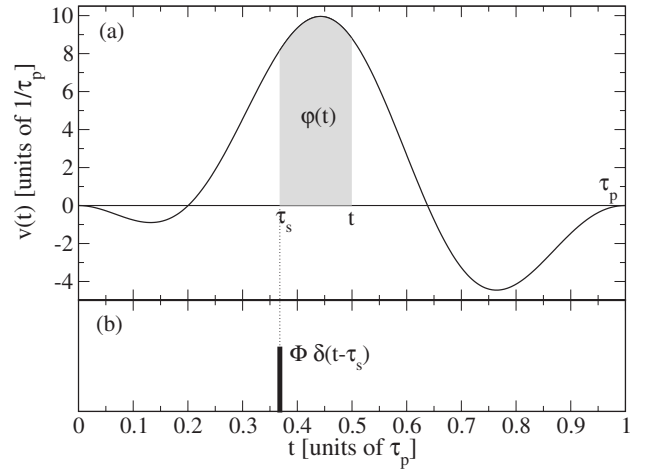


FIG. 1. (a) Plot of a generic pulse $v(t)$. The x - and y -axis values are expressed in units of τ_p and $1/\tau_p$, respectively. The shaded region represents an example for $\varphi(t)$, that is the integrated pulse amplitude between the instant τ_s and a generic instant t (see text). (b) Sketch of the approximately equivalent idealized instantaneous pulse.

very well justified as the effective model in the limit of a large applied magnetic field which implies that other couplings between the quantum bit spin and the bath are averaged out, see for instance, Refs. [26,27].

As an example only one may consider the spin-boson model

$$H = \sum_i \omega_i b_i^\dagger b_i + \sigma_z \sum_i \lambda_i (b_i^\dagger + b_i) \quad (4)$$

with $\lambda := \max_i \lambda_i$, $A = \sum_i (\lambda_i/\lambda) (b_i^\dagger + b_i)$, and $\omega_b := \max_i \omega_i$.

The primitive of the pulse amplitude is

$$\varphi(t) := \int_{\tau_s}^t v(t') dt', \quad (5)$$

where the integration starts from an instant $\tau_s \in [0, \tau_p]$. The intended angle of rotation is given by 2 times the total area under the curve $\theta := 2\Phi = 2[\varphi(\tau_p) - \varphi(0)]$. This area must be kept constant while investigating the limit $\tau_p \rightarrow 0$ so that the amplitude $v(t)$ must tend to infinity as $v(t) \propto 1/\tau_p$. To simplify our notation later, we define also $\psi(t) := 2\varphi(t)$.

The aim is to replace the real pulse given by $v(t)$ by an approximately equivalent instantaneous pulse acting at the instant τ_s , see Fig. 1. The equivalence shall hold up to linear order or quadratic order in τ_p . We highlight that the time evolution before and after the equivalent instantaneous pulse shall be governed by H , i.e., including the decohering interaction between qubit and bath. This shall be accounted for on the higher hierarchical level of appropriate pulse sequences.

III. METHOD AND GENERAL EQUATIONS

A. General equation

Let τ_s be an arbitrary instant inside the interval $[0, \tau_p]$ at which we want to split the time evolution

$$U_p(\tau_p, 0) = U_p(\tau_p, \tau_s)U_p(\tau_s, 0). \quad (6)$$

The guiding idea is shown in Fig. 1(b). We want to replace the full evolution by a first part during $[0, \tau_s]$ where only the Hamiltonian H is active. Then the instantaneous pulse shall follow. Finally, another interval $[\tau_s, \tau_p]$ of the dynamics governed by H terminates the pulse. This motivates the two following ansätze for the two unitary operators in Eq. (6),

$$U_p(\tau_p, \tau_s) = e^{-i(\tau_p - \tau_s)H} e^{-i\sigma_y \int_{\tau_s}^{\tau_p} v(t) dt} U_2(\tau_p, \tau_s), \quad (7a)$$

$$U_p(\tau_s, 0) = U_1(\tau_s, 0) e^{-i\sigma_y \int_0^{\tau_s} v(t) dt} e^{-i\tau_s H}, \quad (7b)$$

which define the operators $U_1(\tau_s, 0)$ and $U_2(\tau_p, \tau_s)$. Both, U_1 and U_2 must be seen as the corrections which are necessary because the left-hand sides of Eqs. (7a) and (7b) do not equal the right-hand sides without them since the pulse and the bath Hamiltonians do not commute. Note that no time ordering is necessary for the exponential of H because it is constant. For the exponential of H_0 no time ordering is necessary despite the time dependence because the commutator $[H_0(t), H_0(t')] = 0$ for any two times t and t' .

If the corrections are small, e.g., $U_2(\tau_p, \tau_s)U_1(\tau_s, 0) = 1 + O(\tau_p^2)$ up to linear order in τ_p , this implies

$$U_p(\tau_p, 0) = e^{-i(\tau_p - \tau_s)H} e^{-i\sigma_y \int_0^{\tau_p} v(t) dt} e^{-i\tau_s H} \quad (8)$$

which corresponds to the ideal, instantaneous pulse sketched in Fig. 1(b) at τ_s while the dynamics before and after τ_s includes both the bath dynamics and the coupling between qubit and bath.

