Optimized dynamical decoupling for time-dependent Hamiltonians

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Abstract
The validity of optimized dynamical decoupling (DD) is extended to analytically time-dependent Hamiltonians. As long as an expansion in time is possible, the time dependence of the initial Hamiltonian does not affect the efficiency of optimized dynamical decoupling (UDD, Uhrig DD). This extension provides the analytic basis for (i) applying UDD to effective Hamiltonians in time-dependent reference frames, for instance in the interaction picture of fast modes and for (ii) its application in hierarchical DD schemes with π pulses about two perpendicular axes in spin space to suppress general decoherence, i.e. longitudinal relaxation and dephasing.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction
Progress in quantum information processing (QIP) requires a complete and coherent control of the dynamics of a quantum bit (spin $S = 1/2$) coupled to an environment (bath). In particular, one must be able to realize the no-operation reliably and coherently for long-time storage of quantum memory. Hence, decoherence must be suppressed. The most general decoherence consists of both transversal dephasing and longitudinal relaxation, i.e. the decoherence rates $1/T_2^*$ and $1/T_1$, respectively, in nuclear magnetic resonance (NMR) language.

So far, only models without explicit time dependence have to our knowledge been considered. The terms in the Hamiltonian $\tilde{H}$ without coherent control (we will call this Hamiltonian henceforth the initial one) do not have any explicit dependence on the time. For such a model, techniques of various degrees of sophistication exist to suppress the dephasing and/or the relaxation [1, 2]. We concentrate here on the dynamical decoupling (DD) [3–11] which generalizes the original ideas on spin echo techniques to open systems and their
application to QIP [12–14]. Intuitively, the interaction between spin (qubit) and bath is averaged to zero by means of repetitive $\pi$ pulses. Each pulse rotates the spin by an angle $\pi$ about a spin axis $\hat{a}$, thus inverting its components perpendicular to $\hat{a}$.

A particularly efficient way to suppress pure dephasing is the optimized DD (Uhrig DD) [7–10, 15–17] where the instants $t_j$ ($j \in \{1, 2, \ldots, N\}$), at which $N$ instantaneous $\pi$ pulses are applied, are given by $t_j = T\delta_j$ where $T$ is the total time of the sequence and

$$\delta_j = \sin^2(j\pi/(2N + 2)).$$

(1)

By efficient suppression it is meant that each pulse helps to suppress dephasing in one additional order in an expansion in $T$, i.e. $N$ pulses reduce dephasing to $O(T^{N+1})$. The existence of an expansion in powers of $T$, at least as an asymptotic expansion, is a necessary assumption.

So far, the derivation of the properties of UDD as defined in equation (1) was given for time-independent initial Hamiltonians [7–10]. The present study extends this derivation to initial Hamiltonians including an analytic time dependence. This extension is a breakthrough because it establishes the applicability of optimized DD for effective Hamiltonians in special reference frames, e.g. rotating frames, which induce an explicit time dependence. Such situations also arise where fast modes are treated in the interaction picture, are averaged over or integrated out so that time-dependent actions result and these actions are sufficiently smooth in time. The condition on smoothness need not always be fulfilled.

Another important application of UDD for time-dependent Hamiltonians is the suppression of general decoherence by the application of $\pi$ pulses around two perpendicular spin axes on two hierarchical levels. If UDD worked only for time-independent initial Hamiltonians, the only known solution for the secondary level would be concatenation of primary UDD sequences [11]. But recent numerical data by West et al showed that also the suppression on the secondary level can be efficiently realized by UDD [18]. They called the scheme quadratic DD (QDD). Hence, the derivation below provides the analytic foundation for the applicability of QDD.

For the sake of simplicity, we first give the extended derivation for pure dephasing, addressing longitudinal relaxation in a second step. Then the applications are discussed again and we provide an explicit derivation of the time dependence of the effective Hamiltonian after the primary application of UDD.

