Corrigendum

Exact results on dynamical decoupling by \( \pi \) pulses in quantum information processes

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An error in the calculation was found that now changes some equations given in the original article to some extent. The phase factors do not occur so that the equations turn out to be even simpler than before.

The statement after equation (13) that the state \(|\uparrow\rangle\) does not change upon the application of the diagonalizing unitary \(U\) does not hold. Instead

\[
U|\uparrow\rangle = \exp(K)|\uparrow\rangle
\]

is valid. Thus, equation (13) becomes

\[
s(t) = \text{Im}\langle\uparrow|U^\dagger \sigma_x^{\text{eff}}(t)\sigma_y^{\text{eff}} \exp(-iH^{\text{eff}} t)U|\uparrow\rangle,
\]

which leads to the altered equations (21)

\[
(21a) \quad s(t) = \text{Im}\langle\uparrow|e^{-K(0)}\sigma_x^{\text{eff}}(t)\sigma_y^{\text{eff}}(0)e^{K(0)}|\uparrow\rangle
\]

\[
(21b) \quad = \text{Im}\langle\downarrow|e^{K(0)}e^{-2K(t)}e^{K(0)}|\downarrow\rangle
\]

\[
(21c) \quad = \text{Re}\langle e^{K(t)}e^{-2K(t)}e^{K(0)}\rangle.
\]

Then equations (23), (25) and (26) become

\[
(23) \quad s(t) = \text{Re}\langle \exp(-2\Delta K) \rangle,
\]

\[
(25) \quad s(t) = \text{Re}\exp(2(\Delta K^2)),
\]

\[
(26) \quad s(t) = \exp(-2\chi(t)).
\]

Note that equation (27) of the original paper is correct but is no longer needed.

Consequently, equations (37)–(40) become

\[
(37) \quad s(t) = \text{Im}\langle\uparrow|e^{-K(0)}\sigma_x^{\text{eff}}(0)\sigma_y^{\text{eff}}(t)e^{K(0)}|\uparrow\rangle.
\]
Figure 1. Various pulse sequences (see the main text) are compared for various values of the cutoff parameter $\gamma$ in $J_\gamma(\omega)$, see (86). All sequences comprise $n = 10$ pulses; this value is chosen for better comparison because level $l = 4$ of the CDD sequence has 10 pulses. The coupling value $\alpha$ in the spectral densities $J_\gamma(\omega)$ is fixed at $1/4$ and the temperature is zero.

Figure 2. Comparison of the performance of the CPMG (dashed lines) and the UDD sequence (solid lines) for various numbers of pulses $n$ (the legend holds for dashed and solid lines) and a spectral density with $\gamma = 8$ corresponding to a cutoff of intermediate hardness. Other values are fixed: $\alpha = 1/4$, $T = 0$. 

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Figure 3. Comparison of the performance of various iterated iUDD\(_{m,c}(t)\) sequences for a total number of \(n = 12\) pulses and various cutoff exponents \(\gamma\). Other values are \(\alpha = 1/4\), \(T = 0\).

\[
\begin{align*}
    s(t) &= \Im \langle e^{K(0)} \ e^{-2K(\delta_1 t)} \ (-i) e^{2K(\delta_2 t)} \ \cdots \ 
            \ (-i) (-1)^n e^{(-1)^n 2K(\delta_1 t)} \\
            &\quad \cdots \ (-i) (-1)^{n+1} e^{(-1)^{n+1} 2K(t)} \\
            &\quad (-i) (-1)^n e^{(-1)^n 2K(\delta_n t)} \\
            &\quad \cdots \ (-i) e^{2K(\delta_2 t)} \ e^{-2K(\delta_1 t) e^{K(0)}}. \\
\end{align*}
\]

(38)

\[
\begin{align*}
    s(t) &= \Re \langle e^{K(0)} \ e^{-2K(\delta_1 t)} \ e^{2K(\delta_2 t)} \ \cdots \\
            &\quad \cdots \ e^{(-1)^n 2K(\delta_n t)} \ e^{(-1)^n 2K(\delta_1 t)} \\
            &\quad \cdots \ e^{2K(\delta_2 t)} \ e^{-2K(\delta_1 t) e^{K(0)}}. \\
\end{align*}
\]

(39)

\[
\begin{align*}
    s(t) &= \Re \langle \exp(2\Delta_n K) \rangle \quad (40a) \\
         &= \exp (-2\chi_n(t)). \quad (40b)
\end{align*}
\]
The sentence before equation (44) should read: Furthermore, the two respective arguments are equal

\[ s(t) = \Re \langle e^{K(0)} e^{\Delta b K - K(0)} e^{\Delta b K - K(0)} e^{K(0)} \rangle \]  

(44)

so that we directly obtain (40) by the BCH formula. The former equations (45) and (46) are correct but are no longer needed. This concludes the changes to the equations. Note that the corrected equations are even simpler than the original ones. No phases are needed. The figures change slightly; the corrected ones are depicted above.

We highlight that the changes relative to the original figures are only minor. No qualitative conclusion of the article is affected.

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Exact results on dynamical decoupling by $\pi$ pulses in quantum information processes

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Abstract. The aim of dynamical decoupling consists in the suppression of decoherence by appropriate coherent control of a quantum register. Effectively, the interaction with the environment is reduced. In particular, a sequence of $\pi$ pulses is considered. Here we present exact results on the suppression of the coupling of a quantum bit to its environment by optimized sequences of $\pi$ pulses. The effect of various cut-offs of the spectral density of the environment is investigated. As a result we show that the harder the cut-off is, the better an optimized pulse sequence can deal with it. For cut-offs which are neither completely hard nor very soft we advocate iterated optimized sequences.

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1. Introduction

Almost six decades ago in 1950, Hahn demonstrated that spin echoes in liquid nuclear magnetic resonance (NMR) can be obtained by applying a $\pi$ pulse in the middle of a time interval [1]. This idea was developed further by Carr and Purcell who proposed iterated cycles of two $\pi$ pulses to reduce the effect of unwanted interactions [2]. Further refinements were introduced by Meiboom and Gill [3]. Since then this technique of coherent control has been established in NMR (see e.g. [4]).

The fascinating possibilities of quantum information have stimulated a great interest in the coherent control of small quantum systems (see e.g. [5]). The idea to preserve coherence by iterated $\pi$ pulses periodic in time was rediscovered in the context of quantum information by Viola and Lloyd [6] and by Ban [7] in 1998 for a spin-boson model and subsequently generalized to open systems [8]; a short review is found in [9]. For symmetry groups with inefficient representations randomized protocols are advocated, see [10] and references therein.

Recently, periodically iterated Carr–Purcell cycles have been advocated for the preservation of the coherence of the electronic spin in quantum dots [11, 12]. Besides periodic iteration of pulse cycles, concatenations of cycles were also proposed and it was shown that they suppress decoherence in higher orders $t^l$ in the length of the time interval $t$ [11], [13]–[15]. But the achieved exponent $l$ grows only logarithmically in the number of pulses $n$.

In parallel, the author showed that neither the iteration nor the concatenation of the Carr–Purcell two-pulse cycle is the optimum strategy for a single-axis bosonic bath [16]. Cycles with $n$ pulses at the instants $\delta_j t$

$$\delta_j = \sin^2[\pi j / (2n + 2)]$$

achieve the optimum suppression of decoherence in the sense that any deviation of the signal occurs with a high power in $t$, namely $t^{2n+2}$ where $n$ is the number of pulses, i.e. only a linear effort is required. The Carr–Purcell cycle is retrieved for $n = 2$. Up to $n \leq 5$ the result (1) was previously shown for general models [17].

Then, Lee et al [18] observed in numerical simulations of spin baths that the pulse sequences obeying equation (1) also suppress the decoherence for spin baths. They could also show analytically that the sequence defined by (1) works for the most general phase decoherence model up to $n = 9$. We have been able to extend this analytical proof up to $n \leq 14$. An unrestricted derivation, however, is still lacking. Lee et al [18] also argued that the optimized sequence (1) works well only when the expansion in time is applicable.