The unitary corrections U_1 and U_2 are determined from the Schrödinger equation. We start analyzing U_2 in (7a). Let τ be a time instant in the interval $[\tau_s, \tau_p]$ such that

$$U_p(\tau, \tau_s) = e^{-i\Delta\tau H} e^{-i\int_{\tau_s}^{\tau} H_0(t) dt} U_2(\tau, \tau_s), \quad (9)$$

where we use the difference

$$\Delta x := x - \tau_s \quad (10)$$

generally for any variable x ; here in particular for $x = \tau$. The Schrödinger equation of $U_p(\tau, \tau_s)$ is the usual one,

$$i\partial_\tau U_p(\tau, \tau_s) = [H_0(\tau) + H]U_p(\tau, \tau_s). \quad (11)$$

Inserting Eq. (9) into (11) one obtains

$$\begin{aligned} & [He^{-i\Delta\tau H} + e^{-i\Delta\tau H}H_0(\tau)]e^{-i\int_{\tau_s}^{\tau} H_0(t) dt} U_2(\tau, \tau_s) \\ & + ie^{-i\Delta\tau H} e^{-i\int_{\tau_s}^{\tau} H_0(t) dt} \partial_\tau U_2(\tau, \tau_s) \\ & = [H_0(\tau) + H]e^{-i\Delta\tau H} e^{-i\int_{\tau_s}^{\tau} H_0(t) dt} U_2(\tau, \tau_s). \end{aligned} \quad (12)$$

It is easy to see that the terms with H cancel so that the differential equation for U_2 becomes

$$i\partial_\tau U_2(\tau, \tau_s) = [\tilde{H}_0(\tau) - H_0(\tau)]U_2(\tau, \tau_s), \quad (13a)$$

where

$$\tilde{H}_0(\tau) := e^{i\int_{\tau_s}^{\tau} H_0(t) dt} e^{i\Delta\tau H} H_0(\tau) e^{-i\Delta\tau H} e^{-i\int_{\tau_s}^{\tau} H_0(t) dt}. \quad (13b)$$

Formal integration leads to

$$U_2(\tau, \tau_s) = T \left[\exp \left(-i \int_{\tau_s}^{\tau} F(t) dt \right) \right], \quad (14a)$$

where

$$F(t) := \tilde{H}_0(t) - H_0(t). \quad (14b)$$

From its definition it is obvious that $F(t)$ vanishes identically if H_0 and H commute. This is the case if there is no coupling between qubit and bath. Closer inspection of Eqs. (13b) and (14b) shows that $F(t) = O(t\lambda v(t))$. More generally, $F(t)$ can be expanded in a series of H , i.e., in the parameters $t\lambda$ and $t\omega$ which amounts up to an expansion in τ_p . Thus, our approach provides the intended expansion in the shortness of the pulse.

With the definitions

$$\sigma_y(\Delta t) := e^{i\Delta t H} \sigma_y e^{-i\Delta t H} \quad (15)$$

and (5) the time-dependent operator $F(t)$ can be written in the compact form

$$F(t) = v(t) [e^{i\sigma_y \varphi(t)} \sigma_y(\Delta t) e^{-i\sigma_y \varphi(t)} - \sigma_y]. \quad (16)$$

Next, we treat U_1 by the analogous procedure solving the Schrödinger equation for (7b). Let τ be a generic instant in the interval $[0, \tau_s]$, the ansatz for this interval is

$$U_p(\tau_s, \tau) = U_1(\tau_s, \tau) e^{i\varphi(\tau) \sigma_y} e^{i\Delta\tau H}. \quad (17)$$

To obtain the Schrödinger equation in the second time argument of $U_1(\tau_s, \tau)$ it is convenient to consider the Hermitian conjugate of (11) yielding

$$-i\partial_\tau U_p(\tau_s, \tau) = U_p(\tau_s, \tau) [H_0(\tau) + H], \quad (18)$$

where the property $U_p^\dagger(t_1, t_2) = U_p(t_2, t_1)$ has been exploited. The procedure is the same as for U_2 with the only difference that now the exponentials occur on the right-hand side of U_1 ,

$$-i\partial_\tau U_1(\tau_s, \tau) = U_1(\tau_s, \tau) F(\tau) \quad (19)$$

with the same $F(t)$ as defined in (14b). Formal integration yields

$$U_1(\tau_s, \tau) = T \left[\exp \left(-i \int_{\tau}^{\tau_s} F(t) dt \right) \right]. \quad (20)$$

Finally, we combine both corrections U_1 and U_2 ,

$$\begin{aligned} U_p(\tau_p, 0) &= U_p(\tau_p, \tau_s) U_p(\tau_s, 0) \\ &= e^{-i(\tau_p - \tau_s)H} e^{-i\sigma_y \varphi(\tau_p)} U_F(\tau_p, 0) e^{i\sigma_y \varphi(0)} e^{-i\tau_s H}, \end{aligned} \quad (21)$$

where

$$\begin{aligned} U_F(\tau_p, 0) &:= U_2(\tau_p, \tau_s) U_1(\tau_s, 0) \\ &= T(e^{-i\int_{\tau_s}^{\tau_p} F(t) dt}) T(e^{-i\int_0^{\tau_s} F(t) dt}) \\ &= T(e^{-i\int_0^{\tau_p} F(t) dt}). \end{aligned} \quad (22)$$

Thus, the total correction U_F is given by the time-ordered product of $F(t)$. Thereby, we have derived the general expression for the difference between the unitary action of the real pulse as sketched in Fig. 1(a) and the idealized, instantaneous pulse in Fig. 1(b).

