Quadratic Dynamical Decoupling: Universality Proof and Error Analysis

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We prove the universality of the generalized QDD$_{N_1 N_2}$ (quadratic dynamical decoupling) pulse sequence for near-optimal suppression of general single-qubit decoherence. Earlier work showed numerically that this dynamical decoupling sequence, which consists of an inner Uhrig DD (UDD) and outer UDD sequence using N_1 and N_2 pulses respectively, can eliminate decoherence to $\mathcal{O}(T^N)$ using $\mathcal{O}(N^2)$ unequally spaced "ideal" (zero-width) pulses, where T is the total evolution time and $N = N_1 = N_2$. A proof of the universality of QDD has been given for even N_1. Here we give a general universality proof of QDD for arbitrary N_1 and N_2. As in earlier proofs, our result holds for arbitrary bounded environments. Furthermore, we explore the single-axis (polarization) error suppression abilities of the inner and outer UDD sequences. We analyze both the single-axis QDD performance and how the overall performance of QDD depends on the single-axis errors. We identify various performance effects related to the parities and relative magnitudes of N_1 and N_2. We prove that using QDD$_{N_1 N_2}$ decoherence can always be eliminated to $\mathcal{O}(T^{\min\{N_1,N_2\}})$.

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I. INTRODUCTION

The inevitable coupling between a quantum system and its environment, or bath, typically results in decoherence [1]. It is essential in quantum information processing (QIP) to find protection against decoherence, as it leads to computational errors which can quickly eliminate any quantum advantage [2, 3]. A powerful technique that can be used to this end, adapted from nuclear magnetic resonance (NMR) refocusing techniques developed since the discovery of the spin echo effect [4, 5], is dynamical decoupling (DD) [6]. It mitigates the unwanted system-bath interactions through the application of a sequence of short and strong pulses, acting purely on the system. DD is an open-loop technique which works when the bath is non-Markovian [1], and bypasses the need for measurement or feedback, in contrast to closed-loop quantum error correction (QEC) [7]. However, while QEC can be made fault tolerant [8, 9], it is unlikely that this holds for DD as a stand-alone method, or that it holds for any other purely open-loop method, for that matter [10]. This notwithstanding, DD can significantly improve the performance of fault tolerant QEC when the two methods are combined [11].

DD was first introduced into QIP in order to preserve single-qubit coherence within the spin-boson model [12–14]. It was soon generalized via a dynamical group symmetrization framework to preserving the states of open quantum systems interacting with arbitrary (but bounded) environments [15, 16]. These early DD schemes work to a given low order in time-dependent perturbation theory (e.g., the Magnus or Dyson expansions [17]). Namely, the effective system-bath interaction following a DD pulse sequence lasting for a total time T only contains terms of order T^{N+1} and higher, where typically N was 1 for the early DD schemes. For general N this is called $N^{\rm th}$-order decoupling. Concatenated DD (CDD) [18], where a given pulse sequence is recursively embedded into itself, was the first explicit scheme capable of achieving arbitrary order decoupling, i.e., CDD allows N to be tuned at will [19]. CDD has been amply tested in recent experimental studies [20–24], and demonstrated to be fairly robust against pulse imperfections. However, the number of pulses CDD requires grows exponentially with N. In order to implement scalable QIP it is desirable to design efficient DD schemes which have as few pulses as possible.

For the one qubit pure dephasing spin-boson model, Uhrig discovered a DD sequence (UDD) which is optimal in the sense that it achieves Nth order decoupling with the smallest possible number of pulses, N or $N+1$, depending on whether N is even or odd [25]. The key difference compared to other DD schemes is that in UDD the pulses are applied at non-uniform intervals. This optimal pulse sequence had also been noticed in [26] for $N \leq 5$. A scheme to protect a known two-qubit entangled state using UDD was given in Ref. [27]. UDD was conjectured to be model-independent ("universal") with an analytical verification up to $N = 9$ [28] and $N = 14$ [29]. A general proof of universality of the UDD sequence was first given in [30] (see also Ref. [31] for an alternative proof). The performance of the UDD sequence was the subject of a wide range of recent experimental studies [21, 32–36]. An interesting application was to the enhancement of magnetic resonance imaging of structured materials such as tissue [37]. However, one conclusion from some of these studies is that the superior convergence of UDD compared to CDD comes at the expense of lack of robustness to pulse imperfections. It is possible

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that recent theoretical pulse shaping developments [38, 39], designed to replace ideal, instantaneous pulses with realistic pulses of finite duration and amplitude while maintaining the suppression properties of UDD, will lead to improved experimental robustness.

The UDD sequence is effective not only against pure dephasing but also against longitudinal relaxation of a qubit coupled to an arbitrary bounded environment [30]. That is, UDD efficiently suppresses pairs of single-axis errors. However, it cannot overcome general, three-axis qubit decoherence. The reason is that UDD uses a single pulse type (e.g., pulses along the x-axis of the qubit Bloch sphere), and system-bath interactions which commute with this pulse type are unaffected by the sequence.

Combining orthogonal single-axis CDD and UDD sequences (CUDD) reduces the number of control pulses required for the suppression of general single-qubit decoherence compared to two-axis CDD [40]. However, CUDD still requires an exponential number of pulses. This scaling problem was overcome with the introduction of the quadratic DD (QDD) sequence by West *et al.*, which nests two UDD sequences with different pulse types and different numbers of pulses N_1 and N_2 [41]. We denote this sequence by $\mathrm{QDD}_{N_1N_2}$, where N_1 and N_2 are the numbers of pulses of the inner and outer UDD sequences, respectively. $\mathrm{QDD}_{N,N}$ (where the inner and outer UDD sequences have the same decoupling order) was conjectured to suppress arbitrary qubit-bath coupling to order N by using $\mathcal{O}(N^2)$ pulses, an exponential improvement over all previously known DD schemes for general qubit decoherence [41]. This conjecture was based on numerical studies for $N \leq 6$ [41], and these were recently extended to $N \leq 24$ [42], in support of the conjecture. An early argument for the universality and performance of QDD (which below we refer to as "validity of QDD"), based on an extension of UDD to analytically time-dependent Hamiltonians [43], fell short of a proof since the effective Hamiltonian resulting from the inner UDD sequences in QDD is not analytic.

The problem of finding a proof of the validity of QDD was first successfully addressed by Wang & Liu [44], though not in complete generality, as we explain below. In fact Ref. [44] considered the more general problem of protecting a set of qubits or multilevel systems against arbitrary system-bath interactions, using a nested UDD (NUDD) scheme, a generalization of QDD to multiple nested UDD sequences. This problem was also studied, for two qubits, by Mukhtar *et al.*, whose numerical results showed, for their specific choice of pulse operators, that the ordering of the nested UDD sequences impacts performance [45]. Wang & Liu's proof is based on the idea of using mutually orthogonal operation (MOOS) sets—mutually commuting or anti-commuting unitary Hermitian system operators—as control pulses [44] (the ordering effect observed in Ref. [45] disappears when using MOOS sets). As in QDD, the decoupling orders of the nested UDD sequences in NUDD can be different, so that different error types can be removed to different orders. Wang & Liu proved the validity of the general QDD/NUDD scheme when the order of all inner UDD sequences is *even* (the order of the outermost sequence can be even or odd) [44]. Their proof is based on MOOS set preservation, and does not apply to QDD, or more generally NUDD, when the order of at least one of the inner UDD sequences is odd. In addition, Wang & Liu pointed out that there are $\mathrm{QDD}_{N_1N_2}$ examples showing that the outer level UDD sequence does not work "as expected" (i.e., does not suppress errors to its order) if N_1 is odd and $N_1 < N_2$. Thus their proof left the actual suppression order of QDD/NUDD with odd order UDD at the inner levels as an open question.

This problem was addressed numerically in Ref. [42], which studied the performance of $\mathrm{QDD}_{N_1N_2}$ for all three single-axis errors. The numerical results show that the suppression ability of the outer UDD sequence is indeed hindered by the inner UDD sequence if N_1 is odd and, surprisingly, smaller than *half* of the order of the outer level UDD sequence. Moreover, Ref. [42] reported that the suppression order of the system-bath interaction which anti-commutes with the pulses of both the inner and outer sequences depends on the parities of both N_1 and N_2.

In this work we provide a complete proof of the validity of $\mathrm{QDD}_{N_1N_2}$. In particular, we also prove the case of odd N_1 left open in Ref. [44]. Moreover, we analyze the single-axis error suppression abilities of both the inner and outer UDD sequences, and thus provide analytical bounds in support of the numerical results of Ref. [42].

We show that the single-axis error which anti-commutes with the pulses of the inner sequence but commutes with those of the outer sequence is always suppressed to the expected order (N_1). The suppression of the two other single-axis errors (the one which commutes with the inner sequence pulses but anti-commutes with the outer sequence pulses, and the one which anti-commutes with both), is more subtle, and depends on the relative size and parity of N_1 and N_2.

Specifically, we show that when N_1 is even, $\mathrm{QDD}_{N_1N_2}$ always achieves at least the expected decoupling order, irrespective of the relative size of N_1 and N_2. However, when N_1 is odd and $N_1 < N_2 - 1$, we show that the decoupling order of the error which commutes with the inner sequence pulses but anti-commutes with those of the outer sequence, is at least $N_1 + 1$, smaller than the expected suppression order (N_2). Nevertheless, for odd N_1 and $N_1 \geq N_2 - 1$, the outer UDD sequence always suppresses the error which commutes with the inner sequence pulses but anti-commutes with those of the outer sequence to the expected order (N_2).

One might expect that the error which anti-commutes with the pulses of both the inner and outer sequences can be suppressed by both sequences. In other words, one might expect this error to be removed at least up to order $\max[N_1, N_2]$. However, we show that this expectation is fulfilled only when N_1 is even. When N_1 is odd, it determines the suppression order. However, interestingly, the parity of N_2 also plays a role, namely, when it is odd the suppression order is one order higher than when N_2 is even.

Despite this complicated interplay between the orders of the inner and outer UDD sequences, resulting in the outer sequence not always achieving its expected decoupling order when N_1 is odd, we show that, overall, $\mathrm{QDD}_{N_1N_2}$ always suppresses all single-qubit errors at least to order $\min[N_1, N_2]$.

A complete summary of our results for the different single-axis suppression orders under $\mathrm{QDD}_{N_1N_2}$ is given in Table IV. Our analytical results are in complete agreement with the numerical findings of Ref. [42], but our proof method underestimates the suppression of of the error which commutes with the inner sequence pulses but anti-commutes with those of the outer sequence: for odd N_1 we find a decoupling order of $\min[N_1+1, N_2]$, while the numerical result is $\min[2N_1+1, N_2]$ for $N_1, N_2 \leq 24$. Explaining this discrepancy is thus still an open problem.

The structure of the paper is as follows. The model of general decoherence of one qubit in the presence of instantaneous QDD pulses is defined in Sec. II. The QDD theorem is stated there as well. We prove the QDD theorem in Sec. III and Sec. IV. A comparison between the numerical results of Ref. [42] and our theoretical bounds is presented in Sec. V. We conclude in Sec. VI. The appendix provide additional technical details.

II. SYSTEM-BATH MODEL AND THE QDD SEQUENCE

A. General $\mathrm{QDD}_{N_1N_2}$ scheme

We model general decoherence on a single qubit via the following Hamiltonian:

$$H = J_0 I \otimes B_0 + J_X \sigma_X \otimes B_X + J_Y \sigma_Y \otimes B_Y + J_Z \sigma_Z \otimes B_Z, \tag{1}$$

where B_λ, $\lambda \in \{0, X, Y, Z\}$, are arbitrary bath-operators with $\|B_\lambda\| = 1$ (the norm is the largest singular value), the Pauli matrices, σ_λ, $\lambda \in \{X, Y, Z\}$, are the unwanted errors acting on the system qubit, and J_λ, $\lambda \in \{0, X, Y, Z\}$, are bounded coupling coefficients between the qubit and the bath.

The $\mathrm{QDD}_{N_1N_2}$ pulse sequence is constructed by nesting a Z-type UDD_{N_1} sequence, designed to eliminate the longitudinal relaxation errors $\sigma_X \otimes B_X$ and $\sigma_Y \otimes B_Y$ up to order T^{N_1+1} by using N_1 or N_1+1 pulses, with an X-type UDD_{N_2} sequence, designed to eliminate the pure dephasing error $\sigma_Z \otimes B_Z$ up to order T^{N_2+1} by using N_2 or N_2+1 pulses. The nesting order does not matter for our analysis, so without loss of generality we choose Z-type UDD_{N_1} to be the inner sequence and X-type UDD_{N_2} to be the outer sequence. We use the notation X and Z to denote control pulses, to distinguish the same operators from the unwanted errors denoted by the Pauli matrices. We also sometimes use the notation σ_0 for the 2×2 identity matrix I.

The X-type UDD_{N_2} pulses comprising the outer layer of the $\mathrm{QDD}_{N_1N_2}$ sequence are applied at the original UDD_{N_2} timing with total evolution time T, $t_j = T\eta_j$ where η_j is the normalized UDD timing (or the normalized $\mathrm{QDD}_{N_1N_2}$ outer sequence timing),

$$\eta_j = \sin^2 \frac{j\pi}{2(N_2+1)} \tag{2}$$

with $j = 1, 2, \ldots, \overline{N}_2$ where $\overline{N}_2 = N_2$ if N_2 even and

	inner order N_1		outer order N_2	
	even	odd	even	odd
no. of pulses	N_1	N_1+1	N_2	N_1+1
no. of intervals	N_1+1	N_1+1	N_2+1	N_2+1

TABLE I: Inner and outer sequence orders N_1 and N_2 *vs* the number of pulses and pulse intervals in the inner and outer sequences.