There is a multitude of experimental results in NMR on coherent control and the suppression of decoherence (see e.g. [4]). We highlight results in the context of quantum information related to pulse sequences [19]; for a overview see [20]. But also in semi-conductor physics there are many encouraging results in prolonging the coherence time of a qubit by $\pi$ pulses [21]–[25]. In an experiment, one must trade off between the advantages of the suppression of decoherence by multiply applied pulses with the detrimental effects of imperfect realizations of pulses, for instance the finite duration of a pulse so that it cannot be regarded as instantaneous [26].

The aim of the present paper is threefold. Firstly, we provide the explicit calculations leading to the important relation (1). Secondly, we generalize the previous result [16] on a particular signal to a statement on the unitary time evolution. Thereby, we provide the general proof for the applicability of (1) for an arbitrary initial quantum state. Thirdly, we use various
spectral densities $J(\omega)$ in the spin-boson model to discuss under which conditions the optimized sequence works well, namely when the high-energy cut-off of the decohering environment is hard enough. To cope with medium hard cutoffs we propose iterated sequences of short optimized cycles of pulses.

The paper is set up as follows: in the following section 2, the explicit calculation for the spin-boson model is presented, both for the signal in a generic decoherence experiment and for the general time evolution. The results are also given for classical noise. The subsequent section 3 treats the general phase decoherence model. Section 4 presents a discussion of the applicability of the optimized sequences and establishes a link to the nature of the high-energy cutoff. The conclusions in section 5 summarize the results and discuss their implications for further developments.

2. Spin-boson model

We consider the model given by the Hamilton operator

$$H = \sum_i \omega_i b_i^\dagger b_i + \frac{1}{2} \sigma_z \sum_i \lambda_i (b_i^\dagger + b_i) + E \quad (2)$$

consisting of a single qubit interpreted as spin $S = 1/2$, whose operators are the Pauli matrices $\sigma_x$, $\sigma_y$ and $\sigma_z$. The environment is given by the bosonic bath with annihilation (creation) operators $b_i^\dagger (b_i)$. The constant $E$ sets the energy offset. The properties of the bath are defined by the set of real parameters $\{\lambda_i, \omega_i\}$. This information is conveniently encoded in the spectral density \[27, 28\]

$$J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i). \quad (3)$$

Obviously, $H$ in (2) does not allow for spin flips since it commutes with $\sigma_z$. Physically this means that the decay time $T_1$ of a magnetization along $z$ is infinite. But the decoherence of a magnetization in the $\sigma_x \sigma_y$-plane is captured by $H$ so that the decay time $T_2$ can be investigated in the framework of this model.

The Hamiltonian $H$ in (2) is analytically diagonalizable. For any operator $A$, we will use the notation

$$A_{\text{eff}} := U A U^\dagger. \quad (4)$$

The unitary transformation $U$ is chosen so that it diagonalizes $H$

$$H_{\text{eff}} = \sum_i \omega_i b_i^\dagger b_i + \Delta E. \quad (5)$$

The appropriate unitary transformation is

$$U = \exp(\sigma_z K). \quad (6)$$

The operator $K$ is anti-Hermitean

$$K = \sum_i \frac{\lambda_i}{2\omega_i} (b_i^\dagger - b_i) \quad (7)$$

so that $U$ is indeed unitary. The energy offset after the transformation reads

$$\Delta E = E - \int_0^\infty \frac{J(\omega)}{\omega} d\omega. \quad (8)$$

But the global energy offset is not measurable, so that its quantitative form does not matter.
2.1. Signal without $\pi$ pulses

Here we discuss the simple experimental setup without any $\pi$ pulses. We start from the state $|\uparrow\rangle$. Then a $\pi/2$ pulse is applied to rotate the spin from the $z$-direction to the $xy$-plane. To be specific, we rotate the spin about $x$ by the angle $\gamma$ with the help of the unitary transformation

$$D_x(\gamma) := \exp(-i\gamma \sigma_x/2),$$

$$= \cos(\gamma/2) + i\sigma_x \sin(\gamma/2).$$

The rotation is best seen by stating that

$$D_x(\gamma)\sigma_z D_x(\gamma)^\dagger = \sigma_z \cos\gamma + \sigma_y \sin\gamma.$$  

For $\gamma = \pi/2$ a spin along $z$ is turned into a spin along $y$. We will use $D_x(\pi/2) = (1 + i\sigma_x)/\sqrt{2}$.

In the $xy$-plane the spin will evolve. After the time $t$ a measurement of $\sigma_y$ yields the signal

$$s(t) = \langle \uparrow| D_x(\pi/2)^\dagger \exp(iHt)\sigma_y \exp(-iHt) D_x(\pi/2)|\uparrow\rangle.$$  

Since $H$ does not induce spin flips and

$$\langle \uparrow|\sigma_y|\uparrow\rangle = \langle \downarrow|\sigma_y|\downarrow\rangle = 0,$$

we know that

$$\langle \uparrow|\sigma_x \exp(iHt)\sigma_y \exp(-iHt)|\uparrow\rangle = 0$$

and

$$\langle \uparrow|\sigma_y \exp(iHt)\sigma_x \exp(-iHt)|\uparrow\rangle = 0.$$  

Hence the signal is given by

$$s(t) = \text{Im}\langle \uparrow| \sigma_x \exp(iHt)\sigma_y \exp(-iHt)|\uparrow\rangle.$$  

To evaluate this expression explicitly we change to the basis in which $H$ is diagonal

$$s(t) = \text{Im}\langle \uparrow| \sigma_x^{\text{eff}} \exp(iH^{\text{eff}}t)\sigma_y^{\text{eff}} \exp(-iH^{\text{eff}}t)|\uparrow\rangle.$$  

Note that the state $|\uparrow\rangle$ is not altered by $U$. For the explicit calculation of the effective operators we use

$$\sigma_{x/y} \sigma_z = -\sigma_z \sigma_{x/y}$$

and obtain

$$\sigma_x^{\text{eff}} = \exp(\sigma_z K)\sigma_x\exp(-\sigma_z K),$$

$$\sigma_y^{\text{eff}} = \exp(2\sigma_z K)\sigma_y.$$  

Hence the action on particular spin states is

$$\sigma_x^{\text{eff}}|\uparrow/\downarrow\rangle = \exp(\mp 2K)|\downarrow/\uparrow\rangle,$$

$$\sigma_y^{\text{eff}}|\uparrow/\downarrow\rangle = \pm i \exp(\mp 2K)|\downarrow/\uparrow\rangle,$$

where either the first spin orientation and the upper sign holds or the second spin orientation and the lower sign holds.

Turning to the time dependence we define generally the time-dependent operators

$$A(t) := \exp(iH^{\text{eff}}t)A \exp(-iH^{\text{eff}}t).$$

Note that $H^{\text{eff}}$ contains only the bosonic degrees of freedom and it is diagonal. Hence it is easy to see that

$$b_i^{\dagger}(t) = b_i^{\dagger} \exp(i\omega_i t),$$

$$b_i(t) = b_i \exp(-i\omega_i t).$$  

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whence
\[ K(t) = \sum_i \frac{\lambda_i}{2\omega_i} (b_i^\dagger \exp(i\omega_i t) - b_i \exp(-i\omega_i t)). \] (19)

With these definitions the identities (16) apply also to the time-dependent operators \( \sigma^{\text{eff}}(t) \) and \( K(t) \)
\[ \sigma^{\text{eff}}(t)|\uparrow/\downarrow\rangle = \exp(\mp 2K(t))|\downarrow/\uparrow\rangle, \] (20a)
\[ \sigma^{\text{eff}}(t)|\uparrow/\downarrow\rangle = \pm i \exp(\mp 2K(t))|\downarrow/\uparrow\rangle. \] (20b)

