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## Universality proof and analysis of generalized nested Uhrig dynamical decoupling

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Nested Uhrig dynamical decoupling (NUDD) is a highly efficient quantum error suppression scheme that builds on optimized single axis UDD sequences. We prove the universality of NUDD and analyze its suppression of different error types in the setting of generalized control pulses. We present an explicit lower bound for the decoupling order of each error type, which we relate to the sequence orders of the nested UDD layers. We find that the error suppression capabilities of NUDD are strongly dependent on the parities and relative magnitudes of all nested UDD sequence orders. This allows us to predict the optimal arrangement of sequence orders. We test and confirm our analysis using numerical simulations. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4769382>]

### I. INTRODUCTION

One of the main obstacles in building a quantum computer is the inevitable coupling between a quantum system and its environment, or bath, which typically results in decoherence and leads to computational errors.<sup>1–3</sup> Adapted from nuclear magnetic resonance (NMR) refocusing techniques,<sup>4,5</sup> dynamical decoupling (DD)<sup>6</sup> is a powerful open-loop technique that can be used to suppress decoherence by applying a sequence of short and strong pulses purely on the system to mitigate unwanted system-bath interactions.

Early schemes, such as periodic DD (PDD),<sup>7–11</sup> using equidistant  $\pi$ -pulses, have been shown to suppress general system-bath interactions up to first order in time-dependent perturbation theory, with respect to the total sequence duration  $T$ , thereby achieving first-order decoupling. Concatenated DD (CDD),<sup>12,13</sup> which recursively embeds PDD into itself, was the first explicit scheme capable of achieving  $N$ th-order decoupling for general single-qubit decoherence, i.e., complete error suppression to order  $T^N$ , and has been amply tested in recent experimental studies.<sup>14–18</sup> However, the number of pulses required by CDD grows exponentially with decoupling order:  $4^N$  pulses are required to attain  $N$ th order error suppression, which is not efficient enough to implement scalable quantum computing when  $N$  is large. For scalable quantum computing to be possible, it is desirable to design a DD sequence which is both accurate (high decoupling order) and efficient (small number of pulses).

For the single-qubit pure dephasing spin-boson model, an optimal scheme called Uhrig DD (UDD),<sup>19,20</sup> achieves  $N$ th order decoupling with the smallest possible number  $N$  of ideal  $\pi$ -pulses, applied at non-equidistant pulse timings,

$$t_j = T \sin^2 \frac{j\pi}{2(N+1)}, \quad j \in \{1, \dots, \bar{N}\}, \quad (1)$$

where  $\bar{N} = N$  or  $N + 1$  depending on whether  $N$  is even or odd.  $N$  is also referred to as the sequence order. The applicability of UDD extends beyond the spin-boson model to models with pure dephasing interactions, with generic bounded baths,<sup>21,22</sup> rendering it model-independent, or “universal.” Moreover, it has also been proven to be applicable to analytically time-dependent Hamiltonians.<sup>23</sup> Extensive numerical and experimental studies of UDD performance can be found in Refs. 15, 18, 24–32, and 33. Rigorous performance bounds for UDD were found in Ref. 22, and for QDD and NUDD in Ref. 34.

While UDD is applicable to single- and two-axis interactions (e.g., pure dephasing and/or pure bit-flip), it cannot overcome general, three-axis single-qubit decoherence. Quadratic DD (QDD)<sup>35</sup> and its generalization Nested UDD (NUDD),<sup>36</sup> which were proposed to tackle general single and multi-qubit decoherence, respectively, exploit the decoupling efficiency of UDD by nesting two- and multi-layer UDD, where sequence orders of different UDD layers can be different in order to address the dominant sources of error more efficiently. In Ref. 36, NUDD (including QDD) with even sequence orders on the inner levels was verified analytically to achieve arbitrary order decoupling with only a polynomial increase in the number of pulses over UDD, an exponential improvement over CDD or CUDD<sup>37</sup> which combines orthogonal single-axis CDD and UDD sequences. A universality proof of NUDD with arbitrary sequence orders was given in Ref. 38. The same result, for QDD with arbitrary sequence orders, was proved independently in our previous work,<sup>39</sup> using a different method. Our universality proof for QDD<sup>39</sup> went beyond quantifying the overall performance of QDD, in that we provided a thorough analytical study of the suppression abilities of the inner- and outer-layer UDD sequences of QDD for each single-axis error, and obtained the decoupling order of each single-axis error. We found the decoupling order dependence on the parities and relative magnitudes of the inner and outer sequence orders. However, the analysis for the performance of NUDD with arbitrary sequence orders on each individual error is still missing. A further restriction concerns the type of control pulses, which in general QDD or NUDD proofs<sup>38,39</sup> have so far been limited to elements of  $SU(2)$  or tensor products thereof. Numerical studies of QDD and NUDD performance are given in Refs. 31, and 40–43.

In this paper, we give a rigorous and compact proof for the universality and performance of NUDD (including QDD) with arbitrary sequence orders. The set of control pulse types is generalized to the mutually orthogonal operation set (MOOS) defined in Ref. 36. The concept of error types is also generalized, in the sense that errors are classified according to the types of control pulses chosen. Most importantly, we obtain the explicit decoupling order formula, a function of the given error type, and the parities and magnitudes of all the sequence orders of NUDD. This formula shows explicitly how each UDD layer contributes to the suppression of a given type of error. An immediate consequence is that the overall suppression order of NUDD with a MOOS as the control pulse set is the minimum among all sequence orders of NUDD. Moreover, our analysis identifies the condition under which the suppression ability of a given UDD layer is being hindered, or rendered totally ineffective, or enhanced by other UDD layers with odd sequence orders. One can thus design a NUDD scheme such that the full power of each UDD layer is fully exploited. Note that our proof also shows that the performance of NUDD schemes with generalized control pulse types and arbitrary sequence orders is universal, as in previous UDD-like schemes with Pauli group elements as control pulses.<sup>21,22,36,38,39</sup> In other words, the performance of general NUDD sequence remains the same for multi-qubit or multi-level systems coupling to arbitrary bounded environments. We present numerical simulations in support of our analytical results for the decoupling order of each error type, for a four-layer NUDD scheme applied to a two-qubit system.

The structure of this paper is as follows. In Sec. II, a general NUDD scheme with MOOS as the control pulse set is formulated. In Sec. III, the results of the performance of NUDD are presented. Specifically, we present the NUDD theorem (Theorem 1), which gives the decoupling order formula for each error type. Corollary 1, along with its proof, gives the overall performance of NUDD. The complete proof of the NUDD theorem is presented in Sec. IV. Numerical results for a 4-layer NUDD scheme on 2 qubits system are demonstrated in Sec. V, in support of our analysis. We conclude in Sec. VI. The Appendixes provide additional technical details.

## II. NUDD FORMULATION

### A. The noise model

We assume a completely general noise Hamiltonian  $H$  acting on the joint system-bath Hilbert space, the only assumption being that  $\|H\| < \infty$ . We allow for arbitrary interactions between the system and the bath, as well as between different parts of the system or between different parts of the bath. We use

$$\|A\| \equiv \sup_{|\psi\rangle} \frac{\sqrt{\langle \psi | A^\dagger A | \psi \rangle}}{\langle \psi | \psi \rangle} \quad (2)$$

to denote the sup-operator norm of any operator  $A$ , i.e., the largest singular value of  $A$ , or the largest eigenvalue (in absolute value) if  $A$  is Hermitian.

### B. NUDD pulse timing

A general  $\ell$ -layer NUDD scheme with a sequence order set  $\{N_1, N_2, \dots, N_\ell\}$  is constructed by concatenating  $\ell$  levels of UDD sequences, where  $N_i$  is the sequence order of the UDD $_{N_i}$  sequence at the  $i$ th level of NUDD. The sequence orders of different UDD layers can assume different values in order to address the dominant sources of error in any particular implementation more efficiently. The control pulse operator set  $\{\Omega_1, \Omega_2, \dots, \Omega_\ell\}$ , where the subscript  $i$  is the layer index, is chosen to be the MOOS defined in Ref. 36, which consists of independent, mutually commuting, or anticommuting system operators, each of which is both unitary and Hermitian. Obviously, each  $\Omega_i$  is required not to commute with the total Hamiltonian, for otherwise it would not have any effect on the noise. Note that the MOOS elements  $\Omega_i$  are not restricted to be single-qubit system operators such as a single-qubit Pauli matrix.

The normalized  $\ell$ -layer NUDD pulse timing  $\eta_{j_\ell, j_{\ell-1}, \dots, j_1}$  is defined as the actual NUDD timing, divided by total evolution time  $T$ , where  $j_i \in \{1, \dots, N_i + 1\}$  is called the  $i$ th layer UDD pulse timing index. With fixed  $\{j_k\}_{k=i+1}^\ell$  and  $\{j_k = N_k + 1\}_{k=1}^{i-1}$ ,  $\eta_{j_\ell, j_{\ell-1}, \dots, j_1}$  with  $j_i$  running from 1 to  $N_i + 1$  constitute one cycle of UDD $_{N_i}$ , of total duration  $s_{j_\ell} s_{j_{\ell-1}} \dots s_{j_{i+1}}$ , i.e.,

$$\begin{aligned} \eta_{j_\ell, \dots, j_{i+1}, j_i} &= \eta_{j_\ell, \dots, j_{i+1}, 0} \\ &+ s_{j_\ell} s_{j_{\ell-1}} \dots s_{j_{i+1}} \sin^2 \frac{j_i \pi}{2(N_i + 1)}, \end{aligned} \quad (3)$$

where

$$\eta_{j_\ell, \dots, j_i} \equiv \eta_{j_\ell, \dots, j_{i+1}, j_i, N_{i-1}+1, \dots, N_1+1} \quad (4a)$$

$$\equiv \eta_{j_\ell, \dots, j_{i+1}, j_i+1, 0, \dots, 0} \quad (4b)$$

with  $\eta_{j_i=0} \equiv 0$ , and

$$s_{j_k} = \sin \frac{\pi}{2(N_k + 1)} \sin \frac{(2j_k - 1)\pi}{2(N_k + 1)} \quad (5)$$

is the  $j_k$ th pulse interval of the normalized UDD $_{N_k}$  sequence. Equations (3)–(5) for the 2-layer NUDD scheme with sequence orders of 4 are illustrated in Fig. 1.

Accordingly, the  $i$ th level  $\Omega_i$  pulses are applied at the timings  $\eta_{j_\ell, \dots, j_i}$  with  $j_i = 1, 2, \dots, \bar{N}_i$ , where  $\bar{N}_i = N_i$  if  $N_i$  even while  $\bar{N}_i = N_i + 1$  if  $N_i$  odd, and  $\{j_k \in \{1, \dots, N_k + 1\}\}_{k=i+1}^\ell$ . The additional pulse applied at the end of the sequence when  $N_i$  is odd, is required in order to make the total number of  $\Omega_i$  pulses even, so that the overall effect of the  $\Omega_i$  pulses at the final time  $T$  will be to leave the qubit state unchanged.<sup>35,39</sup>

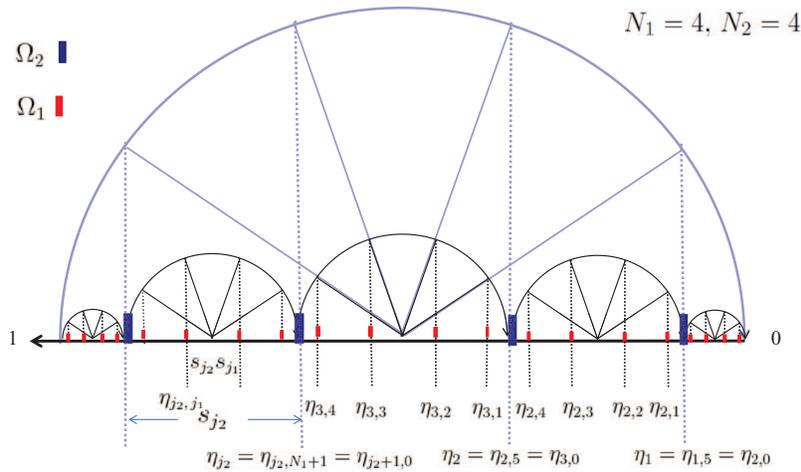


FIG. 1. A graphical way to see the normalized pulse timings and pulse intervals for the 2-layer NUDD scheme where both sequence orders are 4. The red bars indicate the pulse timings of the first UDD layer with control pulse type  $\Omega_1$ , and the blue bars are the pulse timings of the second UDD layer with control pulse type  $\Omega_2$ .

**C.  $(r_1, r_2, \dots, r_\ell)$ -type error**

Each control operator  $\Omega_i$  can divide the total Hamiltonian  $H$  into two parts: one that commutes with  $\Omega_i$  and another that anticommutes with  $\Omega_i$ . Hence, by the procedure provided in Appendix A, the total Hamiltonian can accordingly be divided into  $2^\ell$  independent pieces by the given MOOS  $\{\Omega_1, \Omega_2, \dots, \Omega_\ell\}$ , as

$$H = \sum_{\{r_i=0,1\}_{i=1}^\ell} H_{(r_1, r_2, \dots, r_\ell)}, \tag{6}$$

where

$$\begin{cases} r_i = 1 & \Rightarrow \{\Omega_i, H_{(r_1, r_2, \dots, r_\ell)}\} = 0 \\ r_i = 0 & \Rightarrow [\Omega_i, H_{(r_1, r_2, \dots, r_\ell)}] = 0 \end{cases} \tag{7}$$

with  $i = 1, 2, \dots, \ell$  and

$$\sum_{\{r_i=0,1\}_{i=1}^\ell} \equiv \sum_{r_1=0,1} \sum_{r_2=0,1} \cdots \sum_{r_\ell=0,1} . \tag{8}$$

$H_{(r_1, r_2, \dots, r_\ell)}$  is classified as an  $(r_1, r_2, \dots, r_\ell)$ -type error, a definition which includes all the operators that have the same commuting or anticommuting relation (7) as  $H_{(r_1, r_2, \dots, r_\ell)}$  with respect to a given MOOS  $\{\Omega_1, \Omega_2, \dots, \Omega_\ell\}$ . In particular, the  $\vec{0}_\ell \equiv (0, 0, \dots, 0)$ -type error, which commutes with all control pulses and hence is not suppressed by the NUDD sequence, is called a trivial error. All other error-types are non-trivial.

For example, suppose the first and second pulse types used in 2-layer NUDD (namely, QDD) are Z and X-type pulses, respectively. And the target quantum system we consider is a single qubit subjected to general decoherence, which can always be modeled as

$$H = J_0 I \otimes B_0 + J_x \sigma_x \otimes B_x + J_y \sigma_y \otimes B_y + J_z \sigma_z \otimes B_z, \tag{9}$$

where  $B_\lambda, \lambda \in \{0, X, Y, Z\}$ , are arbitrary bath-operators, the Pauli matrices,  $\sigma_\lambda, \lambda \in \{X, Y, Z\}$ , are the unwanted errors acting on the system qubit, and  $J_\lambda, \lambda \in \{0, X, Y, Z\}$ , are bounded qubit-bath coupling coefficients. Then the MOOS  $\{\sigma_z, \sigma_x\}$  divides the Hamiltonian (9) into four pieces: one trivial error  $H_{(0,0)} = J_0 I \otimes B_0$ , and three non-trivial errors,  $H_{(1,0)} = J_x \sigma_x \otimes B_x$ ,  $H_{(0,1)} = J_z \sigma_z \otimes B_z$ , and  $H_{(1,1)} = J_y \sigma_y \otimes B_y$ .

**D.  $(r_1, r_2, \dots, r_\ell)$ -type error modulation function**

Due to the discreteness of the pulse timings, it is easier to perform the analysis in the toggling frame, i.e., the frame that rotates with the control pulses. Up to  $\pm 1$  factors, the normalized ( $T = 1$ ) control evolution operator is

$$U_c(\eta) = \Omega_\ell^{j_\ell-1} \dots \Omega_2^{j_2-1} \Omega_1^{j_1-1} \tag{10}$$

when  $\eta \in [\eta_{j_\ell, j_{\ell-1}, \dots, j_1-1}, \eta_{j_\ell, j_{\ell-1}, \dots, j_1})$  and  $U_c(1) = I$ , the identity operator.

Note that the commuting and anticommuting relation, Eq. (7), can be reformulated equivalently as follows:

$$\Omega_i H_{(r_1, r_2, \dots, r_\ell)} \Omega_i = (-1)^{r_i} H_{(r_1, r_2, \dots, r_\ell)}, \tag{11}$$

for  $i$  from 1 to  $\ell$ , by using the unitary Hermitian property  $\Omega_i^2 = I$ .

Hence, with Eqs. (10) and (11), we obtain the Hamiltonian in the toggling frame,

$$\begin{aligned} \tilde{H}(\eta) &= U_c^\dagger(\eta) H U_c(\eta) \\ &= \sum_{\{r_i=0,1\}_{i=1}^\ell} (f_1)^{r_1} \dots (f_\ell)^{r_\ell} H_{(r_1, r_2, \dots, r_\ell)}, \end{aligned} \tag{12}$$

where

$$f_i(\eta) = (-1)^{j_i-1} \quad \eta \in [\eta_{j_\ell, \dots, j_i-1}, \eta_{j_\ell, \dots, j_i}) \tag{13}$$

is the normalized  $i$ th-layer modulation function for an  $\ell$ -layer NUDD sequence, which switches sign only when the  $i$ th layer UDD pulse index,  $j_i$ , changes. The factor  $\prod_{i=1}^\ell f_i(\eta)^{r_i}$ , i.e., the coefficient of the  $(r_1, r_2, \dots, r_\ell)$ -type error  $H_{(r_1, r_2, \dots, r_\ell)}$  in Eq. (12), is called an  $(r_1, r_2, \dots, r_\ell)$ -type error modulation function.

Note that since

$$\prod_{p=1}^n f_i(\eta)^{r_i^{(p)}} = f_i(\eta)^{\sum_{p=1}^n r_i^{(p)}} = f_i(\eta)^{\oplus_{p=1}^n r_i^{(p)}}, \tag{14}$$

where  $\oplus$  is the binary addition defined as ordinary integer addition followed by the modulo 2 operation,  $\{f_i^{r_i=0}, f_i^{r_i=1}\}$  forms a  $Z_2$  group under ordinary multiplication. Likewise, for  $(r_1, r_2, \dots, r_\ell)$ -type error modulation functions, we have

$$\prod_{p=1}^n \prod_{i=1}^\ell (f_i(\theta))^{r_i^{(p)}} = \prod_{i=1}^\ell (f_i(\theta))^{\oplus_{p=1}^n r_i^{(p)}}, \tag{15}$$

which indicates that the set of the  $(r_1, r_2, \dots, r_\ell)$ -type error modulation functions constitutes a  $Z_2^{\otimes \ell}$  group.