2. Dephasing

We consider the explicitly time-dependent Hamiltonian

$$\tilde{H}(t) = H_b(t) + \sigma_z A_z(t)$$

(2)

where the time dependences of the bath Hamiltonian $H_b(t)$ and of the coupling operator $A_z(t)$ are required to be analytic, i.e. they can be expanded in $t$. If the system described by (2) is subject to $N$ instantaneous $\pi$ pulses at the instants $\{T\delta_j\}$, $j \in \{1, 2, \ldots, N\}$, about a spin axis perpendicular to the $z$-axis, the effective Hamiltonian $H(t)$ in the basis of unflipped spins reads

$$H(t) = H_b(t) + \sigma_z A_z(t)F(t)$$

(3)

where the switching function $F(t) = \pm 1$ appears which changes sign at the instants $\{T\delta_j\}$. We are interested in the time evolution operator $U(t)$ induced by $H(t)$:

---

1 In the present work, we stick to idealized, instantaneous pulses, but this requirement can be realized in [19].

2
\[ U(T) := \mathcal{T} \exp \left( -i \int_0^T H(t) \, dt \right) \]  
\[ = U_0(T)U_1(T) \]  
(4a)  
(4b)

where \( \mathcal{T} \) is the time-ordering operator. The second line is based on the interaction picture with respect to \( H_0(t) \),

\[ U_0(t) := \mathcal{T} \exp \left( -i \int_0^T H_0(t) \, dt \right) \]  
(5a)  
\[ U_1(t) := \mathcal{T} \exp \left( -i \int_0^T A_1(t)F(t) \, dt \right) \]  
(5b)  
\[ A_1(t) := U_1^\dagger(t)\sigma_z A_z(t)U_0(t). \]  
(5c)

The key observation is that \( A_1(t) \) is analytic as well because \( H_0(t) \) is analytic according to our requirement, and thus \( U_0(t) \) and \( A_z(t) \) again according to our requirement. Thus, we have

\[ A_1(t) = \sum_{p=0}^{\infty} A_pt^p. \]  
(6)

To be precise, to exclude any terms up to a given order \( N \), we only need that \( A_1(t) \) can be represented by the sum in (6) up to \( p = N \) plus a residual function of higher order, i.e. the convergence of the Taylor series is not needed. In general, the operators \( A_p \) are complicated integral expressions of the operators in (2).

Next, the time evolution \( U_1(T) \) is expanded according to the standard time-dependent perturbation theory

\[ U_1(T) = \sum_{n=0}^{\infty} (-i)^n u_n \]  
(7a)  
\[ u_n = \int_0^T F(t_n) \cdots \int_0^{t_1} F(t_1) A_1(t_n) A_1(t_{n-1}) \cdots A_1(t_1) \, dt_1 \, dt_2 \cdots dt_n. \]  
(7b)

Our aim is to show that the powers with \( n \) odd are of order \( T^{N+1} \) because only the odd powers in \( \sigma_z \) affect the qubit spin. Hence, we can follow the reasoning of Yang and Liu [10] from here on. In order to keep the present communication self-contained, we include the main steps. First, we expand in powers of \( T \) by inserting (6) into (7b):

\[ u_n = \sum_{\{p_j\}} T^{n+P_n} A_{p_n} \cdots A_{p_2} A_{p_1} F_{p_1,p_2,\ldots,p_n}, \]  
(8)

where \( p_j \in \mathbb{N} \) and \( P_n := \sum_{j=1}^n p_j \) and

\[ F_{p_1\ldots p_n} := \int_0^1 d\tilde{r}_n \cdots \int_0^{t_1} d\tilde{r}_2 \int_0^{t_2} d\tilde{r}_1 \prod_{j=1}^n F(T\tilde{t})^p_j. \]  
(9)

\[ ^2 \text{We assume that all operators appearing in the derivation are bounded. Alternatively, we require at least that all products of the operators of the system have finite matrix elements. This implies that no divergences at low or high energies are present [9, 21, 22].} \]
We used the dimensionless relative times $\tilde{t} := t/T$. Since the $N$ switching instants are given by $T \delta_j$, the function $F(T \tilde{t})$ does not depend on $T$ for given $\{\delta_j\}$. Hence, the coefficients $F_{p_1 ... p_n}$ do not depend on $T$.