With these identities we can write for the signal
\[ s(t) = \mathfrak{Im} \langle \uparrow|\sigma^{\text{eff}}(0)\sigma^{\text{eff}}(t)|\uparrow\rangle, \] (21a)
\[ = \mathfrak{Im} i \langle \downarrow|\exp(2K(0)) \exp(-2K(t))|\downarrow\rangle, \] (21b)
\[ = \Re \langle \exp(2K(0)) \exp(-2K(t)) \rangle, \] (21c)
where we took the expectation value in the spin sector in (21c) so that only a bosonic expectation value with respect to the bilinear \( H^{\text{eff}} \) must be computed. This is eased by the Baker–Campbell–Hausdorff (BCH) formula
\[ \exp(A) \exp(B) = \exp(A + B + [A, B]/2), \] (22)
which is valid if \([A, B]\) commutes with \(A\) and \(B\). This yields
\[ s(t) = \Re \exp(-2[K(0), K(t)]) \langle \exp(-2\Delta K) \rangle, \] (23)
with \(\Delta K := K(t) - K(0)\). Any expectation value of an exponential of a linear bosonic operator \(A\) with respect to a bilinear \(H^{\text{eff}}\) can be reduced to the exponential of an expectation value by
\[ \langle \exp(A) \rangle = \exp(\langle A^2 \rangle/2). \] (24)
Hence we have
\[ s(t) = \Re \exp(-2[K(0), K(t)]) \exp(2\langle \Delta K^2 \rangle), \] (25)
which simplifies due to the Hermiticity of \(\Delta K^2\) to
\[ s(t) = \cos(2\varphi(t)) \exp(-2\chi(t)), \] (26)
where the phase is given by
\[ \varphi(t) := i[K(0), K(t)], \] (27a)
\[ = -i \sum_i \frac{\lambda_i^2}{4\omega_i} (\exp(i\omega_i t) - \exp(-i\omega_i t)), \] (27b)
\[ = \sum_i \frac{\lambda_i^2}{2\omega_i^2} \sin(\omega_i t), \] (27c)
\[ = \frac{1}{2} \int_0^\infty J(\omega) \frac{\omega}{\omega^2} \sin(\omega t) \, d\omega. \] (27d)
The exponential suppression is given by
\[ \chi(t) := -\langle \Delta K^2 \rangle, \] (28)
where
\[ \Delta K = \sum_i \lambda_i^2 \left[ b_i^\dagger (\text{e}^{i\omega_i t} - 1) - b_i (\text{e}^{-i\omega_i t} - 1) \right], \] (29)
whence we obtain
\[ \chi(t) = \sum_i \frac{\lambda_i^2}{4\omega_i^2} 4 \sin^2(\omega_i t/2) \langle b_i^\dagger b_i + b_i b_i^\dagger \rangle. \] (30)
The bosonic occupation is such that the last expectation value equals \( \text{coth}(\beta \omega_i / 2) \) so that we finally have
\[ \chi(t) = \int_0^\infty J(\omega) \frac{\sin^2(\omega t/2)}{\omega^2} \text{coth}(\beta \omega / 2) \, d\omega. \] (31)
This concludes the derivation of the signal without any dynamical decoupling. The formulae (6) in [16] are rederived in all detail. The above derivation sets the stage for the derivation in the case of dynamical decoupling by sequences of \( \pi \) pulses.

2.2. Signal with \( \pi \) pulses

Here we consider a sequence of \( \pi \) pulses which are applied at the instants of time \( \delta_i t \) with \( i \in \{1, 2, \ldots, n\} \) so that \( n \) pulses are applied and the total time interval \( t \) is divided into \( n+1 \) subintervals. For notational convenience we set \( \delta_0 = 0 \) and \( \delta_{n+1} = 1 \). It is understood that \( \delta_{i+1} > \delta_i \) for all \( i \in \{0, 1, 2, \ldots, n\} \).

The \( \pi \) pulses are taken to be ideal, that means they are instantaneous so that during their application no coupling to the bath needs to be considered. The possible workarounds if this is not justified in the experiment are discussed elsewhere [26]. For simplicity, we take the \( \pi \) pulses to be realized as rotations about \( \sigma_y \):
\[ D_y(\gamma) := \exp(-i\gamma \sigma_y/2), \] (32a)
\[ = \cos(\gamma/2) + i\sigma_y \sin(\gamma/2), \] (32b)
which implies for \( \gamma = \pi \) simply \( D_y(\pi) = i\sigma_y \). Below we will use \( \sigma_y \) only because the factor \( i \) corresponds to an irrelevant global phase shift.

The signal is given in general as before by
\[ s(t) = \Re \langle \uparrow | \sigma_y \tilde{R}^\dagger \sigma_y \tilde{R} | \uparrow \rangle, \] (33)
where the time evolution has changed its form of \( \exp(-iHt) \) in (12) to
\[ \tilde{R} := e^{-iH(\delta_{n+1} - \delta_0)t} \sigma_y e^{-iH(\delta_n - \delta_{n-1})t} \sigma_y \cdots e^{-iH(\delta_2 - \delta_1)t} \sigma_y e^{-iH(\delta_1 - \delta_0)t}. \] (34)
The expression (34) becomes much more compact if written after the diagonalization by \( U \) as given in (6)
\[ \tilde{R}^\text{eff} = e^{-iH^\text{eff}t} R^\text{eff}, \] (35)
where we express \( R^\text{eff} \) based on (17) in the form
\[ R^\text{eff} = \sigma_y^\text{eff}(\delta_n t) \sigma_y^\text{eff}(\delta_{n-1} t) \cdots \sigma_y^\text{eff}(\delta_2 t) \sigma_y^\text{eff}(\delta_1 t). \] (36)

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Then we arrive easily at
\[ s(t) = \Im \langle \uparrow | \sigma_x^{\text{eff}}(0) R^{\text{eff}} \sigma_y^{\text{eff}}(t) R^{\text{eff}} | \uparrow \rangle. \] (37)

Equation (37) can be converted by means of (20) into the following purely bosonic expression
\[ s(t) = \Im \left\{ e^{2K(0)} i e^{-2K(\delta_1 t)} (-i) e^{2K(\delta_2 t)} \ldots (-i)^n e^{(-1)^n 2K(\delta_n t)} \right. \\
\left. \times (-i)(-1)^{n+1} e^{(-1)^{n+1} 2K(t)} (-i)(-1)^n e^{(-1)^n 2K(\delta_n t)} \ldots (-i) e^{2K(\delta_2 t)} i e^{-2K(\delta_1 t)} \right\}. \] (38)

Counting the factors \((-1)\) and \(i\) one finds that they all combine to a single factor \(i\). This is most easily seen by combining the prefactors in front of each of the terms \((-i)(-1)^n e^{(-1)^n 2K(\delta_n t)}\) which all occur twice so that each kind of these terms provides a factor \((-i)^2 = -1\) yielding a total factor \((-1)^n\). This is multiplied with \((-i)(-1)^{n+1}\) from the prefactor of \(e^{(-1)^n 2K(\delta_n t)}\) which is the only term occurring only once. Hence we have
\[ s(t) = \Re \left\{ e^{2K(0)} e^{-2K(\delta_1 t)} e^{2K(\delta_2 t)} \ldots e^{(-1)^n 2K(\delta_n t)} e^{(-1)^{n+1} 2K(t)} e^{(-1)^n 2K(\delta_n t)} \ldots e^{2K(\delta_2 t)} e^{-2K(\delta_1 t)} \right\}. \] (39)

