Rigorous performance bounds for quadratic and nested dynamical decoupling

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We present rigorous performance bounds for the quadratic dynamical decoupling pulse sequence which protects a qubit from general decoherence, and for its nested generalization to an arbitrary number of qubits. Our bounds apply under the assumptions of instantaneous pulses and of bounded perturbing environment and qubit-environment Hamiltonians such as those realized by baths of nuclear spins in quantum dots. We prove that if the total sequence time is fixed then the trace-norm distance between the unperturbed and protected system states can be made arbitrarily small by increasing the number of applied pulses.

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I. INTRODUCTION

The coupling between a quantum system and its environment typically causes decoherence, which is detrimental in quantum-information processing as it results in computational errors [1]. Over the years, various ways of suppressing quantum decoherence have been explored; see, e.g., Ref. [2]. The methodology we study here is dynamical decoupling (DD), which utilizes sequences of strong pulses to decouple the system from its environment [3–7]. Recently, an optimal DD pulse sequence was discovered for the suppression of pure dephasing or longitudinal relaxation of a qubit coupled to a bath with a hard high-frequency cutoff: Uhrig DD (UDD) [8–13]. In UDD, the instants t_j ($j \in \{1,2,\ldots,N\}$) at which N instantaneous π pulses are applied are given by $t_j = T\lambda_j$, where T is the total time of the sequence, and

$$\lambda_j = \sin^2 \frac{j\pi}{2N+2}. \quad (1)$$

By optimal it is meant that each additional pulse suppresses dephasing or longitudinal relaxation to one additional order in an expansion in powers of T, i.e., N pulses reduce dephasing or longitudinal relaxation to $O(T^{N+1})$. Rigorous performance bounds were established in Ref. [14]. In this work we derive performance bounds for more general pulse sequences.

A near-optimal way to suppress general single-qubit decoherence, as opposed to only pure dephasing or pure longitudinal relaxation, is the quadratic DD (QDD) sequence [15–19]. A QDD sequence is obtained by nesting two UDD sequences of pulses which are orthogonal in spin space. When these two UDD sequences comprise the same number of pulses N, a QDD sequence of $(N+1)^2$ pulses will suppress general qubit decoherence to $O(T^{N+1})$, which is known from brute-force symbolic algebra solutions for small N to be near optimal [15]. It has been analytically proven that when the two UDD sequences comprise different numbers of pulses N_1 and N_2, a QDD sequence of $(N_1+1)(N_2+1)$ pulses will suppress general qubit decoherence to $O(T^{\min(N_1,N_2)+1})$, and this is universal, i.e., holds for arbitrary baths and system-bath interactions [16,18,19]. Moreover, the dependence of the suppression order of each single-qubit error type (dephasing, bit flip, or both) on N_1 and N_2 has also been established in detail in terms of both analytical bounds [18] and numerical simulations [17,20].

When the nesting process of UDD sequences is continued, one has the nested UDD (NUDD) sequence, which can protect multiple qubits, or general multilevel quantum systems, against general decoherence [16,19]. It has been proven that NUDD is universal and will suppress general multiqubit decoherence to $O(T^{\min_i(N_i)+1})$, where N_i are the orders of the UDD sequences being nested [19]. However, it is known that NUDD is suboptimal [16].

Our main results in this paper are analytical upper bounds, for QDD and NUDD, on the trace-norm distance between the states of the DD-protected qubit or qubits and the unperturbed qubit or qubits, given as a function of the total evolution time and the norms of the bath operators. Under the assumption that the bath operators have finite norms, the upper bound for NUDD shows that the trace-norm distance can be made arbitrarily small as a function of the minimal decoupling order N of the UDD sequences comprising the NUDD sequence. In the QDD case, a tighter bound is obtained by having different decoupling orders for different types of decoherence errors, using the results of Ref. [18].

The structure of this paper is as follows. We develop our results for QDD and NUDD in parallel, always starting with the simpler case of QDD. We first review the QDD and NUDD sequences in Sec. II. We also derive bounding series for the two sequences in this section. In Sec. III we use the bounding

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series in order to find explicit upper bounds on the different single-axis errors for QDD, and similar explicit upper bounds on different error types for NUDD. These results are then used in Sec. IV to derive the main results of this paper: trace-norm distance upper bounds for QDD and NUDD. We conclude in Sec. V and present additional technical details in the Appendixes.