Our goal is to show that $F_{p_1 ... p_n}$ vanishes for $n$ odd and $N \geq n + P_n$. Based on the UDD choice for the $\{\delta_j\}$ in (1), the substitution $\tilde{t} = \sin^2(\theta/2)$ suggests itself because it renders $f(\theta) := F(T \sin^2(\theta/2))$ particularly simple if the $\{\delta_j\}$ are chosen according to (1). Then $f(\theta) = (-1)^j$ holds for $\theta \in (j \pi/(N + 1), (j + 1)\pi/(N + 1)$ with $j \in \{0, \ldots, N\}$. If we release this constraint on $j$ allowing $j \in \mathbb{Z}$, the function $f(\theta)$ becomes an odd function with antiperiod $\pi/(N + 1)$. Thus, its Fourier series

$$f(\theta) = \sum_{k=0}^{\infty} c_{2k+1} \sin((2k + 1)(N+1)\theta) \quad (10)$$

contains only harmonics $\sin(r \theta)$ with $r$ an odd multiple of $N + 1$. The precise coefficients $c_{2k+1}$ do not matter which can be exploited for other purposes, e.g. to deal with pulses of finite duration [19].

Under the substitution $\tilde{t} = \sin^2(\theta/2)$, the terms $\tilde{t}^p \, dt$ in (9) become $\sin^{2p}(\theta/2) \sin(\theta) \, d\theta$ which can be reexpressed as suitably weighted sum over terms $\sin(\theta q) \, d\theta$ with $q \in \mathbb{Z}$, $|q| \leq p + 1$. Thus, we can achieve our goal if we show that the coefficients

$$f_{q_1 ... q_n} := \int_0^\pi d\theta_n \cdots \int_0^\theta_3 \int_0^\theta_2 \int_0^\theta_1 \prod_{j=1}^n f(\theta_j) \sin(q_j \theta_j) \quad (11)$$

vanish for $n$ odd and $|q_j| \leq p_j + 1$. These coefficients are split up further by inserting the Fourier series (10) for $f(\theta)$ consisting of terms $\sin(r \theta)$ ($r$ odd multiple of $N + 1$). Twice the product of two sine functions is the difference of two cosines whose arguments are the sum and differences of the sine arguments. Thus, we want to show

$$0 = \int_0^\pi d\theta_n \cdots \int_0^\theta_3 \int_0^\theta_2 \int_0^\theta_1 \prod_{j=1}^n \cos((r_j + q_j) \theta_j) \quad (12)$$

where $r_j$ is an odd multiple of $N + 1$ and

$$\sum_{j=0}^n |q_j| \leq \sum_{j=0}^n (p_j + 1) = n + P_n \leq N. \quad (13)$$

It is easy to perform the first two integrations in (12),

$$\cos((r_3 + q_3) \theta_j) \int_0^{\theta_3} d\theta_2 \int_0^{\theta_2} d\theta_1 \prod_{j=1}^2 \cos((r_j + q_j) \theta_j), \quad (14)$$

analytically yielding a lengthy sum over terms of the form $\cos((r_3^j + q_3^j) \theta_3)$ where $r_3^j$ is still an odd multiple of $N + 1$ and $|q_3^j| \leq |q_1^j| + |q_2^j| + |q_3^j|$. Hence, the structure of the expression on the rhs of (12) is preserved, but $n$ is lowered by two. This procedure is iterated till $n = 1$, and we arrive at

$$0 = \int_0^\pi d\theta \cos((R + Q) \theta) \quad (15)$$

because $R$ is an odd multiple of $N + 1$ and $|Q| \leq N$; thus, $|R + Q| \in \mathbb{N}$. This concludes the derivation.
3. Longitudinal relaxation

The above derivation holds also for the odd powers of longitudinal relaxation as observed for constant Hamiltonians before [10]. The Hamiltonian studied is \( H(t) = D_0(t) + D_1(t) \) where

\[
D_0(t) := H_b(t) + \sigma_z A_z(t) \tag{16a}
\]

\[
D_1(t) = \vec{\sigma}_\perp \cdot \vec{A}_\perp(t) = \sigma_x A_x(t) + \sigma_y A_y(t). \tag{16b}
\]

The \( \pi \) pulses are applied around the spin \( z \) axis so that the switching function appears for \( D_1 \), i.e. \( H(t) = D_0(t) + D_1(t) F(t) \). Then all the above steps for dephasing can be repeated identically on substituting \( H_b \to D_0 \) and \( \sigma_z A_z \to D_1 \). Thus, we know that the UDD sequence of \( N \) pulses makes all odd powers up to \( N \) in \( D_1 \) vanish. Thus, it efficiently suppresses longitudinal relaxation also for time-dependent Hamiltonians.