$\overline{N}_2 = N_2 + 1$ if N_2 odd. The additional pulse applied at the end of the sequence when N_2 is odd, is required in order to make the total number of X pulses-type even, so that the overall effect of the X-type pulses at the final time T will be to leave the qubit state unchanged. Note that it is the relative size of the pulse intervals that matters for error cancellations in UDD, not the precise pulse application times. Hence, the most relevant quantities for the outer level UDD_{N_2} are the N_2+1 normalized UDD_{N_2} pulse intervals (or the normalized $\mathrm{QDD}_{N_1N_2}$ outer pulse intervals),

$$s_j \equiv \frac{\tau_j}{T} = \eta_j - \eta_{j-1} \tag{3a}$$

$$= \sin\frac{\pi}{2(N_2+1)} \sin\frac{(2j-1)\pi}{2(N_2+1)} \tag{3b}$$

where $\tau_j \equiv t_j - t_{j-1}$ is the actual pulse interval.

The Z-type pulses of the inner level UDD_{N_1}, applied from t_{j-1} to t_j, are executed at times

$$t_{j,k} = t_{j-1} + \tau_j \sin^2 \frac{k\pi}{2(N_1+1)} \tag{4}$$

with N_1+1 pulse intervals

$$\tau_{j,k} \equiv t_{j,k} - t_{j,k-1}. \tag{5}$$

Even though adding an additional Z-type pulse to the end of each inner sequence with odd N_1 is not required (since instead one can add just one additional Z-type pulse at the end of the $\mathrm{QDD}_{N_1N_2}$ sequence to ensure that the total number of Z pulses at the final time T is even), for simplicity of our later analysis, we let $k = 1, 2, \ldots \overline{N}_1$ where $\overline{N}_1 = N_1$ if N_1 even and $\overline{N}_1 = N_1 + 1$ if N_1 odd. The corresponding normalized $\mathrm{QDD}_{N_1N_2}$ inner pulse timings are

$$\eta_{j,k} \equiv \frac{t_{j,k}}{T} = \eta_{j-1} + s_j \sin^2 \frac{k\pi}{2(N_1+1)} \tag{6}$$

with the normalized $\mathrm{QDD}_{N_1N_2}$ inner pulse interval $\frac{\tau_{j,k}}{T} = s_j \tilde{s}_k$, where $\tilde{s}_k$ is the normalized UDD_{N_1} pulse interval and is the same function as s_j but with different decoupling order N_1. The first subindex stands for the outer interval while the second subindex stands for the inner interval. Moreover, by definition, we have

$$\eta_j = \eta_{j,N_1+1} = \eta_{j+1,0}. \tag{7}$$

To summarize, the evolution operator at the final time T, at the completion of the $\text{QDD}_{N_1N_2}$ sequence, is

$$U(T) = X^{N_2} U_Z(\tau_{N_2+1}) X \cdots X U_Z(\tau_2) X U_Z(\tau_1), \quad (8)$$

with

$$U_Z(\tau_j) = Z^{N_1} U_f(\tau_{j,N_1+1}) Z \cdots Z U_f(\tau_{j,2}) Z U_f(\tau_{j,1}) \quad (9)$$

being the inner UDD_{N_1} sequence evolution, and with U_f being the pulse-free evolution generated by H [Eq. (1)]. Table I summarizes how the number of pulses and pulse intervals in the inner and outer sequences depend on the inner and outer sequence orders N_1 and N_2.

B. Toggling frame

Our QDD proof will be done in the toggling frame. Since our analysis is based on an expansion of powers of the total time T, most quantities we will deal with are functions of the normalized total time 1.

The normalized control Hamiltonian with $\eta \equiv \frac{t}{T}$ is given by,

$$H_c(\eta) = \frac{\pi}{2}[X \sum_{j=1}^{\overline{N}_2} \delta(\eta - \eta_j) + Z \sum_{j=1}^{N_2+1} \sum_{k=1}^{\overline{N}_1} \delta(\eta - \eta_{j,k})]. \quad (10)$$

The normalized control evolution operator,

$$U_c(\eta) = \widehat{T} \exp[-i \int_0^\eta H_c(\eta')\, d\eta'], \quad (11)$$

where $\widehat{T}$ denotes time-ordering, is either I or Z in the odd j outer intervals,

$$\begin{aligned} U_c(\eta) &= I, & [\eta_{j,2\ell}, \eta_{j,2\ell+1}) \quad & (12a)\\ &= Z, & [\eta_{j,2\ell+1}, \eta_{j,2\ell+2}), \quad & (12b) \end{aligned}$$

while in the even j outer intervals,

$$\begin{aligned} U_c(\eta) &= X, & [\eta_{j,2\ell}, \eta_{j,2\ell+1}) \quad & (13a)\\ &= Y, & [\eta_{j,2\ell+1}, \eta_{j,2\ell+2}). \quad & (13b) \end{aligned}$$

Accordingly, the normalized Hamiltonian in the toggling frame for the single-qubit general decoherence model,

$$\begin{aligned} \widetilde{H}(\eta) &= U_c(\eta)^\dagger H U_c(\eta) & (14a)\\ &= f_0 J_0 I \otimes B_0 + f_x(\eta) J_x \sigma_X \otimes B_X & (14b)\\ &\quad + f_y(\eta) J_y \sigma_Y \otimes B_Y + f_z(\eta) J_z \sigma_Z \otimes B_Z, \end{aligned}$$

has four different normalized $\text{QDD}_{N_1N_2}$ modulation functions,

$$\begin{aligned} f_0 &= 1 & [0, 1,), \quad & (15a)\\ f_z(\eta) &= (-1)^{j-1} & [\eta_{j-1}, \eta_j), \quad & (15b)\\ f_x(\eta) &= (-1)^{k-1} & [\eta_{j,k-1}, \eta_{j,k}), \quad & (15c)\\ f_y(\eta) &= (-1)^{k-1}(-1)^{j-1} & [\eta_{j,k-1}, \eta_{j,k}), \quad & (15d)\\ &= f_x(\eta) f_z(\eta) & & (15e) \end{aligned}$$

unlike the single-qubit pure dephasing case, which has only two UDD modulation functions. Because the Z-type pulses on the inner levels anti-commute with the errors σ_X and σ_Y and commute with σ_Z, the modulation functions $f_x(\eta)$ and $f_y(\eta)$ switch sign with the inner interval index k while $f_z(\eta)$ is constant inside each outer interval. On the other hand, the outer X-type pulses anti-commute with the errors σ_Z and σ_Y and commute with the error σ_X, so both $f_z(\eta)$ and $f_y(\eta)$ switch sign with the outer interval index j,while $f_x(\eta)$ doesn't depend on the outer index j.

Each $\text{QDD}_{N_1N_2}$ modulation function $f_\lambda(\eta)$ can be separated naturally as

$$f_\lambda(\eta) = f_{\tilde{\alpha}}(\eta) f_{\tilde{\beta}}(\eta) \quad (16)$$

where $f_{\tilde{\alpha}}(\eta)$ describes the behaviour of $f_\lambda(\eta)$ inside each outer interval and $f_{\tilde{\beta}}(\eta)$ describes the behaviour of $f_\lambda(\eta)$ when the outer interval index j changes. In fact $f_{\tilde{\beta}}(\eta)$ is identified as the normalized UDD_{N_2} modulation function and $f_{\tilde{\alpha}}(\eta)$ covers $N_2 + 1$ cycles of UDD_{N_1} modulation functions with different durations. However, up to a scale factor $f_{\tilde{\alpha}}(\eta)$ is the same function in each of these cycles. Therefore, instead of $f_{\tilde{\alpha}}(\eta)$, we use one cycle of the normalized UDD_{N_1} modulation function denoted as $f_\alpha(\eta)$ to denote the effective inner function of $f_\lambda(\eta)$. Likewise, since $f_{\tilde{\beta}}(\eta)$ is constant inside any jth outer interval s_j, it can be viewed as a function of the outer interval j, and we replace $f_{\tilde{\beta}}(\eta)$ by the notation $f_\beta(j)$. In particular, $f_{\beta=z}(j) = (-1)^{j-1}$. Table II lists the effective inner functions f_α and outer functions f_β for all $\text{QDD}_{N_1N_2}$ modulation functions f_λ and will be used in Sec. III.

f_λ	(f_α, f_β)
f_x	(f_x, f_0)
f_y	(f_x, f_z)
f_z	(f_0, f_z)
f_0	(f_0, f_0)

TABLE II: The effective inner functions f_α and outer functions f_β of the normalized $\text{QDD}_{N_1N_2}$ modulation functions f_λ. Functions in the first column are the normalized $\text{QDD}_{N_1N_2}$ modulation function and those in the second column are the normalized UDD_{N_1} and UDD_{N_2} modulation functions respectively.

In the toggling frame, the unitary evolution operator which

Components \\$n$th order QDD$_{N_1N_2}$ coefficients:	$a_{\lambda_n\cdots\lambda_1=X}$		$a_{\lambda_n\cdots\lambda_1=Y}$		$a_{\lambda_n\cdots\lambda_1=Z}$	
(1) Total # of σ_X and $f_x(\eta)$	odd	even	even	odd	even	odd
(1) Total # of σ_Y and $f_y(\eta)$	even	odd	odd	even	even	odd
(1) Total # of σ_Z and $f_z(\eta)$	even	odd	even	odd	odd	even
(2) Total # of effective inner integrand f_x	odd	odd	odd	odd	even	even
(3) Total # of effective outer integrand f_z	even	even	odd	odd	odd	odd

TABLE III: Number combinations of Pauli matrices (or modulation functions) for each error type (or QDD$_{N_1N_2}$ coefficients). For example, when $\lambda_n\cdots\lambda_1 = X$, there are two possibilities, represented in the two corresponding columns in the rows numbered (1): either there is an odd number of σ_X (and $f_x(\eta)$) along with an even number of both σ_Y (and $f_y(\eta)$) and σ_Z (and $f_z(\eta)$) , or there is an even number of σ_X (and $f_x(\eta)$) along with an odd number of both σ_Y (and $f_y(\eta)$) and σ_Z (and $f_z(\eta)$) . Consulting Table II, in the first case there is an odd number of inner integrand f_x functions from $f_x(\eta)$ and an even number of f_x from $f_y(\eta)$, so that the total number of f_x is odd, as indicated in the first entry in row (2). Likewise, in the second case there is an odd number of outer integrand f_z functions from $f_y(\eta)$ and an odd number of f_z from $f_z(\eta)$, so that the total number of f_z is even, as indicated in the second entry in row (3).

contains a whole QDD$_{N_1N_2}$ sequence at the final time T reads

$$\widetilde{U}(T) \;=\; \widehat{T}\exp[-i\int_0^T \widetilde{H}(t)\,dt] \tag{17a}$$

$$\;=\; \widehat{T}\exp[-iT\int_0^1 \widetilde{H}(\eta)\,d\eta]. \tag{17b}$$

We expand the evolution operator $\widetilde{U}(T)$ into the Dyson series of standard time dependent perturbation theory,

$$\widetilde{U}(T) = \sum_{n=0}^{\infty}\sum_{\vec{\lambda}_n}(-iT)^n J_\lambda^{(n)}\sigma_\lambda^{(n)}\otimes B_\lambda^{(n)} a_{\lambda_n\cdots\lambda_1}, \tag{18}$$

where we use the shorthand notation

$$\sum_{\vec{\lambda}_n} \equiv \sum_{\lambda_n\in\{0,X,Y,Z\}}\;\sum_{\lambda_{n-1}\in\{0,X,Y,Z\}}\cdots\sum_{\lambda_1\in\{0,X,Y,Z\}}, \tag{19}$$

and

$$J_\lambda^{(n)} \equiv \prod_{i=1}^n J_{\lambda_i}, \quad \sigma_\lambda^{(n)} \equiv \prod_{i=1}^n \sigma_{\lambda_i}, \quad B_\lambda^{(n)} \equiv \prod_{i=1}^n B_{\lambda_i}. \tag{20}$$

Finally,

$$a_{\lambda_n\cdots\lambda_1} \equiv \int_0^1 d\eta^{(n)}\ldots\int_0^{\eta^{(2)}} d\eta^{(1)}\prod_{\ell=1}^n f_{\lambda_\ell}(\eta^{(\ell)}) \tag{21}$$

is a dimensionless constant we call the nth order normalized QDD$_{N_1N_2}$ coefficient. These coefficients play a key role in the theory as it is their vanishing which dictates the decoupling properties of the QDD sequence.

The subscript of $a_{\lambda_n\cdots\lambda_1}$ represents a product of Pauli matrices, and we shall write $\lambda_n\cdots\lambda_1 = \lambda$ with λ representing the result of the multiplication up to $\pm1, \pm i$. From Eqs. (18)-(21), this subscript indicates not only its associated operator term $\sigma_{\lambda_n}\ldots\sigma_{\lambda_1}\otimes B_{\lambda_n}\cdots B_{\lambda_1}$ but also its n ordered integrands, $f_{\lambda_n}\cdots f_{\lambda_1}$. Moreover, from Table II, one can also deduce the ordered set of effective inner and outer integrands for a given subscript of $a_{\lambda_n\cdots\lambda_1}$.

C. Error terms

Every product of system operators, $\sigma_\lambda^{(n)} = \sigma_{\lambda_n}\cdots\sigma_{\lambda_1}$ can be either I, σ_X, σ_Y or σ_Z. The summands in the expansion (18) of $\widetilde{U}$ can accordingly all be classified as belonging to one of four groups . If $\sigma_\lambda^{(n)} \in \{\sigma_X, \sigma_Y, \sigma_Z\}$ then the corresponding summand in Eq. (18) decoheres the system qubit.

Definition 1. *A single-axis error of order n and type λ is the sum of all terms in Eq.* (18) *with fixed $\sigma_\lambda^{(n)}$ and $\lambda \in \{X,Y,Z\}$.*

In the UDD case Eq. (18) would include just one type of single-axis error [30].

