Optimized Dynamical Decoupling for Power Law Noise Spectra

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We analyze the suppression of decoherence by means of dynamical decoupling in the pure-dephasing spin-boson model for baths with power law spectra. The sequence of ideal \( \pi \) pulses is optimized according to the power of the bath. We expand the decoherence function and separate the cancelling divergences from the relevant terms. The proposed sequence is chosen to be the one minimizing the decoherence function. By construction, it provides the best performance. We analytically derive the conditions that must be satisfied. The resulting equations are solved numerically. The solutions are very close to the Carr-Purcell-Meiboom-Gill (CPMG) sequence for a soft cutoff of the bath while they approach the Uhrig dynamical-decoupling (UDD) sequence as the cutoff becomes harder.

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I. INTRODUCTION

The dynamics of a spin \( S = 1/2 \), or a quantum bit (qubit), coupled to an environment is one of the longest studied models of quantum decoherence. It finds important applications both in nuclear magnetic resonance (NMR) and in quantum information processing (QIP). The suppression of the decoherence is one of the goals one usually strives for. In order to achieve it, sequences of control pulses are used [1].

There are two ways to address dynamical decoupling (DD) by control pulses. Either the control is modulated continuously, see for instance Ref. 2, or the control consists of short pulses which can be seen as (approximately) instantaneous. In this article, we will focus exclusively on the latter approach which is common in NMR and wide-spread in QIP [3,4,5]. It relies on control pulses to invert the dynamics of the spin. The spin experiences a rotation of an angle \( \pi \) at each pulse. The choice of the appropriate sequence is essential for an enhancement of the suppression of decoherence. A large variety of sequences has been suggested. The majority is characterized by periodic pulses [3,4,6,7,8,9]. The most famous example is the Carr-Purcell-Meiboom-Gill (CPMG) sequence [8,9] where cycles of two \( \pi \) pulses are iterated.

Other sequences proposed are non-equidistant such as the concatenated dynamical decoupling (CDD) [7,10,11] or the Uhrig dynamical decoupling (UDD) [12,13,14]. The CDD consists of concatenations of pulse sequences. It can suppress both transverse relaxation and longitudinal relaxation at the price of a relatively large number of pulses. If \( \ell \) is the largest order in an expansion in the total duration \( t \), in which no decoherence occurs, the required number of pulses grows exponentially with \( \ell \). The UDD eliminates only pure dephasing, but in turn it requires only a linearly growing number of pulses. The concatenation of the UDD sequence (CUDD) allows for the suppression of transverse and longitudinal relaxation again at the price of an exponential growth of the number of pulses, but requiring only the square root of the number of pulses necessary for CDD [14].

We point out that all the above sequences are idealized in the sense that they are based on ideal, instantaneous pulses, i.e., \( \delta \) peaks, though the effect of finite pulse durations is being discussed. Furthermore, sequences of realistic pulses have been proposed [15,16,17,18]. The finite duration of the pulse is a source of additional errors which can be reduced by designing the shape of the pulses appropriately, see for instance Ref. 19 and references therein. In the present paper, however, we will concentrate only on sequences of instantaneous \( \pi \) pulses.

The UDD sequence was discovered first for a spin-boson model [12] where it was observed that no details of the model entered. On the basis of numerical evidence and finite order recursion it was conjectured that UDD is applicable to any dephasing model [13,20]. This claim was finally proven for arbitrary number of pulses in the total duration \( t \) of the sequence [21]. For various classical noise spectra the experimental verification of the theoretical results was achieved by optical control of the transition in Be ions [22,23,24]. It was also shown that the UDD sequence outperforms the CPMG sequence and equidistant sequences in general for pure dephasing baths with hard cutoff while it performs worse for soft cutoffs [13,20,22,23,24]. This shows that the knowledge of the cutoff is an essential piece of information for an optimum suppression of decoherence.

The performance of some pulse sequences for classical noise spectra has already been considered by Cywiński et al. for superconducting qubits subject to gaussian and random telegraph noise [25]. The authors compare the efficiency of different sequences in suppressing pure dephasing. They find that the UDD sequence is optimum in suppressing the decoherence if the gaussian noise displays a hard ultraviolet (UV) cutoff. In situations, however,
where one has to work in the regime of small frequencies (long times) such that the cutoff cannot be reached, the CPMG sequence is the one yielding the best results.

Another proposal for an optimized sequence is put forward by Biercuk et al. [22, 23]. The optimization in the UDD is extended to a locally optimized dynamical decoupling (LODD) sequence which is tailored to a given experimental noise environment. The experimental implementation of LODD for classical noise shows that it performs better than UDD and CPMG. The LODD, however, is limited by the degree to which the spectral function of the noise (or the bath) is known. This caveat is dealt with by an optimized noise-filtration dynamic decoupling (OFDD) [24] where the noise spectrum is approximated by a constant up to a high-energy (UV) cutoff for which sequences of pulses are deduced numerically. For an ohmic bath the OFDD implies about the same factor of ≈ 1.5 of improvement over the UDD sequence than the more cumbersome LODD. But it does not provide a significant improvement for an ambient noise scaling such as ∝ 1/ω^4.