B. Expansion to second order in $\tau_p H$

We want to find the conditions under which $U_F(\tau_p, 0)$ can be approximated by the identity operator. Because $F(t)$ is $O(\lambda)$ for $\lambda \rightarrow 0$ the expansion in F is an appropriate first step. A convenient way to obtain the n th order of an expansion in λ and ω_b is to compute up to the n th order of the Magnus expansion from average Hamiltonian theory [9,28]. Then the resulting expressions are expanded to n th order in λ and ω_b . The advantage of this approach over a direct expansion is that the expansion is done in the argument of the exponential.

The Magnus expansion reads as

$$U_F(\tau_p, 0) = T \left[\exp \left(-i \int_0^{\tau_p} F(t) dt \right) \right] \\ = \exp[-i\tau_p(F^{(1)} + F^{(2)} + F^{(3)} + \dots)], \quad (23)$$

where $F^{(1)} = \frac{1}{\tau_p} \int_0^{\tau_p} F(t) dt$ is the average value of F . The next-leading term $F^{(2)}$ comprises the commutators of F with itself at different times,

$$F^{(2)} = \frac{-i}{2\tau_p} \int_0^{\tau_p} dt_1 \int_0^{t_1} dt_2 [F(t_1), F(t_2)]. \quad (24)$$

Thus from the Magnus expansion we know at least the two leading orders in powers of $F(t)$. Next, we expand $F(t)$ itself which is still a complicated quantity, see Eq. (16). To obtain the two leading orders in H we expand $F(t)$ in powers of H corresponding to an expansion in τ_p . We use the identity [29]

$$\sigma_y(\Delta t) = \sigma_y + \sum_{n=1}^{\infty} \frac{i^n}{n!} (\Delta t)^n [[H, \sigma_y]]_n, \quad (25)$$

where Δt is used as defined in (10). The notation stands for

$$[[H, \sigma_y]]_1 = [H, \sigma_y] = -2i\sigma_x \lambda A,$$

$$[[H, \sigma_y]]_2 = [H, [H, \sigma_y]] = -2i\sigma_x \lambda [H_b, A] + 4\sigma_y \lambda^2 A^2,$$

$$[[H, \sigma_y]]_3 = [H, [H, [H, \sigma_y]]] = \dots, \quad (26)$$

to obtain

$$\sigma_y(\Delta t) - \sigma_y = 2\sigma_x \Delta t \lambda A + (i\sigma_x \lambda [H_b, A] - 2\sigma_y \lambda^2 A^2) (\Delta t)^2 \\ + O(\Delta t^3). \quad (27)$$

Inserting the above expansion in Eq. (16) of $F(t)$ and using the elementary relation

$$e^{i\sigma_y \varphi(t)} \sigma_x e^{-i\sigma_y \varphi(t)} = \cos(\psi) \sigma_x + \sin(\psi) \sigma_z, \quad (28)$$

where $\psi(t) = 2\varphi(t)$ as well as the Magnus expansion (23) allows us to compute the leading orders of U_F in exponential representation

$$U_F(\tau_p, 0) = \exp[-i(\eta^{(1)} + \eta^{(2)} + \dots)] \quad (29)$$

with

$$\eta^{(1)} = (\eta_{11}\sigma_x + \eta_{12}\sigma_z) \lambda A, \quad (30a)$$

$$\eta^{(2)} = i(\eta_{21}\sigma_x + \eta_{22}\sigma_z) \lambda [H_b, A] + \eta_{23}\sigma_y \lambda^2 A^2. \quad (30b)$$

Note that $[H_b, A] = O(\omega_b)$ so that $\eta^{(2)}$ truly represents the desired second order in the shortness of the pulse. The coefficients η_{ij} are given by the integrals

$$\eta_{11} = 2 \int_0^{\tau_p} \Delta t v(t) \cos[\psi(t)] dt, \quad (31a)$$

$$\eta_{12} = 2 \int_0^{\tau_p} \Delta t v(t) \sin[\psi(t)] dt, \quad (31b)$$

$$\eta_{21} = \int_0^{\tau_p} \Delta t^2 v(t) \cos[\psi(t)] dt, \quad (31c)$$

$$\eta_{22} = \int_0^{\tau_p} \Delta t^2 v(t) \sin[\psi(t)] dt, \quad (31d)$$

$$\eta_{23} = -2 \int_0^{\tau_p} (\Delta t)^2 v(t) dt + 4 \int_0^{\tau_p} dt_1 \int_0^{t_1} dt_2 \Delta t_1 \Delta t_2 v_1 v_2 \sin(\psi_1 \\ - \psi_2), \quad (31e)$$

where we used ψ_i for $\psi(t_i)$ and v_i for $v(t_i)$ for $i \in \{1, 2\}$ in the last line. The differences are used as defined in (10). The last line of (31e) results from the commutator (24) yielding

$$[F(t_1), F(t_2)] = \Delta t_1 \Delta t_2 v_1 v_2 ([\sigma_z, \sigma_x] \sin \psi_1 \cos \psi_2 \\ + [\sigma_x, \sigma_z] \cos \psi_1 \sin \psi_2) \lambda^2 A^2, \\ = 2i \Delta t_1 \Delta t_2 v_1 v_2 \sigma_y (\sin \psi_1 \cos \psi_2 \\ - \cos \psi_1 \sin \psi_2) \lambda^2 A^2, \\ = 2i \Delta t_1 \Delta t_2 v_1 v_2 \sigma_y \sin(\psi_1 - \psi_2) \lambda^2 A^2. \quad (32)$$

This concludes the expansion up to second order in $\tau_p H$, i.e., in the shortness of the pulse.