Due to the Pauli matrix identities $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k$ and $\sigma_i^2 = I$, which of the three possible errors a given product $\sigma_\lambda^{(n)}$ becomes is uniquely determined by the parity of the total number of times each Pauli matrix appears in the product. In this sense there are only two possible ways in which each type of error can be generated. Take the error σ_X as an example. One way to generate σ_X is to have an odd number of σ_X operators which generates σ_X itself, along with an even number of σ_Y, an even number of σ_Z, and arbitrary number of I. The other possibility is an odd number of σ_Y with an odd number of σ_Z to generate σ_X, along with an even number of σ_X and arbitrary number of I.

Note that for a given error σ_λ, the parity of the total number of times each modulation function appears in $a_{\lambda_n\cdots\lambda_1=\lambda}$'s integrands $f_{\lambda_n}\cdots f_{\lambda_1}$ is also determined accordingly. For example, consider $\lambda_n\cdots\lambda_1 = Z$. This can be the result of there being an even number of σ_Z [and $f_z(\eta)$] along with an odd number of both σ_X [and $f_x(\eta)$] and σ_Y [and $f_y(\eta)$], a situation summarized in the last column of the block numbered (1) in Table III. In this case, given Table II, the total number of effective inner integrand functions f_x contributed by $f_x(\eta)$ is odd, as is the contribution of effective inner integrand functions f_x from $f_y(\eta)$, so the total number of effective inner integrand functions f_x is even. This situation is summarized by the last "even" entry in row (2) of Table III. This table gives all possible parities of Pauli matrices (or modulation functions) for each type of error (or its associated nth order QDD$_{N_1N_2}$ coefficient). The parity of the total number of identity matrices I (modulation function f_0) is irrelevant for the proof, so is omitted from Table III. With a given number combination of Pauli matrices (or modulation functions) and Table II, one can determine the parity of the total number of effective inner and outer integrands as presented in rows (2) and (3) of Table III. Table III will be referred to often during the proof.

If all of the first Nth order QDD$_{N_1N_2}$ σ_λ coefficients vanish for a given λ, namely $a_{\lambda_n\cdots\lambda_1=\lambda} = 0$ for $n \le N$, we say that the QDD$_{N_1N_2}$ scheme eliminates the error σ_λ to order N, i.e., the error σ_λ is $\mathcal{O}(T^{N+1})$. Naively, one might expect the inner Z-type UDD$_{N_1}$ sequence to eliminate both σ_X and σ_Y errors to order N_1, and the outer X-type UDD$_{N_2}$ sequence to eliminate σ_Z errors and any remaining σ_Y errors to order N_2. The situation is in fact more subtle, and is summarized in the following QDD Theorem whose proof is provided in Sec. III and Sec. IV.

QDD Theorem 1. *Assume that a single qubit is subject to the general decoherence model Eq.* (1). *Then, under the QDD*$_{N_1N_2}$ *sequence Eq.* (8)*, all three types of single-axis errors of order n are guaranteed to be eliminated if $n \le \min[N_1, N_2]$. Higher order single axis errors are also eliminated depending on the parities and relative magnitudes of N_1 and N_2, as detailed in Table IV, the results of which remain valid under any permutation of the labels X, Y, Z along with a corresponding label permutation in Eq.* (8)*.*

Single-axis error type	Inner order N_1	Outer order N_2	Decoupling order
σ_X	arbitrary	arbitrary	N_1
σ_Y	even	even	$\max[N_1, N_2]$
	even	odd	$\max[N_1 + 1, N_2]$
	odd	even	N_1
	odd	odd	$N_1 + 1$
σ_Z	even	arbitrary	N_2
	odd	arbitrary	$\min[N_1 + 1, N_2]$

TABLE IV: Summary of single-axis error suppression. For each error type σ_λ, the nth order QDD$_{N_1N_2}$ coefficients [Eq. (21)] $a_{\lambda_n\cdots\lambda_1=\lambda} = 0\ \forall n \le N$, where N is the decoupling order given in the last column.

An immediate corollary of this Theorem is that the overall error suppression order of QDD$_{N_1N_2}$ is $\min[N_1, N_2]$. This will be reflected in distance or fidelity measures for QDD, such as computed for UDD in Ref. [31].

We shall prove Theorem 1 in two steps. First, in Sec. III we shall prove that for arbitrary values of N_1 and N_2 the QDD$_{N_1N_2}$ sequence eliminates the first N_1 orders of σ_X and σ_Y errors. Secondly, we shall prove that if N_2 is odd, an additional order of the σ_Y error is eliminated, i.e., $N_1 + 1$. We will not show any suppression of the σ_Z error in Sec. III.

Then, in Sec. IV we shall complete the analysis of the effect of the outer sequence, and show that the σ_Z error is suppressed to order N_2 if N_1 is even. If N_1 is odd, σ_Z is suppressed to order N_2 if $N_1 \ge N_2 - 1$, and to order $N_1 + 1$ if $N_1 < N_2 - 1$. Additionally, we show that if N_1 is even, the σ_Y error is suppressed to order N_2, which may be higher than the result of Sec. III alone. Combining the results of the two sections, we find that the error σ_Y is suppressed to order $\max[N_1, N_2]$ if N_2 is even, and to order $\max[N_1 + 1, N_2]$ if N_2 is odd. These results are all summarized in Table IV.

III. SUPPRESSION OF LONGITUDINAL RELAXATION σ_X AND σ_Y

A general proof of the error suppression properties of UDD was first given by Yang & Liu, including for the suppression of longitudinal relaxation errors σ_X and σ_Y [30]. Wang & Liu first proved that the outer sequence does not interfere with the suppression abilities of the inner sequence with the DD pulses chosen as a MOOS set [44]. In this section, we give an alternative non-interference proof which shows explicitly that it is the inner Z-type UDD$_{N_1}$ sequence that makes all longitudinal relaxation related QDD$_{N_1N_2}$ coefficients $a_{\lambda_n\cdots\lambda_1=\sigma_X,\sigma_Y}$ with $n \le N_1$ vanish, regardless of the details of the outer X-type UDD$_{N_2}$ sequence. Moreover, we also show that the outer X-type UDD$_{N_2}$ sequence, when the outer order N_2 is odd, eliminates the σ_Y error to one additional order, i.e., to order $N_1 + 1$. For precise details refer to Table IV.

A. The outer interval decomposition of $a_{\lambda_n\cdots\lambda_1}$

We expect the inner Z-type UDD$_{N_1}$ sequences of QDD$_{N_1N_2}$ to suppress the errors σ_X and σ_Y. Therefore, our strategy for evaluating $a_{\lambda_n\cdots\lambda_1}$ [Eq. (21)] is to split each of its integrals into a sum of sub-integrals over the normalized outer intervals s_j in Eq. (3a). In this way, each resulting segment of $a_{\lambda_n\cdots\lambda_1}$ can be decomposed naturally into an inner part (which contains the action of the inner Z-type UDD$_{N_1}$) times an outer part (which contains the action of the outer X-type UDD$_{N_2}$ sequence). The manner by which the inner Z-type UDD$_{N_1}$ sequences suppress longitudinal relaxations can then be easily extracted.

As we show in Appendix A, after this decomposition $a_{\lambda_n\cdots\lambda_1}$ can be expressed as

$$a_{\lambda_n\cdots\lambda_1} = \sum_{\{r_\ell=\emptyset,*\}_{\ell=1}^{n-1}} \Phi^{\rm in}(r_n f_{\alpha_n} r_{n-1}\dots f_{\alpha_2} r_1 f_{\alpha_1}) \times$$
$$\Phi^{\rm out}(r_n f_{\beta_n} r_{n-1}\dots f_{\beta_2} r_1 f_{\beta_1}). \tag{22}$$

with $r_n \equiv *$. This is just a compact way of writing multiple nested integrals and multiple summations, with a notation we explain next.

First, f_{α_ℓ} and f_{β_ℓ} are the effective inner and outer functions respectively of $a_{\lambda_n\cdots\lambda_1}$'s ℓth integrand f_{λ_ℓ}. From Table II, the effective inner (outer) function of the normalized QDD$_{N_1N_2}$ modulation functions will be either f_x (f_z) or $f_0 = 1$, the normalized UDD$_{N_1}$ (UDD$_{N_2}$) modulations functions in the generic σ_X (σ_Z) pure bit flip (dephasing) model.

Second, the "inner output function" $\Phi^{\rm in}$ generates all the segments' inner parts via the following mapping,

$$r_\ell f_{\alpha_\ell} \overset{\Phi^{\rm in}}{\longmapsto} \begin{cases} \int_0^1 f_{\alpha_\ell}(\eta^{(\ell)})\, d\eta^{(\ell)} & \text{if } r_\ell = * \\ \int_0^{\eta^{(\ell+1)}} f_{\alpha_\ell}(\eta^{(\ell)})\, d\eta^{(\ell)} & \text{if } r_\ell = \emptyset. \end{cases} \tag{23}$$

For example,

$$\Phi^{\rm in}(*f_{\alpha_2}\emptyset f_{\alpha_1}) = \int_0^1 f_{\alpha_2} d\eta^{(2)} \int_0^{\eta^{(2)}} f_{\alpha_1} d\eta^{(1)}, \tag{24}$$

a term which appears in the expansion of $a_{\lambda_2\lambda_1}$.

From Eq. (23), one can see that r_ℓ determines how the integral of $\eta^{(\ell)}$ relates to the integral of its adjacent variable $\eta^{(\ell+1)}$. For the inner part, the relationship between the integrals of two adjacent variables $\eta^{(\ell+1)}$ and $\eta^{(\ell)}$ is either independent ($r_\ell = *$; they appear in separate integrals) or nested ($r_\ell = \emptyset$; they appear together in a time-ordered pair of integrals).

Third, the outer output function $\Phi^{\rm out}$ generates all the segments' outer parts via the following mapping,

$$r_\ell f_{\beta_\ell} \overset{\Phi^{\rm out}}{\longmapsto} \begin{cases} \sum_{j^{(\ell)}=m}^{j^{(\ell+1)}-1} f_{\beta_\ell}(j^{(\ell)})\, s_{j^{(\ell)}} & \text{if } r_\ell = * \\ f_{\beta_\ell}(j^{(\ell+1)})\, s_{j^{(\ell+1)}} & \text{if } r_\ell = \emptyset \end{cases} \tag{25}$$

where $s_{j^{(\ell)}}$ is the $j^{(\ell)}$th normalized outer interval for variable $\eta^{(\ell)}$, and m indicates that r_ℓ is the mth $*$ in $\{r_n r_{n-1} \ldots r_1\}$, counting from r_1. For $r_n f_{\beta_n}$ with $r_n = *$, the upper limit $j^{(\ell)} = j^{(\ell+1)} - 1$ in Eq. (25) should be replaced by $j^{(n)} = N_2 + 1$. For example,

$$\Phi^{\rm out}(*f_{\beta_3} * f_{\beta_2}\emptyset f_{\beta_1}) = \sum_{j^{(3)}=2}^{N_2+1} f_{\beta_3}(j^{(3)}) s_{j^{(3)}} \times \sum_{j^{(2)}=1}^{j^{(3)}-1} f_{\beta_2}(j^{(2)}) s_{j^{(2)}} f_{\beta_1}(j^{(2)}) s_{j^{(2)}}, \tag{26}$$

a term which appears in the expansion of $a_{\lambda_3\lambda_2\lambda_1}$.

From Eq. (25), r_ℓ indicates the relationship between the outer intervals of two adjacent variables $\eta^{(\ell+1)}$ and $\eta^{(\ell)}$. They can either be time-ordered, namely, in different outer intervals ($r_\ell = *$), or in the same interval ($r_\ell = \emptyset$).

Finally,

$$\sum_{\{r_\ell=\emptyset,*\}_{\ell=1}^{n-1}} \equiv \sum_{r_{n-1}\in\{\emptyset,*\}} \sum_{r_{n-2}\in\{\emptyset,*\}} \cdots \sum_{r_1\in\{\emptyset,*\}} \tag{27}$$

includes all possible integration configurations for $\Phi^{\rm in}$ and all possible summation configurations for $\Phi^{\rm out}$. Each such configuration is determined by a given set $\{*, r_{n-1}, r_{n-2}, \ldots, r_1\}$.

Note that the integration pattern of the inner part determines the summation pattern of the outer part and vice versa. The relation between the inner part and its corresponding outer part comes from the time-ordering condition, $\eta^{(n)} \geq \eta^{(n-1)} \geq \ldots \eta^{(2)} \geq \eta^{(1)}$, because $a_{\lambda_n\cdots\lambda_1}$ comprises n time-ordered integrals. More specifically, if the sub-integrals over any two adjacent variables $\eta^{(\ell)}$ and $\eta^{(\ell+1)}$ are already located in time-ordered, different outer intervals, then the sub-integral over $\eta^{(\ell)}$ is not nested inside the sub-integral over $\eta^{(\ell+1)}$, and its integration domain is the entire outer interval. In contrast, if the sub-integrals over any two adjacent variables $\eta^{(\ell)}$ and $\eta^{(\ell+1)}$ are in the same outer interval, it follows that their sub-integrals are nested due to time-ordering.

B. The inner parts $\Phi^{\rm in}$ and the outer parts $\Phi^{\rm out}$ of $a_{\lambda_n\cdots\lambda_1}$

Consider the argument $r_n f_{\mu_n} r_{n-1} f_{\mu_{n-1}} r_{n-2} \ldots f_{\mu_2} r_1 f_{\mu_1}$ of $\Phi^{\rm in}$ or $\Phi^{\rm out}$, where μ can be α or β in Eq. (22). Define a cluster of f's as a contiguous set of f's connected only by $\emptyset$. Different clusters are separated by $*$. For example, $(f_{\mu_5}) * (f_{\mu_4}\emptyset f_{\mu_3}) * (f_{\mu_2}\emptyset f_{\mu_1})$, where the parentheses indicate clusters. In this manner, each integration or summation configuration $\{*r_{n-1}r_{n-2}\ldots r_1\}$ corresponds to a way in which a set of n functions is separated into clusters.