**E. Dyson expansion of the evolution operator in the toggling frame**

With the shorthand notations,

$$\vec{r}_\ell \equiv (r_1, r_2, \dots, r_\ell) \in \{0, 1\}^{\otimes \ell} \tag{16}$$

and

$$\sum_{\vec{r}_\ell} \equiv \sum_{\{r_i=0,1\}_{i=1}^\ell}, \tag{17}$$

where the subscript  $\ell$  of the vector  $\vec{r}_\ell$  indicates that  $\vec{r}_\ell$  has  $\ell$  components, the Dyson series expansion of the evolution propagator in the toggling frame,

$$\tilde{U}(T) = \hat{T} \exp[-iT \int_0^1 \tilde{H}(\eta) d\eta], \tag{18}$$

reads

$$\tilde{U}(T) = \sum_{n=0}^{\infty} \sum_{\{\vec{r}_\ell^{(p)}\}_{p=1}^n} (-iT)^n \prod_{p=1}^n H_{\vec{r}_\ell^{(p)}} F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}, \tag{19}$$

where the operators in this expression are

$$H_{\vec{r}_\ell}^{(n)} \equiv \prod_{p=1}^n H_{\vec{r}_\ell^{(p)}} = H_{\vec{r}_\ell^{(n)}} H_{\vec{r}_\ell^{(n-1)}} \dots H_{\vec{r}_\ell^{(1)}} \tag{20}$$

(note the ordering), and the scalars are

$$F_{\vec{r}_\ell}^{(n)} \equiv F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}} \equiv \prod_{p=1}^n \int_0^{\eta^{(p+1)}} \prod_{i=1}^{\ell} f_i(\eta^{(p)}) r_i^{(p)} d\eta^{(p)} \tag{21}$$

with  $\eta^{(n+1)} = 1$ , and where  $r_i^{(p)}$  is the  $i$ th component of  $\vec{r}_\ell^{(p)}$ . Our task will be to find the conditions under which these  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  coefficients vanish, which will dictate the decoupling orders of the NUDD sequence.

Since

$$\begin{aligned} \Omega_i H_{\vec{r}_\ell}^{(n)} \Omega_i &= \prod_{p=1}^n \Omega_i H_{\vec{r}_\ell^{(p)}} \Omega_i = \prod_{p=1}^n (-1)^{r_i^{(p)}} H_{\vec{r}_\ell^{(p)}} \\ &= (-1)^{\oplus_{p=1}^n r_i^{(p)}} \prod_{p=1}^n H_{\vec{r}_\ell^{(p)}}, \end{aligned} \tag{22}$$

where the first equality is obtained by inserting  $\Omega_i^2 = I$  between any adjacent  $H_{\vec{r}_\ell^{(p)}}$  and the second equality is obtained by using Eq. (11),  $\prod_{p=1}^n H_{\vec{r}_\ell^{(p)}}$  either commutes ( $\oplus_{p=1}^n r_i^{(p)} = 0$ ) or anticommutes ( $\oplus_{p=1}^n r_i^{(p)} = 1$ ) with each control pulses operator  $\Omega_i$ . In other words,  $\prod_{p=1}^n H_{\vec{r}_\ell^{(p)}}$  belongs to an  $\vec{r}_\ell$ -type error whose component  $r_i = \oplus_{p=1}^n r_i^{(p)}$  and can be denoted as either  $H_{\oplus_{p=1}^n \vec{r}_\ell^{(p)} = \vec{r}_\ell}$ , or  $H_{\vec{r}_\ell}^{(n)}$  [as in Eq. (20)] if we only care about the resulting error type  $\vec{r}_\ell$ . Therefore, the set of  $2^\ell$  ( $r_1, r_2, \dots, r_\ell$ )-type errors  $H_{\vec{r}_\ell}^{(n)}$  form a  $Z_2^{\otimes \ell}$  group under multiplication.

Note the key role played by

$$\vec{r}_\ell = (r_1, r_2, \dots, r_\ell), \quad r_i = \oplus_{p=1}^n r_i^{(p)}. \tag{23}$$

There are  $2^\ell$  such vectors, and they completely classify all the summands in the Dyson series (19).

### F. NUDD coefficients

From Eq. (21),  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  is a normalized  $n$ -nested integral (total duration  $T = 1$ ), and the  $\vec{r}_\ell^{(p)}$  in its subscript indicates that the  $p$ th integrand of  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  is the  $\vec{r}_\ell^{(p)} = (r_1^{(p)}, r_2^{(p)}, \dots, r_\ell^{(p)})$ -type error modulation function  $\prod_{i=1}^{\ell} f_i(\eta^{(p)}) r_i^{(p)}$ . According to  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$ 's associated error type  $H_{\oplus_{p=1}^n \vec{r}_\ell^{(p)} = \vec{r}_\ell}$  (or  $H_{\vec{r}_\ell}^{(n)}$  for short), we can also denote  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  as  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)} = \vec{r}_\ell}$  or  $F_{\vec{r}_\ell}^{(n)}$  [Eq. (21)], and name it the  $n$ th order normalized  $\ell$ -layer NUDD  $\vec{r}_\ell$ -type error coefficient. If no confusion can arise we will sometimes call  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)} = \vec{r}_\ell}$  an ‘‘NUDD coefficient’’ for short.

Let us consider a couple of examples. From Eq. (21), the form of the 1-layer NUDD ( $\vec{r}_1 = 1$ )-type error coefficients

$$F_{\oplus_{p=1}^n \vec{r}_1^{(p)} = \vec{r}_1} = \prod_{p=1}^n \int_0^{\eta^{(p+1)}} f_1(\eta^{(p)}) r_1^{(p)} d\eta^{(p)} \tag{24}$$

is exactly the same as the UDD coefficients appearing in Ref. 22 for the pure dephasing model where the dephasing term  $\sigma_z \otimes B_z$  is our ( $\vec{r}_1 = 1$ )-type error and the Pauli matrix  $\sigma_x$  is our control pulse operator.

Moreover, the form of the 2-layer NUDD  $\vec{r}_2 = (r_1, r_2)$ -type error coefficients

$$F_{\oplus_{p=1}^n \vec{r}_2^{(p)} = \vec{r}_2} = \prod_{p=1}^n \int_0^{\eta^{(p+1)}} f_1(\eta^{(p)})^{r_1^{(p)}} f_2(\eta^{(p)})^{r_2^{(p)}} d\eta^{(p)} \tag{25}$$

is exactly the same as the QDD coefficients defined in our earlier work,<sup>39</sup> where  $\sigma_x \otimes B_x$ ,  $\sigma_z \otimes B_z$ , and  $\sigma_y \otimes B_y$  are our (1, 0)-, (0, 1)-, and (1, 1)-type errors, respectively, while the Pauli matrices  $\sigma_z$  and  $\sigma_x$  are our first-layer and second-layer control pulses, respectively.

Note that from Eq. (21), the NUDD coefficients are actually the same no matter what the control pulse operators are, as long as they are independent and constitute a MOOS. Therefore, the proofs for the performance of UDD and QDD sequence in Refs. 22 and 39, which used single qubit Pauli matrices as control pulses, apply directly to 1-layer NUDD and 2-layer NUDD schemes with more general control pulses.

### III. PERFORMANCE OF THE NUDD SEQUENCE

#### A. The decoupling order of each error type

As we observed, the summands in the Dyson series expansion of the evolution propagator Eq. (19) are each classified as one of  $2^\ell$  types of errors. Therefore, for a given  $\vec{r}_\ell$ -type error, if all of its first  $\check{N}_{\vec{r}_\ell}$  NUDD coefficients vanish, then we say that the  $\ell$ -layer NUDD sequence eliminates the  $\vec{r}_\ell$ -type error to order  $\check{N}_{\vec{r}_\ell}$ , i.e.,  $\check{N}_{\vec{r}_\ell}$  is the decoupling order of the  $\vec{r}_\ell$ -type error.

Let us define

$$[x]_2 \equiv (x \bmod 2) \tag{26}$$

and

$$p_\oplus(a, b) \equiv \bigoplus_{k=a}^b r_k [N_k]_2 \text{ if } b \geq a, \text{ otherwise } 0, \tag{27a}$$

$$p_+(a, b) \equiv \sum_{k=a}^b r_k [N_k]_2 \text{ if } b \geq a, \text{ otherwise } 0. \tag{27b}$$

The value of  $[N_k]_2$  indicates the parity of the sequence order  $N_k$  of the  $k$ th UDD layer, i.e.,  $[N_k]_2 = 0$  or  $1$  when  $N_k$  is even or odd, respectively. Hence  $p_\oplus(1, i - 1) \in \{0, 1\}$  gives the parity of the total number of UDD layers, each of which has odd sequence order and control pulses that anticommute with the  $\vec{r}_\ell$ -type error, in the first  $i - 1$  levels of NUDD. Likewise,  $p_+(i + 1, \ell)$  counts the total number of those UDD layers after the  $i$ th UDD layer, with odd sequence orders and control pulses anticommuting with the  $\vec{r}_\ell$ -type error. With this in mind, we shall prove the following theorem in Sec. IV.

**NUDD Theorem 1:** *An  $\ell$ -layer NUDD scheme with a given sequence order set  $\{N_1, N_2, \dots, N_\ell\}$  eliminates  $\vec{r}_\ell = (r_1, r_2, \dots, r_\ell)$ -type errors to order  $\check{N}_{\vec{r}_\ell}$ , i.e.,*

$$F_{\vec{r}_\ell}^{(n)} = 0, \quad \forall n \leq \check{N}_{\vec{r}_\ell} \tag{28}$$

with the decoupling order of the  $\vec{r}_\ell$ -type error being

$$\check{N}_{\vec{r}_\ell} = \max_{i \in \{1, \dots, \ell\}} [r_i(p_\oplus(1, i - 1) \oplus 1)\tilde{N}_i + p_+(i + 1, \ell)], \tag{29}$$

where

$$\tilde{N}_i = \begin{cases} N_i & \text{when } i \leq o_1, \\ \min[N_{\sigma_{\min}^{k' < i}} + 1, N_i] & \text{when } i > o_1, \end{cases} \tag{30}$$

and where the  $o_1$ th layer is the first UDD layer with odd sequence order denoted as  $N_{o_1}$ , and

$$N_{o_{\min}}^{k' < i} \equiv \min_{k' < i} \{N_{k'} \mid [N_{k'}]_2 = 1\}. \tag{31}$$

Let us proceed to explain this theorem before embarking on its proof. First, note that  $N_{o_{\min}}^{k' < i}$  is simply the minimum value among all the odd sequence orders of the first  $(i - 1)$  UDD layers of NUDD. As we shall see,  $\tilde{N}_i$  is the suppression order of the  $i$ th UDD layer, in contrast with the sequence order  $N_i$  of the same layer. By Eq. (30),  $\tilde{N}_i \leq N_i$ . When  $\tilde{N}_i < N_i$  occurs, we have  $\tilde{N}_i = N_{o_{\min}}^{k' < i} + 1$ , which suggests that the suppression order of the  $i$ th UDD layer is partially hindered by the UDD layer with the smallest odd sequence order, which is nested inside the  $i$ th UDD layer.

The coefficient in front of the suppression order  $\tilde{N}_i$  in Eq. (29) is 1 if and only if both  $r_i = 1$  and  $p_{\oplus}(1, i - 1) = 0$  are satisfied, and vanishes otherwise. Accordingly, there are two requirements for the  $i$ th UDD layer to be effective on a given  $\vec{r}_\ell$ -type error. First, the error must anticommute with the control pulses of this UDD layer ( $r_i = 1$ ). Second, the error must anticommute with a total even number of odd order UDD layers among the first  $(i - 1)$  layers [ $p_{\oplus}(1, i - 1) = 0$ ].

In contrast, if an error anticommutes with a total odd number of odd order UDD layers among the first  $(i - 1)$  layers [ $p_{\oplus}(1, i - 1) = 1$ ], then the  $i$ th-layer UDD sequence is totally ineffective in suppressing this error type, even though this error also anticommutes with the control pulses of the  $i$ th UDD layer.

Note that for the trivial error type, the  $\vec{0}_\ell$ -type error, we have  $\tilde{N}_{\vec{0}_\ell} = 0$ , which by Eq. (28) implies  $F_{\vec{0}_\ell}^{(n)} = 0$  for  $n \leq 0$ . This should be interpreted as saying that the vanishing of the  $\vec{0}_\ell$ -type errors cannot be concluded from Theorem 1.

In the following, we discuss the decoupling order formula Eq. (29) for some particular examples of NUDD schemes.

### 1. 1-layer NUDD (UDD)

Since 1-layer NUDD has  $\ell = 1$ , for the decoupling order of  $(\vec{r}_1 = 1)$ -type error, Eq. (29) gives  $\tilde{N}_{\vec{r}_1=1} = \tilde{N}_1$ . By definition of  $\tilde{N}_1$  [Eq. (30)], the suppression order of the first UDD layer  $\tilde{N}_1$  is always equal to its sequence order  $N_1$ , i.e.,  $\tilde{N}_1 = N_1$ , irrespective of  $N_1$ 's parity. Therefore, we have

$$\tilde{N}_{\vec{r}_1=1} = N_1 \tag{32}$$

which shows that the non-trivial error is eliminated up to the UDD's sequence order, in agreement with Refs. 21 and 22.

### 2. 2-layer NUDD (QDD)

For 2-layer NUDD with a sequence order set  $\{N_1, N_2\}$ , the decoupling order formula Eq. (29) simplifies to

$$\tilde{N}_{\vec{r}_2} = \max[r_1 \tilde{N}_1 + r_2 [N_2]_2, r_2 (r_1 [N_1]_2 \oplus 1) \tilde{N}_2]. \tag{33}$$

Specifically, we have

$$\begin{aligned} \tilde{N}_{(1,0)} &= \tilde{N}_1 = N_1, \\ \tilde{N}_{(0,1)} &= \max[[N_2]_2, (0 \oplus 1) \tilde{N}_2] = \tilde{N}_2, \\ \tilde{N}_{(1,1)} &= \max[\tilde{N}_1 + [N_2]_2, ([N_1]_2 \oplus 1) \tilde{N}_2]. \end{aligned} \tag{34}$$

If we identify the (1, 0)-type, (0, 1)-type, and (1, 1)-type errors to be  $\sigma_x, \sigma_z$ , and  $\sigma_y$  errors, respectively, Eq. (34) agrees exactly with the results obtained in our earlier QDD work.<sup>39</sup>

### 3. NUDD with all even sequence orders

For  $\ell$ -layer NUDD with  $[N_i]_2 = 0 \forall i \leq \ell$ , the suppression order of each UDD layer is equal to its corresponding sequence order  $N_i$ ,  $\tilde{N}_i = N_i$  [Eq. (30)]. Therefore, the decoupling order formula

Eq. (29) for this type of NUDD schemes reduces to

$$\check{N}_{\vec{r}_\ell} = \max_{i \in \{1, \dots, \ell\}} [r_i \check{N}_i] = \max_{i \in \{1, \dots, \ell\}} [r_i N_i], \tag{35}$$

which indicates that the suppression ability of the UDD sequence in each layer is unaffected by the other nested UDD sequences, i.e., successive UDD layers do not interfere with one another.

**4. NUDD with all even sequence orders except the outer-most UDD layer**

For  $\ell$ -layer NUDD with  $[N_i]_2 = 0 \forall i < \ell$ , and  $[N_\ell]_2 = 1$ , we again have  $\check{N}_i = N_i$  [Eq. (30)]. Therefore, the decoupling order formula Eq. (29) reads

$$\check{N}_{\vec{r}_\ell} = \max[\{r_i N_i \oplus r_\ell\}_{i=1}^{\ell-1}, r_\ell N_\ell]. \tag{36}$$

From Eq. (36), we can see that if a given error anticommutes with the outer-most UDD layer, namely,  $r_\ell = 1$ , then the outer-most layer boosts the suppression abilities of all inner UDD layers by one additional order. We call this the outer-odd-UDD effect.

**5. NUDD with all odd sequence orders**

For any NUDD scheme with all odd sequence orders, in general,  $\check{N}_i = N_{\text{min}}^{k' < i} + 1 < N_i$  could occur, which suggests that the suppression ability of the  $i$ th UDD layer is hindered by one of the odd order UDD layers inside the  $i$ th layer.

Nevertheless, for the case of  $\ell$ -layer NUDD with a  $[N_i]_2 = 1 \forall i$  and  $N_1 > N_2 > \dots > N_\ell$ ,  $\check{N}_i = N_i$  [Eq. (30)] is guaranteed. Moreover, it is easy to show that

$$N_i + \sum_{k=i+1}^{\ell} r_k > N_j + \sum_{k=j+1}^{\ell} r_k \tag{37}$$

for any  $i < j$ . Accordingly, due to Eq. (37), it turns out that the maximum value in Eq. (29) occurs at the inner-most UDD layer that the error anticommutes with. Suppose the first non-zero component of an  $\vec{r}_\ell$ -type error is  $r_M = 1$ . Then it follows that the  $M$ th UDD layer has the maximum suppression on this error, i.e.,

$$\check{N}_{\vec{r}_\ell} = N_M + \sum_{k=M+1}^{\ell} r_k. \tag{38}$$

The second term of the above equation implies that the outer-odd-UDD suppression effects generated by UDD layers with odd sequence orders outside the  $M$ th layer all add up. In other words, the outer-odd-UDD suppression effect is cumulative.

**B. The overall performance of NUDD scheme**

The overall performance of an  $\ell$ -layer NUDD scheme is quantified by the minimum over the decoupling orders of all error types, i.e., by

$$\check{N}_{\min} \equiv \min_{\{\vec{r}_\ell\}} [\check{N}_{\vec{r}_\ell}]. \tag{39}$$

We call  $\check{N}_{\min}$  the overall decoupling order. The following corollary of the NUDD theorem states the relationship between the overall decoupling order  $\check{N}_{\min}$  and given sequence orders  $\{N_i\}$ .