4. Applications

The first application, of course, is the use of the UDD for Hamiltonians in certain reference frames which imply that the Hamiltonians are effective ones with some time dependence. Examples are a rotating frame, in which a magnetic field is not fully compensated, and an effective Hamiltonian in which fast modes have been averaged by the help of Magnus expansions or they are treated in an interaction picture. In the cases where the resulting time dependence can be considered to be sufficiently smooth (which need not be always true), the previous results establish the applicability of the optimized sequence UDD, in spite of the time dependence of the Hamiltonian.

The second application concerns dynamic decoupling for general decoherence. The nesting of pulse sequences about perpendicular spin axes makes it possible to eliminate all possible couplings between a qubit and its environment provided the expansion in time is possible, see figure 1. A first proposal used iterative concatenation (CDD) without optimization leading to a fast growing number of pulses proportional to \( 4^\ell \) if terms up to \( T^\ell \) were eliminated [6]. If one uses concatenation on the secondary level, but optimized UDD on the primary level (i.e. CUDD), the number of pulses grows only like \( 2^\ell \) improving by a square root [11]. On the primary level, CUDD suppresses longitudinal relaxation by \( N \pi \) pulses about the \( z \) axis such that the time evolution due to a Hamiltonian \( \tilde{H} = D_0 + D_1 \) (for \( D_i \) see (3)) without explicit time dependence is reduced to the time evolution due to an effective Hamiltonian

\[
\tilde{H}_\text{eff}^\ell(t) = D_{0\text{eff}}^\ell(t) \tag{17}
\]
up to correction of the order $O(T_p^{N-1})$. For a discussion of the smoothness of $\dot{\overline{H}}(t)$, we refer the reader to the appendix. The time dependence of $\dot{\overline{H}}(t)$ was seen previously as the decisive obstacle to apply an optimized UDD sequence again on the secondary level [11]. Below we show explicitly that $H^{\text{eff}}(t)$ is indeed time dependent.

Very recent numerical data [18], however, indicate that the use of a UDD sequence also on the secondary level with pulses about $z_\perp$ is in fact a very efficient way to suppress general decoherence. This nesting of two perpendicular UDD sequences of $N_\perp$ pulses about $z$ for each of the $N_\perp + 1$ intervals of a UDD sequence of $N_\perp$ pulses about a perpendicular axis is called quadratic dynamic decoupling (QDD) [18] highlighting the case $N_\perp = N_\perp$. This choice is advantageous if longitudinal relaxation and dephasing are of similar magnitude.

The above derivation of the UDD as optimized sequence for dephasing and longitudinal relaxation for time-dependent Hamiltonians provides the analytic foundation of the QDD proposed by West et al [18]. In spite of the time dependence that the effective Hamiltonian $\dot{\overline{H}}^{\text{eff}}(t)$ acquires under the primary UDD (suppressing longitudinal relaxation up to $T^{N_\perp + 1}$), the secondary UDD (suppressing dephasing up to $T^{N_\perp + 1}$) will still work to the desired order given by the number of pulses$^3$. The reason is that an analytic time dependence, quite surprisingly, does not spoil the analytic properties of the optimized UDD sequences.

5. Time dependence after the primary DD

Applying $\pi$ pulses about the spin axis $z$ to $\tilde{H} = D_0 + D_1$ without explicit time dependence converts $\tilde{H}$ to $H(t) = D_0 + D_1F(t)$, where $F(t) = \pm 1$ is a switching sign at the instants of the pulses (see footnote 1), see figure 1. To find the time dependence of the time evolution $U(T_p)$ due to $H(t)$, the Magnus expansion $U(T_p) = \exp\left\{-i\int_0^{T_p}(H^{(1)} + H^{(2)} + H^{(3)}) + O(T_p^4)\right\}$ is used [1, 20]. The terms are powers in $T_p$; they read $T_p H^{(1)} = \int_0^{T_p} H(t) \, dt$, $T_p H^{(2)} = i/2 \int_0^{T_p} \int_0^{T_p} [H(t_1), H(t_2)] \, dt_1 \, dt_2$ and