Suppose that for a given configuration $\{*r_{n-1}r_{n-2}\ldots r_1\}$, the mth inner cluster, counting from right to left, is $f_{\alpha_p}\emptyset f_{\alpha_{p-1}}\emptyset \ldots \emptyset f_{\alpha_q}$, which has $p-q+1$ elements. Likewise, we have the mth outer cluster $f_{\beta_p}\emptyset f_{\beta_{p-1}}\emptyset \ldots \emptyset f_{\beta_q}$. Applying the rule of Eq. (23) to the mth inner cluster, or the rule of Eq. (25) to the mth outer cluster, we then have, respectively

$$* \;\; f_{\alpha_p}\emptyset \ldots \emptyset f_{\alpha_q}(*) \overset{\Phi^{\rm in}}{\longmapsto} \tag{28a}$$

$$\int_0^1 d\eta^{(p)} \int_0^{\eta^{(p)}} d\eta^{(p-1)} \ldots \int_0^{\eta^{(q+1)}} d\eta^{(q)} \prod_{\ell=q}^{p} f_{\alpha_\ell}(\eta^{(\ell)}) \equiv u_{\alpha_p\alpha_{p-1}\ldots\alpha_q} \tag{28b}$$

$$* \;\; f_{\beta_p}\emptyset \ldots \emptyset f_{\beta_q}(*) \overset{\Phi^{\rm out}}{\longmapsto} \sum_{j_m=m}^{j_{m+1}-1} \prod_{\ell=q}^{p} f_{\beta_\ell}(j_m)\, s_{j_m}^{p-q+1} \tag{28c}$$

where if $p = n$, namely the mth group is the last group (counting from right to left), the upper limit $j_{m+1} - 1$ should be replaced by $j_m = N_2 + 1$. Also note that in Eq. (28c) we have replaced $j^{(p)}$ [according to the notation of Eq. (25)] by the cluster index j_m.

Now recall that the outer effective function $f_{\beta_\ell}(j)$ is either $f_0 = 1$ or $f_z(j) = (-1)^{j-1}$. Therefore, if $\prod_{\ell=q}^{p} f_{\beta_\ell}(j_m)$ contains an odd number of $f_z(j_m)$, we have $\prod_{\ell=q}^{p} f_{\beta_\ell}(j_m) = (-1)^{j_m-1}$, otherwise $\prod_{\ell=q}^{p} f_{\beta_\ell}(j_m) = 1$.

Note that the nested integral $u_{\alpha_p\alpha_{p-1}\ldots\alpha_q}$ in Eq. (28a) is just the $(p-q+1)$th order normalized UDD$_{N_1}$ coefficient for the generic σ_X pure bit flip model, because the effective integrands f_{α_ℓ}, either f_x or f_0, are the normalized UDD$_{N_1}$ modulations functions.

We have now assembled the tools to perform the summation implied in Eq. (22), which is the result of the outer interval decomposition. Different clusters, each of which is given in Eqs. (28a) or (28c), are simply multiplied. To illustrate this, the second order normalized QDD$_{N_1N_2}$ coefficients $a_{\lambda_1\lambda_2}$ are listed in Table V.

Error Type	2nd order normalized QDD$_{N_1N_2}$ coefficients
σ_X	$a_{x0} = u_x\, u_0 \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} s_p + u_{x0} \sum_{j=1}^{N_2+1} s_j^2$
	$a_{0x} = u_0\, u_x \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} s_p + u_{0x} \sum_{j=1}^{N_2+1} s_j^2$
	$a_{zy} = u_0\, u_x \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{0x} \sum_{j=1}^{N_2+1} s_j^2$
	$a_{yz} = u_x\, u_0 \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{x0} \sum_{j=1}^{N_2+1} s_j^2$
σ_Y	$a_{y0} = u_x\, u_0 \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} s_p + u_{x0} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{0y} = u_0\, u_x \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{0x} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{zx} = u_0\, u_x \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} s_p + u_{0x} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{xz} = u_x\, u_0 \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{x0} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
σ_Z	$a_{z0} = u_0\, u_0 \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} s_p + u_{00} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{0z} = u_0\, u_0 \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{00} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{xy} = u_x\, u_x \sum_{j=2}^{N_2+1} s_j \sum_{p=1}^{p<j} (-1)^{p-1} s_p + u_{xx} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$
	$a_{yx} = u_x\, u_x \sum_{j=2}^{N_2+1} (-1)^{j-1} s_j \sum_{p=1}^{p<j} s_p + u_{xx} \sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^2$

TABLE V: The outer decomposition form of $a_{\lambda_1\lambda_2}$. For $n = 2$ we have $r_2r_1 = \{**\}$ or $r_2r_1 = \{*\emptyset\}$. The first summand in each line is the result of the $\{**\}$ expansion, the second is the result of the $\{*\emptyset\}$ expansion.

The following lemmas relate the normalized QDD and UDD coefficients. They are easily concluded from Eq. (28a).

Consider a configuration $\{*r_{n-1}r_{n-2}\dots r_1\}$ with m $*$'s. Correspondingly there are m clusters. Each cluster has associated with it a normalized UDD$_{N_1}$ coefficient of order n' equal to the number of elements (f's) in the cluster, and $1 \leq n' < n$. The sum of all the orders is n. Thus:

Lemma 1. *Consider a configuration $\{*r_{n-1}r_{n-2}\dots r_1\}$ with m $*$'s. The corresponding inner part $\Phi^{\rm in}$ of $a_{\lambda_n\cdots\lambda_1}$ [Eq. (22)] is composed of m normalized UDD$_{N_1}$ coefficients whose integrands are the effective inner ones of $a_{\lambda_n\cdots\lambda_1}$, and the sum of whose orders is equal to n.*

In addition, all of the first nth order UDD$_{N_1}$ coefficients, but not order $n+1$ and above, appear in any given nth order QDD$_{N_1N_2}$ coefficient, i.e.,

Lemma 2. *The only UDD$_{N_1}$ coefficients which can appear in all the inner parts $\Phi^{\rm in}$ of the nth order QDD$_{N_1N_2}$ coefficient $a_{\lambda_n\cdots\lambda_1}$ are those whose orders are between 1 and n.*

C. The first N_1 vanishing orders of the single-axis σ_X and σ_Y error due to the inner Z-type UDD$_{N_1}$ sequences

From the second row of Table III, one can see that the total number of f_x's in the effective inner integrands of the coefficients $a_{\lambda_n\cdots\lambda_1=X}$ and $a_{\lambda_n\cdots\lambda_1=Y}$ is odd. Accordingly, no matter how one divides the inner integrands into clusters, there will always be at least one cluster which has an odd number of f_x. Then, from Lemma 1, it follows that all the inner parts $\Phi^{\rm in}$ of $a_{\lambda_n\cdots\lambda_1=X}$ and $a_{\lambda_n\cdots\lambda_1=Y}$ contain one or more UDD$_{N_1}$ coefficients with an odd number of f_x in the integrands. Recall that UDD$_{N_1}$ coefficients $u_{\lambda_m\dots\lambda_1=X}$, i.e., those associated with the error σ_X, contain an odd number of f_x in their integrands. Therefore, we have

Lemma 3. *After outer interval decomposition, all the inner parts of the nth order QDD$_{N_1N_2}$ coefficients $a_{\lambda_n\dots\lambda_1=X}$ and $a_{\lambda_n\dots\lambda_1=Y}$ contain one or more UDD$_{N_1}$ coefficients $u_{\lambda_m\dots\lambda_1=X}$, where $m \leq n$.*

Now recall:

Lemma 4. *(Yang & Liu [30]) The UDD$_{N_1}$ coefficients $u_{\lambda_m\dots\lambda_1=X} = 0$ when $m \leq N_1$.*

It follows from the last two lemmas that all QDD$_{N_1N_2}$ coefficients associated with longitudinal relaxation $a_{\lambda_n\cdots\lambda_1=X}$ or $a_{\lambda_n\cdots\lambda_1=Y}$ with $n \leq N_1$ vanish. Physically, it is clearly the inner Z-type UDD$_{N_1}$ sequence that is responsible for eliminating the single-axis errors $\sigma_X \otimes B_X$ and $\sigma_Y \otimes B_Y$ up to order T^{N_1+1}. The effect of the outer X-type UDD$_{N_2}$ sequence is entirely contained in the outer output function $\Phi^{\rm out}$ in Eq. (22), and consequently does not interfere with the elimination ability of the inner level control Z-type UDD$_{N_1}$, in agreement with [44].

From row 2 of Table III, unlike $a_{\lambda_n\cdots\lambda_1=X,Y}$, all $a_{\lambda_n\cdots\lambda_1=Z}$ contain an even number of effective inner functions f_x. Accordingly, Lemma 3 does not apply to $a_{\lambda_n\cdots\lambda_1=Z}$ and therefore, the argument that all the inner output functions $\Phi^{\rm in}$ of $a_{\lambda_n\cdots\lambda_1}$ are removed by the Z-type UDD$_{N_1}$ sequences cannot be applied to the pure dephasing terms. This is, of course, due to the fact that the inner Z-type sequence commutes with the the pure dephasing error $\sigma_Z \otimes B_Z$. Instead, this error will be suppressed by the outer X-type UDD$_{N_2}$ sequence.

Note that the outer output functions $\Phi^{\rm out}$ of $a_{\lambda_n\cdots\lambda_1}$ [Eq. (22)], which contain the effect of the outer X-type UDD$_{N_2}$ sequence, are expressed in terms of multiple time-ordered summations [Eq. (28c)], which are not easily analyzed using the current method. Therefore, in order to demonstrate the suppression of the pure dephasing error $\sigma_Z \otimes B_Z$, in Sec. IV we shall deal directly with $a_{\lambda_n\dots\lambda_1=Z}$, rather than a separation into inner and outer parts as we have done in this section.

D. One more order of suppression for the single-axis σ_Y error due to the outer X-type UDD$_{N_2}$ sequence when N_2 is odd

In the previous subsection we proved that $a_{\lambda_n \cdots \lambda_1 = Y} = 0$ when $n \leq N_1$. Now we shall show that also $a_{\lambda_{N_1+1} \ldots \lambda_1 = Y}$ vanishes, due to the outer level X-type UDD$_{N_2}$ sequence, for odd N_2. Essentially, as we now explain in detail, this sequence is responsible for eliminating one remaining term in the expansion of $a_{\lambda_{N_1+1} \ldots \lambda_1 = Y}$.

According to Lemma 2, as applied to $a_{\lambda_{N_1+1} \ldots \lambda_1 = Y}$, the only UDD$_{N_1}$ coefficients which can appear are those with order at most $N_1 + 1$. According to Lemma 4 the first N_1 of these UDD coefficients vanish. The only UDD coefficient (in $a_{\lambda_{N_1+1} \ldots \lambda_1 = Y}$) regarding which at this point we have no information is the $N_1 + 1$th, and indeed, it may be nonvanishing. Using the mapping Eq. (28c), we therefore have

$$a_{\lambda_{N_1+1} \ldots \lambda_1 = Y} = u_{\lambda_{N_1+1} \ldots \lambda_1 = X} \sum_{j=1}^{N_2+1} \prod_{\ell=1}^{N_1+1} f_{\beta_\ell}(j)\, s_j^{N_1+1}. \tag{29}$$

We now show that this vanishes due to the outer part.

According to the third row of Table III, all $a_{\lambda_n \cdots \lambda_1 = Y}$ contain an odd number of effective outer functions $f_z(j) = (-1)^{j-1}$. Consequently, we have $\prod_{\ell=1}^{N_1+1} f_{\beta_\ell}(j) = (-1)^{j-1}$ which simplifies the outer part in Eq. (29) to

$$\sum_{j=1}^{N_2+1} (-1)^{j-1} s_j^{N_1+1}. \tag{30}$$

Note that the UDD pulse intervals are time-symmetric (for the proof see Appendix B). Therefore, the UDD$_{N_2}$ outer intervals s_j satisfy

$$s_j = s_{N_2+2-j} \tag{31}$$

If the decoupling order of the outer UDD sequence N_2 is odd then j and $N_2 + 2 - j$ have opposite parities. Accordingly,

$$\begin{aligned} (-1)^{j-1} s_j^{N_1+1} &= (-1)^{j-1} (s_{N_2+2-j})^{N_1+1} \\ &= -(-1)^{N_2+2-j-1} (s_{N_2+2-j})^{N_1+1}. \end{aligned} \tag{32}$$

Thus, when N_2 is odd the outer part Eq. (30) vanishes due to the mutual cancellation of terms with equal magnitude but opposite sign.

This concludes our proof of the error suppression of σ_X and σ_Y errors to order N_1, and of σ_Y to order $N_1 + 1$ when N_2 is odd. This confirms row one of Table IV and row two of the same Table, disregarding for now N_2 in the last column. In the next Section we set out to complete the proof and confirm all claims made in Table IV.

IV. SUPPRESSION OF THE PURE DEPHASING ERROR σ_Z

In this section we focus on the suppression of the pure dephasing error σ_Z by the outer X-type sequence, and also show that σ_Y can be additionally suppressed by the outer sequence to order N_2 when N_1 is even.

To do so, we shall show that if N_1 is even the inner Z-type UDD$_{N_1}$ sequence does not hinder the suppression ability of the Y and Z-type errors by the outer X-type UDD$_{N_2}$ sequence. For odd N_1 we cannot conclude that the inner sequence does not hinder the outer sequence. However, if N_1 is odd, our method does show that the outer sequence suppresses σ_Z at least to order $\min[N_1 + 1, N_2]$.

A. Linear change of variables

To avoid having to analytically integrate a multiple nested integral with step functions as integrands such as $a_{\lambda_n \cdots \lambda_1}$, we adapt the approach of Refs. [30, 44], which avoids integrating step functions directly but still manages to show $a_{\lambda_n \cdots \lambda_1 = Z} = 0$ up to a certain order.