IV. SHAPING THE PULSES

A. General discussion

1. Linear order

The general idea is that one can shape the pulses such that the leading deviations in U_F from unity vanish. First, we focus on the linear order which requires that $\eta^{(1)}$ vanishes. Hence we have two conditions given by $\eta_{11} = 0$ and $\eta_{12} = 0$. The relation $v(t) = \partial_t \psi(t)/2$ can be exploited to integrate the corresponding integrals (31a) and (31b) by parts yielding

$$0 = (\tau_p - \tau_s) \sin \psi(\tau_p) + \tau_s \sin \psi(0) - \int_0^{\tau_p} \sin \psi dt, \quad (33a)$$

$$0 = (\tau_p - \tau_s) \cos \psi(\tau_p) + \tau_s \cos \psi(0) - \int_0^{\tau_p} \cos \psi dt. \quad (33b)$$

Any pulse which fulfills these two conditions will show only quadratic deviations from the idealized instantaneous pulse. Note that τ_s is not *a priori* fixed and can be considered a free parameter which can be tuned to fulfill the above conditions. Hence one additional free parameter is sufficient to obtain a pulse which is ideal up to linear order. Explicit solutions will be discussed below.

A last general property worth mentioning is the symmetry of Eqs. (33a) and (33b) under the transformation $v(t) \rightarrow v(\tau_p - t)$ which implies $\tau_s \rightarrow \tau_p - \tau_s$ and $\psi(t) \rightarrow -\psi(\tau_p - t)$. Thus, if $v(t)$ fulfills Eqs. (33a) and (33b) for τ_s , then $v(\tau_p - t)$ fulfills them for $\tau_p - \tau_s$ also.

2. Quadratic order

The requirement $\eta^{(2)}$ in quadratic order adds another three integrals for η_{21} , η_{22} , and η_{23} . It is obvious that integration by parts can also be used to make $v(t)$ disappear in the expressions for η_{21} , η_{22} , and η_{23} . The resulting expressions are

$$\eta_{21} = \frac{(\tau_p - \tau_s)^2}{2} \sin \psi(\tau_p) - \frac{\tau_s^2}{2} \sin \psi(0) - \int_0^{\tau_p} \Delta t \sin \psi(t) dt, \quad (34a)$$

$$\eta_{22} = -\frac{(\tau_p - \tau_s)^2}{2} \cos \psi(\tau_p) + \frac{\tau_s^2}{2} \cos \psi(0) + \int_0^{\tau_p} \Delta t \cos \psi(t) dt, \quad (34b)$$

$$\begin{aligned} \eta_{23} = & (\tau_p - \tau_s) \tau_s \sin \theta - \tau_s \int_0^{\tau_p} \sin[\psi(t) - \psi(0)] dt - (\tau_p \\ & - \tau_s) \int_0^{\tau_p} \sin[\psi(\tau_p) - \psi(t)] dt + \frac{1}{2} \int_0^{\tau_p} \int_0^{\tau_p} \sin(\psi_1 \\ & - \psi_2) \text{sgn}(t_1 - t_2) dt_1 dt_2, \end{aligned} \quad (34c)$$

where we used $\theta = \psi(\tau_p) - \psi(0)$.

In view of the five expressions to be set to zero, one needs at least five free parameters including τ_s , in order to obtain pulses which show only cubic deviations from the idealized instantaneous pulse. One way to approach the solution of the above discussed conditions is to consider symmetric pulses aiming at $\tau_s = \tau_p/2$. Then $\psi(t)$ is an odd function about τ_s and the coefficients η_{11} and η_{22} vanish by antisymmetry. Then only three conditions remain to be solved. But the shape of the pulse is already fixed to some extent by its symmetry.

A closer inspection reveals that π pulses cannot be corrected in second order. This statement is proven rigorously by the following consideration. We combine the two real equations (34a) and (34b) to the complex equation

$$0 = \tau_s^2 e^{i\psi(0)} - (\tau_p - \tau_s)^2 e^{i\psi(\tau_p)} + 2 \int_0^{\tau_p} \Delta t e^{i\psi(t)} dt, \quad (35)$$

which leads to

$$\begin{aligned} \tau_s^2 + (\tau_p - \tau_s)^2 &= -2 \int_0^{\tau_p} \Delta t e^{i[\psi(t) - \psi(0)]} dt, \\ &\leq 2 \int_0^{\tau_p} |\Delta t| dt, \\ &\leq \tau_s^2 + (\tau_p - \tau_s)^2. \end{aligned} \quad (36)$$

The equality holds if and only if the exponential factor in the first line of (36) changes its value from -1 to 1 abruptly at $\Delta t = 0$. This implies an instantaneous, ideal pulse with infinite amplitude which is not experimentally realizable. Hence a π pulse cannot be corrected in second order. This no-go result is very remarkable in its general validity.