*Corollary 1: The overall decoupling order  $\check{N}_{\min}$  of an  $\ell$ -layer NUDD scheme with a given sequence order set  $\{N_1, N_2, \dots, N_\ell\}$  is*

$$\check{N}_{\min} = \min_{i \in \{1, \dots, \ell\}} [N_i]. \tag{40}$$

*Proof of Corollary 1:* For a given error type  $\vec{r}_\ell \neq \vec{0}_\ell$ , suppose the inner-most non-zero component is  $r_i = 1$  with  $i \geq 2$ , i.e.,  $r_{k < i} = 0$ , so that  $p_{\oplus}(1, i - 1) = 0$ . By definition for  $i = 1$ , we also have

$p_{\oplus}(1, i - 1) = 0$ . Due to  $r_i(p_{\oplus}(1, i - 1) \oplus 1) = 1$  and  $\check{N}_{\vec{r}_i}$  taking the maximum value over the set displayed in Eq. (29), it follows that

$$\check{N}_{\vec{r}_\ell} \geq r_i(p_{\oplus}(1, i - 1) \oplus 1)\check{N}_i = \check{N}_i. \tag{41}$$

Among  $\vec{r}_\ell \neq \vec{0}_\ell$  error types, there are error types which anti-commute with only one control pulse type denoted as  $\vec{e}_i$  with  $r_i = 1$  and all  $r_{j \neq i} = 0$ . According to Eq. (29), the decoupling order of the  $\vec{e}_i$ -type error is

$$\check{N}_{\vec{e}_i} = \check{N}_i. \tag{42}$$

Owing to Eqs. (41) and (42),  $\check{N}_{\min}$ , the minimum among decoupling orders of all non-trivial error types [Eq. (39)], occurs among the decoupling orders of all  $\vec{e}_i$ -type errors, i.e.,

$$\check{N}_{\min} \equiv \min_{\{\vec{r}_\ell\}} [\check{N}_{\vec{r}_\ell}] = \min_{i \in \{1, \dots, \ell\}} [\check{N}_{\vec{e}_i}] = \min_{i \in \{1, \dots, \ell\}} [\check{N}_i]. \tag{43}$$

Suppose that among the  $\ell$  layers, the  $o_1$ th,  $o_2$ th,  $\dots$ , and  $o_b$ th UDD layers where  $0 < o_1 < o_2 < \dots < o_b \leq \ell$  are the layers with odd sequence orders. By the definition of  $\check{N}_i$  [Eq. (30)], for  $i \leq o_1$ ,  $\check{N}_i = N_i$ , while for  $o_j - 1 < k \leq o_j$  with  $j \in \{2, \dots, b\}$ ,  $\check{N}_k = \min[N_{o_1} + 1, N_{o_2} + 1, \dots, N_{o_{j-1}} + 1, N_k]$ . Then it follows that

$$\min_{i \in \{1, \dots, \ell\}} [\check{N}_i] = \min_{i \in \{1, \dots, \ell\}} [N_i] \tag{44}$$

which proves Eq. (40). □

#### IV. PROOF OF THE NUDD THEOREM

##### A. Synopsis of the proof

Our proof is by induction. To establish the base case, we recall that (as already discussed in Sec. II F) the proofs of the vanishing of UDD coefficients in Ref. 22 and QDD coefficients in our earlier work,<sup>39</sup> which used single qubit Pauli matrices as control pulses, are also valid for the 1-layer and the 2-layer NUDD schemes with a more general set of control pulses (MOOS). From Refs. 22 and 39, the decoupling orders of each error type for UDD and QDD match exactly with Eq. (29). Accordingly, the NUDD theorem holds for the 1-layer and the 2-layer NUDD sequence.

Suppose that Theorem 1 holds for  $(\ell - 1)$ -layer NUDD with an arbitrary integer  $\ell \geq 2$ , i.e.,

$$F_{\vec{r}_{\ell-1}}^{(n)} = 0, \quad \forall n \leq \check{N}_{\vec{r}_{\ell-1}}. \tag{45}$$

Then the remaining task is to show that Theorem 1—in particular Eqs. (28) and (29)—also holds for  $\ell$ -layer NUDD. The procedure is the following.

$F_{\vec{r}_\ell}^{(n)}$  can be re-expressed in two different forms, building on two different methods adapted from our earlier QDD proof:<sup>39</sup> the outer-most-layer interval decomposition (“Method 1”), and the nested integral analysis with certain function types (“Method 2”). Each method allows us to show the vanishing of  $F_{\vec{r}_\ell}^{(n)}$  for some error types, and when put together the two methods complete the proof.

In Sec. IV B, using Method 1, the  $\ell$ -layer NUDD coefficient  $F_{\vec{r}_\ell}^{(n)}$  is expressed in terms of the  $(\ell - 1)$ -layer NUDD coefficients. Then, in Sec. IV C, we show that it is the vanishing of the  $(\ell - 1)$ -layer NUDD coefficients that make the first  $\check{N}_{\vec{r}_{\ell-1}}$  orders of the  $\ell$ -layer NUDD coefficient  $F_{\vec{r}_\ell}^{(n)}$  vanish, i.e.,

$$F_{\vec{r}_\ell = (\vec{r}_{\ell-1}, r_\ell)}^{(n)} = 0, \quad \forall n \leq \check{N}_{\vec{r}_{\ell-1}} \tag{46}$$

due to the inductive assumption Eq. (45).

Further, using the outer-layer interval decomposition form of  $F_{\vec{r}_\ell}^{(n)}$ , we show in Sec. IV D that for the  $(\vec{r}_{\ell-1}, 1)$ -type error, which anticommutes with the control pulses of the  $\ell$ th UDD layer, if the  $\ell$ th sequence order is odd, then due to the anti-symmetry of the  $\ell$ th UDD layer, the first  $(\ell - 1)$  UDD layers in fact suppress the error by one more order, namely,

$$F_{(\vec{r}_{\ell-1}, 1)}^{(\check{N}_{\vec{r}_{\ell-1}}+1)} = 0. \tag{47}$$

Combining Eq. (47) with Eq. (46), Method 1 gives rise to

$$F_{\vec{r}_\ell}^{(n)} = 0, \quad \forall n \leq \check{N}_{\vec{r}_{\ell-1}} + r_\ell[N_\ell]_2. \tag{48}$$

Let us now define two special cases, by parity

$$\vec{v}_i^a \equiv \vec{r}_i \text{ with } p_\oplus(1, i) = a, \quad a \in \{0, 1\}. \tag{49}$$

The decoupling order of the  $(\vec{v}_{\ell-1}^0, 1)$ -type error which by Eq. (49) includes the  $(\vec{0}_{\ell-1}, 1)$ -type error is derived independently by Method 2 in Subsections **IV E–IV G**.

The second part of the NUDD proof is summarized as follows. In Sec. **IV E**, we apply a piecewise linear change of variables to  $F_{\vec{r}_\ell}^{(n)}$ , such that the Fourier expansions of all its integrands,  $\prod_{i=1}^\ell f_i(\eta)^{r_i}$ , belong to certain specific function types. In particular, for NUDD with all even inner sequence orders, there are only two function types,  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}\}$ , while for NUDD with at least one odd sequence order, there are four types,  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}, \zeta_{\text{even}}^{N_\ell, 0}, c_{\text{odd}}^{N_\ell, 0}\}$ . These function types are defined as follows:

*Definition 1: Let  $k, q \in \mathbb{Z}$  with  $|q| \leq n$  and let  $d_{ki} \in \mathbb{R}$  be arbitrary*

<i>Name</i>	<i>Function type</i>
$c_{\text{odd}}^{N_\ell, n}$	$\sum_k d_{k1} \cos[(2k + 1)(N_\ell + 1)\theta + q\theta]$
$c_{\text{even}}^{N_\ell, n}$	$\sum_k d_{k2} \cos[2k(N_\ell + 1)\theta + q\theta]$
$\zeta_{\text{even}}^{N_\ell, n}$	$\sum_k d_{k3} \sin[2k(N_\ell + 1)\theta + q\theta]$
$\zeta_{\text{odd}}^{N_\ell, n}$	$\sum_k d_{k4} \sin[(2k + 1)(N_\ell + 1)\theta + q\theta]$ .

Also, let  $\diamond$  denote the product-to-sum trigonometric function operation.

By utilizing the group properties of  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}\}$  (or  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}, \zeta_{\text{even}}^{N_\ell, 0}, c_{\text{odd}}^{N_\ell, 0}\}$ ), after integrating out the first  $n - 1$  integrals of  $F_{\vec{r}_\ell}^{(n)}$ , we obtain

$$\begin{aligned} F_{(\vec{v}_{\ell-1}^0, 1)}^{(n)} &= \int_0^\pi c_{\text{odd}}^{N_\ell, n} d\theta \\ &= \sum_k d_k \sin[(2k + 1)(N_\ell + 1)\theta + q\theta] \Big|_0^\pi \\ &= 0 \end{aligned} \tag{50}$$

for the  $(\vec{v}_{\ell-1}^0, 1)$ -type error, where  $n \leq N_\ell$  for NUDD with all even inner sequence orders, and  $n \leq \min[N_{\text{min}}^{k' < \ell} + 1, N_\ell]$  for NUDD with at least one odd inner sequence order. The vanishing orders of the other types of errors cannot be deduced from this method and we denote this fact by:  $F_{\vec{r}_\ell \notin (\vec{v}_{\ell-1}^0, 1)}^{(n)} = 0, \quad \forall n \leq 0$ . In conclusion, Method 2 yields

$$F_{\vec{r}_\ell}^{(n)} = 0, \quad \forall n \leq r_\ell[(p_\oplus(1, \ell - 1) \oplus 1)\check{N}_\ell]. \tag{51}$$

Combining Eq. (48) with Eq. (51), we have

$$F_{\vec{r}_\ell}^{(n)} = 0 \quad \forall n \leq \max[\check{N}_{\vec{r}_{\ell-1}} + r_\ell[N_\ell]_2, r_\ell((p_\oplus(1, \ell - 1) \oplus 1)\check{N}_\ell)]. \tag{52}$$

Equation (52) is equivalent to the decoupling order formula Eq. (29) given in Theorem 1, as can be seen by substituting the explicit expression for  $\check{N}_{\vec{r}_{\ell-1}}$ , i.e., Eq. (29) for  $(\ell - 1)$ -layer NUDD, into Eq. (52). Therefore, Theorem 1 also holds for the  $\ell$ -layer NUDD scheme with arbitrary sequence

orders. The induction method also implies that Theorem 1 holds for any number of nested layers of NUDD.

**B. The outer-layer interval decomposition form of  $F_{\vec{r}_\ell}^{(n)}$**

It is expected that the  $(\vec{r}_{\ell-1} \neq \vec{0}_{\ell-1}, r_\ell)$ -type errors, which anticommute with one or more of the first  $(\ell - 1)$  inner-layer control operators, are suppressed mainly by the inner  $(\ell - 1)$ -layer NUDD sequences. In order to extract the action of the inner  $(\ell - 1)$ -layer NUDD scheme and factor out the action of the outer-most ( $\ell$ th-layer) UDD sequence, we employ the outer-layer interval decomposition method, which splits each integral of  $F_{\vec{r}_\ell}^{(n)}$  [Eq. (21)] into a sum of sub-integrals over the  $\ell$ th-layer UDD $_{N_\ell}$  pulse intervals  $s_{j_\ell}$  [Eq. (5)].

The derivation of  $F_{\vec{r}_\ell}^{(n)}$  given in Appendix B shows that each  $\ell$ -layer NUDD coefficient can be expressed in terms of the  $(\ell - 1)$ -layer NUDD coefficients as follows:

$$F_{\vec{r}_\ell=(\vec{r}_{\ell-1}, r_\ell)}^{(n)} \equiv F_{\oplus_{p=1}^n (\vec{r}_{\ell-1}^{(p)}, r_\ell^{(p)})} = \sum_{m=1}^n \sum_{\{\sum_{a=1}^m n_a=n\}} \left( \prod_{a=1}^m F_{\vec{r}_{\ell-1}}^{(n_a)} \right) \left( \prod_{a=1}^m \sum_{j_\ell^{(a)}=a}^{j_\ell^{(a+1)}-1} (-1)^{(j_\ell^{(a)}-1)r_\ell^{(a)}} s_{j_\ell^{(a)}}^{n_a} \right), \tag{53}$$

where  $j_\ell^{(m+1)} - 1 \equiv N_\ell + 1$ , and for given  $m$ ,  $\sum_{\{\sum_{a=1}^m n_a=n\}}$  sums over all possible combinations of  $\{n_a\}_{a=1}^m$  under the condition  $\sum_{a=1}^m n_a = n$ , with  $1 \leq n_a \leq n$ . From the derivation of Eq. (53) in Appendix B, one can see that each segment with a specific configuration  $\{m, \{n_a\}_{a=1}^m\}$  defines a unique way to separate the  $n$  vectors  $\{\vec{r}_\ell^{(p)}\}_{p=1}^n$  into  $m$  clusters. The  $a$ th cluster contains  $n_a$  vectors,  $\{\vec{r}_\ell^{(p)}\}_{p=\sum_{k=1}^{a-1} n_k+1}^{\sum_{k=1}^a n_k+n_a}$  with  $n_0 \equiv 0$ , and  $\vec{r}_\ell^{(a)}$  is the resulting vector of the  $a$ th cluster, i.e.,

$$\vec{r}_\ell^{(a)} \equiv \oplus_{p=\sum_{k=1}^{a-1} n_k+1}^{\sum_{k=1}^a n_k+n_a} \vec{r}_\ell^{(p)}, \tag{54}$$

which implies  $\oplus_{a=1}^m \vec{r}_\ell^{(a)} = \vec{r}_\ell$ , i.e.,

$$\oplus_{a=1}^m \vec{r}_{\ell-1}^{(a)} = \vec{r}_{\ell-1}, \tag{55a}$$

$$\oplus_{a=1}^m r_\ell^{(a)} = r_\ell. \tag{55b}$$

Moreover, the  $a$ th cluster is associated with  $F_{\vec{r}_{\ell-1}}^{(n_a)}$ , an  $n_a$ th order  $(\ell - 1)$ -layer  $\vec{r}_{\ell-1}^{(a)}$ -type error NUDD coefficient, and with  $\sum_{j_\ell^{(a)}=a}^{j_\ell^{(a+1)}-1} (-1)^{(j_\ell^{(a)}-1)r_\ell^{(a)}} s_{j_\ell^{(a)}}^{n_a}$  which contains the outermost ( $\ell$ th) UDD layer's information.

**C. The performance of the inner  $(\ell - 1)$ -layer NUDD**

We shall show that it is the vanishing of the inner  $(\ell - 1)$ -layer NUDD coefficients,  $F_{\vec{r}_{\ell-1}}^{(n_a)} = 0, \forall n_a \leq \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ , that make the first  $\check{N}_{\vec{r}_{\ell-1}}$  orders of  $F_{\vec{r}_\ell=(\vec{r}_{\ell-1}, r_\ell)}^{(n)}$  vanish.

First, we have the following lemma, with the proof given in Appendix C.

*Lemma 1:*  $\check{N}_{\vec{r}_{\ell-1}} \leq \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ , where  $\vec{r}_{\ell-1} = \oplus_{a=1}^m \vec{r}_{\ell-1}^{(a)}$ .

With Lemma 1, for  $F_{\vec{r}_\ell=(\vec{r}_{\ell-1}, r_\ell)}^{(n)}$  with  $n \leq \check{N}_{\vec{r}_{\ell-1}}$ , each  $\prod_{a=1}^m F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $\oplus_{a=1}^m \vec{r}_{\ell-1}^{(a)} = \vec{r}_{\ell-1}$  in Eq. (53) satisfies

$$\sum_{a=1}^m n_a = n \leq \check{N}_{\vec{r}_{\ell-1}} \leq \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}}^{(a)}. \tag{56}$$

From Eq. (56), it follows that there must exist at least one  $a$  from 1 to  $m$  such that  $n_a \leq \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ , because if  $n_a > \check{N}_{\vec{r}_{\ell-1}}^{(a)}$  for all  $a$ , it leads to

$$\sum_{a=1}^m n_a > \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}}^{(a)} \tag{57}$$

which contradicts the assumption Eq. (56). Accordingly, each  $\prod_{a=1}^m F_{\vec{r}_{\ell-1}}^{(n_a)}$  term of  $F_{\vec{r}_{\ell}=(\vec{r}_{\ell-1}, r_{\ell})}^{(n)}$  with  $n \leq \check{N}_{\vec{r}_{\ell-1}}$  contains at least one  $F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $n_a \leq \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ , which turns out to be zero due to the assumption Eq. (45) for  $(\ell - 1)$  NUDD coefficients. Therefore, the first step  $F_{\vec{r}_{\ell}=(\vec{r}_{\ell-1}, r_{\ell})}^{(n)} = 0$  for all  $n \leq \check{N}_{\vec{r}_{\ell-1}}$ . Eq. (46) is proven.

From the proof, one can see that the effect of the outer  $\ell$ -layer UDD sequence which is entirely contained in the outer part  $\prod_{a=1}^m \sum_{j_{\ell}^{(a)}=a}^{j_{\ell}^{(a+1)}-1} (-1)^{(j_{\ell}^{(a)}-1)r_{\ell}^{(a)}} s_{j_{\ell}^{(a)}}^{n_a}$  in Eq. (53) does not interfere with the elimination ability of the inner  $(\ell - 1)$ -layer NUDD sequence.

Note that for the  $\vec{r}_{\ell} = (\vec{0}_{\ell-1}, 1)$ -type error,  $N_{\vec{0}_{\ell-1}} = 0$  by Eq. (29) gives rise to  $F_{(\vec{0}_{\ell-1}, 1)}^{(n)} = 0$  for all  $n \leq N_{\vec{0}_{\ell-1}} = 0$  [Eq. (46)]. However, this does not mean that  $F_{(\vec{0}_{\ell-1}, 1)}^{(n)} \neq 0$  in our context, but rather that the vanishing of  $F_{(\vec{0}_{\ell-1}, 1)}^{(n)}$  cannot be deduced by the just-mentioned method, which only considers the contribution of the first  $(\ell - 1)$  UDD layers. This makes sense because the  $\vec{r}_{\ell} = (\vec{0}_{\ell-1}, 1)$ -type error, which commutes with all the control pulses of the inner  $(\ell - 1)$  UDD layers, is supposed to be suppressed by the  $\ell$  th-layer UDD sequence.