First, we make an appropriate variable transformation from $\eta \in [0, 1)$ to $\theta \in [0, \pi)$, with the result that the outer pulse intervals are all equal. This is required to make the modulation functions f_x, f_y, f_z, and f_0 (possible integrands that can occur in $a_{\lambda_n \cdots \lambda_1}$) become periodic functions so that each of their Fourier expansions is either a Fourier sine or Fourier cosine series.

The variable transformation introduced by [44] to tackle the QDD$_{N_1 N_2}$ sequence is to apply the corresponding linear transformation to each outer pulse interval $[\eta_{j-1}, \eta_j)$ with duration s_j,

$$\theta = \frac{\pi}{N_2 + 1} \left(\frac{\eta - \eta_{j-1}}{s_j} \right) + \frac{(j-1)\pi}{N_2 + 1}. \tag{33}$$

The timing of the outer X-type pulses becomes

$$\theta_j = \frac{j\pi}{N_2 + 1} \tag{34}$$

so that $f_z(\theta)$ becomes a periodic function with period of $\frac{2\pi}{N_2+1}$,

$$\begin{aligned} f_z(\theta) &= (-1)^{j-1} \qquad\qquad [\theta_{j-1}, \theta_j) \\ &= \sum_{k=0}^{\infty} d_k^z \sin[(2k+1)(N_2+1)\theta], \end{aligned} \tag{35}$$

where the second equality is the Fourier sine-series expansion, and $d_k^z = \frac{4}{(2k+1)\pi}$.

When we apply the piecewise linear transformation (33) to the inner pulse timings $\eta_{j,k}$ [Eq. (6)] the UDD$_{N_1}$ structure is preserved

$$\theta_{j,k} = \frac{\pi}{N_2 + 1} \sin^2 \left(\frac{k\pi}{2(N_1 + 1)} \right) + \theta_{j-1}. \tag{36}$$

In fact all the inner pulse sequences become identical as they have the same total duration $\frac{\pi}{N_2+1}$. It follows that $f_x(\theta) = (-1)^{k-1}$ within $[\theta_{j,k-1}, \theta_{j,k})$ is a periodic function with period of $\frac{\pi}{N_2+1}$.

The parity of the decoupling order N_1 of the inner UDD$_{N_1}$ sequence determines whether $f_x(\theta)$ is even or odd inside each outer interval (Appendix C). Inside each outer interval the parity of $f_x(\theta)$ equals that of N_1. Hence, we have

$$f_x(\theta) = \begin{cases} \sum_{k=0}^{\infty} d_k^x \cos[2k(N_2+1)\theta] & N_1 \text{ even} \\ \sum_{k=1}^{\infty} d_k^x \sin[2k(N_2+1)\theta] & N_1 \text{ odd} \end{cases} \tag{37}$$

The relation $f_y(\theta) = f_z(\theta) f_x(\theta)$, Eqs. (35) and (37), and the product-to-sum rules of the trigonometric functions,

$$\sin a \sin b = \frac{1}{2}\left[\cos(a-b) - \cos(a+b)\right], \tag{38a}$$

$$\cos a \sin b = \frac{1}{2}\left[\sin(a+b) - \sin(a-b)\right], \tag{38b}$$

$$\cos a \cos b = \frac{1}{2}\left[\cos(a+b) + \cos(a-b)\right], \tag{38c}$$

yield the following Fourier expansions of $f_y(\theta)$

$$f_y(\theta) = \begin{cases} \sum_{k=0}^{\infty} d_k^y \sin[(2k+1)(N_2+1)\theta] & N_1 \text{ even} \\ \sum_{k=0}^{\infty} d_k^y \cos[(2k+1)(N_2+1)\theta] & N_1 \text{ odd} \end{cases} \tag{39}$$

Note that while the Fourier expansion coefficients in the even and odd cases are in fact different, we use the notation d_k^x or d_k^y for both since the exact values of these coefficients are irrelevant for our proof.

It follows from Eq. (33) that $d\eta = \frac{N_2+1}{\pi} s_j\, d\theta = G(\theta) d\theta$, where $G(\theta)$ is the step function whose step heights are proportional to the QDD$_{N_1 N_2}$ outer intervals,

$$G(\theta) = \frac{N_2+1}{\pi} s_j \qquad \theta \in [\theta_{j-1}, \theta_j) \tag{40a}$$

$$= \sum_{k=0}^{\infty} \sum_{q=-1,1} g_{k,q} \sin[(2k)(N_2+1)\theta + q\theta], \tag{40b}$$

as shown in Appendix D.

With Eqs. (35), (37)-(40b), and $f_0 = 1$, the nth order QDD$_{N_1 N_2}$ coefficients (21) can be rewritten as

$$a_{\lambda_n \cdots \lambda_1} = \int_0^{\pi} d\theta_n \int_0^{\theta_n} d\theta_{n-1} \cdots \int_0^{\theta_2} d\theta_1 \prod_{\ell=1}^{n} \tilde{f}_{\lambda_\ell}(\theta_\ell) \tag{41}$$

with $\tilde{f}_{\lambda_\ell}(\theta_\ell) \equiv G(\theta_\ell) f_{\lambda_\ell}(\theta_\ell)$, where

$$\tilde{f}_0 = \sum_{k=0}^{\infty} \sum_{q=-1,1} g_{k,q} \sin[2k(N_2+1)\theta + q\theta], \tag{42}$$

$$\tilde{f}_z = \sum_{k=0}^{\infty} \sum_{q=-1,1} d_{k,q}^z \cos[(2k+1)(N_2+1)\theta + q\theta]. \tag{43}$$

When the inner decoupling order N_1 is even,

$$\tilde{f}_x = \sum_{k=0}^{\infty} \sum_{q=-1,1} d_{k,q}^x \sin[2k(N_2+1)\theta + q\theta], \tag{44}$$

$$\tilde{f}_y = \sum_{k=0}^{\infty} \sum_{q=-1,1} d_{k,q}^y \cos[(2k+1)(N_2+1)\theta + q\theta], \tag{45}$$

while if it is odd,

$$\tilde{f}_x = \sum_{k=0}^{\infty} \sum_{q=-1,1} d_{k,q}^x \cos[2k(N_2+1)\theta + q\theta], \tag{46}$$

$$\tilde{f}_y = \sum_{k=0}^{\infty} \sum_{q=-1,1} d_{k,q}^y \sin[(2k+1)(N_2+1)\theta + q\theta]. \tag{47}$$

Observe that all the integrands of $a_{\lambda_n \cdots \lambda_1}$ are composed of sums of either purely cosine functions or purely sine functions, i.e., none of the integrands is a mixed sum. This fact is key to our ability to perform the nested integral, as we show next.

B. Procedure to evaluate nested multiple integrals with integrands being either a cosine series or a sine series

Suppose that, up to an order N which depends on N_1 and N_2, all the normalized QDD$_{N_1,N_2}$ coefficients $a_{\lambda_n \cdots \lambda_1}$ [multiple nested integral Eq. (21)] can be reduced to a single integral as either

$$\sum_{P \in \mathbb{Z}} \int_0^{\pi} \sin[P\theta] d\theta \qquad \text{or} \tag{48}$$

$$\sum_{P \in \mathbb{Z} \setminus 0} \int_0^{\pi} \cos[P\theta] d\theta \tag{49}$$

where we omit prefactors for simplicity. We shall show in the following subsections that this form arises in the evaluation of the QDD$_{N_1 N_2}$ coefficients.

Moreover, we shall show in the following subsections that all $a_{\lambda_n \cdots \lambda_1 = Z}$ coefficients with order $n \leq N$ are of the form of Eq. (49), and hence that $a_{\lambda_n \cdots \lambda_1 = Z}$ vanishes since

$$\sum_{P \in \mathbb{Z} \setminus 0} \sin[P\theta]|_0^{\pi} = 0 \tag{50}$$

after performing the last integral. Therefore, the dephasing errors σ_Z can be eliminated at least up to a remaining error of $\mathcal{O}(T^{N+1})$.

We first note that regardless of the integration limits, all $a_{\lambda_n \cdots \lambda_1}$ coefficients can be viewed as one integral nested with one order lower ($n-1^{th}$ order) coefficient,

$$a_{\lambda_n \cdots \lambda_1} = \int_0^{\pi} d\theta_n \tilde{f}_{\lambda_n}(\theta_n)\, a_{\lambda_{n-1} \cdots \lambda_1}^{\theta_n} \tag{51}$$

where the superscript θ_n indicates that the upper integration limit of $a^{\theta_n}_{\lambda_{n-1}\cdots\lambda_1}$ is θ_n, not π. Now assume that all the $n-1^{th}$ order coefficients $a_{\lambda_{n-1}\cdots\lambda_1}$ are of the form of Eq. (48) or Eq. (49). Then one could just proceed to the next order by substituting Eq. (48) or Eq. (49) (with upper integration limits π replaced by θ_n for the $n-1^{th}$ order coefficient $a^{\theta_n}_{\lambda_{n-1}\cdots\lambda_1}$) into Eq. (51), with the n-level nested integral having been reduced to a two-fold nested integral. Therefore, under the assumption above, two-fold nested integrals are the basic units for evaluating multiple nested integrals.

It follows from the result in the previous subsection that all $\tilde{f}_{\lambda_n}$ are sums of purely sine or purely cosine functions. Combining this with Eq. (51) and the assumption that all the $n-1^{th}$ order coefficients $a_{\lambda_{n-1}\cdots\lambda_1}$ are of the form of Eq. (48) or Eq. (49), there are only four possible types of two-fold nested integrals, which are presented on the left hand sides of Eq. (52). The results, on the right, follow simply from evaluation of the θ_{n-1} integrals, followed by application of the product-to-sum trigonometric formulas (38a)-(38c).

$$\int d\theta_n \sin[p_s\theta_n] \int_0^{\theta_n} d\theta_{n-1} \cos[P_c\theta_{n-1}] \sim \int d\theta_n \cos[(p_s \pm P_c)\theta_n] \tag{52a}$$

$$\int d\theta_n \cos[p_c\theta_n] \int_0^{\theta_n} d\theta_{n-1} \sin[P_s\theta_{n-1}] \sim \int d\theta_n \cos[(p_c \pm P_s)\theta_n] \tag{52b}$$

$$\int d\theta_n \cos[p_c\theta_n] \int_0^{\theta_n} d\theta_{n-1} \cos[P_c\theta_{n-1}] \sim \int d\theta_n \sin[(p_c \pm P_c)\theta_n] \tag{52c}$$

$$\int d\theta_n \sin[p_s\theta_n] \int_0^{\theta_n} d\theta_{n-1} \sin[P_s\theta_{n-1}] \sim \int d\theta_n \sin[(p_s \pm P_s)\theta_n] \tag{52d}$$

where the $\pm$ symbol is shorthand for, e.g., $\int d\theta_n \cos[(p_s \pm P_c)\theta_n] \equiv \int d\theta_n \cos[(p_s + P_c)\theta_n] + \int d\theta_n \cos[(p_s - P_c)\theta_n]$, and where we have omitted irrelevant prefactors in front of all integrals.

Note that the $\cos$ integrands on the right hand side of Eq. (52). will yield 1 if their arguments happen to vanish. This conflicts with the requirement of Eq. (49), and would prevent us from proving that $a_{\lambda_n\cdots\lambda_1=Z}$ vanishes. Likewise, in order to proceed to the next order, say order n, none of the $n-1^{\text{th}}$ order coefficients $a^{\theta_n}_{\lambda_{n-1}\cdots\lambda_1}$ in Eq. (51) may contain constant terms when expressed as a single integral of a cosine series. The reason that a constant is problematic is that it behaves differently from a cosine function under integration. The integral of a cosine function with non-zero argument gives rise to a sine function, but the integral of a constant gives rise to a linear function. Therefore, if the integrand is a cosine series including a constant term, then after integration the result will not be a pure sine series any more. Furthermore, the problem cannot be resolved by carrying out the next integral. On the other hand, one need not worry about sine functions because sine functions with arbitrary angles will always result in cosine functions after integration.

Therefore, proceeding from $n-1^{\text{th}}$ order to n^{th} order, suppose none of $n-1^{\text{th}}$ order coefficients $a^{\theta_n}_{\lambda_{n-1}\cdots\lambda_1}$ contain a constant term. From Eq. (52), due to the product-to-sum trigonometric formula, the problematic constant term will be generated when the new resulting argument $p_s \pm P_c$ in the cosine functions happens to vanish. When this happens to any one of the n^{th} order coefficients $a_{\lambda_n\cdots\lambda_1}$, there is no advantage, when using our proof method, in proceeding to the $n+1^{th}$ order; this order is where the cosine arguments may start to be zero, and hence it sets a lower bound on the suppression order of the pure dephasing term.

C. The suppression ability of the outer X-type UDD$_{N_2}$ sequence when N_1 is even

Let us define four function types we shall encounter in our proof.

Definition 2. *c^n_{odd}, c^n_{even}, ζ^n_{even}, and ζ^n_{odd} function types. Let $k, q \in \mathbb{Z}$ with k arbitrary and $|q| \le n$.*
A c^n_{odd}-type function is an arbitrary linear combination of $\cos[(2k+1)(N_2+1)\theta + q\theta]$ terms.
A c^n_{even}-type function is an arbitrary linear combination of $\cos[2k(N_2+1)\theta + q\theta]$ terms.
A ζ^n_{even}-type function is an arbitrary linear combination of $\sin[2k(N_2+1)\theta + q\theta]$ terms.
A ζ^n_{odd}-type function is an arbitrary linear combination of $\sin[(2k+1)(N_2+1)\theta + q\theta]$ terms.