Applying the BCH formula (22) yields
\[ s(t) = \Re \exp(2i \varphi_n(t)) \langle \exp(2 \Delta_n K) \rangle, \] (40a)
\[ = \cos(2 \varphi_n(t)) \exp(-2 \chi_n(t)), \] (40b)

where we used the identity (24) to obtain the second line. Therein the suppression \(\chi_n(t) := -\langle \Delta_n K^2 \rangle\) results from
\[ \Delta_n K := K(0) + (-1)^{n+1} K(t) + 2 \sum_{i=1}^{n} (-1)^n K(\delta_i t), \] (41a)
\[ = \sum_{i} \frac{\lambda_i}{2\omega_i} \left( b_i^+ y_n(\omega_i t) - b_i y_n^*(\omega_i t) \right), \] (41b)

where
\[ y_n(z) := 1 + (-1)^{n+1} e^z + 2 \sum_{j=1}^{n} (-1)^j e^{ijz}. \] (42)

Thereby we arrive at
\[ \chi_n(t) = \sum_{i} \frac{\lambda_i^2}{4\omega_i^2} |y_n(\omega_i t)|^2 \langle b_i^+ b_i + b_i b_i^+ \rangle, \] (43a)
\[ = \int_0^\infty J(\omega) \left\{ \frac{|y_n(\omega t)|^2}{4\omega^2} \right\} \coth(\beta\omega/2) \, d\omega. \] (43b)

The phase \(\varphi_n(t)\) in (40) can easily be computed by the following method. Using (22) we combine the second and third factors in (39), i.e. the two exponentials \(e^{-2K(\delta_1 t)} e^{2K(\delta_2 t)}\), to one exponential \(and\) the last and last-but-one factor, i.e. \(e^{2K(\delta_2 t)} e^{-2K(\delta_1 t)}\). Obviously, the occuring phases cancel. This procedure can be repeated by including the factor \(e^{-2K(\delta_1 t)}\) next in both the growing last exponential and in the second exponential. Iteration up to and including the
factor \( e^{(-1)^{n+1}2K(\delta_n,t)} \), which can be thought as being split into \( e^{(-1)^{n+1}2K(\delta_n,t)/2} e^{(-1)^{n+1}2K(\delta_n,t)/2} \), leads to two exponentials whose respective arguments contain all term \( K(\delta_n,t) \) except the very first \( K(0) \). Furthermore, the two respective arguments are equal so that the exponentials can be combined without further phase yielding

\[
s(t) = \mathcal{R} \{ e^{2K(0)} e^{2\Delta_n K - 2K(0)} \}.
\]  

(44)

From this equation we arrive at (40a) by defining

\[
\varphi_n(t) := -i[K(0), \Delta_n K],
\]

(45a)

\[
= i \sum_i \frac{\lambda_i^2}{4\omega_i^2} (y_n(\omega_i t) - y_n^*(\omega_i t)),
\]

(45b)

\[
= i \int_0^\infty \frac{J(\omega)}{4\omega^2} (y_n(\omega t) - y_n^*(\omega t)) \, d\omega,
\]

(45c)

\[
= \int_0^\infty \frac{J(\omega)}{2\omega^2} x_n(\omega t) \, d\omega,
\]

(45d)

where we used (41b) in the second line (45b). The last line (45d) reproduces equation (8b) in [16] with

\[
x_n(z) := i(y_n(z) - y_n^*(z))/2,
\]

(46a)

\[
= -3y_n(z),
\]

(46b)

\[
= (-1)^n \sin(z) + 2 \sum_{j=1}^{n} (-1)^{j+1} \sin(z\delta_j),
\]

(46c)

where the last line (46c) corrects equation (9) in [16] in the factor 2 in front of the sum.

Thereby, we have derived all the results used in the analysis in the previous paper [16].

2.3. Optimization of the sequence of \( \pi \) pulses

A particular asset of the equations (40b), (43) and (45) together with (46a) is that it is obvious that any deviation of the signal \( s(t) \) from unity is kept as low as possible if \( |y_n(z)| \) is kept as small as possible. Note that this strategy holds equally well for \( \varphi_n \) and for \( \chi_n \).

If \( y_n \) is of the order \( p \) in some small parameter \( p \), for instance \( p = t^{n+1} \), then \( \chi_n = \mathcal{O}(p^2) \) whence we deduce \( \exp(-2\chi_n) = 1 - \mathcal{O}(p^2) \). In analogy, we find \( \varphi_n = \mathcal{O}(p) \) whence we deduce \( \cos(-2\varphi_n) = 1 - \mathcal{O}(p^2) \) so that both factors are close to unity in the same way. Hence the total signal \( s(t) \) is close to unity in this order \( s(t) = 1 - \mathcal{O}(p^2) \).

So our aim is to choose the \( n \) instants \( \{\delta_j\} \) such that \( y_n(z) \) is as small as possible. The best way to do so is to make the first \( n \) derivatives of \( y_n(z) \) vanish. Note that \( y_n(0) = 0 \) for any sequence \( \{\delta_j\} \). The \( m \)th derivative reads \( m > 0 \)

\[
\delta^m z |_{z=0} = i^m \left( (-1)^{n+1} + 2 \sum_{j=1}^{n} (-1)^j \delta^m_j \right).
\]

(47)
Hence we have to solve the set of nonlinear equations

$$0 = (-1)^{n+1} + 2 \sum_{j=1}^{n} (-1)^j \delta_j^n$$

(48)

for \( m \in \{1, 2, \ldots, n\} \). For finite \( n \), solutions can easily be found analytically \([17]\) and numerically. Closer inspection of these numerical solutions reveals that they are excellently described by the condition (1).

Indeed, we can prove that (1) is a valid solution for the set of equations (48). To do so we choose a little detour by considering

$$\tilde{y}_n(h)|_{h=\pm 2} := \exp(-iz/2)y_n(z).$$

(49)

Obviously the equivalence

$$y_n(z) = \mathcal{O}(z^{n+1}) \iff \tilde{y}_n(h) = \mathcal{O}(h^{n+1})$$

(50)

holds so that the vanishing of the first \( n \) derivatives of \( y_n(z) \) is equivalent to the vanishing of the first \( n \) derivatives of \( \tilde{y}_n(h) \). The choice (1) implies by standard trigonometric identities

$$\delta_j = 1/2 - \cos(\pi j/(n+1))/2.$$

(51)

Inserting this choice into \( \tilde{y}_n(h) \) yields

$$\tilde{y}_n(h) = e^{-ih} + (-1)^{n+1} e^{ih} + 2 \sum_{j=1}^{n} (-1)^j \exp[-ih \cos(\pi j/(n+1))].$$

(52a)

$$= \sum_{j=-n-1}^{n} (-1)^j \exp[-ih \cos(\pi j/(n+1))].$$

(52b)

Obviously \( \tilde{y}_n(0) = 0 \). The \( m \)th derivative \((m > 0)\) reads

$$\partial^m_h \tilde{y}_n|_{h=0} = (-i)^m \sum_{j=-n-1}^{n} (-1)^j \cos^m(\pi j/(n+1)).$$

(53)

We compute explicitly \( d_m := (2i)^m \partial^m_h \tilde{y}_n|_{h=0} \)

$$d_m = \sum_{j=-n-1}^{n} (-1)^j [e^{i\pi j/(n+1)} - e^{-i\pi j/(n+1)}]^m,$$

(54a)

$$= \sum_{v=0}^{m} \binom{m}{v} \sum_{j=-n-1}^{n} \exp \left( \frac{i\pi j (2v - m + 1)}{n + 1} \right).$$

(54b)

The last sum, however, vanishes for \( m < n + 1 \)

$$\sum_{j=-n-1}^{n} \exp \left( \frac{i\pi j (2v - m + 1)}{n + 1} \right) = (-1)^{n+1} \frac{\exp(-i\pi (2v - m)) - \exp(i\pi (2v - m))}{1 + \exp((i\pi (2v - m))/(n+1))} = 0,$$

(55)

since the denominator in (55) remains finite in this range. Hence \( d_m = 0 \) and we know \( \tilde{y}_n(h) = \mathcal{O}(h^n) \) and hence \( y_n(z) = \mathcal{O}(z^n) \). This concludes the formal proof that (1) represents a valid solution of the set of nonlinear equations (48). We have not presented a proof that this is the only solution. But we presume that it is the only one which is physically meaningful with consecutive values \( \delta_{j+1} > \delta_j \).
2.4. Classical noise with $\pi$ pulses

In [16], we argued that the fact that the optimized sequence (1) works independently from the precise temperature indicates that it applies also to classical, Gaussian noise. The argument runs qualitatively as follows. Because (1) is the optimum sequence for all temperatures it also holds for $T \to \infty$. In this limit, the thermal fluctuations dominate over all the quantum effects and the bath behaves completely classically.