In this paper we generalize the OFDD from a constant spectrum to an arbitrary power law without UV cutoff. This problem can be analysed to a large extent analytically. The resulting optimized dynamic decoupling sequences for power law spectra (PLODD) are universal in the sense that the relative instants \( \{ \delta_j = t_j / t \} \) of the pulses depend only on the power law exponent \( p \). The gist of our finding is that the PLODD sequences resemble CPMG sequences for slowly decreasing noise spectra while they approach UDD sequences for fast decreasing noise spectra. This agrees with the qualitative expectations based on other investigations [13, 22, 23, 24, 25].

Our results provide an important guideline in the choice of sequences to be applied in experiments on the suppression of decoherence.

From an experimental point of view, the noise used to test the dynamical decoupling sequences - classical noise, ohmic spectrum, as well as the 1/ω^4 noise spectrum - is in general governed by a power law spectrum. Analytically, power law spectra approximate any spectrum either for very small or for very large frequencies which in turn correspond to long or short durations, respectively. Moreover, power law spectra are the perfect tool to analyze the influence of baths characterized by different cutoffs on the optimized pulse sequence. By varying the exponent of the power law of the spectrum we can simulate both baths with soft and hard cutoffs and we can interpolate smoothly between them.

In order to render an analytical investigation possible we consider the spin-boson model with pure dephasing. We start from the decoherence function \( \chi(t) \) (defined in Eq. (1)) which measures the size of the decoherence. The advantage is that the decoherence function at the same time embodies both the characteristics of the bath and of the sequence of \( \pi \) pulses. Hence one has to minimize \( \chi(t) \).

The article is organized as follows. In Sect. [III] the model is introduced and the decoherence function for a sequence of \( \pi \) pulses is defined and discussed. In the following Sect. [IV] we study and solve the problem of the diverging terms in the integration yielding the decoherence function. Then we derive the final equations in Sect. [V] and solve them numerically in Sect. [VI] where also examples of the PLODD are shown. At last the conclusions are drawn in Sect. [VI].

### II. CONVERGENCE OF THE DECOHERENCE FUNCTION

We consider the spin-boson model with pure dephasing

\[
H = \sum_i \omega_i b_i^\dagger b_i + \frac{1}{2} \sigma_z \sum_i \lambda_i \left( b_i^\dagger + b_i \right) + E
\]

(1)

describing a single qubit as a spin \( S = 1/2 \) coupled linearly to a bosonic bath. The spin is represented by the Pauli matrix \( \sigma_z \), while the \( b_i^\dagger \) are the annihilation (creation) operators of the bath. The constant \( E \) sets the energy offset. The properties of the bath are defined by the set of parameters \( \{ \lambda_i, \omega_i \} \). This information is conveniently encoded in the spectral density [26, 27]

\[
J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i).
\]

(2)

We recall that the quantum mechanical time evolution \( p^n \) of a sequence with \( n \) \( \pi \) pulses about the \( x \) axis of the spin reads

\[
p^n = f_{t-\delta_n} X f_{\delta_n-\delta_{n-1}} X \ldots X f_{\delta_3-\delta_2} X f_{\delta_2-\delta_1} X f_{\delta_1},
\]

(3)

where \( X \) stands for the spin operator of the rotation due to the pulse [14, 21]. Such a sequence suppresses the relaxation along \( z \) [14, 21]. If \( t \) is the total duration of the sequence, the instant \( t_j \), at which the pulse \( j \) is applied, is given by \( t_j = t \delta_j \). By definition \( \delta_0 := 0 \) and \( \delta_{n+1} := 1 \) although there is no pulse neither at the very beginning nor at the very end. The notation \( f_{\delta_i-\delta_{i-1}} \) stands for the free evolution of the system in the interval \( t(\delta_i - \delta_{i-1}) \) between two successive pulses.

In Refs. [14, 13] it is shown that the free induction decay is proportional to \( e^{-2\chi(t)} \) where the decoherence function is defined by

\[
\chi(t) := \int_0^\infty \frac{S(\omega)}{\omega^2} |y_n(\omega t)|^2 d\omega.
\]

(4)

Here the noise spectrum \( S(\omega) \) is related to the spectral density \( J(\omega) \) in (2) by

\[
S(\omega) := \frac{1}{4} J(\omega) \coth(\beta \omega / 2),
\]

(5)

where \( \beta \) is the inverse temperature. The filter function \( y_n(z) \) (\( z := \omega t \)) for \( n \) pulses is given by

\[
y_n(z) := \sum_{j=0}^{n+1} 2^j (-1)^j e^{i \delta j},
\]

(6)
with

$$q_j := \begin{cases} 0 & \text{if } j = 0, n + 1 \\ 1 & \text{if } j \in \{1, 2, \ldots, n - 1, n\} \end{cases}.$$  \hspace{1cm} (7)

Obviously, it encodes the properties of the sequence.