For $\pi/2$ pulses we found solutions which make η_{21} and η_{22} vanish. In spite of our intensive search we have not succeeded in finding solutions which additionally make η_{23} vanish. Hence, we conjecture that no such solution exists. But to our knowledge, there is no mathematical proof stating the impossibility to correct $\pi/2$ pulses in second order.

In this context, the reader may wonder whether one cannot combine two $\pi/2$ pulses to obtain a π pulse. But this is indeed not possible within the present framework. According to (21) there is always some decoherent time evolution before and after the ideal pulse. Hence no direct combination of pulses with small angles to pulses with larger angles is possible. But pulse sequences with finite time intervals between the pulses as in dynamic decoupling are well possible [1–8].

3. Possibility of $\tau_s = \tau_p$

We return to the corrections in linear order (33a) and (33b). Inspired from discussions with experimentalists in NMR, we pose the question whether it is possible to shape a pulse such that it corresponds to an ideal, instantaneous pulse at the end of the real pulse, i.e., $\tau_s = \tau_p$. If such a pulse existed it could be used to measure the response of systems at delay times much shorter than the duration τ_p of the initial pulse. Clearly, this would represent a promising experimental tool.

Unfortunately, it is impossible to construct such a pulse. Again, we can prove this rigorously by inserting $\tau_s = \tau_p$ into Eqs. (33a) and (33b) which we combine to one single complex equation using $\exp(i\psi) = \cos \psi + i \sin \psi$,

$$0 = \tau_p \exp[i\psi(0)] - \int_0^{\tau_p} \exp[i\psi(t)] dt. \quad (37)$$

We find again a rigorous estimate

$$\tau_p = \int_0^{\tau_p} \exp\{i[\psi(t) - \psi(0)]\} dt \leq \int_0^{\tau_p} 1 dt = \tau_p, \quad (38)$$

which is fulfilled if and only if $\psi(t)$ is a piecewise constant with jumps of 2π . But such a $\psi(t)$ represents via $\partial_t \psi(t) = 2v(t)$ instantaneous pulses with infinite amplitudes. Thus, there cannot be a real pulse with bounded amplitude which is close to an ideal pulse at the end of its duration in linear order of the bath parameters.

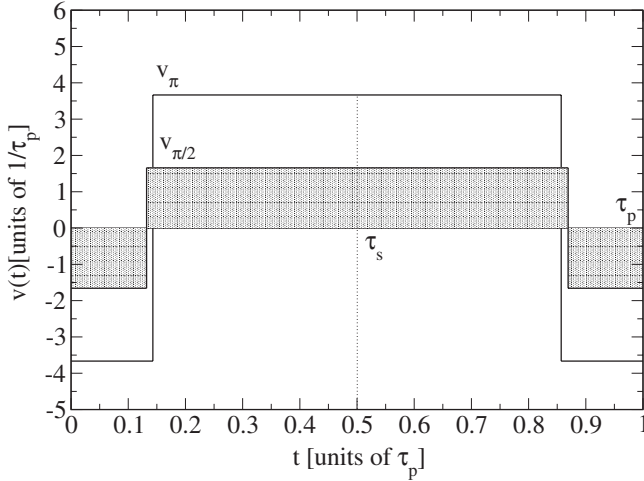


FIG. 2. Composite π and $\pi/2$ pulses with piecewise constant amplitude in the symmetric case. In the π pulse, the sign changes occur at $\tau_1 = \tau_p/7$ ($6\tau_p/7$, respectively) and the amplitude is $a_{\max} = 7\pi/6[1/\tau_p]$. In the $\pi/2$ pulse, the sign changes occur at $\tau_1 = 0.13155\tau_p$ ($\tau_p - \tau_1$, respectively) and the amplitude is $a_{\max} = 1.65765[1/\tau_p]$.

One can only approximate the desired situation by aiming at a τ_s close to τ_p . To this end, asymmetric pulses will be considered below.

B. Solutions

In view of the above general discussion we focus here only on the correction in linear order. First, we consider so-called composite pulses which consist of piecewise constant pulses of maximally positive or negative amplitude $\pm a_{\max}$. Second, continuously shaped pulses made from sines and cosines are investigated. In each class, we look at symmetric pulses with $\tau_s = \tau_p/2$ first and then at asymmetric pulses.

1. Composite pulses

(a) *Symmetric pulses.* For symmetric pulses with $\tau_s = \tau_p/2$ there is only one equation to be solved, namely (33b), because (33a) is fulfilled by antisymmetry. We need only one free parameter and take the instant τ_1 , at which the pulse changes first, to be this free parameter. Another sign change occurs by symmetry at $t = \tau_p - \tau_1$. Figure 2 depicts the solutions for a π pulse and for a $\pi/2$ pulse. The parameters are given in the caption.