**D. One more order suppression of the  $(\vec{r}_{\ell-1}, 1)$ -type error**

In Sec. IV C, we proved that  $F_{\vec{r}_{\ell}=(\vec{r}_{\ell-1}, r_{\ell})}^{(n)} = 0$  for all  $n \leq \check{N}_{\vec{r}_{\ell-1}}$  [Eq. (46)]. Now we shall show that for  $(\vec{r}_{\ell-1}, 1)$ -type error, there is an additional order suppression, i.e.,  $F_{(\vec{r}_{\ell-1}, 1)}^{(\check{N}_{\vec{r}_{\ell-1}}+1)} = 0$  [Eq. (47)], if  $N_{\ell}$  is odd. First, we need the following lemma.

*Lemma 2: For  $\sum_{a=1}^m n_a = n = \check{N}_{\vec{r}_{\ell-1}} + 1$  with  $m \geq 2$ , there must exist at least one  $a$  such that  $n_a \leq \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ .*

*Proof of Lemma 2:* With Lemma 1, we have

$$\sum_{a=1}^m n_a \leq \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}}^{(a)} + 1. \tag{58}$$

For  $m \geq 2$ , pick an arbitrary  $n_{a'}$  among  $\{n_a\}_{a=1}^m$ . If  $n_{a'} \leq \check{N}_{\vec{r}_{\ell-1}}^{(a')}$ , then Lemma 2 is true. On the other hand, if  $n_{a'} \geq \check{N}_{\vec{r}_{\ell-1}}^{(a')} + 1$ , subtracting  $n_{a'}$  from Eq. (58) leads to

$$\sum_{a \neq a'} n_a \leq \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}}^{(a)} + 1 - n_{a'} \leq \sum_{a \neq a'} \check{N}_{\vec{r}_{\ell-1}}^{(a)}. \tag{59}$$

Accordingly, by the same counterargument mentioned in Sec. IV C, there must exist at least one  $a'' \neq a'$  such that  $n_{a''} \leq \check{N}_{\vec{r}_{\ell-1}}^{(a'')}$ , for otherwise we would obtain  $\sum_{a \neq a'} n_a \geq \sum_{a \neq a'} \check{N}_{\vec{r}_{\ell-1}}^{(a)}$  which contradicts Eq. (59).  $\square$

With Lemma 2, it follows that for the outer-layer decomposition form of  $F_{(\vec{r}_{\ell-1}, 1)}^{(\check{N}_{\vec{r}_{\ell-1}}+1)}$  Eq. (53), in each  $\prod_{a=1}^m F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $m \geq 2$  and  $\sum_{a=1}^m n_a = n = \check{N}_{\vec{r}_{\ell-1}} + 1$ , there must exist at least one  $F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $n_a \leq \check{N}_{\vec{r}_{\ell-1}}^{(a)}$ . Due to the induction assumption Eq. (45), all  $\prod_{a=1}^m F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $m \geq 2$  in Eq. (53) vanish. Therefore, only the  $\{m = 1, n_a = n\}$  term,  $F_{\vec{r}_{\ell-1}}^{(\check{N}_{\vec{r}_{\ell-1}}+1)}$ , remains in the outer-layer decomposition form

of  $F_{\vec{r}_\ell}^{(\check{N}_{\vec{r}_{\ell-1}}+1)}$ . In particular, for the  $(\vec{r}_{\ell-1}, 1)$ -type error, we have

$$F_{(\vec{r}_{\ell-1}, 1)}^{(\check{N}_{\vec{r}_{\ell-1}}+1)} = F_{\vec{r}_{\ell-1}}^{(\check{N}_{\vec{r}_{\ell-1}}+1)} \sum_{j_\ell=1}^{N_\ell+1} (-1)^{(j_\ell-1)} s_{j_\ell}^n. \tag{60}$$

Despite  $F_{\vec{r}_{\ell-1}}^{(\check{N}_{\vec{r}_{\ell-1}}+1)}$ , the outer part  $\sum_{j_\ell=1}^{N_\ell+1} (-1)^{(j_\ell-1)} s_{j_\ell}^n$  turns out to be zero due to the cancellation of opposite signs between  $j_\ell$  and  $N_\ell + 2 - j_\ell$  when  $N_\ell$  is odd, but otherwise equal terms  $s_{j_\ell} = s_{N_\ell+2-j_\ell}$  (time-symmetric property of UDD) in the sum. Therefore,  $F_{(\vec{r}_{\ell-1}, 1)}^{(\check{N}_{\vec{r}_{\ell-1}}+1)} = 0$  and Eq. (47) is proven. Combining Eq. (47) with Eq. (46), which we proved in Sec. IV C, leads to  $F_{\vec{r}_\ell}^{(n)} = 0$  for  $n \leq \check{N}_{\vec{r}_{\ell-1}} + r_\ell[N_\ell]_2$ , i.e., Eq. (48).

From the proof, one can see that the anti-symmetry of the  $\ell$ th outer-most UDD layer with odd sequence order can help the inner  $(\ell - 1)$  NUDD sequences to suppress the  $(\vec{r}_{\ell-1}, 1)$ -type error by one more order.

**E. Fourier expansion after linear change of variables**

We shall complete the proof of Theorem 1 by another approach which analyzes the nested integral with certain Fourier function types. First apply a piecewise linear transformation,

$$\theta = \frac{\pi}{N_\ell + 1} \left( \frac{\eta - \eta_{j_\ell-1}}{s_{j_\ell}} \right) + \frac{(j_\ell - 1)\pi}{N_\ell + 1} \quad \eta \in [\eta_{j_\ell-1}, \eta_{j_\ell}] \tag{61}$$

with  $j_\ell \in \{1, \dots, N_\ell\}$ , to the  $n$ -fold nested integral  $F_{\vec{r}_\ell}^{(n)}$ . With  $d\eta = G_1(\theta) d\theta$ ,  $F_{\vec{r}_\ell}^{(n)} = F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  Eq. (21) is re-expressed as

$$F_{\vec{r}_\ell}^{(n)} = \prod_{p=1}^n \int_0^{\theta^{(p+1)}} G_1(\theta^{(p)}) \prod_{i=1}^{\ell} f_i(\theta^{(p)}) r_i^{(p)} d\theta^{(p)} \tag{62}$$

with

$$\theta^{(n+1)} = \pi, \tag{63}$$

$$f_i(\theta) = (-1)^{j_i-1} \quad \theta \in [\theta_{j_\ell, \dots, j_i-1}, \theta_{j_\ell, \dots, j_i}], \tag{64}$$

$$G_1(\theta) = \frac{N_\ell + 1}{\pi} s_{j_\ell} \quad \theta \in [\theta_{j_\ell-1}, \theta_{j_\ell}], \tag{65}$$

where  $\theta_{j_\ell, \dots, j_i}$  is the new pulse timing.

The advantage of using the piecewise linear transformation Eq. (61) is that all the modulation functions become periodic functions. Consequently, as explained in Appendix D, it turns out that the Fourier expansion of each function appearing in  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  belongs to one of the function types from Definition 1,

$$\Psi(f_\ell(\theta)) = \zeta_{\text{odd}}^{N_\ell, 0}, \tag{66}$$

$$\Psi(f_{i < \ell}(\theta)) = \begin{cases} c_{\text{even}}^{N_\ell, 0} & \text{when } N_i \text{ even,} \\ \zeta_{\text{even}}^{N_\ell, 0} & \text{when } N_i \text{ odd,} \end{cases} \tag{67}$$

$$\Psi(G_1(\theta)) = \zeta_{\text{even}}^{N_\ell, 1}, \tag{68}$$

where  $\Psi$  maps a function to the function type of its Fourier expansion up to unimportant coefficients.

Note that the sets  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}\}$  and  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}, \zeta_{\text{even}}^{N_\ell, 0}, c_{\text{odd}}^{N_\ell, 0}\}$  constitute  $Z_2$  and  $Z_2 \times Z_2$  groups with  $c_{\text{even}}^{N_\ell, 0}$  as identity, respectively, under the binary operation  $\diamond$  (the product-to-sum trigonometric

TABLE I. The first column classifies  $2^\ell \vec{r}_\ell$ -type errors into four groups by two values,  $\oplus_{k=1}^{\ell-1} r_k [N_k]_2$  and  $r_\ell$ , where  $\vec{v}_{\ell-1}^0$  and  $\vec{v}_{\ell-1}^1$  are defined in Eq. (49). The second column shows the function types of the Fourier expansion of the  $\vec{r}_\ell$ -type error modulation functions.

Error type $\vec{r}_\ell$	$\Psi(\prod_{i=1}^{\ell} f_i(\theta)^{r_i})$
(1) $(\vec{v}_{\ell-1}^0, 0)$ : $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 0,$ $r_\ell = 0$	$c_{\text{even}}^{N_\ell, 0}$
(2) $(\vec{v}_{\ell-1}^0, 1)$ : $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 0,$ $r_\ell = 1$	$\zeta_{\text{odd}}^{N_\ell, 0}$
(3) $(\vec{v}_{\ell-1}^1, 0)$ : $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 1,$ $r_\ell = 0$	$\zeta_{\text{even}}^{N_\ell, 0}$
(4) $(\vec{v}_{\ell-1}^1, 1)$ : $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 1,$ $r_\ell = 1$	$c_{\text{odd}}^{N_\ell, 0}$

formula). Then one can obtain the function types of the  $\vec{r}_\ell$ -type error modulation functions by employing the group algebra of  $Z_2$  and  $Z_2 \times Z_2$  to

$$\Psi\left(\prod_{i=1}^{\ell} f_i(\theta)^{r_i}\right) = \diamond_{i=1}^{\ell} \Psi(f_i(\theta)^{r_i}), \tag{69}$$

where  $\Psi(f_i(\theta)^0) = 1 = c_{\text{even}}^{N_\ell, 0}$  for all  $i$ . For example, for the  $\vec{v}_{\ell-1}^1$ -type error [see Eq. (49)], its  $\diamond_{i=1}^{\ell-1} \Psi(f_i(\theta)^{r_i})$  would result in  $\zeta_{\text{even}}^{N_\ell, 0}$ , because the condition  $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 1$ , that the components of  $\vec{v}_{\ell-1}^1$  satisfy, implies that there is a total odd number of  $r_i = 1$  associated with  $[N_i]_2 = 1$  such that  $\Psi(f_i(\theta)^{r_i}) = \zeta_{\text{even}}^{N_\ell, 0}$ . It turns out that  $\Psi(\prod_{i=1}^{\ell} f_i(\theta)^{r_i})$  is determined by only two values,  $\oplus_{k=1}^{\ell-1} r_k [N_k]_2$  and  $r_\ell$ , (see Table I).

Note that for the  $\ell$ -layer NUDD with  $[N_i]_2 = 0 \forall i \leq \ell - 1$ ,  $\oplus_{k=1}^{\ell-1} r_k [N_k]_2$  is zero for all  $2^\ell \vec{r}_\ell$ -type errors. Therefore,  $\Psi(\prod_{i=1}^{\ell} f_i(\theta)^{r_i})$  for all error types in this case is either  $\zeta_{\text{odd}}^{N_\ell, 0}$  or  $c_{\text{even}}^{N_\ell, 0}$ , the first two rows in Table I. On the other hand, for the  $\ell$ -layer NUDD with at least one UDD layer with odd sequence order, there are four functions types as shown in Table I.

The following expression of  $F_{\vec{r}_\ell}^{(n)}$  focuses on the function types of the integrands, while the coefficients in their Fourier expansion are unimportant in the proof

$$F_{\vec{r}_\ell}^{(n)} = \diamond_{p=1}^n \int_0^{\theta^{(p+1)}} d\theta^{(p)} \Psi\left(\prod_{i=1}^{\ell} f_i(\theta^{(p)})^{r_i^{(p)}}\right) \diamond \Psi(G_1(\theta^{(p)})). \tag{70}$$

As a matter of fact, due to

$$\begin{aligned} &\Psi\left(\prod_{i=1}^{\ell} f_i(\theta)^{r_i^{(1)}}\right) \diamond \Psi\left(\prod_{i=1}^{\ell} f_i(\theta)^{r_i^{(2)}}\right) \\ &= \Psi\left(\prod_{i=1}^{\ell} f_i(\theta)^{r_i^{(1)}} * \prod_{i=1}^{\ell} f_i(\theta)^{r_i^{(2)}}\right) = \Psi\left(\prod_{i=1}^{\ell} f_i(\theta)^{\oplus_{p=1}^2 r_i^{(p)}}\right), \end{aligned} \tag{71}$$

$\Psi$  is a homomorphism from the  $Z_2^{\otimes \ell}$  group  $\{\prod_{i=1}^{\ell} f_i(\theta)^{r_i}\}$  to either the  $Z_2$  group  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}\}$  or the  $Z_2 \times Z_2$  group  $\{c_{\text{even}}^{N_\ell, 0}, \zeta_{\text{odd}}^{N_\ell, 0}, \zeta_{\text{even}}^{N_\ell, 0}, c_{\text{odd}}^{N_\ell, 0}\}$ .

### F. Integrating out the first $n - 1$ integrals of $F_{\vec{r}_\ell}^{(n)}$

We shall prove the following lemma.

*Lemma 3: For all  $n \leq \Lambda + 1$ , the form of  $F_{\vec{r}_\ell}^{(n)}$  after  $n - 1$  integrations becomes*

$$F_{\vec{r}_\ell}^{(n)} = \int_0^\pi d\theta^{(n)} \Psi\left(\prod_{i=1}^{\ell} f_i(\theta^{(n)})^{r_i}\right) \diamond \Psi(G_n(\theta^{(n)})) \tag{72}$$

TABLE II. The second column shows the function type of the resulting integrand of  $F_{\vec{r}_\ell}^{(n)}$  after  $n - 1$  integrations. The third column shows the maximum order  $\Lambda_{\vec{r}_\ell}$  up to which the function type of the resulting integrand of  $F_{\vec{r}_\ell}^{(n)}$  does not contain a constant term.

Error type $\vec{r}_\ell$	The resulting integrand of $F_{\vec{r}_\ell}^{(n)}$	$\Lambda_{\vec{r}_\ell}$
(1) $(\vec{v}_{\ell-1}^0, 0)$ :	$\zeta_{\text{even}}^{N_\ell, n}$	$\infty$
(2) $(\vec{v}_{\ell-1}^0, 1)$ :	$c_{\text{odd}}^{N_\ell, n}$	$N_\ell$
(3) $(\vec{v}_{\ell-1}^1, 0)$ :	$c_{\text{even}}^{N_\ell, n}$	$\tilde{N}_{\vec{r}_{\ell-1}}$
(4) $(\vec{v}_{\ell-1}^1, 1)$ :	$\zeta_{\text{odd}}^{N_\ell, n}$	$\infty$

up to different unimportant coefficients in the Fourier expansion, where  $\Psi(G_n(\theta^{(n)})) \equiv \zeta_{\text{even}}^{N_\ell, n}$ . With  $\Psi(\prod_{i=1}^\ell f_i(\theta^{(n)})^{r_i})$  given explicitly in Table I, all the possible function types of the resulting integrands of  $F_{\vec{r}_\ell}^{(n)}$ ,  $\Psi(\prod_{i=1}^\ell f_i(\theta^{(n)})^{r_i}) \diamond \Psi(G_n(\theta^{(n)}))$ , in Eq. (72) are listed in Table II.

$\Lambda_{\vec{r}_\ell}$  is defined as the maximum order such that the function type of the resulting integrand of  $F_{\vec{r}_\ell}^{(n)}$  does not contain any constant term, and

$$\Lambda \equiv \min\{\{\Lambda_{\vec{r}_\ell}\}\}. \tag{73}$$

The proof of Lemma 3 is done by induction. It is trivial that Lemma 3 is true for the first order  $F_{\vec{r}_\ell}^{(1)}$  based on the form of Eq. (70). Suppose Lemma 3 holds for all the  $(n - 1)$ th order NUDD coefficients where  $n - 1 \leq \Lambda$ , i.e.,

$$F_{\vec{r}_\ell}^{(n-1)} = \int_0^\pi d\theta^{(n-1)} \Psi\left(\prod_{i=1}^\ell f_i(\theta^{(n-1)})^{r_i}\right) \diamond \Psi(G_{n-1}(\theta^{(n-1)})), \tag{74}$$

where  $\Psi(\prod_{i=1}^\ell f_i(\theta^{(n-1)})^{r_i}) \diamond \Psi(G_{n-1}(\theta^{(n-1)}))$  belongs to one of  $\{c_{\text{even}}^{N_\ell, n-1}, \zeta_{\text{odd}}^{N_\ell, n-1}, \zeta_{\text{even}}^{N_\ell, n-1}, c_{\text{odd}}^{N_\ell, n-1}\}$ .

To proceed to the next order, first compare the forms of Eq. (70) between the  $n$ th order and the  $(n - 1)$ th order NUDD coefficients. One can see that the  $n$ th order NUDD coefficients can actually be viewed as one integral nested with one order lower  $[(n - 1)\text{th-order}]$  NUDD coefficients, i.e.,

$$F_{\vec{r}_\ell}^{(n)} = \int_0^\pi d\theta^{(n)} \Psi\left(\prod_{i=1}^\ell f_i(\theta^{(n)})^{r_i^{(n)}}\right) \diamond \Psi(G_1(\theta^{(n)})) \diamond F_{\vec{r}'_\ell}^{(n-1), \theta^{(n)}}, \tag{75}$$

where  $\vec{r}_\ell = \vec{r}_\ell^{(n)} \oplus \vec{r}'_\ell$  implies that  $\vec{r}'_\ell$  could be a different vector from  $\vec{r}_\ell$ , and the extra superscript  $\theta^{(n)}$  of  $F_{\vec{r}'_\ell}^{(n-1)}$  indicates that the upper integration limit,  $\pi$ , of the last integral of  $F_{\vec{r}'_\ell}^{(n-1)}$  is replaced by  $\theta^{(n)}$ . Therefore, we can just substitute the results of  $F_{\vec{r}'_\ell}^{(n-1)}$  [Eq. (74)] directly into Eq. (75) to evaluate  $F_{\vec{r}_\ell}^{(n)}$ .