A crucial corollary is that the pulse sequence can be used for all kinds of baths at elevated temperatures because all physical systems behave like classical, Gaussian baths at high temperatures. Hence the applicability extends beyond the spin-boson model discussed so far. We will discuss the general validity of (1) in more detail in the next section.

Here we present the calculation for classical noise in order to establish a quantitative relation. We consider the decoherence due to

$$H = f(t) \sigma_z,$$

(56)

where $f(t)$ is a random variable with Gaussian distribution\(^1\). It is characterized by the expectation values

$$\langle f(t) \rangle = 0,$$  \hspace{1cm} (57a)

$$\langle f(t_1) f(t_2) \rangle = g(t_1 - t_2).$$  \hspace{1cm} (57b)

Note the translational invariance in time. Then the signal $s(t)$ after a $\pi/2$ pulse reads

$$s(t) = \langle |\uparrow\rangle D_x(\pi/2) \sigma_z \sigma_y e^{-iF(t)} D_x(\pi/2) |\uparrow\rangle,$$

(58)

where $F(t) := \int_0^t f(t') dt'$ is the primitive of $f(t)$. Since $\sigma_{x,y}$ only flips the spin, see for instance equation (16) for $K = 0$, we may write

$$s(t) = \langle e^{-iF(t)} e^{-iF(t')} \rangle,$$  \hspace{1cm} (59a)

$$= e^{-2\langle (F(t))^2 \rangle},$$  \hspace{1cm} (59b)

where we exploited the properties of Gaussian random variables to obtain the second line (59b).

The exponent can be computed easily

$$\langle (F(t))^2 \rangle = \int_0^t dt_1 \int_0^t dt_2 \langle f(t_1) f(t_2) \rangle,$$  \hspace{1cm} (60a)

$$= 2 \int_0^t dt_1 \int_0^{t_1} dt' g(t'),$$  \hspace{1cm} (60b)

$$= \frac{4}{\pi} \int_0^\infty \frac{p(\omega)}{\omega^2} \sin^2(\omega t/2) d\omega,$$  \hspace{1cm} (60c)

where we used $g(t') = g(-t')$ to obtain (60b) and the Fourier representation for (60c)

$$g(t) = \frac{1}{\pi} \int_0^\infty p(\omega) \cos(\omega t) d\omega,$$  \hspace{1cm} (61)

\(^1\) Note that we have changed the definition of $f(t)$ by a factor of 2 relative to our previous work [16] to keep the notation concise.
based on the power spectrum $p(\omega)$. The comparison with the quantum mechanical result (26) and (31) yields exactly the same form except that $\varphi(t) = 0$ because there are no operators which might not commute with themselves. The argument of the exponential $\chi(t) = \langle F(t)^2 \rangle$ is identical if we identify

$$\left(\frac{4}{\pi}\right) p(\omega) = J(\omega) \coth(\beta \omega/2).$$

(62)

This provides the quantitative correspondence between the classical calculation and the general quantum mechanical one.

The extension to the signal in presence of the $\pi$ pulses is also straightforward. The signal is given as in (33) except that the time evolution $\bar{R}_{cl}$ is classically given by

$$\bar{R}_{cl} = e^{-i\sigma_y \int_{t_0}^{t_{n+1}} f(t) dt} \sigma_x e^{-i\sigma_y \int_{t_n}^{t_{n-1}} f(t) dt} \sigma_y \ldots e^{-i\sigma_y \int_{t_1}^{t_0} f(t) dt} \sigma_x e^{-i\sigma_y \int_{t_0}^{t_{j+1}} f(t) dt}.$$

(63)

Again, the dynamics of the spin is easily computed since it flips at each $\sigma_y$ or $\sigma_x$ according to (16). The final result is $s(t) = e^{-2(F_n(t))^2}$ where $F_n(t)$ is given by

$$F_n(t) := \int_{-\infty}^{\infty} f(t') s_n(t') dt',$$

(64)

where $s_n(t')$ switches the sign according to

$$s_n(t') := \begin{cases} 0, & \text{for } t' \leq 0, \\ (-1)^j, & \text{for } \delta_j t < t' \leq \delta_{j+1} t, \\ 0, & \text{for } t' > t, \end{cases}$$

(65)

for $j \in \{0, 1, 2, \ldots, n\}$. Note that the Fourier transform $s_n(\omega)$ of $s_n(t')$ is given essentially by $y_n(\omega t)$

$$\int_{-\infty}^{\infty} s_n(t') \exp(i\omega t') dt' = \frac{i}{\omega} y_n(\omega t).$$

(66)

Next, $\langle F_n(t)^2 \rangle$ is expressed as a convolution and integral

$$\langle F_n(t)^2 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt_1 dt_2 s_n(t_1) g(t_1 - t_2) s_n(t_2).$$

(67a)

$$= \frac{1}{\pi} \int_{0}^{\infty} |y_n(\omega t)|^2 \frac{P(\omega)}{\omega^2} d\omega.$$

(67b)

For the last line, Fourier transformation, Parseval identity and the symmetry of the integrand are used. Again, we retrieve the quantum mechanical result (40b) and (43b) except for the phase $\varphi_n(t)$ which does not occur at all in the classical framework. The necessary identification is the same as before (62).

We conclude that the classical decoherence and the decoherence due to a quantum bosonic bath coincide except for the phases if the power spectrum $4p(\omega)/\pi$ is identified with the product of spectral density $J(\omega)$ and bosonic occupation factor $\coth(\beta \omega/2)$. Hence the optimization of the quantum model applies equally to the classical problem. Therefore, the optimization (1) applies to all models with (commuting) Gaussian fluctuations.
2.5. Unitary time evolution with $\pi$ pulses

So far we focused on the signal $s(t)$ as it results from a measurement of $\sigma_y$ after a $\pi/2$ pulse around $\sigma_x$. This appears to be a special choice. But in view of the spin rotational symmetry about the $z$-axis it is sufficiently general to guarantee that the coherence of an arbitrary initial state is preserved by the optimized pulse sequence. To corroborate this point and to prepare for the discussion of the most general model for phase coherence we discuss the time evolution operator $\hat{R}$ of the spin-boson model in this section.

The unitary operator $\hat{R}$ is defined in (34). Using the identities (4) and (35) we get

$$\hat{R} = U^\dagger e^{-iH_{\text{eff}}t} R_{\text{eff}} U,$$

(68a)

$$= e^{-iH_{\text{eff}}t} R,$$

(68b)

with

$$R = e^{-\sigma_z K(t)} R_{\text{eff}} e^{\sigma_z K(0)}.$$  

(68c)

Inserting the time-dependent version of (15b) (cf also equation (20b))

$$\sigma_y^{\text{eff}}(t) = \exp(2\sigma_z K(t)) \sigma_y$$

(69)

into (36) and using (14) yields for $n$ even

$$R|_{n\text{ even}} = e^{-\sigma_z K(t)} e^{2\sigma_z K(\delta_{n-1}t)} \cdots e^{2\sigma_z K(\delta_1t)} e^{-2\sigma_z K(\delta_n t)} e^{\sigma_z K(0)},$$

(70)

while for $n$ odd we arrive at

$$R|_{n\text{ odd}} = \sigma_y e^{\sigma_z K(t)} e^{-2\sigma_z K(\delta_{n-1}t)} \cdots e^{2\sigma_z K(\delta_1t)} e^{-2\sigma_z K(\delta_n t)} e^{\sigma_z K(0)}.$$  

(71)

These results are combined to yield for the total time evolution

$$\tilde{R} = \left\{ \begin{array}{l}
1 \\
\sigma_y
\end{array} \right\} \exp(-iH_{\text{eff}}t) \exp(-i\phi_n(t)) \exp(\sigma_z \Delta_n K),$$

(72)

where the upper entry in the curly brackets refers to $n$ even and the lower one to $n$ odd. The multiple difference is defined and computed in (41). Combining all the exponents to a single one makes a phase $\phi_n(t)$ occur which can be computed by commuting the various expression $K(\delta_j t)$ as required in (22). We do not give the explicit expression because we do not need it here. What is important is that this phase is a global one. It is just a real number and it does not depend on the spin; no Pauli matrix occurs because $\sigma_z^2 = 1$. Similarly, $H_{\text{eff}}$ does not depend on the spin.