It is noteworthy that the symmetric π pulse found is exactly the one that Cummins *et al.* named SCORPSE [23,24]. Do our results reproduce theirs generally? The answer is “no” because the goals are different. While Cummins *et al.* aim at finding a pulse shape such that

$$U_p(\tau_p, 0) \approx U_\theta \quad (39)$$

our aim is to approximate as closely as possible

$$U_p(\tau_p, 0) \approx \exp[-i(\tau_p - \tau_s)H]U_\theta \exp(-i\tau_s H), \quad (40)$$

where U_θ stands for the ideal θ pulse evolution operator. In other words, the authors of Refs. [23,24] aim at making the

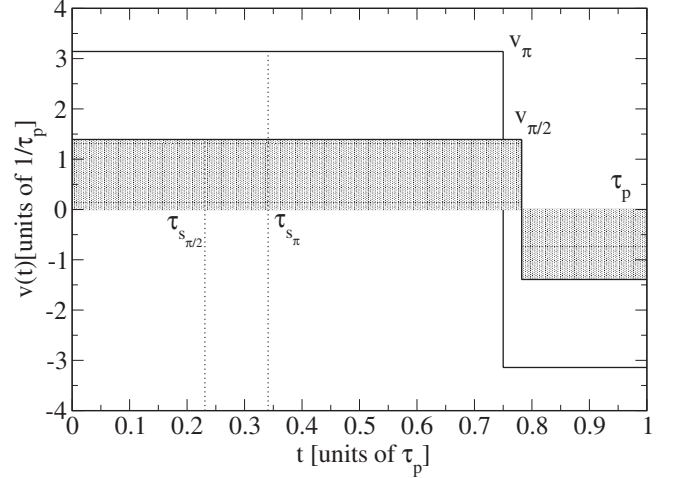


FIG. 3. Composite π and $\pi/2$ pulses with piecewise constant amplitude made from two elementary pulses in the asymmetric case. For the π pulse, the sign change occurs at $\tau_1 = 3\tau_p/4$, the amplitude is $a_{\max} = \pi[1/\tau_p]$, and the instant of the equivalent ideal pulse is $\tau_s = (\tau_p/2)(1 - 1/\pi)$. For the $\pi/2$ pulse, $\tau_1 = 0.78220\tau_p$, the amplitude is $a_{\max} = 1.39156[1/\tau_p]$ and the instant of the equivalent ideal pulse is $\tau_s = 0.23128\tau_p$.

imperfections vanish completely while our aim is more modest: We aim at separating the bath and the pulse evolution. We are convinced that our aim is more realistic, in particular for general dynamic baths without static components so that no averaging to zero is possible. The compensation of the coupling between qubit and bath for longer storage times shall be done by dynamic decoupling [1–8] on the basis of the optimized pulses discussed here.

But for static couplings $H \propto \sigma_z$ and a π pulse with $\tau_s = \tau_p/2$ both aims (39) and (40) happen to coincide,

$$e^{-i\tau_p H/2} U_\pi e^{-i\tau_p H/2} = U_\pi e^{i\tau_p H/2} e^{-i\tau_p H/2} = U_\pi. \quad (41)$$

Note that the argument does not require that the pulse is symmetric but only that the splitting time τ_s is in the middle of the pulse so that the first half of the evolution under H compensates the second half. Indeed, the CORPSE pulse [23,24] fulfills our conditions (33a) and (33b) as well (see Fig. 4).

(b) *Asymmetric pulses.* On considering asymmetric pulses there is no reason to restrict oneself to $\tau_s = \tau_p/2$. Hence, there is another free parameter to tune. In this way, it is possible to find composite pulses which consist only of two constant regions. Figure 3 depicts the simplest solutions, but there can be many more. For the π pulse, for instance, we have found an infinite set of solutions with the time $\tau_1 = (2n+1)\tau_p/(4n)$ at which the jump occurs and the amplitude $a_{\max} = \pi n/\tau_p$, where n is a positive integer. The corresponding splitting time reads $\tau_s/\tau_p = 1/2 + (-1)^n/(2n\pi)$. The solution depicted corresponds to $n=1$.

The pulses depicted in Fig. 3 are the most asymmetric ones for given maximum amplitude. This is reflected by the values for τ_s which are not close to $\tau_p/2$. If one is looking for a pulse shape which allows the measurement of a signal as soon as possible after an ideal pulse the inverted pulses

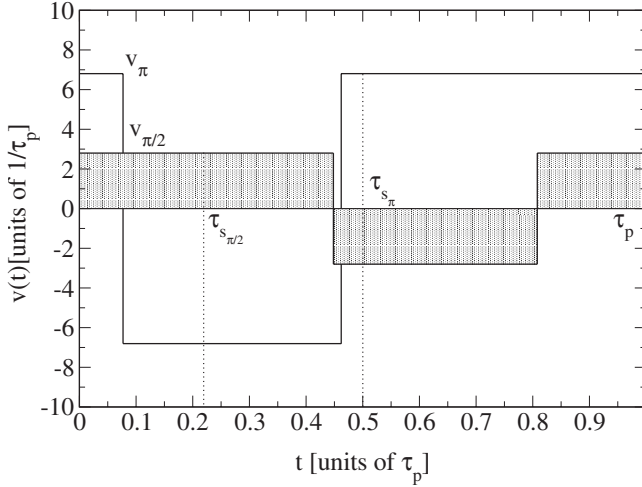


FIG. 4. Composite π and $\pi/2$ pulses with piecewise constant amplitude made from three elementary pulses in the asymmetric case. For the π pulse, the sign changes occur at $\tau_1 = \tau_p/13$ and at $\tau_2 = 6\tau_p/13$, the amplitude is $a_{\max} = 13\pi/6[1/\tau_p]$, and the instant of the equivalent ideal pulse is $\tau_s = \tau_p/2$. For the $\pi/2$ pulse, the sign changes occur at $\tau_1 = 0.44834\tau_p$ and at $\tau_2 = 0.80813\tau_p$, the amplitude is $a_{\max} = 2.80074[1/\tau_p]$, and the instant of the equivalent ideal pulse is $\tau_s = 0.219\tau_p$.