Equation (4) is the starting point for the evaluation of the optimized sequences. The aim is to keep $e^{-2x(t)}$ close to the unity as long as possible. In Ref. [12] the condition was enforced that the first $n$ derivatives of the filter function should vanish at $\omega t = 0$ for a sequence with $n$ pulses. Thus the function $y_n$ would increase very slowly close to zero. The condition on the derivatives implies the following set of non-linear equations

$$0 = \sum_{j=1}^{n+1} 2^q (-1)^j \delta_j^p$$  \hspace{1cm} (8)

for $p \in \{1, 2, \ldots, n\}$. For $p = 0$, Eq. (5) is also zero [12], which is equivalent to $y_n(0) = 0$. The solution of the Eqs. (5) reads [12]

$$\delta_j^{\text{UDD}} = \sin^2 \left[ j \pi / (n + 1) \right].$$  \hspace{1cm} (9)

The UDD sequence suppresses the decoherence best for baths with a hard cutoff rather than for baths with a very soft cutoff. This was tested by means of numerical simulations [20], analytical analyses [13, 25], and experiments with classical noise [22, 22].

![Figure 1: (color online) Schematic visualization of the filter function (black dashed line) and of the spectral function $S(\omega)$ for a soft and for a hard cutoff. $\omega_D$ stands for the ultraviolet cutoff. The plot illustrates that the overlap between the filter function and the spectral density remains significant for a soft cutoff, even if $|y_n(\omega t)|^2$ shifts to the right. This is in contrast to the situation for a hard cutoff where the overlap becomes extremely small for $n \to \infty$ or $t \to 0.$](image)

The efficiency of UDD depends on the applicability of an expansion in powers of $t$ of $\chi(t)$ [13, 20]. This expansion implies the expansion of $y_n(z)$ in powers of $z = \omega t$. This is always possible since $y_n(z)$ as defined in (6) is analytical. But the existence of the integrals of the resulting series in powers of $\omega t$, as required by (4), depends on the UV cutoff of $S(\omega)$ [13].

In the derivation of Eq. (9) only the existence of the derivatives of $y_n(\omega t)$ and not the existence of the integral over the frequency $\omega$ is required. The decoherence function consists of the product of the function $S(\omega)$ times the square modulus of the filter function. The function $\chi(t)$ is minimum if the overlap between $S(\omega)$ and $|y_n(z)|^2$ is minimum. The significance of the UV cutoff is illustrated in Fig. (1).

From now on we focus on power law spectra

$$\frac{S(\omega)}{\omega^2} = \frac{S_0}{\omega^{\alpha+1}}.$$  \hspace{1cm} (10)

Then the decoherence function reads

$$\chi(t) = S_0 \int_0^\infty \frac{1}{\omega^{\alpha+1}} |y_n(\omega t)|^2 d\omega$$  \hspace{1cm} (11)

It is required that $\alpha$ is strictly positive to ensure the convergence for $\omega \to \infty$. This is true because the filter function is bounded from above $|y_n(\omega t)|^2 \leq 2(n+1)$. The prefactor $S_0$ incorporates all the constants of the spectral density.

For $\omega \to 0$ (infrared (IR) limit), $\chi(t)$ converges if $y_n(\omega t) \propto (\omega)^m$ for $m$ large enough. This in turn depends on the choice of the sequence $\{\delta_j\}$. For arbitrary sequences $\{\delta_j\}$ we have $y_n(0) = 0$ so that the IR convergence is guaranteed for $\alpha < 2$. For larger $\alpha$, we require that the first $m$ derivatives of the filter function vanish, implying

$$|y_n(\omega t)|^2 \propto (\omega)^{2(m+1)},$$  \hspace{1cm} (12)

which is similar, but not identical, to the requirement for the UDD in Eq. (8). The convergence of $\chi(t)$ is guaranteed for

$$\alpha < 2m + 2.$$  \hspace{1cm} (13)

In Ref. [12] it was argued that UDD applies independently of the temperature. This indicates that UDD can be equally used to suppress classical gaussian noise [13, 25]. For high temperature $\beta \to 0$ the thermal fluctuations dominate over the quantum fluctuations such that $S(\omega) \propto 1/\omega$ for $J(0) \neq 0$. This is the famous $1/f$ noise, which corresponds to $\alpha = 2$ in our notation. The case $S(\omega) \propto 1/\omega^4$ is experimentally relevant for ions in a Penning trap [22, 23]. This case corresponds to $\alpha = 5$ in the above notation.

The basic 2-pulse cycle of the CPMG sequence coincides with the UDD sequence for $n = 2$. It makes the first two derivatives of the filter function vanish [12]. According to Eq. (13) its applicability is restricted to baths characterized by $\alpha < 6$.