To assess to which extent the time evolution depends on the spin state we consider the difference between the evolution of an $\uparrow$ and of a $\downarrow$ state. We define for $n$ even

$$\tilde{R}_\uparrow := \langle \uparrow | \tilde{R} | \uparrow \rangle_{\text{spin}},$$

(73a)

$$\tilde{R}_\downarrow := \langle \downarrow | \tilde{R} | \downarrow \rangle_{\text{spin}},$$

(73b)

and for $n$ odd

$$\tilde{R}_\uparrow := -i\langle \downarrow | \tilde{R} | \uparrow \rangle_{\text{spin}},$$

(74a)

$$\tilde{R}_\downarrow := i\langle \uparrow | \tilde{R} | \downarrow \rangle_{\text{spin}},$$

(74b)
where the subscript ‘spin’ signifies that we compute the expectation value only with respect to the Hilbert space of the spin. The bosonic operators remain unaltered. Then we consider

$$\Delta(t) := \tilde{R}_+ - \tilde{R}_-,$$

$$= e^{-i H_{\text{eff}} t} e^{-i \varphi_n(t)} \left[ e^{t \alpha K} - e^{- t \alpha K} \right].$$

as proposed by Lee et al [18]. From the last formula and (41b) it is obvious that the influence of the spin state is small for general sets \(\{\omega_i, \lambda_i\}\) if and only if \(y_n(z)\) is small. Quantitatively, one has

$$y_n(z) = \mathcal{O}(z^{n+1}) \iff \Delta(t) = \mathcal{O}(t^{n+1}).$$

Thereby, we have shown explicitly that the condition \(y_n(z) = \mathcal{O}(z^{n+1})\) implies generally that the coupling between any spin state, i.e. any state of the quantum bit, and the bosonic bath is efficiently suppressed if the pulse sequence obeys (1). Note that this holds for all choices of \(\{\omega_i, \lambda_i\}\).

3. General quantum bath

So far we considered the spin-boson model (2). One might think that the optimized sequence (1) is useful only for this model [14]. This is not the case.

The first piece of evidence for the general applicability of (1) is the fact that classical Gaussian noise can equally well be suppressed, see section 2.4. Conventional wisdom has it that any generic model with fluctuations will display Gaussian fluctuations in its high temperature limit. If this is true the optimized sequence (1) is applicable generally for high temperatures. Note that the ‘high’ temperatures need not be really high. The inter-spin coupling of nuclear spins is so low that already 1 K is sufficient to put a system of nuclear spins at high temperatures.

The second piece of evidence was found by Lee et al [18]. They observed analytically for up to \(n = 9\) that an expansion of \(\Delta(t)\) in powers of \(t\) for a general model yields vanishing coefficients for the optimized sequence (1). On the basis of this observation they conjectured that the optimized sequence (1) is generally applicable for the generic model for phase decoherence, also called single-axis decoherence model

$$H = \sigma_z A_1 + A_0,$$

where \(A_0\) and \(A_1\) contain only operators from the bath. Below we use the notation \(H_\pm = \pm \sigma_z A_1 + A_0\).

This model does not include spin flips; hence it implies an infinite life time \(T_1\) as a completely general decoherence model would do. But the phase decoherence of a precessing spin in the \(xy\)-plane is described in full generality because we do not specify for which operator \(A_1\) stands and the bath dynamics is fully unspecified. It is described by \(A_0\). Such a model is experimentally 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 [29, 30].

We investigate the time evolution \(\tilde{R}\) from 0 to \(t\) with \(\pi\) pulses at the instants \(\delta_j t\) where \(j \in \{1, 2, \ldots, n\}\). The \(\pi\) pulses are assumed to be ideal; they are given by \(\sigma_y\) so that \(\tilde{R}\) is given again by (34). Next, using (14), we shift all the factors \(\sigma_y\) to the far left side yielding

$$\tilde{R} = \frac{1}{\sigma_y} \left( e^{-i H_{-1} t (\delta_n - \delta_0) t} \cdots e^{-i H_1 t (\delta_1 - \delta_2) t} e^{-i H_0 t (\delta_0)} \right),$$

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where the upper entry between curly brackets refers to an even number \( n \) of pulses and the lower one to an odd number.

We define the unitary operators \( U_p \) as the product of the \( p + 1 \) rightmost factors on the right-hand side of equation (78), that means for \( 0 \leq p \leq n \)

\[
U_p(t) := e^{-iH_{\pi p}(\delta_{p-1} - \delta_p)t} e^{-iH_{\pi (p-1)}(\delta_{p-2} - \delta_{p-1})t} \cdots e^{-iH_{\pi 1}(\delta_0 - \delta_1)t}.
\] (79)

This operator can be expanded in a Taylor expansion with coefficients \( C^m_p \)

\[
U_p(t) = \sum_{j=0}^{\infty} (-it)^j \sum_{m \in B_j} \sigma_z^{|m|} C^m_p A_{m_j} A_{m_{j-1}} \cdots A_{m_2} A_{m_1}.
\] (80)

The set \( B_j \) contains all binary words \( m \) with \( j \) letters, i.e. \( m_i \in \{0, 1\} \) where \( m_i \) is the \( i \)th letter, \( i \in \{1, 2, \ldots, j\} \). Note that leading zeros also count. We use \( |m| \) for the checksum of \( m \), i.e. the sum over all letters \( |m| := \sum_{i=1}^{j} m_i \). The number of letters \( j \) of \( m \) shall be denoted by \( \|m\| \).

Using \( B \) as the union of all \( B_j \) with \( j \geq 0 \) we may denote the expansion by

\[
U_p(t) = \sum_{m \in B} (-it)^{|m|} \sigma_z^{|m|} C^m_p A_{m_1} \cdots A_{m_2} A_{m_1}.
\] (81)

Obviously, the coefficients which matter in the end are those for \( p = n \). The statement \( \Delta(t) = O(t^{n+1}) \) corresponding to (76) for the spin-boson model is equivalent to the vanishing of all the coefficients which are prefactors of terms depending on the spin state. This means that all \( C^m_p \) with \( |m| \) odd have to vanish as long as \( n \geq \|m\| \).

So far no general proof is available that these coefficients vanish for the sequence (1). But for finite \( n \) the calculation can be done explicitly by computer algebra. Lee et al [18] carried out such a calculation up to \( n = 9 \). We succeeded in reaching \( n = 14 \) with the help of the following recursion.

Clearly, we know from the expansion of a single exponential that

\[
C^m_0 = \frac{1}{\|m\|!} (\delta_1 - \delta_0)^{|m|!}.
\] (82)

This serves as starting point of our recursion which relies on

\[
U_{p+1}(t) = e^{-iH_{\pi (p+1)}(\delta_{p+2} - \delta_{p+1})t} U_p(t)
\]

\[
= \sum_{w \in B} \left\{ (-it)^{|w|} (\sigma_z)^{|w|} \frac{((\delta_{p+2} - \delta_{p+1})^{|w|} \cdot A_{w_1} \cdots A_{w_2} A_{w_1})}{|w|!} \right\}
\]

\[
\times \sum_{m \in B} (-it)^{|m|} \sigma_z^{|m|} C^m_p A_{m_1} \cdots A_{m_2} A_{m_1}.
\] (83)

The comparison of the arising coefficients with those in (81) leads to the recursion relation

\[
C^m_{p+1} = \sum_{(w, m) = v} \frac{(-1)^{(p+1)|w|}}{|w|!} (\delta_{p+2} - \delta_{p+1})^{|w|} C^m_p,
\] (84)

where the sum over \((w, m) = v\) means that all splittings of the binary word \( v \) in two subwords \( w \) for the first part and \( m \) for the second part are considered. Given \( v \) with \( \|v\| \) letters there are \( \|v\| + 1 \) such splittings.