$v(\tau_p - t)$ with $\tau_s \approx 0.77$ for the $\pi/2$ pulse and with $\tau_s \approx 0.66$ for the π pulse should be used.

Beyond the composite pulses consisting of two constant regions we consider also the more commonly discussed composite pulses consisting of three constant regions. Figure 4 shows generic results. The π pulse depicted is the CORPSE pulse proposed previously [23,24] which happens to fulfill also our conditions as explained above. The solution is arbitrary in the sense that other values for τ_s are also possible.

The same is true for the $\pi/2$ pulse for which we have chosen τ_s at will. Many other values are also possible. For $\tau_s = \tau_p/2$, however, we have not found any asymmetric solution.

2. Continuous pulses

The above composite pulses are advantageous because they are fairly simple to generate and because they use the maximally possible amplitudes most efficiently. But they are not optimum in view of their frequency selectivity due to the jumps. It is well known that the faithful representation of jumps requires particularly broad frequency bands. Hence, it is important to demonstrate that our conditions (33a) and (33b) can be also fulfilled by continuous pulses. We choose ansätze inspired from Fourier series which ensure even continuity of the derivative $v'(t)$.

(a) *Symmetric pulses.* For symmetric pulses our ansatz reads as

$$v(t) = \theta/2 + a \cos(2\pi t/\tau_p) - (a + \theta/2)\cos(4\pi t/\tau_p). \quad (42)$$

The coefficients are chosen such that $v(0) = v(\tau_p) = 0$ and $v'(0) = v'(\tau_p) = 0$. Of course, higher cosine terms could be added. But the constraints in linear order (33a) and (33b) can be fulfilled already by the above ansatz. Figure 5 displays the

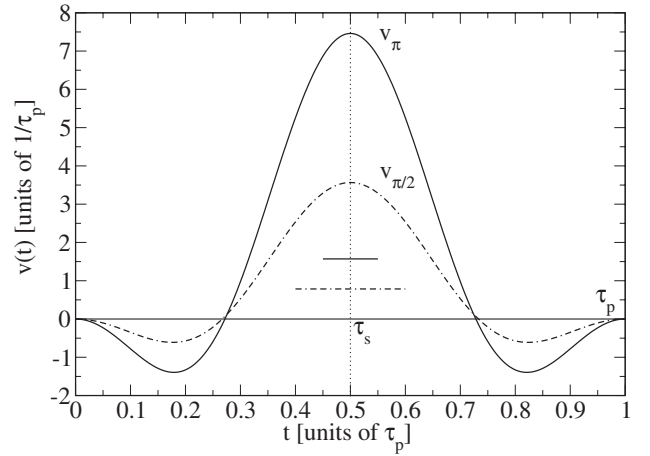


FIG. 5. Continuous π and $\pi/2$ pulses in the symmetric case. The parameter a as defined in the ansatz (42) takes the value $-3.73002/\tau_p$ for the π pulse and the value $-1.78259/\tau_p$ for the $\pi/2$ pulse. The horizontal lines indicate the amplitude for a totally constant, uncorrected π pulse (solid line) and $\pi/2$ pulse (dashed-dotted line), respectively.

resulting pulse shapes. Note that the instant of the equivalent ideal pulse is $\tau_s = \tau_p/2$. Comparing Fig. 2 and Fig. 5 the above statement is illustrated that the composite pulses require only smaller amplitudes. But the continuous pulses in Fig. 5 are much smoother and, hence, do not spread so much in frequency space. It depends on the actual constraints in experiment which kind of pulse is the most advantageous.

(b) *Asymmetric pulses.* For completeness, we also consider an ansatz allowing for asymmetric continuous pulses

$$v(t) = (\theta/2)[1 - \cos(2\pi t/\tau_p)] + a \sin(2\pi t/\tau_p) - (a/2)\sin(4\pi t/\tau_p). \quad (43)$$

The resulting solutions of the conditions (33a) and (33b) are plotted in Fig. 6. The values of the parameters are given in the caption. Naturally, the instant of the equivalent instantaneous pulse is no longer in the middle of the pulse $\tau_s \neq \tau_p$.

V. CONCLUSIONS

In this paper, we have investigated under which conditions it is possible to shape the pulses implementing single qubit gates such that they correspond to ideal, instantaneous pulses (cf. Fig. 1). To this end, we computed the corrections in powers of H , the Hamiltonian containing the coupling to the bath and the dynamics of the bath, to the equivalence

$$U_p(\tau_p, 0) = e^{-i(\tau_p - \tau_s)H} U_\theta e^{-i\tau_s H} + O(H). \quad (44)$$

The expansion in powers of H is an expansion in the shortness of the total pulse. No assumption about the nature of the bath is made so that our results are very generally applicable.