From the definition of  $\Lambda$ , the resulting integrands of  $F_{\vec{r}'_\ell}^{(n-1)}$  for all possible  $\vec{r}'_\ell$  are guaranteed to contain no constant term for  $n - 1 \leq \Lambda$ . Accordingly, it is straightforward to check that the operation

$$\Psi(G_1(\theta^{(n)})) \diamond \int_0^{\theta^{(n)}} d\theta^{(n-1)} \tag{76}$$

maps  $\{c_{\text{even}}^{N_\ell, n-1}, \zeta_{\text{odd}}^{N_\ell, n-1}, \zeta_{\text{even}}^{N_\ell, n-1}, c_{\text{odd}}^{N_\ell, n-1}\}$  to its corresponding  $\{c_{\text{even}}^{N_\ell, n}, \zeta_{\text{odd}}^{N_\ell, n}, \zeta_{\text{even}}^{N_\ell, n}, c_{\text{odd}}^{N_\ell, n}\}$  regardless of the unimportant change of the coefficients in the linear combination. Therefore, up to different coefficients in the linear combination, the operation Eq. (76) gives rise to the following mapping:

$$\Psi\left(\prod_{i=1}^\ell f_i(\theta^{(n-1)})^{r'_i}\right) \diamond \Psi(G_{n-1}(\theta^{(n-1)})) \rightarrow \Psi\left(\prod_{i=1}^\ell f_i(\theta^{(n)})^{r'_i}\right) \diamond \Psi(G_n(\theta^{(n)})). \tag{77}$$

By substituting Eq. (77) into Eq (75), the resulting integrand of  $F_{\tilde{r}_\ell}^{(n)}$  becomes

$$\Psi\left(\prod_{i=1}^{\ell} f_i(\theta^{(n)})r_i^{(n)}\right) \diamond \Psi\left(\prod_{i=1}^{\ell} f_i(\theta^{(n)})r_i'\right) \diamond \Psi(G_n(\theta^{(n)})). \tag{78}$$

Applying the homomorphism property Eq. (71) to the above equation, we obtain Eq. (72) for the  $n$ th order where  $n \leq \Lambda + 1$ .

For the order  $n = \Lambda + 1$ , the resulting integrands of  $F_{\tilde{r}_\ell}^{(n)}$  for some of the errors begin to contain a constant term. Then the operation  $\Psi(G_1(\theta^{(n+1)})) \diamond \int_0^{\theta^{(n+1)}} d\theta^{(n)}$  will map them to different functions other than a purely cosine series or a purely sine series. Hence, it follows that Eq. (72) or the second column of Table II are no longer true for the  $\Lambda + 2$  or higher order NUDD coefficients.

Now let us prove the claimed values of  $\Lambda_{\tilde{r}_\ell}$  shown in the last column of Table II. By Definition 1,  $c_{\text{odd}}^{N_\ell, n}$ , which is the function type of the resulting integrand of the  $(\tilde{v}_{\ell-1}^0, 1)$ -type error NUDD coefficients in Table II, does not contain a cosine function with zero argument (a constant 1 term) when  $n \leq N_\ell$ . Therefore,  $\Lambda_{(\tilde{v}_{\ell-1}^0, 1)} = N_\ell$ . Neither  $\zeta_{\text{even}}^{N_\ell, n}$  nor  $\zeta_{\text{odd}}^{N_\ell, n}$  ever have constant terms, which indicates that  $\Lambda_{(\tilde{v}_{\ell-1}^0, 0)} = \Lambda_{(\tilde{v}_{\ell-1}^1, 1)} = \infty$ . Only for the  $(\tilde{v}_{\ell-1}^1, 0)$ -type error,  $c_{\text{even}}^{N_\ell, n}$  is in general (by definition) allowed to have a cosine function with zero argument, a constant term. However, in Sec. IV C, we already showed that  $F_{\tilde{r}_\ell}^{(n)} = 0$  for all  $n \leq \check{N}_{\tilde{r}_{\ell-1}}$  [Eq. (48)]. Hence, with Eq. (48),

$$F_{\tilde{r}_\ell \in (\tilde{v}_{\ell-1}^1, 0)}^{(n)} = 0 = \int_0^\pi c_{\text{even}}^{N_\ell, n} d\theta \quad \forall n \leq \check{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1} \tag{79}$$

suggests that  $c_{\text{even}}^{N_\ell, n}$  in Eq. (79) has no constant term for the first  $\check{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1}$  orders. Accordingly,

$$\Lambda_{\tilde{r}_\ell \in (\tilde{v}_{\ell-1}^1, 0)} = \check{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1}. \tag{80}$$

**G. The vanishing of the  $(\tilde{v}_{\ell-1}^0, 1)$ -type error**

According to Lemma 3, for the  $(\tilde{v}_{\ell-1}^0, 1)$ -type error,  $F_{(\tilde{v}_{\ell-1}^0, 1)}^{(n)} = \int_0^\pi c_{\text{odd}}^{N_\ell, n} d\theta$ , where  $c_{\text{odd}}^{N_\ell, n}$  does not contain any constant term, for all  $n \leq \min[\Lambda + 1, N_\ell]$ , where  $n \leq \Lambda + 1$  ensures that the function type of the resulting integrand of  $F_{(\tilde{v}_{\ell-1}^0, 1)}^{(n)}$  is  $c_{\text{odd}}^{N_\ell, n}$ , and  $n \leq \Lambda_{(\tilde{v}_{\ell-1}^0, 1)} = N_\ell$  ensures that there is no constant term in it. Then as shown in Eq. (50), it follows that  $F_{(\tilde{v}_{\ell-1}^0, 1)}^{(n)} = 0$  for

$$n \leq \min[\Lambda + 1, N_\ell], \tag{81}$$

where the value of  $\Lambda$  expressed explicitly in terms of the sequence orders shall be determined as follows.

For the NUDD with  $[N_i]_2 = 0$  for all  $i < \ell$ ,  $\oplus_{k=1}^{\ell-1} r_k [N_k]_2 = 0$  is always true for all errors, so there are only two error types,  $(\tilde{v}_{\ell-1}^0, 0)$ - and  $(\tilde{v}_{\ell-1}^0, 1)$ -type errors in this case. Therefore, from the definition of  $\Lambda$  [Eq. (73)], we have

$$\Lambda = \min[\Lambda_{(\tilde{v}_{\ell-1}^0, 0)}, \Lambda_{(\tilde{v}_{\ell-1}^0, 1)}] = \min[\infty, N_\ell] = N_\ell, \tag{82}$$

which leads to  $\min[N_\ell + 1, N_\ell] = N_\ell$  in Eq. (81). Therefore, we have proven that

$$F_{(\tilde{v}_{\ell-1}^0, 1)}^{(n)} = 0 \quad \forall n \leq N_\ell \tag{83}$$

for the NUDD with all even inner sequence orders.

For NUDD with at least one odd sequence order in the first  $\ell - 1$  UDD layers, from the definition of  $\Lambda$  Eq. (73),

$$\begin{aligned} \Lambda &= \min[\Lambda_{(\tilde{v}_{\ell-1}^0, 0)}, \Lambda_{(\tilde{v}_{\ell-1}^0, 1)}, \Lambda_{\tilde{r}_\ell \in (\tilde{v}_{\ell-1}^1, 0)}, \Lambda_{(\tilde{v}_{\ell-1}^1, 1)}] \\ &= \min[\infty, N_\ell, \{\check{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1}\}, \infty] \\ &= \min[N_\ell, \{\check{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1}\}]. \end{aligned} \tag{84}$$

Due to the following.

*Lemma 4:*  $\min[\{\tilde{N}_{\tilde{r}_{\ell-1} \in \tilde{v}_{\ell-1}^1}\}] = N_{o_{\min}}^{k' < \ell}$ ,  
which we prove in Appendix E, Eq. (84) reads

$$\Lambda = \min[N_{\ell}, N_{o_{\min}}^{k' < \ell}], \quad (85)$$

which gives rise to

$$\begin{aligned} \min[\Lambda + 1, N_{\ell}] &= \min[\min[N_{\ell}, N_{o_{\min}}^{k' < \ell}] + 1, N_{\ell}] \\ &= \min[N_{o_{\min}}^{k' < \ell} + 1, N_{\ell}] \end{aligned} \quad (86)$$

in Eq. (81). Therefore, we have proven that

$$F_{(\tilde{v}_{\ell-1}^0, 1)}^{(n)} = 0 \quad \forall n \leq \min[N_{o_{\min}}^{k' < \ell} + 1, N_{\ell}] \quad (87)$$

for NUDD with at least one odd inner sequence order.

Combining Eqs. (83) and (87) with the fact that the vanishing of the other error types cannot be deduced from this approach due to their function types (shown in Table II), we obtain  $F_{\tilde{r}_{\ell}}^{(n)} = 0$  for all  $n \leq r_{\ell}[(p_{\oplus}(1, \ell - 1) \oplus 1)\tilde{N}_{\ell}]$  [Eq. (51)], where  $\tilde{N}_{\ell} = N_{\ell}$  for NUDD with all even inner sequence orders, and  $\tilde{N}_{\ell} = \min[N_{o_{\min}}^{k' < \ell} + 1, N_{\ell}]$  for NUDD with at least one odd inner sequence order, which is equivalent to the definition given in Eq. (30). This completes the proof of the NUDD theorem.

## V. NUMERICAL RESULTS: 4-LAYER NUDD

In this section, numerical simulations are employed to examine the performance of a 4-layer NUDD scheme for two contrasting MOOS. Given the UDD sequence order set  $\{N_j\}_{j=1}^4$ , the proof given above ensures a minimum suppression of all non-trivial error types to at least  $N = \min[N_1, N_2, N_3, N_4]$ , resulting in  $U(T) \sim \mathcal{O}(T^{N+1})$ . We reconcile our analytical results with numerical simulations to confirm the predicted scaling of  $U(T)$  and show that this scaling is indeed MOOS-independent. Furthermore, we analyze the scaling of all  $2^4$  individual error types to convey the validity of the decoupling order formula Eq. (29).

### A. Model

We consider a 2-qubit system coupled to a generic quantum bath to analyze the performance of the 4-layer NUDD. The total Hamiltonian, which includes a pure-bath term and system-bath interactions, is given by

$$H = \sum_{\lambda_1=0,x,y,z} \sum_{\lambda_2=0,x,y,z} J_{\lambda_1\lambda_2} \sigma_{\lambda_1} \otimes \sigma_{\lambda_2} \otimes B_{\lambda_1\lambda_2}, \quad (88)$$

where  $\sigma_{\lambda_j}$  are the standard Pauli matrices with  $\sigma_0 \equiv I$  for the  $j = 1, 2$  system qubits,  $B_{\lambda_1\lambda_2}$  are arbitrary bath-operators with  $\|B_{\lambda_1\lambda_2}\| = 1$ , and  $J_{\lambda_1\lambda_2}$  are bounded coupling coefficients between the qubits and the bath.

Modeling the environment as a spin bath consisting of four spin-1/2 particles with randomized couplings between them, the operator  $B_{\lambda_1\lambda_2}$  is given by

$$B_{\lambda_1\lambda_2} = \sum_{\lambda_3, \lambda_4, \lambda_5, \lambda_6} c_{\lambda_1\lambda_2}^{\lambda_3\lambda_4\lambda_5\lambda_6} \sigma_{\lambda_3} \otimes \sigma_{\lambda_4} \otimes \sigma_{\lambda_5} \otimes \sigma_{\lambda_6}, \quad (89)$$

where the interactions are non-restrictive, i.e., 1- to 4-local interactions are permitted. The index  $\lambda_j = 0, x, y, z$  where  $j = 3, 4, 5, 6$  stands for the bath qubit and coefficients  $c_{\lambda_1\lambda_2}^{\lambda_3\lambda_4\lambda_5\lambda_6} \in [0, 1]$  are chosen randomly from a uniform distribution.

We focus on the case of uniform coupling,  $J_{\lambda_1\lambda_2} = J \forall \lambda_j$  except  $\lambda_1 = \lambda_2 = 0$ , where we discriminate between the strength of the system-bath interactions and the pure bath dynamics  $J_{00}$ . For all simulations,  $J = 1$  MHz and  $J_{00} = 1$  kHz are considered so that  $J_{00} \ll J$ . In this particular

regime, DD has been shown to be the most beneficial since the environment dynamics are effectively static with respect to system-environment interactions.<sup>35,40</sup>

## B. Overall decoupling order

The overall performance of NUDD is quantified with respect to the state-independent distance measure

$$D = \frac{1}{\sqrt{d_S d_B}} \min_{\Phi} \|U(T) - I \otimes \Phi\|_F, \quad (90)$$

where  $d_S$  is the system Hilbert space dimension,  $d_B$  is the environment dimension, and  $\Phi$  is a bath operator.<sup>44</sup> The minimum order scaling of NUDD is expected to be  $D \sim \mathcal{O}[(JT)^{N+1}]$  for a total sequence duration  $T$ . Therefore, the overall numerical decoupling order of the NUDD scheme,  $n_{\min}$ , is obtained by

$$n_{\min} = (\log_{10} D) - 1. \quad (91)$$

In the subsequent simulations, the scaling of  $D$  is extracted by varying the minimum pulse delay  $\tau \equiv T s_{j_{\ell=1}} s_{j_{\ell-1}=1} \dots s_{j_2=1} s_{j_1=1}$  instead of the total time  $T$ . We utilize  $\tau$  since this quantity is usually the most relevant experimental time constraint.

## C. $\vec{r}_4 = (r_1, r_2, r_3, r_4)$ -type error

Given a MOOS  $\{\Omega_j\}_{j=1}^4$ , the general 2-qubit Hamiltonian (88) can be partitioned into  $2^4$  error types  $H_{\vec{r}_4} = H_{(r_1, r_2, r_3, r_4)}$  [Eq. (6)] via the procedure discussed in Appendix A. We also note that it is possible to generate  $\{H_{(r_1, r_2, r_3, r_4)}\}$  using  $H_{(1, 0, 0, 0)}$ ,  $H_{(0, 1, 0, 0)}$ ,  $H_{(0, 0, 1, 0)}$ , and  $H_{(0, 0, 0, 1)}$  as the generators of the  $Z_2^{\otimes 4}$  group, where the complete set of error types can be obtained by all possible products of the error generators:  $H_{\vec{r}_4^{(1)}} H_{\vec{r}_4^{(2)}} = H_{\vec{r}_4^{(1)} \oplus \vec{r}_4^{(2)}}$ . We explicitly display the 16 error types in Table III, where each error type is generated by a product of the corresponding outer-most column and row elements.

In order to illustrate the procedure by which the error types are generated, we consider the two MOOS sets utilized to convey the unbiased nature of the minimum scaling for NUDD. The first,

$$\{I \otimes \sigma_z, I \otimes \sigma_x, \sigma_z \otimes I, \sigma_x \otimes I\} \quad (92)$$

is composed of single-qubit operators with the corresponding error generators

$$\begin{aligned} H_{(1,0,0,0)} &= I \otimes \sigma_x, & H_{(0,1,0,0)} &= I \otimes \sigma_z, \\ H_{(0,0,1,0)} &= \sigma_x \otimes I, & H_{(0,0,0,1)} &= \sigma_z \otimes I, \end{aligned} \quad (93)$$

up to arbitrary bath operators which are omitted in the above equations. Substituting Eq. (93) into Table III, we obtain the explicit forms for all error types, as shown in Table IV.

The second MOOS is chosen similarly as

$$\{\sigma_z \otimes \sigma_z, I \otimes \sigma_x, \sigma_z \otimes I, \sigma_x \otimes I\}, \quad (94)$$

TABLE III. 16 error types  $\vec{r}_4$  for the 4-layer NUDD scheme.

*	$H_{(0,0,0,0)}$	$H_{(0,0,1,0)}$	$H_{(0,0,0,1)}$	$H_{(0,0,1,1)}$
$H_{(0,0,0,0)}$	$H_{(0,0,0,0)}$	$H_{(0,0,1,0)}$	$H_{(0,0,0,1)}$	$H_{(0,0,1,1)}$
$H_{(1,0,0,0)}$	$H_{(1,0,0,0)}$	$H_{(1,0,1,0)}$	$H_{(1,0,0,1)}$	$H_{(1,0,1,1)}$
$H_{(0,1,0,0)}$	$H_{(0,1,0,0)}$	$H_{(0,1,1,0)}$	$H_{(0,1,0,1)}$	$H_{(0,1,1,1)}$
$H_{(1,1,0,0)}$	$H_{(1,1,0,0)}$	$H_{(1,1,1,0)}$	$H_{(1,1,0,1)}$	$H_{(1,1,1,1)}$

TABLE IV. The 16 error types  $\vec{r}_4$  for the 4-layer NUDD scheme with the MOOS  $\{I \otimes \sigma_z, I \otimes \sigma_x, \sigma_z \otimes I, \sigma_x \otimes I\}$ .

*	$I \otimes I$	$\sigma_x \otimes I$	$\sigma_z \otimes I$	$\sigma_y \otimes I$
$I \otimes I$	$I \otimes I$	$\sigma_x \otimes I$	$\sigma_z \otimes I$	$\sigma_y \otimes I$
$I \otimes \sigma_x$	$I \otimes \sigma_x$	$\sigma_x \otimes \sigma_x$	$\sigma_z \otimes \sigma_x$	$\sigma_y \otimes \sigma_x$
$I \otimes \sigma_z$	$I \otimes \sigma_z$	$\sigma_x \otimes \sigma_z$	$\sigma_z \otimes \sigma_z$	$\sigma_y \otimes \sigma_z$
$I \otimes \sigma_y$	$I \otimes \sigma_y$	$\sigma_x \otimes \sigma_y$	$\sigma_z \otimes \sigma_y$	$\sigma_y \otimes \sigma_y$

where we replace the  $\sigma_z \otimes I$  operator with a two-qubit  $\sigma_z \otimes \sigma_z$  operator. The error generators for this MOOS, up to arbitrary bath operators, are

$$\begin{aligned} H_{(1,0,0,0)} &= I \otimes \sigma_x, & H_{(0,1,0,0)} &= I \otimes \sigma_z, \\ H_{(0,0,1,0)} &= \sigma_x \otimes \sigma_x, & H_{(0,0,0,1)} &= \sigma_z \otimes I \end{aligned} \quad (95)$$

and the error types are given in Table V.

#### D. Decoupling order of each error type

The decoupling order for each error type is extracted using an equivalent procedure to Ref. 40, where

$$E_{\vec{r}_4} = \|\text{Tr}_S(U(T)H_{\vec{r}_4})\|_F, \quad (96)$$

represents the effective error for error type  $H_{\vec{r}_4}$  present at the end of the DD evolution  $U(T)$ . Here,  $\|A\|_F$  is the Frobenius norm of  $A$ ,

$$\|A\|_F = \text{Tr}\sqrt{A^\dagger A}, \quad (97)$$

the sum of singular values of  $A$ . (The choice of norm is somewhat arbitrary; we could have used any other unitarily invariant norm as well, e.g., the trace norm.)