The recursion (84) can be easily implemented in computer algebra programmes such as MAPLE. With about 2 GB RAM the verification of the vanishing of the \( C^n_v \) with odd checksum \( |v| \) for the optimum sequence (1) up to the order \( n = 14 \) was feasible. Nevertheless, a general mathematical proof would be highly desirable.

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4. Influence of the high-energy cutoff

Lee et al [18] observed that the optimized sequence (1), henceforth abbreviated UDD, works very well in numerical simulations for GaAs quantum dots where it does better than the concatenated sequence (concatenated dynamical decoupling (CDD)) proposed by Khodjasteh and Lidar [13, 14]2. But they found that qubits made from phosphorous impurities in silicon are better dynamically decoupled by the CDD sequence. They relate this result to the applicability of an expansion in time. Their model consists of a qubit coupled to a spin bath so that a direct applicability of results obtained for the spin-boson model is not possible. Yet the question is intriguing whether one can mimic the qualitative aspects of the spin bath by a bosonic bath.

From the way the general single-axis model is treated to derive the effect of the UDD sequence (see previous section) it is clear that the expansion in powers of \(t\) plays the crucial role. If such an expansion in time does not work, for instance because the resulting expansion is only asymptotically valid, there is no justification to use the UDD sequence.

The analytically accessible spin-boson model allows us to investigate the question of the expansion in time in a concrete example. Inspecting equations (40b), (43b) and (45d) one realizes that the existence of the expansion of the signal \(s(t)\) depends on the existence of the expansions of \(\chi_n(t)\) and \(\phi_n(t)\). In order that \(\chi_n(t) = \mathcal{O}(t^{n+1})\) the first \(n\) derivatives of \(\chi_n(t)\) must exist and vanish and the \(n + 1\)st derivative must exist. From (43b) we see that the expansion of \(\chi_n(t)\) in powers of \(t\) is directly related to the expansion of \(y_n(z)\) as in (42) in powers of \(z\) since \(z = \omega t\). In section 2.3 and in [16] we considered only the existence and the vanishing of the derivatives of \(y_n(z)\). The existence of the integral over the frequencies is no issue as long as a completely hard cutoff at \(\omega_D\) is considered

\[
J_\infty(\omega) := 2\alpha\omega\Theta(\omega_D - \omega)
\]

(85)

for which no ultraviolet (UV) divergence can appear. Hence all derivatives with respect to time exist for \(\chi_n(t)\) and for \(\phi_n(t)\). This also remains true if the UV cutoff is exponential.

But the physical systems might be such that the UV cutoff is soft because the spectral density displays power-law behavior. We consider

\[
J_\gamma(\omega) := \frac{2\alpha\omega}{1 + (\omega/\omega_D)^\gamma}
\]

(86)

as a generic form for this situation. Note that \(\gamma = \infty\) amounts up to the completely hard cutoff. The vanishing of the first \(n\) derivatives of \(y_n(z)\) implies \(y_n(z) = A(\omega t)^{n+1}\) plus higher terms. But in order to be able to conclude that \(\chi_n(t) = Ct^{2n+2}\) plus higher terms the integral

\[
C = \frac{A^2}{4} \int_0^\infty \omega^{2n} J(\omega) \coth(\beta\omega/2) \, d\omega
\]

(87)

must exist, i.e. converge. For \(J_\gamma(\omega)\) this strictly requires

\[
\gamma > 2n + 2.
\]

(88)

The equivalent consideration for the phase \(\varphi_n(t)\) leads to a less strict condition. If \(y_n(z) = A(\omega t)^{n+1}\) plus higher terms one has \(\varphi_n(t) = Dt^{n+1}\) which contributes the same order \(t^{2n+2}\) as

\[\text{2 It should be mentioned that the CDD was originally proposed for the general decoherence model where all Pauli matrices of the qubit are coupled to the bath. In the present paper, we consider the special case of CDD for single axis models for phase decoherence.}\]
\[
\exp(-2\chi_n) \to 1 - s(t) \text{ because of the cosine in which it appears, see (40b). The coefficient } D \text{ is given by the integral}
\]
\[
D = -\frac{3A}{2} \int_0^\infty \omega^{n-1} f(\omega) d\omega. \tag{89}
\]

Its existence requires only
\[
\gamma > n + 1 \tag{90}
\]
for \(J_\gamma(\omega)\). Hence we conclude that the condition for the smallness of the deviations resulting from \(\chi_n\) implies the condition for the smallness of the deviations resulting from \(\varphi_n\). For this reason, we will focus on the condition for the smallness of the exponential suppression by \(\chi_n\).

For practical purposes, the existence or non-existence of certain derivatives is not the ultimate criterion. So below we compare the effect of various pulse sequences on the signal \(s(t)\). Firstly, we look at the sequence \(UDD_n(t)\) which is characterized by (1). It leads via (42) for an even number of pulses \(n\) to
\[
\begin{align*}
y^\text{UDD}_n(z) &= -2i e^{i z/2} \left\{ \sin \left(\frac{z}{2}\right) + 2 \sum_{j=1}^{n/2} (-1)^j \sin \left(\frac{z}{2} \cos \left(\frac{j\pi}{n+1}\right)\right) \right\}. \tag{91}
\end{align*}
\]

Recall equation (76) stating the order \(y^\text{UDD}_n(z) = O(z^{n+1})\).

Secondly, we consider the concatenated sequence (CDD) [13, 14]. The zeroth level \(\text{CDD}_0(t)\) is the evolution without pulse. Higher levels are defined recursively by
\[
\begin{align*}
\text{CDD}_{l+1}(t) &= \text{CDD}_l \left(\frac{t}{2}\right) \circ \text{CDD}_l \left(\frac{t}{2}\right) & \forall l \text{ odd,} \tag{92a} \\
\text{CDD}_{l+1}(t) &= \text{CDD}_l \left(\frac{t}{2}\right) \circ \Pi \circ \text{CDD}_l \left(\frac{t}{2}\right) & \forall l \text{ even,} \tag{92b}
\end{align*}
\]
where \(\circ\) stands for the concatenation and \(\Pi\) for a \(\pi\) pulse. We obtain for the CDD sequence
\[
\begin{align*}
y^\text{CDD}_l(z) &= (-2i)^l e^{iz/2} \sin(2^{-l-1}z) \prod_{k=1}^l \sin(2^{-k-1}z), \tag{93}
\end{align*}
\]
where \(l\) now stands for the level which is exponentially related to the number of pulses \(n \approx 2^l\). From (93) it is easy to see that \(y^\text{CDD}_l(z) = O(z^{l+1})\) holds.

Thirdly, we consider the first suggestion [6, 7], namely the periodic bang–bang (BB) control with \(n\) pulses and
\[
\delta_j = j/(n + 1) \tag{94}
\]
implying (for even \(n\))
\[
y^\text{BB}_n(z) = -2i e^{iz/2} \cos(z/2) \tan(z/(2n + 2)). \tag{95}
\]
From this equation one learns \(y^\text{BB}_n(z) = O(z)\).