$$T_p H^{(3)} = -\frac{1}{6} \int_0^{T_p} \int_0^{T_p} \int_0^{T_p} \left[[H(t_1), [H(t_2), H(t_3)]\right]$$

$$+[[H(t_2), [H(t_1), H(t_3)]]] \, dt_1 \, dt_2 \, dt_3. \quad (18)$$

The first-order term $H^{(1)}$ contains the integral $I_1 := \int_0^{T_p} F(t) \, dt$ which vanishes for any reasonable DD sequence with at least one pulse; thus, one has $H^{(1)} = D_0$ without time dependence.

The second-order term $H^{(2)}$ involves the commutator $[H(t_1), H(t_2)]$. We find

$$T_p H^{(2)} = \frac{1}{2} \left\langle \tilde{\eta}^{(2)} \right\rangle \int_0^{T_p} \int_0^{T_p} (F(t_2) - F(t_1)) \, dt_1 \, dt_2, \quad (19)$$

where the operator $\tilde{\eta}^{(2)}$ induces dephasing,

$$\tilde{\eta}^{(2)} := \sum_{i,j=x,y} \sigma_i ([H_0, A_j] - ie^{ij/2} [A_x, A_j]), \quad (20)$$

with $e^{ij/2}$ being the Levi-Civita operator and $[,]$ the anti-commutator. Since the rhs of (19) is linear in $F(t)$, we know from the general derivations given above or in [10] that the double integral vanishes if a UDD sequence with two or more pulses is applied since the total order of the term is $T_p^4$.

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3 One can equally suppress dephasing on the primary level and relaxation on the secondary level.

4 For symmetric pulse sequences, e.g. UDD sequences with an even number of pulses, a general theorem on the Magnus expansion precludes a finite second order term anyway [1]; note our non-standard counting of the orders.
The third order finally yields a non-vanishing time dependence. There is a linear and a quadratic term in $F(t)$:

$$T_p H^{(3)} = -\frac{1}{6} \{ I_{3,1} [D_0, \eta^{(2)}] + I_{3,2} [D_1, \eta^{(2)}] \}$$  \hspace{1cm} (21a)

$$I_{3,1} := \int_0^{T_p} \int_0^{t_1} \int_0^{t_2} \left( F(t_3) + F(t_1) - 2F(t_2) \right) dt_1 dt_2 dt_3$$ \hspace{1cm} (21b)

$$I_{3,2} := \int_0^{T_p} \int_0^{t_1} \int_0^{t_2} \left( 2F(t_1)F(t_3) - F(t_2)F(t_1) + F(t_2)F(t_3) \right) dt_1 dt_2 dt_3.$$ \hspace{1cm} (21c)

We do not give the first commutator in (21a) explicitly because $I_{3,1}$ is linear in $F(t)$. Hence, it is zero for any UDD with three or more pulses. But $I_{3,2}$ is quadratic in $F(t)$ so that the UDD sequence does not make any statement on its value. Hence, it will generally be finite. Indeed, we verify numerically for $N_z$ pulses the examples $I_{3,2}^{N_z=3} = -0.0303 T_p^3$ and $I_{3,2}^{N_z=5} = -0.0068 T_p^3$ for $N_z$ odd, and $I_{3,2}^{N_z=6} = -0.0084 T_p^3$ and $I_{3,2}^{N_z=8} = -0.0052 T_p^3$ for $N_z$ even. This implies a finite quadratic dependence of the effective Hamiltonian $H_{eff}$ which we aimed to establish.

For completeness, we compute the corresponding operator $[D_1, \eta^{(2)}]$ which introduces corrections to dephasing and to the bath dynamics as expected:

$$[D_1, \eta^{(2)}] = \sum_{i,j=x,y} \left( [A_i, [H_b, A_j]] - i \epsilon_{ijz} [A_i, A_j] \right) + i \sigma_z [A_i, \epsilon_{ijz} [H_b, A_j]] + i[A_z, A_i]).$$ \hspace{1cm} (22)

Obviously, these terms do not vanish except for very special choices of bath $H_b$ and the coupling operator $A$. This completes the derivation that the effective Hamiltonians are indeed time dependent. Thus, the analytic argument in [18] for the validity of the QDD does not hold.