The expected scaling for each effective error type can be shown to follow

$$E_{\vec{r}_4} \sim \mathcal{O}[(JT)^{\check{N}_{\vec{r}_4}+1}] \sim \mathcal{O}[(J\tau)^{\check{N}_{\vec{r}_4}+1}], \quad (98)$$

where  $\check{N}_{\vec{r}_4}$  is given by the Eq. (29). Therefore, the numerical decoupling order of  $\vec{r}_4$ -type error,  $n_{\vec{r}_4}$ , is obtained by

$$n_{\vec{r}_4} = (\log_{10} E_{\vec{r}_4}) - 1. \quad (99)$$

#### E. Comparison of analytical predictions with numerical results

In order to convey the MOOS-independent scaling of NUDD performance, we consider the case where the three inner-most layers contain the same number of pulses, i.e.,  $N_{123} = N_j$ ,  $j = 1, 2, 3$ , for both MOOS sets given above; see Eqs. (92) and (94). We choose the NUDD

TABLE V. The 16 error types  $\vec{r}_4$  for the 4-layer NUDD scheme with the MOOS  $\{\sigma_z \otimes \sigma_z, I \otimes \sigma_x, \sigma_z \otimes I, \sigma_x \otimes I\}$ .

*	$I \otimes I$	$\sigma_x \otimes \sigma_x$	$\sigma_z \otimes I$	$\sigma_y \otimes \sigma_x$
$I \otimes I$	$I \otimes I$	$\sigma_x \otimes \sigma_x$	$\sigma_z \otimes I$	$\sigma_y \otimes \sigma_x$
$I \otimes \sigma_x$	$I \otimes \sigma_x$	$\sigma_x \otimes I$	$\sigma_z \otimes \sigma_x$	$\sigma_y \otimes I$
$I \otimes \sigma_z$	$I \otimes \sigma_z$	$\sigma_x \otimes \sigma_y$	$\sigma_z \otimes \sigma_z$	$\sigma_y \otimes \sigma_y$
$I \otimes \sigma_y$	$I \otimes \sigma_y$	$\sigma_x \otimes \sigma_z$	$\sigma_z \otimes \sigma_y$	$\sigma_y \otimes \sigma_z$

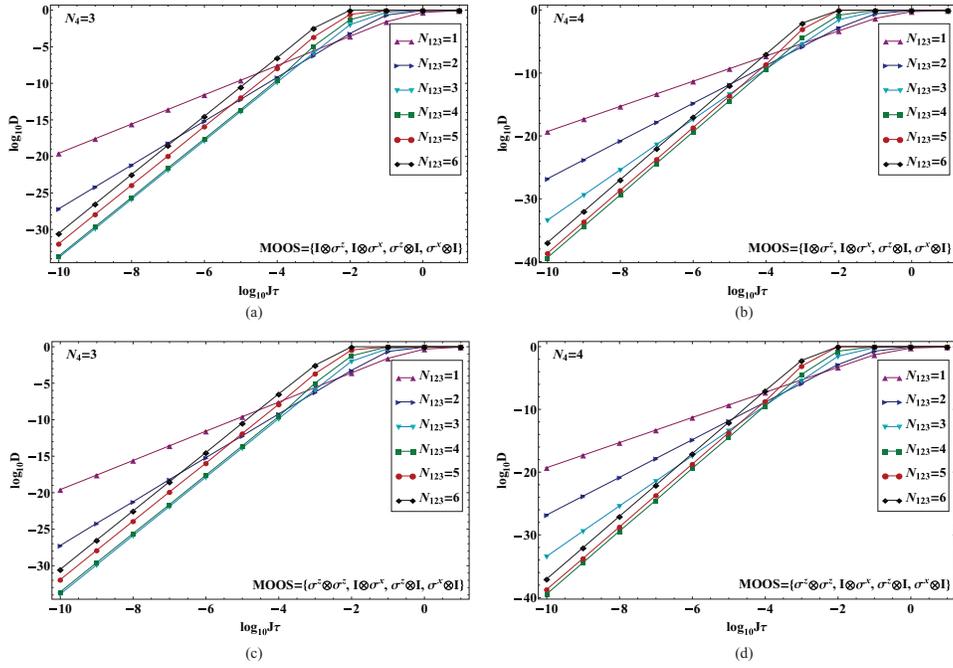


FIG. 2. Performance of NUDD as a function of the minimum pulse interval  $\tau$  for the two-qubit system specified by Eqs. (88) and (89), averaged over 15 random realizations of  $B_{\lambda_1\lambda_2}$ . Error bars are included, but are very small. A four-layer construction is utilized to address all system-bath interactions, where the MOOS sets are chosen as Eq. (92) in (a) and (b), and Eq. (94) in (c) and (d). The orders of the first three layers are identical:  $N_j = N_{123}$ ,  $j = 1, 2, 3$  and are varied as  $N_{123} = 1, 2, \dots, 6$ . In particular, the outer layer sequence order is chosen as  $N_4 = 3$  in (a) and (c), and  $N_4 = 4$  in (b) and (d). Linear interpolation from  $\log_{10}J\tau = -10$  to approximately  $\log_{10}J\tau = -2$  confirms the MOOS-independent scaling  $D \sim \mathcal{O}[(J\tau)^{n_{\min}+1}]$ ,  $n_{\min} = \min\{N_j\}_{j=1}^4$ , for all simulations.

layering such that the right-most control pulse operator corresponds to the outer-most UDD sequence with sequence order  $N_4$  and the left-most operator generates the inner-most UDD sequence with sequence order  $N_1$ . Fixing the sequence order for the outer-most layer,  $N_4$ , and varying  $N_{123}$ , a qualitative and quantitative similarity can be expected between the QDD analysis given in Ref. 40 and the 4-layer NUDD construction considered here. Hence, the expected scaling of the distance measure described by Eq. (90) is  $D \sim \mathcal{O}[(J\tau)^{n_{\min}+1}]$ , where  $n_{\min} = \min[N_4, N_{123}]$ .

In Fig. 2, the performance is shown as a function of the minimum pulse interval  $\tau$  for both MOOS sets in the case of  $N_4 = 3$  in (a) and (c), and  $N_4 = 4$  in (b) and (d). The inner sequence orders are  $N_{123} = 1, 2, \dots, 6$  for all simulations, which are averaged over 15 random realizations of  $B_{\lambda_1\lambda_2}$  using 120 digits of precision.

TABLE VI. For the case with  $N_1 = 2, N_2 = 4, N_3 = 6, N_4 = 8$ , analytical and numerical decoupling orders for all error types are in complete agreement. The analytical overall decoupling order  $\check{N}_{\min} = \min[2, 4, 6, 8] = 2$  also agrees with the actual overall decoupling order.

$\check{N}_{(0,0,0,0)}$	$\check{N}_{(0,0,1,0)}$	$\check{N}_{(0,0,0,1)}$	$\check{N}_{(0,0,1,1)}$
0	6	8	8
$\check{N}_{(1,0,0,0)}$	$\check{N}_{(1,0,1,0)}$	$\check{N}_{(1,0,0,1)}$	$\check{N}_{(1,0,1,1)}$
2	6	8	8
$\check{N}_{(0,1,0,0)}$	$\check{N}_{(0,1,1,0)}$	$\check{N}_{(0,1,0,1)}$	$\check{N}_{(0,1,1,1)}$
4	6	8	8
$\check{N}_{(1,1,0,0)}$	$\check{N}_{(1,1,1,0)}$	$\check{N}_{(1,1,0,1)}$	$\check{N}_{(1,1,1,1)}$
4	6	8	8

TABLE VII. For the case with  $N_1 = 2, N_2 = 4, N_3 = 6, N_4 = 3$ , analytical and numerical decoupling order (displayed in normal font) are in complete agreement for all error types. The analytical overall decoupling order  $N = \min[2, 4, 6, 3] = 2$  also agrees with the actual overall decoupling order. The difference between the naive (displayed in italics) and the actual decoupling orders comes from outer-odd-UDD suppression effect.

$\check{N}_{(0,0,0,0)}$	$\check{N}_{(0,0,1,0)}$	$\check{N}_{(0,0,0,1)}$	$\check{N}_{(0,0,1,1)}$
0	6	3	6, 7
$\check{N}_{(1,0,0,0)}$	$\check{N}_{(1,0,1,0)}$	$\check{N}_{(1,0,0,1)}$	$\check{N}_{(1,0,1,1)}$
2	6	3	6, 7
$\check{N}_{(0,1,0,0)}$	$\check{N}_{(0,1,1,0)}$	$\check{N}_{(0,1,0,1)}$	$\check{N}_{(0,1,1,1)}$
4	6	4, 5	6, 7
$\check{N}_{(1,1,0,0)}$	$\check{N}_{(1,1,1,0)}$	$\check{N}_{(1,1,0,1)}$	$\check{N}_{(1,1,1,1)}$
4	6	4, 5	6, 7

Comparing Figs. 2(a) and 2(c), we find that variations in the MOOS do not change the qualitative features of NUDD performance. Furthermore, we can confirm by linear interpolation that the slope of each curve indeed satisfies  $n_{\min} = \min[N_{123}, N_4]$ . Similar results are obtained for  $N_4 = 4$  in Figs. 2(b) and 2(d) as well. By this comparison, we show that NUDD is a MOOS-independent construction and confirm this result for two specific even and odd parity values of  $N_4$ . We expect the scaling to remain consistent for general 4-layer NUDD, where the scaling becomes  $n_{\min} = \min[N_1, N_2, N_3, N_4]$ , and for more general multi-layer NUDD as well.

The scaling for each error type is characterized as a function of the minimum pulse interval using Eq. (96) specifically for the MOOS given by Eq. (92). For each error type, we display the decoupling order in tabular form, following the format described in Sec. V C. The numerically obtained decoupling order is denoted in normal font, analytical prediction from Eq. (29) in boldface and the “naive” decoupling order in italics. If a boldface (italics) number is absent, it means our analytical decoupling order (naive decoupling order) is exactly the same as the actual decoupling order. We refer to

$$\check{N}_{\vec{r}_i} = \max[\{r_i N_i\}_{i=1}^{\ell}] \quad (100)$$

as the “naive” decoupling order since it assumes that each nested layer acts independently. A previous analysis for QDD has shown that inter-layer interference may alter the expected UDD efficiency even when the layers do not provide decoupling for the same error type.<sup>40</sup> We expect a similar characteristic for NUDD as well and seek to identify the conditions when the naive decoupling order is incorrect.

Tables VI–VIII contain typical examples where our analytically predicted decoupling orders for all error types exactly match those obtained numerically. Note that in these particular NUDD schemes, the suppression order of each UDD layer is equal to its sequence order, i.e.,  $\check{N}_i = N_i$ . In Table VI, all sequence orders are even parity, i.e.,  $[N_i]_2 = 0 \forall i$ . Specifically, we consider  $N_1 = 2, N_2 = 4, N_3 = 6$ , and  $N_4 = 8$ , although we expect equivalent results for arbitrary even parity  $N_j$ . According

TABLE VIII. For the case with  $N_1 = 7, N_2 = 5, N_3 = 3, N_4 = 1$  analytical and numerical decoupling order for all error types are in complete agreement. The analytical overall decoupling order  $\check{N}_{\min} = \min[7, 5, 3, 1] = 1$  also agrees with the actual overall decoupling order. The difference between the naive (marked in italics) and the actual decoupling orders (in normal font) comes from outer-odd-UDD suppression effect.

$\check{N}_{(0,0,0,0)}$	$\check{N}_{(0,0,1,0)}$	$\check{N}_{(0,0,0,1)}$	$\check{N}_{(0,0,1,1)}$
0	3	1	3, 4
$\check{N}_{(1,0,0,0)}$	$\check{N}_{(1,0,1,0)}$	$\check{N}_{(1,0,0,1)}$	$\check{N}_{(1,0,1,1)}$
7	7, 8	7, 8	7, 9
$\check{N}_{(0,1,0,0)}$	$\check{N}_{(0,1,1,0)}$	$\check{N}_{(0,1,0,1)}$	$\check{N}_{(0,1,1,1)}$
5	5, 6	5, 6	5, 7
$\check{N}_{(1,1,0,0)}$	$\check{N}_{(1,1,1,0)}$	$\check{N}_{(1,1,0,1)}$	$\check{N}_{(1,1,1,1)}$
7, 8	7, 9	7, 9	7, 10

to Eq. (29), the decoupling order formula for such cases coincides with the naive decoupling order formula Eq. (100); interference between layers is not observed. The analytical overall decoupling order  $N = \min[2, 4, 6, 8] = 2$  is found to agree with the actual overall decoupling order as well.

The second example we consider, Table VII, is one of the cases with all even sequence orders except the outer-most UDD layer. Analytical and numerical decoupling orders (normal font) are in complete agreement for all error types. There is one order difference between the naive decoupling order (italics) and the actual decoupling order (normal font) in the last column and the last two entries in the third column. From the decoupling order formula Eq. (36), the difference comes from the fact that the outermost (4th) UDD layer with odd order 3 boosts the decoupling order for error types that are also addressed by one of the inner layers. Clearly, the deviation from the standard UDD scaling can be attributed to the asymmetry of the outer layer.

The third example, shown in Table VIII, is for all odd sequence orders such that  $N_1 > N_2 > N_3 > N_4$  with  $[N_i]_2 = 1$  for all  $i$ . The analytical decoupling order formula is given in Eq. (38). The second term in Eq. (38) is called the outer-odd-UDD suppression effect, which implies a direct relationship between the number of odd parity layers which address the error, and the additional orders of error suppression achievable for a particular error type. Comparing the analytical/numerical results with the naive decoupling order, we find that the increase in decoupling order is attributed to this outer-odd-UDD suppression effect.

Discrepancies between numerical results and analytical predictions occur when the inner UDD layers contain odd parity sequence orders that are smaller than the outer layers beyond the odd order. In Tables IX and X, we consider two cases where deviations from the analytical predictions occur. It is important to note that although the numerical and analytical decoupling orders differ, we do not predict error suppression beyond what is achieved. The formula given by Eq. (29) can be thought of as a lower bound for the actual decoupling order. Essentially, we are predicting the minimum order of error suppression for each error type.

Table IX is an example where the third layer is the only odd parity layer; the sequence orders are chosen specifically as  $N_1 = 2, N_2 = 4, N_3 = 1, N_4 = 6$ . Our analytical prediction from Eq. (29) is

$$\check{N}_{r_4} = \max[\{r_i N_i + r_3\}_{i=1}^2, r_3 N_3, r_4(r_3[N_3]_2 \oplus 1)\tilde{N}_4], \tag{101}$$

where the suppression ability of the fourth UDD layer,  $\tilde{N}_4 = \min[N_4, N_3 + 1]$ , is hindered by the third UDD layer if  $N_3 < N_4 - 1$ . For the particular sequence orders we consider here, the analytical prediction is  $\tilde{N}_4 = \min[6, 1 + 1] = 2$ . Comparing the analytical results to numerical simulations, it appears that the analytical decoupling orders (denoted in boldface) are lower than the numerically calculated values for certain error types; see column 3 in Table IX. However, despite the discrepancy Eq. (101) captures the inhibiting characteristics of the odd parity inner sequence order on the decoupling order of the outer-most layer. As analytically predicted, the outer-odd-UDD suppression effects are observed on the error types, which anticommute with the third and its inner UDD layers, in the second column by comparing their naive and the numerical decoupling orders. For the error

TABLE IX. For the case with  $N_1 = 2, N_2 = 4, N_3 = 1, N_4 = 6$ , the analytical overall decoupling order  $\check{N}_{\min} = \min[2, 4, 1, 6] = 1$  agrees with the actual overall decoupling order. However, the numerical decoupling order (marked in normal font) and our analytical predictions (marked in boldface) have different values for error types in the third column. Naive decoupling order is marked in italics.

$\check{N}_{(0,0,0,0)}$	$\check{N}_{(0,0,1,0)}$	$\check{N}_{(0,0,0,1)}$	$\check{N}_{(0,0,1,1)}$
0	1	<b>6, 3, 2</b>	6, 1
$\check{N}_{(1,0,0,0)}$	$\check{N}_{(1,0,1,0)}$	$\check{N}_{(1,0,0,1)}$	$\check{N}_{(1,0,1,1)}$
2	2, 3	<b>6, 5, 2</b>	6, 3
$\check{N}_{(0,1,0,0)}$	$\check{N}_{(0,1,1,0)}$	$\check{N}_{(0,1,0,1)}$	$\check{N}_{(0,1,1,1)}$
4	4, 5	<b>6, 6</b>	6, 5
$\check{N}_{(1,1,0,0)}$	$\check{N}_{(1,1,1,0)}$	$\check{N}_{(1,1,0,1)}$	$\check{N}_{(1,1,1,1)}$
4	4, 5	<b>6, 4</b>	6, 5

TABLE X. For the case with  $N_1 = 1, N_2 = 3, N_3 = 5, N_4 = 7$ , the analytical overall decoupling order  $\check{N}_{\min} = \min[1, 3, 5, 7] = 1$  agrees with the actual overall decoupling order. However, for some error types, our analytical predictions (marked in boldface) only provide lower bounds for their exact decoupling orders (marked in normal font). “Naive” decoupling orders are marked in italics.

$\check{N}_{(0,0,0,0)}$	$\check{N}_{(0,0,1,0)}$	$\check{N}_{(0,0,0,1)}$	$\check{N}_{(0,0,1,1)}$
0	5, 3, <b>2</b>	7, 3, <b>2</b>	7, 4, <b>3</b>
$\check{N}_{(1,0,0,0)}$	$\check{N}_{(1,0,1,0)}$	$\check{N}_{(1,0,0,1)}$	$\check{N}_{(1,0,1,1)}$
1	5, 2	7, 2	7, 5, <b>3</b>
$\check{N}_{(0,1,0,0)}$	$\check{N}_{(0,1,1,0)}$	$\check{N}_{(0,1,0,1)}$	$\check{N}_{(0,1,1,1)}$
3, <b>2</b>	5, 4, <b>3</b>	7, 4, <b>3</b>	7, <b>4</b>
$\check{N}_{(1,1,0,0)}$	$\check{N}_{(1,1,1,0)}$	$\check{N}_{(1,1,0,1)}$	$\check{N}_{(1,1,1,1)}$
3, 2	5, <b>5</b>	7, 5, <b>3</b>	7, 6, <b>4</b>

types with  $r_3 = r_4 = 1$  in the fourth column of Table IX, due to  $r_3[N_3]_2 \oplus 1 = 0$ , our analytical formula Eq. (101) shows that the fourth layer of UDD is totally ineffective due to the odd sequence order of the third UDD layer. Indeed, the numerical decoupling order for the error types in the fourth column of Table IX is smaller than 6, the sequence order of the fourth UDD layer.