Fourthly, we consider the Carr–Purcell–Meiboom–Gill (CPMG) sequence [2–4]. This sequence results from the \(k\)-fold iteration of a two-pulse cycle of length \(\tau = t/k\). The pulses occur at \(\tau/4\) and \(3\tau/4\). This cycle corresponds in fact to \(UDD_2(\tau)\) [16]. We will come back later to iterations of UDD sequences. Here we state that CPMG is characterized by
\[
\delta_j = (j - 1/2)/n \tag{96}
\]
implying (for even \( n \))

\[
y_n^{\text{CPMG}}(z) = 4ie^{iz/2} \sin^2(z/(4n)) \frac{\sin(z/2)}{\cos(z/(2n))}.
\] (97)

From this equation it is clear that \( y_n^{\text{CPMG}}(z) = O(z^2) \).

In figure 1, the four sequences are compared for 10 \( \pi \) pulses at a fixed value \( \alpha = 1/4 \) of the coupling to the bath. The results for other values of \( \alpha \) are very similar. Furthermore, the temperature is fixed to \( T = 0 \) because the precise value of the temperature matters only for small frequencies \( \omega \to 0 \) while we focus here on high frequencies and the UV cutoff.

In all six panels, it is obvious that the BB sequence does worst in accordance with the power law which is only linear. This inefficient suppression of decoherence also implies that
phase effects in the signal $s(t)$ due to $\varphi_n$ in equation (40b) are seen most strongly leading to the bumps in figure 1. We conclude that one should always try to use one of the other sequences.

Comparing the CDD and the CPMG sequences the CPMG sequence is almost advantageous everywhere. Only for very low deviations $1 - s(t)$ the CDD does better because its curve is steeper reflecting a higher order in $t$: $y_{CDD}^{4}(z) = \mathcal{O}(z^3)$, whereas $y_{CDD}^{CPMG}(z) = \mathcal{O}(z^5)$.

Comparing the CDD and the UDD sequences the UDD sequence always yields lower deviations, except for very soft cutoffs ($\gamma = 2$) where both sequences behave equally. We conclude that we cannot explain the behavior found by Lee et al [18] where the CDD sequence seemed to outperform the UDD on the basis of the spin-boson model. Note that the slope of both sequences in figure 1 seems to be similar though this is difficult to tell from the depicted range of parameters. But the analytic results clearly states $y_{4}^{CDD}(z) = \mathcal{O}(z^5)$, whereas $y_{10}^{UDD}(z) = \mathcal{O}(z^{11})$ for the same number of pulses, namely $n = 10$.

The interesting issue is a comparison of the CPMG and the UDD sequences. For very soft cutoffs, i.e. low values of $\gamma$, the CPMG sequence is slightly better. This was also observed in a model of classical Gaussian noise [31]. The UDD sequence, however, performs better for large values of $\gamma$. Indeed, this finding supports our analytical condition (88). As long as $\gamma \lesssim 2n$ the CPMG sequence with its relatively low order $t^3$ (in $y_n(\omega t)$) does slightly better than the high-order UDD with $t^{11}$. But for $\gamma \gtrsim 2n$ the UDD outperforms the CPMG, especially for low deviations $1 - s(t)$ which matter most for quantum information processing.

We substantiate the comparison between the UDD and the CPMG sequences further by figure 2. The results go in the same direction as before. As long as $n \lesssim \gamma/2$ the UDD does significantly better than the CPMG. For $n \approx \gamma$ the UDD does better than the CPMG at low values of $1 - s(t) \approx 10^{-4}$ while the CPMG is advantageous at higher values $1 - s(t) \approx 10^{-1}$. For $n > \gamma$, the CPMG does slightly better than the UDD except for very small values of $1 - s(t)$. This constitutes a clear message for applications.
One may wonder whether there is a way to combine the advantages of the UDD and of the CPMG sequence. Indeed, this is possible by resorting to hybrid solutions proposed earlier [16, 17]. The UDD cycles with low values of \( n \) can be iterated. We denote such a sequence by \( \text{iUDD}_{m,c}(t) \) where \( m \) stands for the number of pulses within one cycle and \( c \) for the number of cycles so that \( n = mc \) is the total number of pulses. This means we consider the concatenation

\[
\text{iUDD}_{m,c}(t) = (\text{UDD}_m(t/c))^c.
\]  

\[ (98) \]
A quantitative comparison for iterated iUDD sequences is given in figure 3 for a total of 12 \( \pi \) pulses. Note that iUDD\(_{2,6}\) is equivalent to CPMG, whereas iUDD\(_{12,1}\) is equivalent to the UDD sequence. The guideline here is the corollary

\[ \gamma > 2m + 2, \]  

(99)

of (88) where \( m \) is the number of pulses within one cycle. It results from the observation that \( y_{iUDD}^{(m,c)}(z) \) is of order \( z^{m+1} \) independent from the number of cycles.

If the condition (99) is not valid the use of any sequence of higher order does not pay. This is clearly seen in the uppermost panel for \( \gamma = 4 \) (very soft cutoff) in figure 3. All curves are almost on top of each other. The CPMG, i.e. iUDD\(_{2,6}\), is slightly better than the other pulse sequences.

In the middle panel for \( \gamma = 8 \) (intermediate cutoff) in figure 3 the situation has changed. For low deviations \( 1 - s(t) \) the use of the iUDD\(_{3,4}\) or the iUDD\(_{4,3}\) sequence pays while the implementation of a larger value of \( m \) hardly pays.

In the lowermost panel for \( \gamma = \infty \) (hard cutoff) in figure 3 the implementation of higher order sequences is always useful for low values of \( 1 - s(t) \) as was to be expected.

Figure 3 illustrates that one can gain considerably in coherence without implementing the fully optimized pulse sequence (1). Already the implementation of periodic cycles with a moderate number of pulses can be very helpful. In practice, this strategy is generally much easier to realize since not so many special instants in time need to be fine-tuned.

Another remark for experimental realizations is in order. If the pulses are not ideally tailored then the advantages of dynamical decoupling will be thwarted by accumulated pulse errors. So in practice one always will be faced with the need to find the optimum tradeoff. Note, however, that this fact makes it particularly interesting to reach an optimum suppression of decoherence with a small number of pulses.

5. Conclusions

We investigated the suppression of decoherence by sequences of ideal, instantaneous \( \pi \) pulses. The model under study is a spin-boson model valid for pure dephasing, i.e. for a finite \( T_2 \) but an infinite \( T_1 \). But also the most general model for phase decoherence (single-axis decoherence) is considered.

Firstly, we have provided the detailed derivation of the equations which were used in our previous paper in [16]. In particular, it was rigorously shown that the sequence (1) (UDD) makes the first \( n \) derivatives vanish. Furthermore, it was shown that the results transfer also to the classical case of Gaussian fluctuations.

Secondly, it was shown that the UDD sequence is advantageous for any initial state. This important finding was achieved by analyzing the corresponding time evolution operator.

Thirdly, we considered the most general model for phase decoherence and extended the analytical results of Lee et al to the 14th order in the time. This was achieved on the basis of an efficient recursion scheme suitable for implementation in a computer algebra programme.

Fourthly, we investigated the influence of the high-energy cutoff in the framework of the single-axis spin-boson model. We compare various pulse sequences which are currently under debate, namely the periodic BB sequence, the CDD, the well-established CPMG sequence and the general iUDD cycles.
The most important observation is that decoherence due to baths with very soft cutoffs are much more difficult to suppress than decoherence due to baths with hard cutoffs. For soft cutoffs, the simpler sequences (CPMG = iUDD\(_{2,c}\) or iUDD\(_{m,c}\) with low values of \(m\)) are completely sufficient. Higher order sequences do not pay. We established a rule of thumb when the implementation of a more intricate sequence is appropriate. The number of pulses \(m\) in one cycle should not exceed \(\gamma / 2\) where \(\gamma\) is the exponent of the high-energy power law of the decohering spectral density \(J_\gamma(\omega)\), see equation (86).

By the above results, we have elucidated the possibilities of dynamical decoupling. Mathematically, important derivations are provided. Practically, important guidelines are established as to which sequences are most appropriate under which conditions.

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