6. Summary

We extended the derivation of the optimized properties of Uhrig dynamic decoupling to initial Hamiltonians with time dependence. First, this establishes the applicability of optimized dynamic decoupling also for the large class of effective Hamiltonians which inherit an explicit time dependence from special reference frames or from the treatment of fast modes in the interaction picture, by average Hamiltonian theory, or by integrating them out. Second, our finding provides the analytic reason for the advantageous properties of quadratic dynamic decoupling for the suppression of general decoherence including both dephasing and longitudinal relaxation. This scheme was recently proposed by West et al [18]. Thus, the road is paved for a much broader applicability of optimized dynamic decoupling.

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Appendix. Effective Hamiltonian from the primary level of QDD

Here we discuss in more detail how $\tilde{H}_{eff}(t)$ arises from the time evolution on the primary level in QDD. In particular, we discuss why this operator is smooth or even analytic in $t$ although it arises from the integration of $H(t) = D_0 + D_1 F(t)$ where $F(t)$ is a switching function which changes sign at the pulses of the primary level.
Let us denote by $U(t)$ the time evolution operator on the primary level, i.e. within one of the intervals of the secondary level, see figure 1. It reads

$$U(t) = T \exp \left( -i \int_0^t H(t') \, dt' \right)$$

(A.1)

and the domain of integration is illustrated in the upper panel of figure A1 by the range of the switching function $F(t)$ encountered. If we define the dimensionless relative time $\tilde{t} := t/T_p$ and the corresponding Hamiltonian $H^{\text{rel}}(\tilde{t}) := H(T_p \tilde{t})$, the previous equation becomes

$$U(t) = \tilde{T} \exp \left( -i T_p \int_0^{t/T_p} H^{\text{rel}}(\tilde{t}) \, d\tilde{t} \right)$$

(A.2)

where $\tilde{T}$ stands for the time ordering according to the relative time $\tilde{t}$. Equation (A.2) is given here for comparison with the subsequent effective time evolution operator.

To consider what happens on the secondary level, we need $U^{\text{eff}}(t)$. Its defining property is $U^{\text{eff}}(T_p) = U(T_p)$. But if its argument is varied $T_p \to t$, it is implied that the primary sequence is scaled accordingly. That is its decisive difference to $U(t)$, which is illustrated in the lower panel of figure A1. Note that this scaling is exactly what is done when the primary sequences are applied in each of the time intervals of varying duration of the secondary level, see figure 1.

$U^{\text{eff}}(t)$ is given by

$$U^{\text{eff}}(t) = \tilde{T} \exp \left( -it \int_0^1 H^{\text{rel}}(\tilde{t}) \, d\tilde{t} \right).$$

(A.3)

From this equation it is obvious that $U^{\text{eff}}(t)$ is generically smooth in the variable $t$. If the parts of the Hamiltonian are bounded, $U^{\text{eff}}(t)$ is analytic because the exponential is analytic.

The final step is to define the corresponding effective Hamiltonian $\tilde{H}^{\text{eff}}(t)$. As usual, the Hamiltonian is retrieved from the time evolution as its infinitesimal generator

$$\tilde{H}^{\text{eff}}(t) := i[\partial_t U^{\text{eff}}(t)][U^{\text{eff}}(t)]^{-1}.$$  

(A.4)

If $U^{\text{eff}}(t)$ is analytic, then $\tilde{H}^{\text{eff}}(t)$ is analytic as well. If $U^{\text{eff}}(t)$ can be expanded up to and including the power $t^{N+1}$, then $\tilde{H}^{\text{eff}}(t)$ can be expanded up to and including the power $t^N$. 

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Figure A1. Ranges of integration (range of solid curve) and behavior of the switching function $F(t)$ for the calculation of $U(t)$ (upper panel) and of the effective $U^{\text{eff}}(t)$ (lower panel).
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