As a final example, we consider the sequence orders  $N_1 = 1, N_2 = 3, N_3 = 5$ , and  $N_4 = 7$ . Since  $\check{N}_j = \min[N_1 + 1, N_j] = 2 < N_j$  for  $j = 2, 3, 4$ , this indicates that the suppression abilities of the outer UDD layers are diminished due to the  $N_1 = 1$  sequence order of the inner-most UDD layer. Indeed, the numerical decoupling orders are lower than the naive UDD scaling for a substantial fraction of error types, indicating interference between layers. However, we find that the analytically predicted decoupling orders still differ from the numerically obtained values. It appears that the actual decoupling order is not only determined by the sequence orders, but also by the error types in a complicated fashion not fully captured by the analytical decoupling formula, which, however, continues to provide a reliable lower bound on the decoupling order for each error type, as discussed earlier.

## VI. CONCLUSIONS

The NUDD scheme, which nests multiple layers of UDD sequences, is the most efficient scheme currently known for general multi-qubit decoherence suppression, assuming ideal pulses and a bath with a sharp cutoff, or bounded operator norm. In this work, we have given a rigorous analysis, along with a compact formulation, of the universality and performance of general NUDD sequence with a MOOS as the control pulse set. We proved that the overall suppression order of NUDD with general control pulses is the minimum of all the sequence orders of the individual UDD sequences comprising the NUDD scheme. Moreover, we also obtained lower bounds on the decoupling order of each type of error, given a sequence order set. Our decoupling order formula Eq. (29) shows that only for NUDD sequences with all even sequence orders, all UDD layers work independently, i.e., the suppression ability of each UDD layer is unaffected by the presence of the other layers. For all other NUDD schemes, with at least one odd sequence order, the interference phenomenon between UDD layers appears and is summarized as follows:

1. For a given UDD layer, say the  $i$ th UDD layer with sequence order  $N_i$ , if there are inner layers with odd sequence order and the lowest odd order is smaller than  $N_i - 1$ , then the suppression ability of the  $i$ th UDD layer is hindered by this inner UDD layer with lowest odd order, i.e., it cannot achieve  $N_i$ th-order decoupling. [ $\check{N}_i = N_{\min}^{k' < i} + 1 < N_i$  in Eq. (29).]
2. For the  $i$ th UDD layer to be effective against a given error type, this error needs to not only anticommute with the control pulses of the  $i$ th UDD layer ( $r_i = 1$ ) but also anticommute with an even number of UDD layers with odd sequence orders before the  $i$ th UDD layer ( $p_{\oplus}(1, i - 1) = 0$ ).
3. For a given error type, if there is a total odd number of UDD layers with odd sequence orders before the  $i$ th UDD layer that the error anticommutes with ( $p_{\oplus}(1, i - 1) = 1$ ), then the

$i$ th UDD layer is totally ineffective ( $p_{\oplus}(1, i - 1) \oplus 1 = 0$ ) irrespective of whether this error anticommutes with this layer or not.

4. For a given error type, each odd order UDD layer that the error anticommutes with and is nested outside the  $i$ th UDD layer, can enhance the suppression ability of the  $i$ th UDD layer by one more order (outer-odd-UDD effect) on this error type. In other words, the outer-odd-UDD suppression effect is cumulative and is responsible for the  $p_{+}(i + 1, \ell)$  term in the decoupling order formula Eq. (29).

Since our analysis identifies the conditions under which the suppression ability of a given UDD layer is inhibited, or made totally ineffective, or rather enhanced by other UDD layers with odd sequence orders, one can use it to design an *optimally ordered* NUDD scheme that exploits the full power of each UDD layer. To be more specific, suppose one would like to design a NUDD scheme from some UDD sequences whose control pulse types and sequence orders are given. From the analysis presented here, in order to reach optimal efficiency, first one should nest all the UDD layers with even sequence orders together, where the nesting orders can be arbitrary, and denote this resulting sequence as NUDD<sub>e</sub>; second, nest all the UDD layers with odd sequence orders together such that the sequence orders from the inner-most to the outer-most layers are decreasing, and denote this resulting sequence as NUDD<sub>o</sub>; the final and optimal NUDD scheme is constructed by nesting NUDD<sub>e</sub> as the inner sequence with NUDD<sub>o</sub> as the outer sequence.

An important challenge is to generalize the analysis we have presented here to the setting of non-ideal, finite width pulses.

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## APPENDIX A: PROCEDURE TO OBTAIN $H_{(r_1, r_2, \dots, r_\ell)}$

Starting with the control pulse operator composing the first UDD layer,  $\Omega_1$ , the Hamiltonian can be partitioned into

$$H = \sum_{r_1=0,1} H_{(r_1)}, \quad (\text{A1})$$

where

$$H_{(r_1)} \equiv \frac{H + (-1)^{r_1} \Omega_1 H \Omega_1}{2}. \quad (\text{A2})$$

The Hamiltonian  $H_{(0)}$  commutes with  $\Omega_1$ , while  $H_{(1)}$  anticommutes with  $\Omega_1$ . Continuing the procedure for the next layer of NUDD, each  $H_{(r_1)}$ , with  $r_1 = 0$  or 1, can be divided further into commuting and anticommuting parts for the control pulse operator  $\Omega_2$  as

$$H_{(r_1, r_2)} \equiv \frac{H_{(r_1)} + (-1)^{r_2} \Omega_2 H_{(r_1)} \Omega_2}{2}. \quad (\text{A3})$$

Using Eq. (A2) iteratively for the first  $l$  layers, we have

$$H_{(r_1, \dots, r_\ell)} \equiv [H_{(r_1, \dots, r_{\ell-1})} + (-1)^{r_\ell} \Omega_\ell H_{(r_1, \dots, r_{\ell-1})} \Omega_\ell] / 2, \quad (\text{A4})$$

which commutes with  $\Omega_i$  if  $r_i = 0$  and anticommutes with  $\Omega_i$  if  $r_i = 1$ , where  $i \in \{1, \dots, \ell\}$ .

**APPENDIX B: THE OUTER-MOST UDD INTERVAL DECOMPOSITION**

We shall derive Eq. (53) by splitting each integral of  $F_{\oplus_{p=1}^n \tilde{r}_\ell^{(p)}}$  [Eq. (21)] into a sum of sub-integrals over the normalized outer-most layer intervals  $s_{j_\ell}$ . Since  $F_{\oplus_{p=1}^n \tilde{r}_\ell^{(p)}}$  comprises a series of time-ordered nested integrals, our procedure for decomposing  $F_{\oplus_{p=1}^n \tilde{r}_\ell^{(p)}}$  is to evaluate each nested integrals one by one, from  $\eta^{(n)}$  to  $\eta^{(1)}$ .

We call the sub-integral over the  $j_\ell$ th outer-most interval “sub-integral- $j_\ell$ .” Suppose the integral of the integration variable  $\eta^{(p)}$  follows the sub-integral- $j_\ell^{(p+1)}$  of the previous variable  $\eta^{(p+1)}$ . By splitting up the integral of  $\eta^{(p)}$  with respect to the normalized outer-most intervals  $s_{j_\ell}$ , we have

$$\int_0^{\eta^{(p+1)}} \prod_{i=1}^{\ell} f_i(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)} \tag{B1}$$

$$= \sum_{j_\ell^{(p)}=1}^{j_\ell^{(p+1)}-1} f_\ell(j_\ell^{(p)})^{r_\ell^{(p)}} \int_{\eta_{j_\ell^{(p)}-1}^{(p)}}^{\eta_{j_\ell^{(p)}}^{(p)}} \prod_{i=1}^{\ell-1} f_i(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)} + f_\ell(j_\ell^{(p+1)})^{r_\ell^{(p)}} \int_{\eta_{j_\ell^{(p+1)}-1}^{(p+1)}}^{\eta^{(p+1)}} \prod_{i=1}^{\ell-1} f_i(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)},$$

where  $\eta_{j_\ell^{(p)}}^{(p)}$  is UDD $_{N_\ell}$  pulse timing and  $f_\ell(j_\ell^{(p)}) = (-1)^{j_\ell^{(p)}-1}$ .

For each sub-integral with the integration domain from  $[\eta_{j_\ell^{(p)}-1}^{(p)}, \eta_{j_\ell^{(p)}}^{(p)})$ , with pulse interval  $s_{j_\ell^{(p)}}$ , we make the following linear change of variable:

$$\tilde{\eta}^{(p)} = \frac{\eta^{(p)} - \eta_{j_\ell^{(p)}-1}^{(p)}}{s_{j_\ell^{(p)}}} \tag{B2}$$

to normalize the integration domain to 1. Accordingly, each  $f_i(\tilde{\eta}^{(p)})$  with  $i \leq \ell - 1$  becomes the normalized  $i$ th-layer modulation function for  $\ell - 1$  layers of NUDD, and is the same function for all of the outermost pulse intervals. Consequently, the summands in Eq. (B1) become

$$\int_0^1 d\tilde{\eta}^{(p)} \prod_{i=1}^{\ell-1} f_i(\tilde{\eta}^{(p)})^{r_i^{(p)}} \sum_{j_\ell^{(p)}=1}^{j_\ell^{(p+1)}-1} f_\ell(j_\ell^{(p)})^{r_\ell^{(p)}} s_{j_\ell^{(p)}}, \tag{B3a}$$

$$+ \int_0^{\tilde{\eta}^{(p+1)}} d\tilde{\eta}^{(p)} \prod_{i=1}^{\ell-1} f_i(\tilde{\eta}^{(p)})^{r_i^{(p)}} f_\ell(j_\ell^{(p+1)})^{r_\ell^{(p)}} s_{j_\ell^{(p+1)}}, \tag{B3b}$$

where  $\int_0^1 \prod_{i=1}^{\ell-1} f_i(\tilde{\eta}^{(p)})^{r_i^{(p)}} d\tilde{\eta}^{(p)}$  is taken out of the summation.

It is possible to rewrite Eq. (B3a) and Eq. (B3b) in similar form by introducing the configuration number  $\xi_p$ , where  $\xi_p = 0$  stands for Eq. (B3a), while  $\xi_p = 1$  stands for Eq. (B3b). In this notation, Eq. (B3a) becomes

$$\int_0^{(\eta^{(p+1)})^{\xi_p}} \prod_{i=1}^{\ell-1} f_i'(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)} \times \sum_{j_\ell^{(p)}=1}^{j_\ell^{(p+1)} - (\xi_p \oplus 1)} f_\ell(j_\ell^{(p)})^{r_\ell^{(p)}} s_{j_\ell^{(p)}}, \tag{B4}$$

where  $f_i'(\eta^{(p)}) \equiv f_i(\tilde{\eta}^{(p)})$ , and Eq. (B3b) with  $\xi_p = 1$  becomes

$$\int_0^{(\eta^{(p+1)})^{\xi_p}} \prod_{i=1}^{\ell-1} f_i'(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)} \times \sum_{j_\ell^{(p)}=\xi_p j_\ell^{(p+1)}}^{j_\ell^{(p+1)} - (\xi_p \oplus 1)} f_\ell(j_\ell^{(p)})^{r_\ell^{(p)}} s_{j_\ell^{(p)}}, \tag{B5}$$

where

$$\sum_{j_\ell^{(p)}=\xi_p j_\ell^{(p+1)}}^{j_\ell^{(p+1)} - (\xi_p \oplus 1)} = \sum_{j_\ell^{(p)}=j_\ell^{(p+1)}}^{j_\ell^{(p+1)}} \tag{B6}$$

which means that  $j_\ell^{(p)} = j_\ell^{(p+1)}$ .

Note that both forms of Eqs. (B4) and (B5) are naturally decomposed into an inner part, which is an integral of the first  $\ell - 1$  modulation functions for  $(\ell - 1)$ -layer NUDD, and an outer part, which is sum over the outer-most ( $\ell$ th) layer modulation function.

Each integral of  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$  can be split into Eqs. (B4) and (B5), with one exception: if  $j_\ell^{(p+1)} = 1$  the subsequent sub-integrals from  $\eta^{(p)}$  to  $\eta^{(1)}$  will only contain Eq. (B5), whose configuration number is 1.

By substituting Eqs. (B4) and (B5) into each integral of  $F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}}$ , in sequence from  $\eta^{(n)}$  to  $\eta^{(1)}$  (taking the exception into account) and collecting all the inner (outer) parts of all sub-integrals accordingly, we obtain

$$F_{\oplus_{p=1}^n \vec{r}_\ell^{(p)}} = \sum_{\{\xi_k=0,1\}_{k=1}^{n-1}} \Phi_{\xi_n \dots \xi_1}^{\text{in}}(\{\vec{r}_{\ell-1}^{(p)}\}_{p=1}^n) \Phi_{\xi_n \dots \xi_1}^{\text{out}}(\{r_\ell^{(p)}\}_{p=1}^n),$$

where

$$\Phi_{\xi_n \dots \xi_1}^{\text{in}}(\{\vec{r}_{\ell-1}^{(p)}\}_{p=1}^n) = \prod_{p=1}^n \int_0^{(\eta^{(p+1)})^{\xi_p}} \prod_{i=1}^{\ell-1} f'_i(\eta^{(p)})^{r_i^{(p)}} d\eta^{(p)} \tag{B7}$$

and

$$\begin{aligned} \Phi_{\xi_n \dots \xi_1}^{\text{out}}(\{r_\ell^{(p)}\}_{p=1}^n) = & \\ & \left( \sum_{j_\ell^{(n)}=\sum_{k=1}^n (\xi_k \oplus 1)}^{N_\ell+1} f_\ell(j_\ell^{(n)})^{r_\ell^{(n)}} s_{j_\ell^{(n)}} \right) \times \prod_{p=1}^{n-1} \sum_{j_\ell^{(p)}=\xi_p j_\ell^{(p+1)} + (\xi_p \oplus 1) \sum_{k=1}^p (\xi_k \oplus 1)}^{j_\ell^{(p+1)} - (\xi_p \oplus 1)} f_\ell(j_\ell^{(p)})^{r_\ell^{(p)}} s_{j_\ell^{(p)}} \end{aligned} \tag{B8}$$

with  $\sum_{\{\xi_k=0,1\}_{k=1}^{n-1}}$  summing over all possible nested integration (sum) configurations  $\xi_n \dots \xi_2 \xi_1$  with  $\xi_n \equiv 0$  for the inner part  $\Phi_{\xi_n \dots \xi_1}^{\text{in}}$  (the outer part  $\Phi_{\xi_n \dots \xi_1}^{\text{out}}$ ).

Note that in Eq. (B8) for  $\xi_p = 1$ ,

$$\sum_{j_\ell^{(p)}=j_\ell^{(p+1)}+(1\oplus)\sum_{k=1}^p(\xi_k\oplus 1)}^{j_\ell^{(p+1)}-(1\oplus)} = \sum_{j_\ell^{(p)}=j_\ell^{(p+1)}}^{j_\ell^{(p+1)}} , \tag{B9}$$

which means that the variables  $\eta^{(p)}$  and  $\eta^{(p+1)}$  in Eq. (21) are in the same interval  $j_\ell^{(p)} = j_\ell^{(p+1)}$ , while for  $\xi_p = 0$ ,

$$\sum_{j_\ell^{(p)}=0+(0\oplus)\sum_{k=1}^p(\xi_k\oplus 1)}^{j_\ell^{(p+1)}-(0\oplus)} = \sum_{j_\ell^{(p)}=\sum_{k=1}^p(\xi_k\oplus 1)}^{j_\ell^{(p+1)}-1} . \tag{B10}$$

In the latter case, the variable  $\eta^{(p)}$  in Eq. (21) is located in the earlier interval than the variable  $\eta^{(p+1)}$ , namely,  $j_\ell^{(p)} < j_\ell^{(p+1)}$ .  $\sum_{k=1}^p (\xi_k \oplus 1)$  counts the number of  $\xi_k = 0$  from  $k = 1$  to  $k = p$ .

Furthermore, each  $\Phi_{\xi_n \dots \xi_1}^{\text{in}}(\{\vec{r}_{\ell-1}^{(p)}\}_{p=1}^n)$  is a product of multiple nested integrals with the modulation functions of  $\ell - 1$  layers of NUDD as integrands. In fact, each nested integral contained in  $\Phi_{\xi_n \dots \xi_1}^{\text{in}}(\{\vec{r}_{\ell-1}^{(p)}\}_{p=1}^n)$  is actually one of the  $(\ell - 1)$ -layers NUDD coefficients. For example, an inner term appearing in the expansion of the 8th order  $\ell$ -layers NUDD coefficients  $F_{\oplus_{p=1}^8 \vec{r}_\ell^{(p)}}$  reads

$$\begin{aligned} \Phi_{01101011}^{\text{in}}(\{\vec{r}_{\ell-1}^{(p)}\}_{p=1}^8) &= F_{\oplus_{p=6}^8 \vec{r}_{\ell-1}^{(p)}} F_{\oplus_{p=4}^5 \vec{r}_{\ell-1}^{(p)}} F_{\oplus_{p=1}^3 \vec{r}_{\ell-1}^{(p)}} \\ &= F_{\vec{r}_{\ell-1}^{(3)}} F_{\vec{r}_{\ell-1}^{(2)}} F_{\vec{r}_{\ell-1}^{(3)}} , \end{aligned} \tag{B11}$$

where  $\vec{r}_{\ell-1}''' = \bigoplus_{p=6}^8 \vec{r}_{\ell-1}^{(p)}$ ,  $\vec{r}_{\ell-1}'' = \bigoplus_{p=4}^5 \vec{r}_{\ell-1}^{(p)}$ , and  $\vec{r}_{\ell-1}' = \bigoplus_{p=1}^3 \vec{r}_{\ell-1}^{(p)}$ . Its corresponding outer part reads

$$\begin{aligned} & \Phi_{01101011}^{\text{out}}(\{r_{\ell}^{(p)}\}_{p=1}^8) \\ &= \left( \sum_{j_{\ell}^{(8)}=3}^{N_{\ell}+1} f_{\ell}(j_{\ell}^{(8)})^{\bigoplus_{p=6}^8 r_{\ell}^{(p)}} s_{j_{\ell}^{(8)}}^3 \right) \times \left( \sum_{j_{\ell}^{(5)}=2}^{j_{\ell}^{(8)}-1} f_{\ell}(j_{\ell}^{(5)})^{\bigoplus_{p=4}^5 r_{\ell}^{(p)}} s_{j_{\ell}^{(5)}}^2 \right) \times \left( \sum_{j_{\ell}^{(3)}=1}^{j_{\ell}^{(5)}-1} f_{\ell}(j_{\ell}^{(3)})^{\bigoplus_{p=1}^3 r_{\ell}^{(p)}} s_{j_{\ell}^{(3)}}^3 \right), \end{aligned} \quad (\text{B12})$$

where we used Eq. (14).