II. MODEL

In this section we give a formal description of the QDD and NUDD sequences, and the decoherence they suppress.

A. QDD

We describe QDD as a nesting of two UDD sequences. The inner UDD sequence, denoted UDD_{N_1}, comprises N_1 Z-type pulses, meaning N_1 instantaneous rotations by π about the z axis of the qubit Bloch sphere, i.e., $Z = ie^{-i(\pi/2)\sigma_z}$. Similarly, the outer UDD sequence, denoted UDD_{N_2}, comprises N_2 X-type pulses, where $X = ie^{-i(\pi/2)\sigma_x}$. We denote the resulting QDD sequence by QDD_{N_1,N_2}. To make sure that the qubit state is unaltered by the sequence itself, we append an additional pulse at the conclusion of the sequence if N_1 or N_2 is odd. Thus, if N_i' denotes the number of pulses in UDD_{N_i}, where $i \in \{1,2\}$, then

$$N_i' = N_i + (N_i \mod 2). \tag{2}$$

We define the dimensionless relative time $s := t/T$, so that the X-type pulses are applied at times

$$\lambda_j = \sin^2 \frac{j\pi}{2N_2+2}, \tag{3}$$

where $j = 1,2,\ldots,N_2'$ and the Z-type pulses are applied at times

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

with $k = 1,2,\ldots,N_1'$.

We consider the most general form of "bounded" time-independent single-qubit decoherence, which is described by the Hamiltonian

$$\widetilde{H} = \sum_{\alpha\in\{0,x,y,z\}} \sigma_\alpha \otimes B_\alpha, \tag{5}$$

where $\sigma_0 = \mathbb{1}_S$ is the identity operator on the system. The operators B_α with $\alpha \in \{0,x,y,z\}$ are arbitrary except for the requirement that their sup-operator norms, i.e., the largest eigenvalue of $(B_\alpha^\dagger B_\alpha)^{1/2}$, are finite,

$$J_\alpha := \|B_\alpha\| < \infty. \tag{6}$$

To decouple the qubit from the bath, we apply the QDD_{N_1,N_2} sequence, assuming Eq. (5). See Fig. 1 for a schematic depiction of a $\text{QDD}_{3,3}$ sequence.

The QDD_{N_1,N_2} sequence is generated by the control Hamiltonian

$$H_c(s) = \frac{\pi}{2}\sigma_x \sum_{j=1}^{N_2'} \delta(s-\lambda_j) + \frac{\pi}{2}\sigma_z \sum_{j=1}^{N_2+1}\sum_{k=1}^{N_1'} \delta(s-\lambda_{j,k}). \tag{7}$$

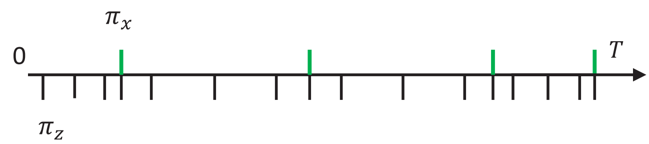

FIG. 1. (Color online) Illustration of $\text{QDD}_{3,3}$. Time flows from left to right. The switching instants are distributed according to Eqs. (3) and (4). The pulses π_z and π_x are rotations about the z and x axes, respectively, by the angle π. The total sequence time is T.

The corresponding control time-evolution operator is

$$U_c(s) = \mathcal{T}\exp\left(-i\int_0^s H_c(s')ds'\right), \tag{8}$$

where $\mathcal{T}$ is the time-ordering operator. Thus, the toggling-frame Hamiltonian reads

$$H(s) = U_c^\dagger(s)\widetilde{H}U_c(s) \tag{9a}$$

$$= \sum_{\alpha\in\{0,x,y,z\}} f_\alpha(s)\sigma_\alpha \otimes B_\alpha, \tag{9b}$$

where the switching functions are

$$f_0(s) = 1 \quad s \in [0,1], \tag{10a}$$

$$f_x(s) = (-1)^{k-1} \quad s \in [\lambda_{j,k-1},\lambda_{j,k}), \tag{10b}$$

$$f_y(s) = (-1)^{k-1}(-1)^{j-1} \quad s \in [\lambda_{j,k-1},\lambda_{j,k}), \tag{10c}$$