When $n \le N_2$ we have $(2k+1)(N_2+1)+q \neq 0$. Therefore, by definition, all c^n_{odd}-type functions will in this case have no constant 1 (the problematic term). The c^n_{even}-type functions are allowed to have a constant term.

From Eqs. (42)-(45), for even inner decoupling order N_1, there are only two kinds of integrands: $\widetilde{f}_0$ and $\widetilde{f}_x$ are ζ^1_{even}-type functions while $\widetilde{f}_z$ and $\widetilde{f}_y$ are c^1_{odd}-type functions which, as we just remarked, do not have the constant 1 term. Therefore, it immediately follows from Eqs. (49) and (50) that the first order normalized QDD$_{N_1,N_2}$ coefficients $a_Z = \int_0^{\pi} \widetilde{f}_z\, d\theta$ and $a_Y = \int_0^{\pi} \widetilde{f}_y\, d\theta$ vanish.

Next, let us consider the second order terms (two-fold nested integrals), as in Eq. (52). We introduce a binary operation $\odot$ which (1) evaluates the first integrand, (2) multiplies the outcome with the second integrand, (3) applies the appropriate product-to-sum trigonometric formula. Substituting the c^1_{odd} or ζ^1_{even}-type functions into Eq. (52), we then have

$$\zeta^1_{\text{even}} \odot c^1_{\text{odd}} = c^2_{\text{odd}} \tag{53a}$$
$$c^1_{\text{odd}} \odot \zeta^1_{\text{even}} = c^2_{\text{odd}} \tag{53b}$$
$$c^1_{\text{odd}} \odot c^1_{\text{odd}} = \zeta^2_{\text{even}} \tag{53c}$$
$$\zeta^1_{\text{even}} \odot \zeta^1_{\text{even}} = \zeta^2_{\text{even}} \tag{53d}$$

where we omitted the second integration symbol.

If we disregard the n superscript of $c^n_{\rm odd}$ and $\zeta^n_{\rm even}$ in Eq. (53), the set $\{\zeta_{\rm even}, c_{\rm odd}\}$ constitutes the abelian group Z_2 under the binary operation $\odot$, with the identity element $\zeta_{\rm even}$.

On the other hand, the superscript of the resulting function, $c^2_{\rm odd}$ or $\zeta^2_{\rm even}$ in Eq. (53), is just the sum of the superscripts of the first and second integrands ($c^1_{\rm odd}$ or $\zeta^1_{\rm even}$). Accordingly, the binary operation $\odot$ acts as integer addition for the superscript n.

Let us now consider the n-fold nested integral implied by Eq. (51). Because of the closure property of the group Z_2, integer addition of the superscripts n of $c^n_{\rm odd}$, and $\zeta^n_{\rm even}$, and the fact that no $c^n_{\rm odd}$-type function with $n \le N_2$ contains the constant 1, we can conclude that such an n-fold nested integral with $n \le N_2$ and with each integrand being either $c^1_{\rm odd}$-type or $\zeta^1_{\rm even}$-type functions can be reduced to be either $\int c^n_{\rm odd} d\theta_n$ or $\int \zeta^n_{\rm odd} d\theta_n$.

More specifically, note that in Eq. (53) the first two lines have an odd number of $c^1_{\rm odd}$ functions and result in $c^2_{\rm odd}$, while the last two lines have an even number of $c^1_{\rm odd}$ functions and result in $\zeta^2_{\rm even}$. When we continue the nesting process using these rules, the odd or even property is maintained while the n superscript grows by one unit each time. In other words, due to Z_2 group multiplication rules [Eq. (53) without the superscripts n], we have the following lemma:

Lemma 5. *Provided $n \le N_2$, all n-fold nested integrals, with each integrand being either a $c^1_{\rm odd}$-type or $\zeta^1_{\rm even}$-type function, can be written as*

1. $\int c^n_{\rm odd}\, d\theta_n$ *if there is an* odd *total number of $c^1_{\rm odd}$-type integrands in the n-fold nested integral,*
2. $\int \zeta^n_{\rm even}\, d\theta_n$ *if there is an* even *total number of $c^1_{\rm odd}$-type integrands in the n-fold nested integral.*

Next, let us determine the parity of the number of $c^1_{\rm odd}$-type functions appearing in the QDD$_{N_1N_2}$ coefficients. Consider, e.g., $a_{\lambda_n\cdots\lambda_1=Z}$. Recall that $\widetilde{f}_0$ and $\widetilde{f}_x$ are $\zeta^1_{\rm even}$-type functions while $\widetilde{f}_z$ and $\widetilde{f}_y$ are $c^1_{\rm odd}$-type functions. Consulting the last column of Part 1 of Table III (the second $a_{\lambda_n\cdots\lambda_1=Z}$ column), we see that there is an odd number of f_x ($\zeta^1_{\rm even}$) and f_y ($c^1_{\rm odd}$), and an even number of f_z ($c^1_{\rm odd}$). Therefore, in this case, we have an odd+even=odd number of $c^1_{\rm odd}$-type functions in $a_{\lambda_n\cdots\lambda_1=Z}$. Similarly, consulting all other columns of Part 1 of Table III, it turns out that all possible combinations generating $a_{\lambda_n\cdots\lambda_1=Z}$ or $a_{\lambda_n\cdots\lambda_1=Y}$ contain an odd number of $c^1_{\rm odd}$-type functions. It now follows from Lemma 5 and then Eq. (50) that all $a_{\lambda_n\cdots\lambda_1=Z} = a_{\lambda_n\cdots\lambda_1=Y} = 0$ if the order $n \le N_2$. [Note that this counting argument is unaffected by the move from f to $\tilde{f}$, since this move was due to a change of integration variables—see Eq. (41).]

In conclusion, the inner UDD$_{N_1}$ sequences with even order N_1 do not affect the suppression effect of the outer UDD$_{N_2}$ sequence, i.e., the σ_Z error is always removed up to the expected order N_2 when the order N_1 of the inner sequence is even. This proves the first row of the σ_Z part of Table IV.

In addition, we have just shown that when the inner order N_1 is even, the outer X-type UDD$_{N_2}$ sequence also eliminates the σ_Y error up to the outer decoupling order N_2. Since we have shown in Sec. III that the σ_Y error is suppressed to order N_1 when N_2 is even, or N_1+1 when N_2 is odd, one can conclude that when the inner order N_1 is even, σ_Y is suppressed to order $\max[N_1, N_2]$ when N_2 is even, and to order $\max[N_1+1, N_2]$ when N_2 is odd. This completes the proof of the σ_Y part in Table IV.

D. The suppression ability of the outer X-type UDD$_{N_2}$ sequence when N_1 is odd

The main difference between the analysis in this subsection and the previous one is that $\tilde{f}_x$ and $\tilde{f}_y$ are interchanged in terms of which function is cosine or sine—see Eqs. (44)-(47).

Also, note that, from Eqs. (42), (43), (46), and (47), for odd inner decoupling order N_1, $\tilde{f}_0$ is a $\zeta^1_{\rm even}$-type function, $\tilde{f}_z$ is a $c^1_{\rm odd}$-type function, $\tilde{f}_x$ is a $c^1_{\rm even}$-type, and $\tilde{f}_y$ is a $\zeta^1_{\rm odd}$-type. We shall use these facts throughout this subsection.

Our procedure is to start from the first order QDD coefficients, then the second order, and finally the general, nth order.

1. The first order terms a_{λ_1}

It immediately follows from the fact that $\tilde{f}_z$ is a $c^1_{\rm odd}$-type function and from Eq. (49) that $a_Z = \int_0^\pi \tilde{f}_z\, d\theta = 0$. It also immediately follows from the function types that $\tilde{f}_0$ and $\tilde{f}_y$ are of the form of Eq. (48). The only function that deserves special attention is $\tilde{f}_x$.

As discussed in Sec. IV B, in order to proceed to second order, none of the modulation functions can contain a constant 1 term. However, Definition 2 allows $c^1_{\rm even}$-type functions to have such a term. Accordingly, before applying Eq. (51) to the second order case, we should check whether $\tilde{f}_x(\theta)$ has a constant term.

Suppose $\tilde{f}_x(\theta)$ has a constant 1 term and then separate the constant 1 from the other cosine functions with non-zero arguments as follows,

$$\tilde{f}_x(\theta) = \sum_{p\neq 0} d_p \cos[\,p\,\theta\,] + r \tag{54}$$

where $p = 2k(N_2+1) \pm q$ with $|q| \le 1$ an integer, r a coefficient of the constant 1 term, and d_p coefficients of $\cos[\,p\,\theta\,]$. Then the first order normalized QDD$_{N_1N_2}$ coefficient of the σ_X error reads

$$\begin{aligned} a_X &= \int_0^\pi \tilde{f}_x(\theta)\, d\theta \\ &= \sum_{p\neq 0} d_p \sin[\,p\,\theta\,]|_{\theta=0}^{\theta=\pi} + r\theta|_{\theta=0}^{\theta=\pi} \\ &= 0 + r\pi \end{aligned} \tag{55}$$

Now, since we already proved in Section III that $a_{\lambda_n\ldots\lambda_1=X} = 0$ for $n \le N_1$, and since in the first order case $n = 1$ and hence $n \leq N_1$ always holds, it follows that $r = 0$. Therefore, $\tilde{f}_x$ does not contain a constant 1 term.

In summary, now that we have shown that $a_{\lambda_1=Z} = 0$ and that all the first order normalized QDD_{N_1,N_2} coefficients a_{λ_1} are of the form of either Eq. (48) or Eq. (49), we can proceed to the second order case.

2. The second order terms $a_{\lambda_2\lambda_1}$

From Eq. (51), the second order normalized QDD_{N_1,N_2} coefficients is

$$a_{\lambda_2\lambda_1} = \int_0^\pi d\theta_2 \tilde{f}_{\lambda_2}(\theta_2)\, a_{\lambda_1}^{\theta_2}. \tag{56}$$

After additionally applying the trigonometric product-to-sum transformation, and using the operation $\odot$ defined above Eq. (53), we can write

$$a_{\lambda_2\lambda_1} = a_{\lambda_2} \odot a_{\lambda_1}^{\theta_2} \tag{57}$$

Next, in Eq. (57), let us substitute ζ_{even}^1 into the integrand of a_I, c_{even}^1 into a_X, ζ_{odd}^1 into a_Y, and c_{odd}^1 into a_Z. The resulting set of all $a_{\lambda_2\lambda_1}$ can be arranged into a multiplication table, Table VI, where the entries in the top row are the types of the first integrand and the entries in the left-most column are the types of the second integrand. The remaining entries are the results of applying the binary operation $\odot$ between the elements of the first row and column.

From Table VI, the superscript of the resulting function is again the sum of the superscripts of the first and second integrands. Hence the binary operation $\odot$ again acts as integer addition for the superscripts. Moreover, disregarding the superscripts n, Table VI shows that the set $\{\zeta_{\text{even}}, c_{\text{even}}, \zeta_{\text{odd}}, c_{\text{odd}}\}$ forms the abelian Klein four-group, i.e., the $Z_2 \times Z_2$ group, under the binary operation $\odot$. The key observation from Table VI is that the algebra of the subscripts $\lambda_2\lambda_1$ of $a_{\lambda_2\lambda_1}$ works as the *Pauli algebra without the anti-commutativity property*, which is isomorphic to the Klein four-group algebra by mapping the identity I to ζ_{even}, X to c_{even}, Y to ζ_{odd}, and Z to c_{odd}.

Accordingly, the results of Table VI can be summarized as follows,

$$\begin{aligned}
a_{\lambda_2\lambda_1=Z} &= \int_0^\pi c_{\text{odd}}^2\, d\theta && (58a)\\
a_{\lambda_2\lambda_1=X} &= \int_0^\pi c_{\text{even}}^2\, d\theta && (58b)\\
a_{\lambda_2\lambda_1=Y} &= \int_0^\pi \zeta_{\text{odd}}^2\, d\theta && (58c)\\
a_{\lambda_2\lambda_1=I} &= \int_0^\pi \zeta_{\text{even}}^2\, d\theta. && (58d)
\end{aligned}$$

We can conclude that $a_{\lambda_2\lambda_1=Z} = 0$ if $N_2 \geq 2$, since then (by definition) c_{odd}^2 does not contain a constant 1 term.

We have already proved in Section III that $a_{\lambda_2\lambda_1=X} = 0$ if $N_1 \geq 2$. By the same argument as Eq. (55), this implies that the integrand c_{even}^2 does not have a constant 1 term if $N_1 \geq 2$.

In order to proceed to the next order none of the integrands may contain a constant. Therefore, our results show that if $N_1, N_2 \geq 2$, one can indeed proceed to the next order. On the other hand, if $N_1 = N_2 = 1$ we can only conclude that $a_{\lambda_1=Z} = 0$, while if $N_1 = 1$ and $N_2 \geq 2$, we can only conclude that $a_{\lambda_1=Z} = a_{\lambda_2\lambda_1=Z} = 0$, but not that the third or higher order Z-type QDD coefficients are zero.

3. The n^{th} order terms $a_{\lambda_n\cdots\lambda_1}$

The procedure we described for the first and second orders applies to higher orders, until one reaches the order N where some resulting integrands begin to include constant 1 terms.

To obtain the nth order $\mathrm{QDD}_{N_1N_2}$ coefficients we proceed by induction on n. We have already established the case of $n = 1$ and $n = 2$. Let us assume that

$$\begin{aligned}
a_{\lambda_n\cdots\lambda_1=Z} &= \int_0^\pi c_{\text{odd}}^n\, d\theta && (59a)\\
a_{\lambda_n\cdots\lambda_1=X} &= \int_0^\pi c_{\text{even}}^n\, d\theta && (59b)\\
a_{\lambda_n\cdots\lambda_1=Y} &= \int_0^\pi \zeta_{\text{odd}}^n\, d\theta && (59c)\\
a_{\lambda_n\cdots\lambda_1=I} &= \int_0^\pi \zeta_{\text{even}}^n\, d\theta. && (59d)
\end{aligned}$$

where none of these integrals contains a constant 1 term in their integrand, and prove that the same integrand form holds for $n + 1$ (but not necessarily that there is no constant 1). Indeed, using the definition of the $\odot$ operation and Eq. (51), we have

$$a_{\lambda_{n+1}\cdots\lambda_1} = a_{\lambda_{n+1}} \odot a_{\lambda_n\cdots\lambda_1}^{\theta_{n+1}} \tag{60}$$

Due to the induction assumption [Eq. (59)] the situation is now identical to the one we analyzed for $n = 2$, in particular in Eq. (58). Therefore Eq. (59) holds with n replaced by $n+1$.