In order to study general power laws we proceed as follows. We substitute $z = \omega t$ in the decoherence function $\chi(t)$ in (4) obtaining

$$\chi(t) = S_0 t^\alpha I_n$$  \hspace{1cm} (14)
with
\[ I_n := \int_0^\infty \frac{|y_n(z)|^2}{z^{\alpha+1}} \, dz. \]  
(15)

This simple substitution reveals that the optimum \( \{\delta_j\} \) are independent of the total duration \( t \) of the sequence. All the time-dependence of \( \chi(t) \) is a simple power of \( t \) as in (14). Its exponent is determined by the power law spectrum of the bath. The precise sequence \( \{\delta_j\} \) determines the factor \( I_n \).

The condition for the first \( m \) derivatives to vanish is given by the set of the first \( m \)-non-linear equations in (8), i.e., for \( p \in \{1, 2, \ldots, m\} \). These conditions are the same as those leading to the UDD sequence (12) except that they do not need to be fulfilled up to \( p = n \) but only up to \( p = m \). For a sequence of \( n > m \) pulses we still have \( n - m \) degrees of freedom left. This freedom is used to minimize \( I_n \) and hence the decoherence function \( \chi(t) \).

In this minimization the \( m \) Eqs. (8) act as additional constraints. Hence, we have to study the variation
\[ \frac{\partial}{\partial \delta_j} \left[ I_n - \sum_{i=1}^{m} \lambda_i \left. \frac{\partial y_n(z)}{\partial z} \right|_{z=0} \right] = 0, \]  
(16)

where \( m \) Lagrange multipliers \( \lambda_i \) appear due to the \( m \) constraints.

### III. DIVERGING TERMS

The integral \( I_n \) (15) converges if the condition \( \alpha < 2(m+1) \) is fulfilled. But the integration in (14) cannot be carried out analytically. To make analytical progress we split the square modulus of the filter function into a sum of exponential terms according to
\[ |y_n(z)|^2 = \sum_{i,j=0}^{n+1} 2^{n+q_i} (-1)^{i+j} e^{iz\Delta_{ij}}, \]  
(17)

where we use the notation \( \Delta_{ij} := i(\delta_i - \delta_j) - 0^+ \) for \( (i,j) = 0,n+1 \); the summand \( -0^+ \) stands for an infinitesimal negative real part which is required later on for convergence for \( z \to +\infty \). The integral \( I_n \) is given by the limit of the sum
\[ I_n = \lim_{x \to 0^+} I_n(x) \]  
(18a)
\[ I_n(x) := \sum_{i,j=0}^{n+1} 2^{n+q_i} (-1)^{i+j} I_{ij}(x) \]  
(18b)

where the integrals
\[ I_{ij}(x) := \int_{x}^{\infty} \frac{e^{iz\Delta_{ij}}}{z^{\alpha+1}} \, dz. \]  
(19)

UV convergence is ensured by the infinitesimal negative real part of \( \Delta_{ij} \), see definition below Eq. (17).

The regularization by a finite IR cutoff \( x \) is required because the limit \( x \to 0 \) does not exist for the individual terms \( I_{ij}(x) \). Each term \( I_{ij}(x) \) can be reduced to an analytical expression by the substitution \( z \to -z/\Delta_{ij} \)
\[ I_{ij}(x) = (-\Delta_{ij})^\alpha \int_{-x\Delta_{ij}}^{\infty} \frac{e^{-z}}{z^{\alpha+1}} \, dz \]  
(20a)
\[ = (-\Delta_{ij})^\alpha \Gamma(-\alpha, -\Delta_{ij}x) \]  
(20b)

where \( \Gamma(-\alpha, -\Delta_{ij}x) \) is the incomplete Gamma function (28).

For later use we state that the vanishing of the first \( m \) derivatives of the filter functions \( y_n(z) \) at \( z = 0 \) implies (12) and thus
\[ \partial_z^p |y_n(z)|^2 \big|_{z=0} = \sum_{i,j=0}^{n+1} 2^{n+q_i} (-1)^{i+j} (\Delta_{ij})^p \]  
(21a)
\[ = 0 \]  
(21b)

for \( 0 \leq p \leq 2m+1 \). Eq. (21b) asserts that the weighted sum of powers of \( \Delta_{ij} \) vanishes. We will utilize this cancellation to find the relevant contributions to \( I_n \) analytically.