As suggested by Eqs. (B11) and (B12), one can see that each configuration  $\xi_n \dots \xi_1$  defines a way to separate the  $n$  vectors  $\{\vec{r}_{\ell}^{(p)}\}_{p=1}^n$  into several clusters with order configuration numbers and error vectors as  $\xi_n \vec{r}_{\ell}^{(n)} \dots \xi_1 \vec{r}_{\ell}^{(1)}$ . A cluster of vectors is defined as a contiguous set of vectors only connected by configuration numbers whose value is 1. Different clusters are separated by configuration numbers whose value is 0. For  $\xi_8 \dots \xi_1 = 01101011$  in Eqs. (B11) and (B12) as an example, we have

$$0 \vec{r}_{\ell}^{(8)} 1 \vec{r}_{\ell}^{(7)} 1 \vec{r}_{\ell}^{(6)} 0 \vec{r}_{\ell}^{(5)} 1 \vec{r}_{\ell}^{(4)} 0 \vec{r}_{\ell}^{(3)} 1 \vec{r}_{\ell}^{(2)} 1 \vec{r}_{\ell}^{(1)}, \quad (\text{B13})$$

which divides the 8 vectors into three clusters. Suppose for a given configuration  $\xi_n \dots \xi_2 \xi_1$ , which separates the  $n$  vectors into  $m$  clusters, the  $a$ th cluster (counting from right to left) contains  $n_a$  vectors  $\{\vec{r}_{\ell}^{(p)}\}_{p=\nu}^{\mu}$  with  $n_a = \mu - \nu + 1$ . Then, according to the result of  $\bigoplus_{p=\nu}^{\mu} \vec{r}_{\ell}^{(p)}$ , its corresponding inner part is  $F_{\vec{r}_{\ell-1}}^{(n_a)}$  with  $\vec{r}_{\ell-1}^{(a)} \equiv \bigoplus_{p=\nu}^{\mu} \vec{r}_{\ell-1}^{(p)}$  and the corresponding outer part is  $\sum_{j_{\ell}^{(a)}=a}^{j_{\ell}^{(a+1)}-1} f_{\ell}(j_{\ell}^{(a)})^{r_{\ell}^{(a)}} s_{j_{\ell}^{(a)}}^{n_a}$  with  $r_{\ell}^{(a)} \equiv \bigoplus_{p=\nu}^{\mu} r_{\ell}^{(p)}$ . Note that for the last cluster,  $a = m$ , the upper bound of the sum  $j_{\ell}^{(m+1)} - 1$  is replaced by  $N_{\ell} + 1$ . Therefore, Eq. (B7) can be re-expressed in the more compact form of Eq. (53).

### APPENDIX C: $F_{\vec{r}_{\ell}}^{(n)}$ IN TERMS OF $F_{\vec{r}_{\ell-1}}^{(n')}$

We prove Lemma 1:  $\check{N}_{\vec{r}_{\ell-1}} \leq \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}^{(a)}}$ , where  $\vec{r}_{\ell-1} = \bigoplus_{a=1}^m \vec{r}_{\ell-1}^{(a)}$ .

*Proof of Lemma 1:* For a given  $\vec{r}_{\ell-1}$ -type error with  $\vec{r}_{\ell-1} = \bigoplus_{a=1}^m \vec{r}_{\ell-1}^{(a)}$  [Eq. (55a)], its decoupling order is [Eq. (29)],

$$\check{N}_{\vec{r}_{\ell-1}} = \max_{i \in \{1, \dots, \ell-1\}} [r_i(p_{\oplus}(1, i-1) \oplus 1) \check{N}_i + p_+(i+1, \ell-1)]. \quad (\text{C1})$$

Suppose the maximum occurs at the  $M$ th UDD layer, i.e.,

$$\check{N}_{\vec{r}_{\ell-1}} = \check{N}_M + p_+(M+1, \ell-1), \quad (\text{C2})$$

where the coefficient of  $\check{N}_M$  is equal to 1, implying that

$$r_M = 1, \quad (\text{C3a})$$

$$p_{\oplus}(1, M-1) = 0. \quad (\text{C3b})$$

With Eqs. (55a), (C3a), and (C3b) we have the following equalities and inequality. First,

$$\bigoplus_{a=1}^m r_M^{(a)} = r_M = 1, \quad (\text{C4})$$

second,

$$\begin{aligned} p_{\oplus}(1, M-1) &= \bigoplus_{k=1}^{M-1} r_k [N_k]_2 = \bigoplus_{k=1}^{M-1} (\bigoplus_{a=1}^m r_k^{(a)}) [N_k]_2 \\ &= \bigoplus_{a=1}^m (\bigoplus_{k=1}^{M-1} r_k^{(a)}) [N_k]_2 \\ &= \bigoplus_{a=1}^m |v_M^{(a)}|, \end{aligned} \quad (\text{C5})$$

where to keep the notation more compact we defined

$$|v_i^{(a)}| \equiv \oplus_{k=1}^{i-1} r_k^{(a)} [N_k]_2. \tag{C6}$$

Thus, using Eq. (C3b),

$$\oplus_{a=1}^m |v_M^{(a)}| = 0, \tag{C7}$$

and third,

$$\begin{aligned} p_+(M+1, \ell-1) &= \sum_{k=M+1}^{\ell-1} r_k [N_k]_2 \\ &= \sum_{k=M+1}^{\ell-1} (\oplus_{a=1}^m r_k^{(a)}) [N_k]_2 \\ &\leq \sum_{k=M+1}^{\ell-1} \sum_{a=1}^m r_k^{(a)} [N_k]_2 \\ &\leq \sum_{a=1}^m \sum_{k=M+1}^{\ell-1} r_k^{(a)} [N_k]_2. \end{aligned} \tag{C8}$$

By using the properties  $\max [A, B, C] \geq \max [A, B]$  and  $\max [A + c, B + c] = \max [A, B] + c$ , we have

$$\begin{aligned} \sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}^{(a)}} &= \sum_{a=1}^m \max[\{r_i^{(a)}(|v_i^{(a)}| \oplus 1)\tilde{N}_i + \sum_{k=i+1}^{\ell-1} r_k^{(a)} [N_k]_2\}_{i=1}^{\ell-1}] \\ &\geq \sum_{a=1}^m \max[\{r_i^{(a)}(|v_i^{(a)}| \oplus 1)\tilde{N}_i + \sum_{k=i+1}^{\ell-1} r_k^{(a)} [N_k]_2\}_{i=1}^M] \\ &\geq \sum_{a=1}^m \max[\{r_i^{(a)}(|v_i^{(a)}| \oplus 1)\tilde{N}_i + \sum_{k=i+1}^M r_k^{(a)} [N_k]_2\}_{i=1}^M] + \sum_{a=1}^m \sum_{k=M+1}^{\ell-1} r_k^{(a)} [N_k]_2. \end{aligned} \tag{C9}$$

Equivalently,

$$\sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}^{(a)}} \geq \sum_{a=1}^m \check{N}_{\vec{r}_M^{(a)}} + \sum_{a=1}^m \sum_{k=M+1}^{\ell-1} r_k^{(a)} [N_k]_2. \tag{C10}$$

In light of the inequality (C8), the remaining task is to show

$$\sum_{a=1}^m \check{N}_{\vec{r}_M^{(a)}} \geq \tilde{N}_M, \tag{C11}$$

which will immediately lead to Lemma 1:  $\sum_{a=1}^m \check{N}_{\vec{r}_{\ell-1}^{(a)}} \geq \check{N}_{\vec{r}_{\ell-1}}$ .

The condition  $\oplus_{a=1}^m r_M^{(a)} = r_M = 1$  [Eq. (C4)] implies that there must exist at least one  $a'$  such that  $r_M^{(a')} = 1$ . For this  $\vec{r}_M^{(a')}$  vector with  $r_M^{(a')} = 1$ , its first  $M - 1$  components either satisfy  $|v_M^{(a')}| = 0$  or  $|v_M^{(a')}| = 1$ .

For the  $\vec{r}_M^{(a')}$ -type error with  $r_M^{(a')} = 1$  and  $|v_M^{(a')}| = 0$ , the coefficient  $r_M^{(a')}(|v_M^{(a')}| \oplus 1)$  of  $\tilde{N}_M$  in  $\check{N}_{\vec{r}_M^{(a)'}}$  [Eq. (29)] is not zero. Therefore,

$$\check{N}_{\vec{r}_M^{(a)'}} = \max[\{\dots\}_{i=1}^{M-1}, \tilde{N}_M] \geq \tilde{N}_M, \tag{C12}$$

which leads to Eq. (C11).

However, for the  $\vec{r}_M^{(a)}$ -type error with  $r_M^{(a)} = 1$  and  $v_M^{(a)} = 1$ , the coefficient  $r_M^{(a)}(|v_M^{(a)}| \oplus 1)$  of  $\tilde{N}_M$  in Eq. (29) ends up vanishing, leading to

$$\check{N}_{\vec{r}_M^{(a)}} = \max\{\{\dots\}_{i=1}^{M-1}, 0\} \tag{C13}$$

which cannot determine whether  $\check{N}_{\vec{r}_M^{(a)}} \geq \tilde{N}_M$ . This notwithstanding,  $v_M^{(a)} \equiv \oplus_{k=1}^{M-1} r_k^{(a)} [N_k]_2 = 1$  indicates that among the  $M - 1$  components of the vector  $\vec{r}_M^{(a)}$ , there is a total odd number of components each of which is equal to 1, and associates with an odd sequence order. Suppose the  $o'$  component is the outermost non-zero component  $r_{o'} = 1$  with  $[N_{o'}]_2 = 1$  of  $\vec{r}_M^{(a)}$ . Accordingly,

$$|v_{o'}^{(a)}| = \oplus_{k=1}^{o'-1} r_k^{(a)} [N_k]_2 = 0, \tag{C14a}$$

$$\sum_{k=o'+1}^M r_k^{(a)} [N_k]_2 = 0. \tag{C14b}$$

With Eq. (C14a) and Eq. (C14b), it follows that

$$\check{N}_{\vec{r}_M^{(a)}} = \max\{\{\dots\}_{i=1}^{o'-1}, \tilde{N}_{o'}, \{\dots\}_{i=o'+1}^{M-1}\} \geq \tilde{N}_{o'} \geq \tilde{N}_M - 1, \tag{C15}$$

where the last inequality is derived as follows:

$$\begin{aligned} \tilde{N}_M &= \min[N_M, N_{o_{\min}}^{k < o'} + 1] = \min[N_M, N_{o_{\min}}^{k < o'} + 1] \\ &\leq N_{o_{\min}}^{k < o'} + 1 = \min[N_{o_{\min}}^{k < o'-1} + 1, N_{o'} + 1] \\ &\leq \tilde{N}_{o'} + 1. \end{aligned} \tag{C16}$$

Moreover, if  $v_M^{(a)} = 1$ , Eq. (C7) implies that there is another vector  $\vec{r}_M^{(a'')}$  such that  $|v_M^{(a'')}| \equiv \oplus_{k=1}^{M-1} r_k^{(a'')} [N_k]_2 = 1$ . Using the same argument, there must exist a  $r_{o''} = 1$  with  $v_{o''}^{(a'')} = 0$  with an odd sequence order  $N_{o''}$ ,  $o'' < M$ . It follows that

$$\check{N}_{\vec{r}_M^{(a'')}} = \max\{\{\dots\}_{i=1}^{o''-1}, \tilde{N}_{o''}, \{\dots\}_{i=o''+1}^M\} \geq \tilde{N}_{o''} \geq 1. \tag{C17}$$

Therefore, with Eqs. (C15) and (C17),

$$\sum_{a=1}^m \check{N}_{\vec{r}_M^{(a)}} \geq \check{N}_{\vec{r}_M^{(a')}} + \check{N}_{\vec{r}_M^{(a'')}} \geq \tilde{N}_M, \tag{C18}$$

which proves Eq. (C11). □

#### APPENDIX D: FOURIER EXPANSIONS AFTER LINEAR CHANGE OF VARIABLE

The  $\ell$ th-layer modulation function  $f_\ell(\theta)$ , which alternates in sign with the new outer-most-layer pulse timing  $\theta_{j_\ell} = \frac{j_\ell \pi}{N_\ell + 1}$ , has a period of  $\frac{2\pi}{N_\ell + 1}$  since the outer-most-layer pulses are now equally spaced. Therefore,  $f_\ell(\theta)$  has a simple Fourier expansion

$$f_\ell(\theta) = \sum_{k=0}^{\infty} d_k^\ell \sin[(2k + 1)(N_\ell + 1)\theta] \tag{D1}$$

with  $d_k^\ell = \frac{4}{(2k+1)\pi}$ . The remaining modulation functions such as  $f_i(\theta)$  with  $i < \ell$ , which switch sign with the inner-layer UDD pulse timing  $\theta_{j_\ell, \dots, j_i}$ , all have the same period  $\frac{\pi}{N_\ell + 1}$ . This is because the inner  $(\ell - 1)$ -layers NUDD pulse timing structure inside each  $[\theta_{j_\ell-1}, \theta_{j_\ell})$  is still preserved and each are actually identical to each other, in that Eq. (61) just rescales the outer-most layer interval

$[\theta_{j_{\ell-1}}, \theta_{j_\ell}]$  linearly. In addition, due to the time-symmetric structure of NUDD pulse timings, it follows that inside each  $[\theta_{j_{\ell-1}}, \theta_{j_\ell}]$ ,  $f_i(\theta)$  for  $i < \ell$  is an even function when  $N_i$  is even, and odd when  $N_i$  is odd. Therefore, it follows that the Fourier expansion of  $f_i(\theta)$  has the following form:

$$f_i(\theta) = \begin{cases} \sum_{k=0}^{\infty} d_k^i \cos[2k(N_\ell + 1)\theta], & N_i \text{ even} \\ \sum_{k=1}^{\infty} d_k^i \sin[2k(N_\ell + 1)\theta], & N_i \text{ odd} \end{cases} \quad (\text{D2})$$

for  $i < \ell$ . Note that the Fourier expansion coefficients  $d_k^i$  in the even and odd cases are, in fact, different. However, we use the same notation for both since the exact values of these coefficients are irrelevant for our proof. Finally, the Fourier expansion of  $G_1(\theta)$  is

$$G_1(\theta) = \sum_{k=0}^{\infty} \sum_{q=-1,1} g_{k,q} \sin[2k(N_\ell + 1)\theta + q\theta] \quad (\text{D3})$$

whose detailed calculations can be found in Ref. 39. In accordance with Definition 1, the function types of  $f_\ell(\theta)$ ,  $f_{\Omega_{i < \ell}}(\theta)$ , and  $G_1(\theta)$  [Eq. (D1)–(D3)] are identified as Eqs. (66)–(68), respectively.

**APPENDIX E:  $\min[\{\check{N}_{\vec{r}_{\ell-1} \in \vec{v}_{\ell-1}^1}\}] = N_{\text{Omin}}^{k' < \ell}$**

We prove Lemma 4:  $\min[\{\check{N}_{\vec{r}_{\ell-1} \in \vec{v}_{\ell-1}^1}\}] = N_{\text{Omin}}^{k' < \ell}$ .

*Proof of Lemma 4:* For all  $\vec{r}_{\ell-1} \in \vec{v}_{\ell-1}^1$ , their components satisfy, by definition, the condition  $p_{\oplus}(1, \ell - 1) = 1$ , which implies that the total number of non-zero components with odd sequence orders in  $\vec{r}_{\ell-1}$  is odd. Suppose that before the  $\ell$ th-layer, the  $o_1$ th,  $o_2$ th,  $\dots$ , and  $o_j$ th UDD layers where  $0 < o_1 < o_2 < \dots < o_j < \ell$  are the layers with odd sequence orders, namely,  $[N_{o_i}]_2 = 1$  for  $i = 1, 2, \dots, j$ .

Define  $\vec{e}_{o_i}$  as the  $\vec{r}_{\ell-1}$ -type errors with  $r_{o_i} = 1$  and all  $r_{j \neq o_i} = 0$ . For  $\vec{e}_{o_i}$ -type errors which obviously belong to the  $\vec{v}_{\ell-1}^1$ -type error, we have  $\check{N}_{\vec{e}_{o_i}} = \tilde{N}_{o_i}$  according to the decoupling order formula Eq. (29).

For the remaining  $\vec{v}_{\ell-1}^1$  vectors, they have 3 or more non-zero components associated with odd orders. For a given  $\vec{r}_{\ell-1} \neq \vec{e}_{o_i} \in \vec{v}_{\ell-1}^1$ , suppose the inner-most component with odd order is  $r_{o_i} = 1$ . Then its decoupling order follows:

$$\begin{aligned} \check{N}_{\vec{r}_{\ell-1} \neq \vec{e}_{o_i} \in \vec{v}_{\ell-1}^1} &= \max[\dots, \tilde{N}_{o_i} + \sum_{k=o_i+1}^{\ell-1} r_k [N_k]_2, \dots] \\ &\geq \tilde{N}_{o_i} = \check{N}_{\vec{e}_{o_i}}. \end{aligned} \quad (\text{E1})$$

Therefore,  $\min[\{\check{N}_{\vec{r}_{\ell-1} \in \vec{v}_{\ell-1}^1}\}]$  will occur among the decoupling orders of the errors which has only one non-zero component with odd sequence order, i.e.,

$$\begin{aligned} \min[\{\check{N}_{\vec{r}_{\ell-1} \in \vec{v}_{\ell-1}^1}\}] &= \min[\check{N}_{\vec{e}_{o_1}}, \check{N}_{\vec{e}_{o_2}}, \dots, \check{N}_{\vec{e}_{o_j}}] \\ &= \min[\tilde{N}_{o_1}, \tilde{N}_{o_2}, \dots, \tilde{N}_{o_j}] \\ &= \min[N_{o_1}, N_{o_2}, \dots, N_{o_j}]. \end{aligned} \quad (\text{E2})$$

Equation (E2) is the same expression as  $N_{\text{Omin}}^{k' < i} \equiv \min_{k' < i} \{N_{k'} \mid [N_{k'}]_2 = 1\}$  [Eq. (31)], which completes the proof of Lemma 4. □

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