This can also be understood without induction as being due to the isomorphism between the set $\{\zeta_{\text{even}}, c_{\text{even}}, \zeta_{\text{odd}}, c_{\text{odd}}\}$ and the set $\{I, X, Y, Z\}$ (the subscripts of $a_{\lambda_n\cdots\lambda_1}$), and the addition of superscripts under the $\odot$ operation.

To figure out up to which order N Eq. (59) holds, one must examine when the c_{odd}^n or c_{even}^n-type functions begin to have constant 1 terms. The c_{odd}^n-type functions will by definition not contain constant 1 terms until order $n = N_2 + 1$. On the other hand, due to Eq. (59b) and $a_{\lambda_n\cdots\lambda_1=X} = 0$ for $n \leq N_1$ (proven in Sec. III), c_{even}^n in Eq. (59b) is guaranteed to have no constant 1 term until order $n = N_1 + 1$, by a similar argument as that leading to Eq. (55). In conclusion,

Lemma 6. *For $\mathrm{QDD}_{N_1N_2}$ with odd N_1, all nth order normalized $\mathrm{QDD}_{N_1N_2}$ coefficients $a_{\lambda_n\cdots\lambda_1}$ with $n \leq \min[N_1 + 1, N_2 + 1]$ can be written as Eq.* (59)*, and none of the integrands in Eq.* (59) *contain a constant* 1 *term when $n \leq \min[N_1, N_2]$.*

$\odot$	$a_I : \zeta^1_{\text{even}}$	$a_X : c^1_{\text{even}}$	$a_Y : \zeta^1_{\text{odd}}$	$a_Z : c^1_{\text{odd}}$
$a_I : \zeta^1_{\text{even}}$	$a_{II=I} : \zeta^2_{\text{even}}$	$a_{IX=X} : c^2_{\text{even}}$	$a_{IY=Y} : \zeta^2_{\text{odd}}$	$a_{IZ=Z} : c^2_{\text{odd}}$
$a_X : c^1_{\text{even}}$	$a_{XI=X} : c^2_{\text{even}}$	$a_{XX=I} : \zeta^2_{\text{even}}$	$a_{XY=Z} : c^2_{\text{odd}}$	$a_{XZ=Y} : \zeta^2_{\text{odd}}$
$a_Y : \zeta^1_{\text{odd}}$	$a_{YI=Y} : \zeta^2_{\text{odd}}$	$a_{YX=Z} : c^2_{\text{odd}}$	$a_{YY=I} : \zeta^2_{\text{even}}$	$a_{YZ=X} : c^2_{\text{even}}$
$a_Z : c^1_{\text{odd}}$	$a_{ZI=Z} : c^2_{\text{odd}}$	$a_{ZX=Y} : \zeta^2_{\text{odd}}$	$a_{ZY=X} : c^2_{\text{even}}$	$a_{ZZ=I} : \zeta^2_{\text{even}}$

TABLE VI: The group structure associated with the second order QDD$_{N_1N_2}$ coefficient $a_{\lambda_2\lambda_1} = a_{\lambda_2} \odot a^{\theta_2}_{\lambda_1}$.

It follows immediately from Lemma 6 and Eq. (50) that the first $\min[N_1, N_2]$ orders of $a_{\lambda_n\cdots\lambda_1=Z}$ vanish. However, in fact we can show more, namely that $a_{\lambda_n\cdots\lambda_1=Z} = 0$ for all $n \leq \min[N_1+1, N_2]$. Suppose that $N_1 < N_2$ and consider the special case $n = N_1+1$. In this case it follows from Lemma 6 that $a_{\lambda_{N_1+1}\cdots\lambda_1=Z} = \int_0^\pi c^{N_1+1}_{\text{odd}}\, d\theta$; the argument of the function $c^{N_1+1}_{\text{odd}}$ is $(2k+1)(N_2+1)\theta + q\theta$, and $|q| \leq N_1+1$. Since $N_1 < N_2$ this argument cannot vanish, and it follows that $a_{\lambda_{N_1+1}\cdots\lambda_1=Z} = 0$. In conclusion, $a_{\lambda_n\cdots\lambda_1=Z} = 0$ for all $n \leq \min[N_1+1, N_2]$, which proves the last row in Table IV.

In summary, if the inner decoupling order N_1 is odd and $N_2 \leq N_1+1$, the outer UDD$_{N_2}$ sequence always suppresses the dephasing error Z to the expected decoupling order N_2, as then $\min[N_1+1, N_2] = N_2$. In contrast, if the inner decoupling order N_1 is odd and $N_2 > N_1+1$, the outer UDD$_{N_2}$ sequence suppresses the dephasing error Z (at least) up to order N_1+1, which may be smaller than the expected outer decoupling order N_2. Thus, if the order of inner level UDD$_{N_1}$ sequence is odd, this may inhibit the suppression ability of the outer UDD$_{N_2}$ sequence.

V. COMPARISON BETWEEN OUR THEORETICAL BOUNDS AND NUMERICAL RESULTS

In Ref. [42] the QDD sequence was analyzed numerically and the scaling of the single-axis errors was determined on the basis of simulations, for N_1 and N_2 in the range $\{1, \ldots, 24\}$. These simulations are in complete agreement with our analytically bounds for n_x and n_y, as given in Table IV. They are also in complete agreement with our bound for n_z when N_1 is even. Thus we can conclude that it is likely that our bounds are in fact tight in these cases. There is, however, one discrepancy: when N_1 is odd our analytical bound yields $n_z = \min[N_1+1, N_2]$, while the numerical result found in Ref. [42] is $n_z = \min[2N_1+1, N_2]$. Thus, in this case our bound is not tight. We attribute this to the fact that the method we used in Sec. IV does not use the full information contained in the integrands, i.e., we discard all Fourier coefficients. Specifically, if $a_{\lambda_n\ldots\lambda_1=Z}$ contains a constant term, namely, $\cos[P\theta]$ with $P = 0$, or does not end up in the form of Eq. (49), it is still possible that $a_{\lambda_n\ldots\lambda_1=Z}$ vanishes because a sum of non-zero terms could be zero when combined with the right Fourier coefficients. Thus, our method of analysis merely yields a lower bound on the decoupling order of the pure dephasing error. It is an interesting open problem to try to improve this bound so that it matches the numerical results of Ref. [42].

VI. SUMMARY AND CONCLUSIONS

The QDD sequence, introduced in Ref. [41], is, to date, the most efficient pulse sequence known for suppression of single-qubit decoherence. In this work we provided a complete proof of the validity of this sequence, i.e., we proved its universality (independence of details of the environment) and performance. Our work complements an earlier proof [44], which was restricted to even order inner UDD sequences. However, our results go beyond a validity proof of QDD. For, in this work we also elucidated the dependence of single-axis error suppression on the orders N_1 and N_2 of the inner X-type and outer Z-type UDD sequences comprising QDD$_{N_1N_2}$, respectively. Our results are stated in Theorem 1. Let us briefly summarize our method and main findings.

Our general proof idea was to analyze the conditions under which, for each error type σ_λ, the nth order QDD$_{N_1N_2}$ coefficients [Eq. (18)] vanish. We used two complementary methods. In the first method, we expressed the QDD coefficients $a_{\lambda_n\cdots\lambda_1}$ in terms of UDD coefficients by splitting each of $a_{\lambda_n\cdots\lambda_1}$'s nested integrals into a sum of sub-integrals over normalized outer intervals. We were then able to conclude that $a_{\lambda_n\cdots\lambda_1=X}$ and $a_{\lambda_n\cdots\lambda_1=Y}$ vanish when $n \leq N_1$ due to the vanishing of the UDD$_{N_1}$ contributions. For the σ_Y error, still as part of the first method, we showed that an additional order vanishes due to a parity cancellation effect involving the outer sequence. However, this additional cancellation cannot be attributed to the vanishing of a corresponding UDD coefficient. In the second method we considered the case of $a_{\lambda_n\cdots\lambda_1=Z}$, for which we provided an analysis based on the evaluation of integrals of trigonometric functions. We showed that their properties under nested integration can be mapped to the Abelian groups Z_2 (for even N_1) and $Z_2\times Z_2$ (for odd N_1). Using this we provided a proof by induction for the vanishing of $a_{\lambda_n\cdots\lambda_1=Z}$, and, when N_1 is even, also for $a_{\lambda_n\cdots\lambda_1=Y}$.

The overall summary of our results is that $a_{\lambda_n\cdots\lambda_1=\lambda} = 0$ $\forall n \leq N$, where N is the decoupling order given in the last column of Table IV. We now provide a recap of these results, including a semi-intuitive explanation based on the idea of interference between the modulation functions.

Starting from the simplest case, we showed explicitly that independently of the order of the outer X-type sequence, the inner Z-type UDD$_{N_1}$ sequence always achieves its expected error suppression order, i.e., the σ_X and σ_Y errors are suppressed to the inner decoupling order N_1. Since σ_X errors commute with the pulses of the outer sequence they are not suppressed any further.

The story is more complicated for the σ_Y and σ_Z errors, as they are both suppressed by the outer sequence.

For the σ_Y error, the parities of the inner and outer sequence orders cause the decoupling order to vary between N_1, N_1+1, and N_2. Consider first the even N_2 case. An intuitive explanation for the corresponding parity effects is the following. For even N_1, the modulation functions f_y and f_z are *in phase*, namely both have a $\sin[(2k+1)(N_2+1)\theta]$ dependence [recall Eqs. (35) and (39)]. The outer X-type UDD$_{N_2}$ sequence, with its f_z modulation function, is then fully effective at eliminating the σ_Y error, with the result that σ_Y is eliminated to the expected decoupling order $\max[N_1, N_2]$. However, when N_1 is odd, f_y has a $\cos[(2k+1)(N_2+1)\theta]$ dependence, which is 90 degrees out of phase with f_z. In this case f_y and f_z interfere destructively with one another, and the outer sequence does not help to further suppress σ_Y. The result is that σ_Y is only eliminated to order N_1.

Now consider the case of odd N_2. This case gives rise to the anomalous N_1+1 suppression order. The reason is that when N_2 is odd, the modulation function f_z is odd with respect to the midpoint of the total sequence duration, while f_x and f_y are both even. It is this oddness of the outer sequence modulation function (f_z) which helps to suppress the error σ_Y to one more order, due to a cancellation of terms with equal magnitude but opposite sign [Eq. (32)]. This gives rise to a cancellation to order $\max[N_1+1, N_2]$ when N_1 is even and the inner sequence does not interfere with the outer sequence, or to order N_1+1 when N_1 is odd and the inner sequence does interfere with the outer sequence.

Thus, suppose we fix N_2 so that it is even (odd) and greater than N_1 (N_1+1). We should then see the suppression order of σ_Y switch between N_1 (N_1+1) and N_2, as N_1 is increased from 1 to N_2, a phenomenon which was indeed observed in the numerical simulations of Ref. [42].

If the inner order N_1 is even, the outer X-type UDD$_{N_2}$ sequence always suppresses σ_Z to the expected decoupling order N_2. This has the same intuitive origin as the σ_Y case. Namely, for even N_1, f_y and f_z are in phase, i.e., both have a $\sin[(2k+1)(N_2+1)\theta]$ dependence, and so are able to suppress σ_Z to the expected order. However, when N_1 is odd, the dependence of f_y is $\cos[(2k+1)(N2+1)\theta$, which is 90 degrees out of phase with f_z. Therefore again f_y and f_z interference destructively, and the outer sequence does not suppress the error σ_Z to the expected order.

In more detail, if the inner order N_1 is odd and $N_2 > N_1+1$, our proof method shows that the outer X-type UDD$_{N_2}$ sequence suppresses the σ_Z error at least to order N_1+1, which is less than the expected outer decoupling order N_2. Hence, if this lower bound is saturated, one can see a saturation effect in the decoupling order of σ_Z, which starts at $N_2 = N_1+2$ when we fix odd N_1 and increase N_2. Thus, odd N_1 can hinder the suppression ability of the outer sequence.

The numerical results of Ref. [42] confirm that odd N_1 can hinder the suppression ability of the outer X-type UDD$_{N_2}$ sequence. However, the actual saturation effect in the decoupling order of σ_Z begins at $N_2 = 2N_1+2$, higher than our lower bound of $N_2 = N_1+2$. A new method may be needed to explain the remaining vanishing orders from N_1+2 to $2N_1+1$.

The inhibitory effect of odd inner decoupling order N_1 disappears when N_1 is large enough. Specifically, whenever $N_1 \geq N_2 - 1$ the outer X-type UDD$_{N_2}$ sequence suppresses σ_Z to the expected decoupling order N_2. This makes intuitive sense because when N_1 is large enough the outer X-type UDD$_{N_2}$ sequence "views" the effective Hamiltonian resulting from the inner Z-type UDD$_{N_1}$ sequence—which has time dependence $\mathcal{O}(T^{N_1+1\geq N_2})$—as time-independent relative to its "error cancellation power" $\mathcal{O}(T^{N_2})$.