#### A. Expansion of the incomplete Gamma function

a. Non-Integer Exponents Starting from the definition of the incomplete Gamma function \( \Gamma(a,x) \) with \( -a = \alpha \notin \mathbb{N}_0 \) we integrate by parts \( \ell \) times and write
\[ \Gamma(a,x) = T_1 + T_2, \]  
(22)
with
\[ T_1 = -e^{-x} \sum_{p=0}^{\ell-1} x^{a+p} \frac{(a-1)!}{(a+p)!} \]  
(23)
and
\[ T_2 = \frac{(a-1)! \Gamma(a+\ell, x)}{(a+\ell-1)!}. \]  
(24)

For \( a \leq 0 \) the limit \( \lim_{x \to 0^+} \Gamma(a,x) \) is not defined. We choose \( \ell \) such that
\[ a + \ell > 0 > a + \ell - 1. \]  
(25)

For non-integer \( a \) this is possible. The first inequality ensures that \( \lim_{x \to 0^+} \Gamma(a+\ell, x) = \Gamma(a+\ell) \). The recurrence relation \( \Gamma(z+1) = z\Gamma(z) \) implies
\[ \lim_{x \to 0^+} T_2 = \Gamma(a). \]  
(26)

Now we concentrate on the term \( T_1 \). Since the exponential function \( e^{-x} \) can be expanded in powers of \( x \), \( T_1 \) has a well-defined expansion
\[ T_1(x) = x^a \sum_{p=0}^{\infty} \alpha_p x^p. \]  
(27)
The coefficients \( \{ \alpha_p \} \) depend on the coefficients of \( T_1 \) and on those of the expansion of the exponential. Their explicit form does not matter here. The powers diverge in the limit \( x \to 0 \) for \( p \in \{ 0, \ldots, \ell - 1 \} \). For \( p \geq \ell \) they vanish for \( x \to 0 \).

Finally we write the integral \( I_n(x) \) in terms of the integrals \( I_{ij}(x) \) defined in Eq. (19) and evaluated in Eq. (20):

\[
I_n(x) = \sum_{p=0}^{\ell-1} \alpha_p x^{p-\alpha} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p + \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p \Gamma(-\alpha) + O(x^{\ell-\alpha}).
\]

(28)

The last term \( O(x^{\ell-\alpha}) \) comprises all the contributions which vanish for \( x \to 0 \), recall (25) for \( a = -\alpha \). The first term (28a) contains the diverging terms. But they cancel one another completely because the inner sum in (28a) vanishes due to (21b). To see this one must use (13) and (24) to arrive at \( p \leq \ell - 1 \leq 2m + 1 \). This rather formal argument simply reflects the fact that (13) guarantees the IR convergence of the integration in (31). Hence all IR divergent terms appearing in intermediate calculations have to cancel finally.

From the above the only remaining and thus relevant contribution to \( I_n = \lim_{x \to 0} I_n(x) \) is (28b)

\[
I_n = \Gamma(-\alpha) \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p. \quad (29)
\]

This is the result for non-integer \( \alpha \). Note that \( \Gamma(-\alpha) \) is only a global prefactor which does not depend on \( \Delta_{ij} \).

b. Integer Exponents

Next we consider the case of \( \alpha = N_0 \). We use Eqs. (24) with \( \ell = \alpha = -\alpha \)

\[
\Gamma(-\alpha, x) = - e^{-x} \sum_{p=0}^{\alpha-1} x^{p-\alpha} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p \left( \frac{\alpha - 1 - p!}{\alpha!} \right)
\]

(30)

Thus Eq. (28) now reads

\[
I_n(x) = - \sum_{p=0}^{\alpha-1} \alpha_p x^{p-\alpha} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p + \left( \frac{-\alpha}{\alpha!} \right) \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p \Gamma(0, -\Delta_{ij} x). \quad (31a)
\]

\[
+ \frac{(-1)^{\alpha}}{\alpha!} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (-\Delta_{ij})^p \Gamma(0, -\Delta_{ij} x). \quad (31b)
\]

As before the inner sum in (31a) cancels because of (21b) and because (13) implies \( p \leq \alpha - 1 \leq 2m \). Note that (13) and (21b) additionally imply that the weighted sum of the powers \( \Delta_{ij}^p \) vanishes. This will help to simplify further in the limit \( x \to 0 \). We expand the incomplete Gamma function

\[
\Gamma(0, -\Delta_{ij} x) = - \gamma - \ln(x) - \ln(-\Delta_{ij}) + O(x), \quad (32)
\]

where \( \gamma \) is the Euler-Mascheroni constant. Hence in the limit \( x \to 0 \) the only non-vanishing contribution to \( I_n = \lim_{x \to 0} I_n(x) \) is

\[
I_n = -\frac{1}{\alpha!} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} \Delta_{ij}^\alpha \ln(-\Delta_{ij}). \quad (33)
\]

B. Example for \( \alpha = 2 \)

For \( \alpha = 2 \) we explicitly write the expansion of the incomplete Gamma function and show that the diverging terms cancel. For \( x \to 0 \) we have

\[
\Delta_{ij}^2 \Gamma(-2, \Delta_{ij} x) = \frac{\Delta_{ij}^2}{4} (3 - 2\gamma - 2 \ln(-\Delta_{ij} x)) + \frac{1}{2x^2} + \frac{\Delta_{ij}}{x} + O(x) \quad (34a)
\]

\[
= I_{ij}^{(-2)}(x) + I_{ij}^{(-1)}(x) + I_{ij}^{(0)} \quad (34b)
\]

\[
- \frac{\Delta_{ij}^2}{2} \ln(-\Delta_{ij}) + O(x) \quad (34b)
\]