We have derived the explicit expression for the corrections in linear order in H as well as those quadratic in H . In the evaluation of the expressions found we focused on the π pulse and the $\pi/2$ pulse. They are by far the most important ones for all kinds of applications. The π pulse is used to flip

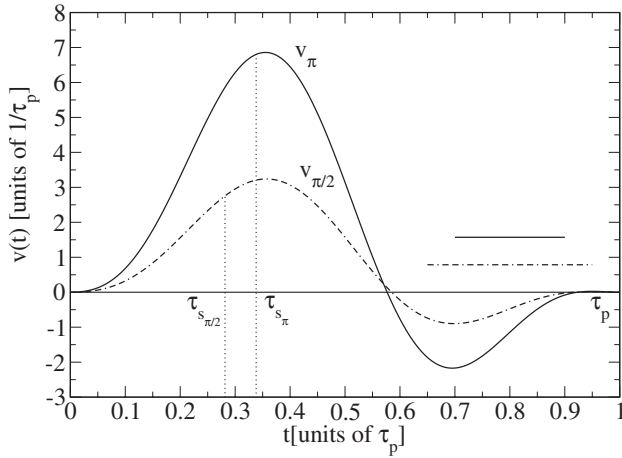


FIG. 6. Continuous π and $\pi/2$ pulses in the asymmetric case. For the π pulse, the parameter a as defined in the ansatz (43) takes the value $3.393\,08/\tau_p$ and the position τ_s of the equivalent ideal pulse takes the value $0.338\,06\tau_p$. For the $\pi/2$ pulse, the parameter a is $1.547\,14/\tau_p$ and the position τ_s of the equivalent ideal pulse is $0.280\,93\tau_p$. The horizontal lines indicate the amplitude for a totally constant, uncorrected π pulse (solid line) and $\pi/2$ pulse (dashed-dotted line), respectively.

spins or qubits. An important application are spin-echo experiments and, more generally, dynamic decoupling of two-level systems from their environment [1–8]. The $\pi/2$ pulse generates in NMR experiments the precessing magnetic field and is used in many intricate pulse sequences to suppress the effect of unwanted interactions [9]. In the context of quantum information, the $\pi/2$ pulse realizes the important Hadamard gate.

We found and showed a multitude of pulse shapes which are correct in linear order, i.e.,

$$U_p(\tau_p, 0) = e^{-i(\tau_p - \tau_s)H} U_\theta e^{-i\tau_s H} + O(H^2). \quad (45)$$

The pulses can be chosen piecewise constant which requires the lowest amplitudes. They imply, however, jumps which deteriorate the frequency selectivity [10]. Continuous and continuously differentiable pulses can also be realized and they have a much better frequency selectivity. Their drawback is that the maximum amplitude required is larger than for the piecewise constant pulses.

We noted that our objective (45) happens to coincide with the one of earlier work [22–24] for a π pulse with $\tau_s = 1/2$ applied to a completely static bath, i.e., a bath without internal dynamics. One reason for this coincidence is that in leading order the internal bath dynamics does not play a role. The commutators between different bath operators occur only in second order. Hence, the corresponding CORPSE and SCORPSE pulse fulfill also the conditions derived in the present paper. In general, however, the coincidence does not hold, i.e., if $\tau_s \neq \tau_p/2$ or if the bath is not static in the above sense or if pulses with angles θ different from π are consid-

ered. Moreover, we emphasize that for dynamic baths without static components, i.e., baths with internal dynamics, the aim to make the coupling between qubit and bath vanish altogether, i.e., $U_p(\tau_p, 0) \approx U_\theta$, cannot be fulfilled for general angle $\theta \neq \pi$.

Investigating the quadratic order, we could prove that π pulses cannot be corrected in this order. For $\pi/2$ pulses we have not found any solution in spite of intensive search. Hence we are led to conjecture that no such solution exists. It would be interesting to find a mathematical foundation for this conjecture. Even in linear order, it is not possible to shape the pulse in such a way that it corresponds to an ideal, instantaneous pulse at the very end of the real pulse. This would have been a nice property for NMR measurements since it would have permitted us to measure directly after a given pulse without further delay. One may, however, use asymmetric pulses which correspond to ideal pulses at about 77% of the total pulse length.

The message from our findings is that pulses can be shaped such that they approximate ideal, instantaneous pulses. The required pulse shapes must fulfill rather simple analytic integrals so that everyone can fine-tune his pulse shape easily himself. The optimized π pulses are an excellent starting point for optimized dynamic decoupling schemes [8].

Möttönen *et al.* [20] have posed themselves a similar question for π pulses as we have done. The main differences are that they investigated classical noise numerically while we tackled a fully quantum mechanical model by analytical means. Another difference is that they aimed at $U_p(\tau_p, 0) \approx U_\pi$ whereas our goal was not to make the bath vanish, but to disentangle it from the actual pulse, i.e., the coupling between qubit and bath is still present before and after the idealized pulse. Of course, in a model of classical noise there are no bath operators which do not commute so the mere disentanglement is trivially given in the model studied by Möttönen *et al.* We found that $U_p(\tau_p, 0) \approx U_\pi$ and $U_p(\tau_p, 0) = e^{-i(\tau_p/2)H} U_\pi e^{-i(\tau_p/2)H}$ coincide for baths without internal dynamics. For these special cases, our pulse shapes agree with those previously found [20,23,24]. For instance, the SCORPSE pulse appears to be a very good choice.

Further work should simulate the proposed pulse shapes in specific models in order to understand better how important the neglected corrections in second order really are. It is to be expected that for small values of λ (generic coupling to the bath) and ω_b (generic frequency of the bath) the corrected pulses are superior to the simple, uncorrected ones. But if the characteristic times of the bath are too short, presumably the simple pulses will be better.

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