Despite this complicated interplay between N_1 and N_2, our proof yields the simple result that the QDD$_{N_1N_2}$ sequence suppresses all single-qubit errors to an order $\geq \min[N_1, N_2]$. This matches the numerical results in [42], so that our bounds appear to be optimal in this regard. We conclude that to attain the highest order decoupling from the QDD$_{N_1N_2}$ sequence with ideal, zero-width pulses, one should use either an even order inner UDD sequence, or ensure that $N_1 \geq N_2 - 1$ if N_1 is odd.

A natural generalization of the work presented here is to NUDD with different sequence orders [46]. We look forward to experimental tests of the properties of the QDD$_{N_1N_2}$ pulse sequence predicted in this work.

Note added: After this work was completed and while it was being written up for publication we became aware of a different, elegant proof of the universality of NUDD and in particular QDD [47]. Our approach differs not only in methodology but also in providing a complete analysis of the single-axis errors.

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Appendix A: The form of $a_{\lambda_n\cdots\lambda_1}$ after outer interval decomposition

We shall derive Eq. (22) by splitting each integral of $a_{\lambda_n\cdots\lambda_1}$ [Eq. (21)] into a sum of sub-integrals over the normalized outer intervals s_j in Eq. (3a). Since $a_{\lambda_n\ldots\lambda_1}$ comprises a series of time-ordered, nested integrals, our procedure for decomposing $a_{\lambda_n\ldots\lambda_1}$ is to split its nested integrals one by one, from $\eta^{(n)}$ to $\eta^{(1)}$.

We call the sub-integral over the jth outer interval "sub-integral-j". Suppose the integral of the integration variable $\eta^{(\ell)}$ follows the sub-integral-$j^{(\ell+1)}$ of the previous variable $\eta^{(\ell+1)}$. By splitting the integral of $\eta^{(\ell)}$ with respect to the normalized outer intervals and using Eq. (16), we have

$$\int_0^{\eta^{(\ell+1)}} f_{\lambda_\ell}(\eta^{(\ell)})\, d\eta^{(\ell)}$$

$$= \sum_{j^{(\ell)}=1}^{j^{(\ell+1)}-1} f_{\beta_\ell}(j^{(\ell)}) \int_{\eta_{j^{(\ell)}-1}}^{\eta_{j^{(\ell)}}} f_{\tilde{\alpha}_\ell}(\eta^{(\ell)})\, d\eta^{(\ell)} \quad \text{(A1a)}$$

$$+ f_{\beta_\ell}(j^{(\ell+1)}) \int_{\eta_{j^{(\ell+1)}-1}}^{\eta^{(\ell+1)}} f_{\tilde{\alpha}_\ell}(\eta^{(\ell)})\, d\eta^{(\ell)} \quad \text{(A1b)}$$

$$= \int_0^1 f_{\alpha_\ell}(\tilde{\eta}^{(\ell)})\, d\tilde{\eta}^{(\ell)} \sum_{j^{(\ell)}=1}^{j^{(\ell+1)}-1} f_{\beta_\ell}(j^{(\ell)}) s_{j^{(\ell)}} \quad \text{(A1c)}$$

$$+ \int_0^{\tilde{\eta}^{(\ell+1)}} f_{\alpha_\ell}(\tilde{\eta}^{(\ell)})\, d\tilde{\eta}^{(\ell)} f_{\beta_\ell}(j^{(\ell+1)}) s_{j^{(\ell+1)}} \quad \text{(A1d)}$$

To obtain Eqs. (A1c) and (A1d) we rescaled $f_{\tilde{\alpha}_\ell}(\eta^{(\ell)})$ in Eq. (A1a) and (A1b) individually with

$$\tilde{\eta}^{(\ell)} = \frac{\eta - \eta_{j^{(\ell)}-1}}{s_{j^{(\ell)}}} \quad \text{(A2)}$$

for each outer interval $s_{j^{(\ell)}}$, thus obtaining $f_{\alpha_\ell}(\tilde{\eta}^{(\ell)})$. In this manner $f_{\alpha_\ell}(\tilde{\eta}^{(\ell)})$ is the same function for all the outer intervals, so that $\int_0^1 f_{\alpha_\ell}(\tilde{\eta}^{(\ell)})\, d\tilde{\eta}^{(\ell)}$ can be taken out from the summation, as shown in Eqs. (A1c) and (A1d).

Recall the time-ordering condition, $\eta^{(n)} \geq \eta^{(n-1)} \geq \ldots \eta^{(2)} \geq \eta^{(1)}$. It has a consequence that in Eq. (A1d), subintegrals over any two adjacent variables $\eta^{(\ell)}$ and $\eta^{(\ell+1)}$ are nested, as they are in the same outer interval, number $j^{(\ell+1)}$. In this case $\eta^{(\ell)} \leq \eta^{(\ell+1)}$.

In contrast, if the sub-integrals are in different outer intervals (automatically time-ordered), then the sub-integral over $\eta^{(\ell)}$ is not nested inside the subintegral over $\eta^{(\ell+1)}$, but integrated over its entire outer interval independently, as in Eq. (A1c).

Let $r_\ell = *$ denote the time-ordering of outer intervals as in Eq. (A1c), and let $r_\ell = \emptyset$ denote the integral time-ordering inside a given outer interval as in Eq. (A1d). Accordingly, r_ℓ describes the relation between the adjacent variables $\eta^{(\ell+1)}$ and $\eta^{(\ell)}$.

As we have just shown, each integral of $a_{\lambda_n \ldots \lambda_1}$ can always be split into two parts, Eq. (A1c) and (A1d), with one exception: if $j^{(\ell+1)} = 1$, the subsequent sub-integral of variables $\eta^{(\ell)}$ will only contain the term Eq. (A1d). Moreover, both Eq. (A1c) and (A1d) contain an effective inner part (the part that depends on f_{α_ℓ}) and an effective outer part (the part that depends on f_{β_ℓ}). Therefore, by substituting Eqs. (A1c) and (A1d) into each integral of $a_{\lambda_n \ldots \lambda_1}$, in sequence from $\eta^{(n)}$ to $\eta^{(1)}$, $a_{\lambda_n \ldots \lambda_1}$ can be written as an inner part Φ^{in} [Eq. (23)] multiplying an outer part Φ^{out} [Eq. (25)] over all the possible integration and summation configurations. Each such configuration can be denoted by an ordered set of symbols $\{r_{n-1} r_{n-2} \ldots r_1\}$. Thereby, we obtain Eq. (22) as the representation of $a_{\lambda_n \ldots \lambda_1}$ after this decomposition.

Appendix B: Time symmetry of the UDD pulse intervals

Due to the identity $\sin\theta = \sin[\pi - \theta]$, $\sin[\frac{(2j-1)\pi}{2(N+1)}]$ in s_j Eq. (3a) satisfies

$$\begin{aligned}\sin\frac{(2j-1)\pi}{2(N+1)} &= \sin[\pi - \frac{(2j-1)\pi}{2(N+1)}] \\ &= \sin[\frac{(2N+2-2j+1)\pi}{2(N+1)}] \\ &= \sin[\frac{(2(N+2-j)-1)\pi}{2(N+1)}]\end{aligned}$$

Therefore, we have proved that $s_j = s_{N+2-j}$ [Eq. (31)], which shows that the UDD pulse intervals are time symmetric. There is, however, a difference between even and odd N: when N is odd every interval to the left of center is paired with an interval to the right of center. When N is even the central interval is unpaired. E.g., for $N = 1$ we have two, paired intervals: $s_1 = s_2$. When $N = 2$ we have two paired intervals, $s_1 = s_3$, and an unpaired interval s_2.

Appendix C: The parity of the inner order N_1 determines the parity of f_x

Since the inner pulse sequences under the piecewise linear variable transformation Eq. (33) still have the UDD$_{N_1}$ structure, the rescaled inner pulse intervals remain time symmetric:

$$\theta_{j,k} - \theta_{j,k-1} = \theta_{j,N_1+2-k} - \theta_{j,N_1+1-k}. \quad \text{(C1)}$$

When the inner decoupling order N_1 is even, the parities of $N_1 + 2 - k$ and k are the same, so that

$$f_x(\theta) = \begin{cases} (-1)^{k-1} & \theta \in [\theta_{j,k-1}, \theta_{j,k}) \\ (-1)^{N_1+2-k-1} & \theta \in [\theta_{j,N_1+1-k}, \theta_{j,N_1+2-k}) \end{cases} \quad \text{(C2)}$$

Hence $f_x(\theta)$ is even inside each outer interval.

When the inner decoupling order N_1 is odd,

$$f_x(\theta) = \begin{cases} (-1)^{k-1} & \theta \in [\theta_{j,k-1}, \theta_{j,k}) \\ (-1)^{N_1+2-k} & \theta \in [\theta_{j,N_1+1-k}, \theta_{j,N_1+2-k}) \end{cases} \quad \text{(C3)}$$

where the sign difference between the second lines of Eq. (C2) and Eq. (C3) arises from the opposite parities of $N_1 + 2 - k$ and k. Accordingly, $f_x(\theta)$ is odd inside each outer interval.

Note that the sequence of rescaled inner intervals $\{\theta_{j,k}\}_{k=1}^{N_1+1}$ is repeated for all values of $j \in \{1, \ldots, N_2+1\}$. As a result the three modulation functions $f_x(\theta), f_y(\theta), f_z(\theta)$ are periodic, with respective periods $\frac{\pi}{N_2+1}, \frac{2\pi}{N_2+1}, \frac{2\pi}{N_2+1}$. In this sense, the variable transformation $\eta = \sin^2(\theta/2)$ introduced in [30], which emerges naturally from the time structure of UDD sequence Eq. (2), is unsuitable for our QDD proof. The reason is that despite the fact that the outer X-type pulses intervals are rescaled to be equal, the timing patterns of the inner sequences in different outer intervals are no longer the same.

Appendix D: Fourier expansions of $G(\theta)$

$G(\theta)$ in Eq. (40b) takes the following form up to a multiplicative constant: $G(\theta) = s_j$, where $\theta \in [\frac{(j-1)\pi}{N+1}, \frac{j\pi}{N+1})$. The symmetry property (31) implies that $G(\theta)$ can be written as

$$G(\theta) = \sum_{\ell=1}^{\infty} g_\ell \sin \ell\theta. \tag{D1}$$

Let us now compute the expansion coefficients:

$$\begin{aligned} g_\ell &\equiv \frac{1}{\pi/2}\int_0^\pi G(\theta)\sin\ell\theta d\theta \\ &= \frac{2}{\pi}\sum_{j=1}^{N+1} s_j \int_{\theta_{j-1}}^{\theta_j} \sin\ell\theta d\theta \\ &= -\frac{2}{\pi\ell}\sin\frac{\pi}{2(N+1)}\sum_{j=1}^{N+1}\sin\frac{(2j-1)\pi}{2(N+1)}\times \\ &\quad (\cos\ell\theta_j - \cos\ell\theta_{j-1}) \\ &= -\frac{2}{\pi\ell}\sin\frac{\pi}{2(N+1)}\sum_{j=1}^{N+1}\sin\frac{(2j-1)\pi}{2(N+1)}\times \\ &\quad (-2)\sin\ell\frac{\theta_j+\theta_{j-1}}{2}\sin\ell\frac{\theta_j-\theta_{j-1}}{2} \end{aligned} \tag{D2}$$

where we used the sum-to product formula in the third equality. Due to $\frac{\theta_j-\theta_{j-1}}{2} = \frac{\pi}{2(N+1)}$ and the product-to sum formula, we have

$$\begin{aligned} g_\ell &= \frac{4}{\pi\ell}\sin\frac{\pi}{2(N+1)}\sin\frac{\ell\pi}{2(N+1)}\times \\ &\quad \sum_{j=1}^{N+1}\sin\frac{(2j-1)\pi}{2(N+1)}\sin\ell\frac{(2j-1)\pi}{2(N+1)} \\ &= \frac{4}{\pi\ell}\sin\frac{\pi}{2(N+1)}\sin\frac{\ell\pi}{2(N+1)}\times \\ &\quad \frac{1}{2}\sum_{j=1}^{N+1}\cos\frac{(\ell-1)(2j-1)\pi}{2(N+1)} - \cos\frac{(\ell+1)(2j-1)\pi}{2(N+1)}. \end{aligned} \tag{D3}$$

Considering the sum over j we have

$$\begin{aligned} &\sum_{j=1}^{N+1}\cos\frac{(\ell\pm1)(2j-1)\pi}{2(N+1)} \\ &= \sum_{j=1}^{N+1}\cos[\frac{(\ell\pm1)j\pi}{(N+1)} - \frac{(\ell\pm1)\pi}{2(N+1)}] \\ &= \mathrm{Re}[e^{-i\frac{(\ell\pm1)\pi}{2(N+1)}}\sum_{j=1}^{N+1}e^{i\frac{(\ell\pm1)j\pi}{(N+1)}}] \\ &= \mathrm{Re}[e^{-i\frac{(\ell\pm1)\pi}{2(N+1)}}e^{i\frac{(\ell\pm1)\pi}{N+1}}\frac{1-e^{i(\ell\pm1)\pi}}{1-e^{i\frac{(\ell\pm1)\pi}{N+1}}}] \\ &= \mathrm{Re}[\frac{1-\cos(\ell\pm1)\pi - i\sin(\ell\pm1)\pi}{e^{-i\frac{(\ell\pm1)\pi}{2(N+1)}} - e^{i\frac{(\ell\pm1)\pi}{2(N+1)}}}] \\ &= \frac{\sin(\ell\pm1)\pi}{2\sin\frac{(\ell\pm1)\pi}{2(N+1)}}, \end{aligned} \tag{D4}$$

where in the third equality we used the geometric series formula. The last expression vanishes if $\ell \neq 2k(N+1)\mp1$. The only values of ℓ for which g_ℓ does not vanish are $2k(N+1)\mp1$. Therefore, finally

$$G(\theta) = \sum_{k=0}^{\infty}\sum_{q=\pm1} g_{k,q}\sin[2k(N+1)\theta + q\theta]. \tag{D5}$$

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