The function \( I_{ij}^{(k)}(x) \) is the sum of the \( I_{ij}^{(k)}(x) \) weighted according to the right hand side of (18b). These contributions vanish. For \( I_{ij}^{(-2)}(x) \) we can write

\[
I_{ij}^{(-2)}(x) = \frac{1}{2x^2} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} \quad (35a)
\]

\[
= \frac{1}{2x^2} \sum_{i=0}^{n+1} 2^{q_i} (-1)^i \sum_{j=0}^{n+1} 2^{q_j} (-1)^j \quad (35b)
\]

\[
= 0. \quad (35c)
\]

The vanishing of (35c) is guaranteed by Eq. (25) for \( p = 0 \) or, equivalently, by the property \( y_n(0) = 0 \). Because of the sum over all \( \{ij\} \) we have

\[
I_{ij}^{(-1)}(x) = \frac{1}{x} \sum_{i,j=0}^{n+1} 2^{q_i + q_j} (-1)^{i+j} (\delta_i - \delta_j) \quad (36a)
\]

\[
= \frac{1}{x} \sum_{j=0}^{n+1} 2^{q_j} (-1)^j \sum_{i=0}^{n+1} 2^{q_i} (-1)^i \delta_i \quad (36b)
\]

\[
- \frac{1}{x} \sum_{i=0}^{n+1} 2^{q_i} (-1)^i \sum_{j=0}^{n+1} 2^{q_j} (-1)^j \delta_j \quad (36c)
\]

\[
= 0. \quad (36c)
\]

Similarly one obtains for \( I_{ij}^{(0)}(x) \)

\[
I_{ij}^{(0)}(x) = 2 + \ln(x) - 3 \sum_{j=0}^{n+1} 2^q (-1)^{i+j} (\delta_i - \delta_j)^2 \quad = 0. \quad (37)
\]

The last equation vanishes because of Eq. (38) at \( p = 0 \) or at \( p = 1 \). This is because \( (\delta_i - \delta_j)^2 = \delta_i^2 + \delta_j^2 - 2\delta_i \delta_j \). Eq. (38) has to hold for \( p = 0 \) and \( p = 1 \) because these values fulfill \( p \leq m \) since \( m \geq 1 \) is required by (13) for \( \alpha = 2 \).
IV. RELEVANT TERMS AND FINAL EQUATIONS

Eqs. 29-33 provide the analytical results for $I_n$. One further simplification stems from the fact that $I_n$ is real. Hence only the real parts of the summands in 29-33 need to be included since the imaginary parts cancel. We analyze the case $\alpha \in \mathbb{N}_0$, where we distinguish even and odd exponents, and the case $\alpha \notin \mathbb{N}_0$ separately.

A. Integer Exponent

c. $\alpha$ even. We use $\Delta_{ij} := i\varphi_{ij} - 0^+$ with $\varphi_{ij} = \delta_i - \delta_j$ and $\ln(\text{Re} e^{i\theta}) = \ln(r) + i\theta$ with $r > 0$ and $|\theta| < \pi$ to obtain

$$\text{Re} \Delta_{ij}^\alpha \ln(-\Delta_{ij}) = (-1)^{\alpha/2} \varphi_{ij}^\alpha \text{Re} \left( \ln |\varphi_{ij}| - i\frac{\pi}{2} \text{sgn} \varphi_{ij} \right)$$

$$= (-1)^{\alpha/2} \varphi_{ij}^\alpha \ln |\varphi_{ij}|.$$  (38)

The sum over all $i \neq j$ as required by 33 reads

$$I_{\text{even}} = \frac{(-1)^{1+\frac{\pi}{2}}}{\alpha!} \sum_{i,j=0}^{n+1} 2^{n+\eta_i} (-1)^{i+j} |\delta_i - \delta_j|\alpha \ln |\delta_i - \delta_j|.$$  (39)

d. $\alpha$ odd. Starting from

$$\text{Re} \Delta_{ij}^\alpha \ln(-\Delta_{ij}) = (-1)^{\frac{\alpha+1}{2}} \varphi_{ij}^\alpha \text{Re} \left[ i \left( \ln |\varphi_{ij}| - i\frac{\pi}{2} \text{sgn} \varphi_{ij} \right) \right]$$

$$= (-1)^{\frac{\alpha+1}{2}} |\varphi_{ij}|^{\alpha} \frac{\pi}{2}.$$  (40)

the final integral $I_n$ becomes

$$I_{\text{odd}} = (-1)^{\frac{\alpha+1}{2}} \frac{\pi}{2} \sum_{i,j=0}^{n+1} 2^{n+\eta_i} (-1)^{i+j} |\delta_i - \delta_j|\alpha.$$  (41)

B. $\alpha$ Non-Integer

For positive non-integer $\alpha$ we consider

$$\text{Re} (-\Delta_{ij})^\alpha = |\varphi_{ij}|^\alpha \text{Re} \left( e^{-i(\pi/2)\alpha} \text{sgn} \varphi_{ij} \right)$$

$$= \cos((\pi/2)\alpha) |\varphi_{ij}|^\alpha.$$  (42a)

which implies

$$I_n^{\text{ni}} = \cos((\pi/2)\alpha) \Gamma(-\alpha)\times \sum_{i,j=0}^{n+1} 2^{n+\eta_i} (-1)^{i+j} |\delta_i - \delta_j|^{\alpha}.$$  (43)

where the superscript ‘ni’ of $I_n^{\text{ni}}$ stands for ‘non-integer’.

V. NUMERICAL RESULTS

The power law optimized dynamical decoupling (PLODD) is a batch-optimized sequence depending on the exponent $\alpha$ only. For various values of $\alpha$, we numerically
solve the system of non-linear equations

\[
0 = \sum_{j=1}^{n+1} 2^q (-1)^j \delta_j^p \tag{44a}
\]

\[
0 = \frac{\partial}{\partial \delta_j} \left[ I_n - \sum_{i=1}^{[\alpha/2]} \lambda_i \frac{\partial y_n(z)}{\partial z} \right]_{z=0} \tag{44b}
\]

where \( p \in \{1, \ldots, \lceil \frac{\alpha}{2} \rceil \} \); here \( \lceil x \rceil \) stands for the largest integer not larger than \( x \in \mathbb{R} \) and \( [\alpha/2] \) results from \( \lceil x \rceil \). The prefactor \( I_n \) is computed analytically both in the case of integer and of non-integer values of \( \alpha \); it is given in Eqs. \( \textbf{59} \) and \( \textbf{43} \).

In the sequel, we restrict ourselves to symmetric sequences for two reasons. First, the main results in dynamical decoupling are derived for symmetric sequences. Second, we searched for asymmetric optimized sequences for small number of pulses, but those sequences found did not perform better than the symmetric ones. Here we focus on symmetric sequences fulfilling \( \delta_{n+1-j} = 1 - \delta_j \). In this case one has to deal with a system of \( n/2 + [\alpha/2] \) equations, solved for \( n/2 \) variables \( \{\delta_j\} \) and \( [\alpha/2] \) Lagrange multipliers \( \lambda_n \). For example, for \( \alpha = 4 \) the system consists of \( n/2 + 2 \) equations.

Figure 2 shows the resulting PLODD sequences for \( \alpha = 4 \) for various number of pulses \( n \). The PLODD sequences are very close to the CPMG ones. We recall that \( \delta_{\text{CPMG}} = (2j - 1)/2n \). No relevant dependence of the PLODD instants as functions of the number of pulses \( n \) can be observed. The concatenated sequence CDD for pure dephasing is also shown for comparison for \( n = 10 \). We recall its recursion \( p_{n+1}^{\text{CDD}} = p_n^{\text{CDD}} X p_n^{\text{CDD}} \) for even \( n \) while \( p_{n+1}^{\text{CDD}} = p_n^{\text{CDD}} p_n^{\text{CDD}} \) holds for odd \( n \); \( p_0 \) stands for the free evolution without pulse.

In Fig. 3 the evaluation of the prefactor \( I_n \) shows that PLODD performs slightly better than CPMG for \( \alpha = 4 \) while for \( \alpha = 2 \) the data for PLODD and for CPMG coincide. It is interesting to notice how the performance changes with \( \alpha \). For \( \alpha = 2 \) we see that CDD and UDD provide almost the same results while for \( \alpha = 4 \) UDD performs better than CDD, though still outperformed by CPMG and PLODD. In addition, Fig. 3 indicates that \( I_n \) decreases if \( \alpha \) increases. We will come back to this point below.

The log-log plot in Fig. 5 shows that \( I_n \) scales like a power law in \( n \). The regression \( \ln I_n = a_1 \ln n + a_0 \) yields \( a_0 = -(2.33 \pm 0.01) \) and \( a_1 = -(3.041 \pm 0.003) \) for PLODD and \( a_0 = -(2.231 \pm 0.009) \) and \( a_1 = -(3.062 \pm 0.003) \) for CPMG. We can compare these results with Eq. \( \text{(25)} \) in Ref. \( \text{25} \) derived by Cywiński et al. Cywiński’s formula was derived for a \textit{de facto} infinite UV cutoff for \( 1.5 \leq \alpha \leq 2.5 \) (or \( 0.5 \leq \alpha_{\text{Cyw}} \leq 1.5 \) in the notation of Ref. \( \text{25} \)). It shows that \( \chi(t) \) scales like \( n^{\alpha-1} \).

As a further check we calculated \( I_n \) versus \( n \) for CPMG for \( 1/f \) noise, i.e., \( \alpha = 2 \). We find \( a_1 = -(0.9899 \pm 0.0008) \) and \( a_0 = -(0.199 \pm 0.002) \), which is close to the corresponding value \( \ln C_1 \simeq -0.163 \) reported in Ref. \( \text{25} \).

Cywiński et al. concluded that in the range \( 0.5 \leq \alpha_{\text{Cyw}} \leq 1.5 \) CPMG is to be preferred over UDD for the prolongation of qubit coherence. The UDD outperforms the other sequences in the range where a finite UV cutoff makes itself felt. Our systematic minimization confirms the results by Cywiński et al. It extends them by putting them on a systematic basis leading to the optimum power law dynamic decouling and because a larger range of exponents is treated.

If we consider higher values of \( \alpha \), the PLODD sequence approaches the UDD one. This is illustrated in Fig. 4. The instants of the PLODD sequence appear to be bounded from below by the instants of the CPMG sequence and from above by the those of the UDD one. For \( \alpha \geq 6 \) CPMG does not satisfy the condition \( \text{(13)} \) any more which is required for the convergence of \( \chi(t) \) so that no comparison to PLODD or UDD is possible. For small values of \( \alpha, [\alpha/2] \) is also small. This implies that the conditions \( \text{(11a)} \) are less important than the conditions \( \text{(14d)} \) resulting from the minimization of the prefactor \( I_n \). This finding confirms what was already expected from studies on UDD \( \text{13, 22, 22, 25} \), namely that the suppression of decoherence is more efficient for baths with a hard cutoff.

As \( \alpha \) increases the PLODD sequences tend to coincide with the UDD sequences. We computed the maximum difference between the \( \{\delta_i\} \) of the PLODD and of the UDD as a function of \( \alpha \). The results are depicted in Fig. 6. Clearly, the maximum difference decreases as \( \alpha \) increases. This supports that the PLODD tends to recover the UDD for large values of \( \alpha \). This can also be seen in Fig. 4.

The inset of Fig. 5 shows that \( \ln I_n \) decreases linearly with \( \alpha \) for fixed values of \( n \). Combined with the power law scaling shown in Fig. 8 we deduce that

\[
I_n \propto (C_n, \alpha/n)^{\alpha-1} \tag{45}
\]
investigated for various powers ($\alpha$ holds for the PLODD sequences where the factor of the inset is in logarithmic scale. Our approach extends previous results in several ways. This is that the convergence of the decoherence function is depicted. Note that the $y$ axis of the inset is in logarithmic scale.

holds for the PLODD sequences where the factor $C_{n,\alpha}$ depends only very weakly on $n$ and $\alpha$.

VI. CONCLUSIONS

We analyzed the supression of decoherence by means of sequences of instantaneous $\pi$ pulses. The work horse is the spin-boson model with pure dephasing which can be treated analytically. The sequences are optimized for power law spectra. The main difference to the already known optimized sequences, for instance UDD or OFDD, is that the convergence of the decoherence function $\chi(t)$ is investigated for various powers ($\alpha$) of the noise spectrum. Our approach extends previous results in several ways.

The OFDD sequences proposed by Uys et al. are optimized for a constant spectrum ($\alpha = 1$ in our notation) with finite UV cutoff [22]. In our study we sent the UV cutoff to infinity and treated general power law spectra characterized by the exponent $\alpha > 0$. Hence the proposed PLODD sequences are optimized for arbitrary, but fixed, exponent. They are universal in the sense that their relative switching instants $\delta_j = t_j/t$ depend only on $\alpha$, but not on the total duration $t$ of the sequence.

In their investigation of classical noise with exponents $\alpha \in \{1.5, 2.5\}$, Cywiński et al. observed that the well-known CPMG sequence works well in the regime where the UV cutoff is infinite for practical purposes. The UDD does not provide an improvement [23]. One of the authors generalized this investigation to the quantum mechanical spin-boson model and cutoffs with arbitrary power law behavior [13].

In the present work we extended these findings further by the systematic optimization of the sequence on the basis of analytical results for arbitrary power law spectra. The softer the UV behavior of the power law spectrum is, i.e., the smaller its exponent $\alpha$ is, the more the PLODD approaches the CPMG. Vice versa, the harder the UV behavior of the power law spectrum is, i.e., the larger its exponent $\alpha$ is, the more the PLODD approaches the UDD.

Hence, the findings of previous investigations are corroborated. There is no completely different sequence which displays a significantly better performance for pure dephasing other than PLODD. The PLODD has the limiting cases CPMG (soft UV behavior) and UDD (hard UV behavior).

We also investigated how the decoherence function $\chi(t)$ scales with $\alpha$ and $n$, the number of pulses. From Eqs. (14) and (45) we obtain

$$\chi(t) \propto n(C_{n,\alpha} t/n)^\alpha,$$

which generalizes the result in Ref. [25] to arbitrary exponent and a quantum mechanical model. Here $C_{n,\alpha}$ is a factor which depends only weakly on $n$ and $\alpha$.

We reckon that the results of this work represent a useful contribution to the technique of dynamic decoupling. The optimization of the pulse sequence in relation to the specific baths is of vital importance in many applications in high precision nuclear magnetic resonance and quantum information processing.

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