$$f_z(s) = (-1)^{j-1} \quad s \in [\lambda_{j-1},\lambda_j). \tag{10d}$$

For later use, we note that

$$f_y(s) = f_x(s)f_z(s). \tag{11}$$

Next, we consider the total time evolution given by the unitary operator

$$U(T) = \mathcal{T}\exp\left(-iT\int_0^1 H(s)ds\right). \tag{12}$$

Standard time-dependent perturbation theory provides the following Dyson series for $U(T)$:

$$U(T) = \sum_{n=0}^{\infty}(-iT)^n \sum_{\{\vec{\alpha};\dim(\vec{\alpha})=n\}} f_{\vec{\alpha}}\widehat{Q}_{\vec{\alpha}}, \tag{13a}$$

$$f_{\vec{\alpha}} := \int_0^1 ds_n f_{\alpha_n}(s_n)\int_0^{s_n} ds_{n-1} f_{\alpha_{n-1}}(s_{n-1}) \times \cdots$$

$$\times \int_0^{s_3} ds_2 f_{\alpha_2}(s_2)\int_0^{s_2} ds_1 f_{\alpha_1}(s_1), \tag{13b}$$

$$\widehat{Q}_{\vec{\alpha}} := (\sigma_{\alpha_n}\otimes B_{\alpha_n})\cdots(\sigma_{\alpha_1}\otimes B_{\alpha_1}) \tag{13c}$$

$$= r\sigma_0^{n_0}\sigma_x^{n_x}\sigma_y^{n_y}\sigma_z^{n_z} \otimes B_{\alpha_n}\cdots B_{\alpha_1}. \tag{13d}$$

The notation $\dim(\vec{\alpha}) = n$ in Eq. (13a) means that the vector $\vec{\alpha}$ is restricted to having n components $\{\alpha_n,\ldots,\alpha_1\}$. The components are $\alpha_k \in \{0,x,y,z\}$ for $1 \leqslant k \leqslant n$. Each integer $n_\alpha \geqslant 0$, $\alpha \in \{0,x,y,z\}$ counts how many times the operator $\sigma_\alpha \otimes B_\alpha$ appears in $\widehat{Q}_{\vec{\alpha}}$. For a given dimension n of $\vec{\alpha}$, we have $n = n_0 + n_x + n_y + n_z$. In this way, the complete sum over all possible sequences of B_0, B_x, B_y, and B_z is considered. The rearrangement of the noncommuting product of Pauli matrices in Eq. (13c) into the canonical form (13d) gives rise to $r = (-1)^v$, where v counts the number of times two different

Pauli matrices have to pass each other based on $\sigma_\alpha\sigma_\beta = -\sigma_\beta\sigma_\alpha$ if $\alpha \neq \beta$.

Our goal is to find an upper bound for each term $f_{\vec\alpha}\widehat{Q}_{\vec\alpha}$ separately. We exploit $|f_\alpha(s)| = 1$, $\|\sigma_\alpha\| = 1$, and

$$\|\widehat{Q}_{\vec\alpha}\| \leqslant J_{\vec\alpha}, \tag{14a}$$

$$J_{\vec\alpha} := J_{\alpha_n}J_{\alpha_{n-1}}\cdots J_{\alpha_1} \tag{14b}$$

to obtain the upper-bounding series given below for the series (13a) term by term:

$$\|U(T)\| \leqslant \sum_{n=0}^{\infty} T^n F_n \sum_{\{\vec\alpha;\dim(\vec\alpha)=n\}} J_{\vec\alpha} \tag{15a}$$

$$=: S_{\mathrm{Q}}(T) \tag{15b}$$

$$= \exp[(J_0 + J_x + J_y + J_z)T], \tag{15c}$$

where

$$F_n := \int_0^1 ds_n \int_0^{s_n} ds_{n-1}\cdots\int_0^{s_3} ds_2 \int_0^{s_2} ds_1 = \frac{1}{n!}. \tag{16}$$

The equality between (15a) and (15c) is most easily seen by realizing that the right-hand side of (15a) is the Dyson series of (15c) as obtained by time-dependent perturbation theory. This series will be used extensively when we compute the performance bounds in Sec. III which generalize the UDD results in Ref. [14].

B. NUDD

The NUDD sequence is a generalization of the UDD and QDD sequences that suppresses decoherence for a multiqubit system. Assume that the system comprises m qubits. We consider the most general form of "bounded" time-independent m-qubit decoherence. Subject only to the constraint on the bath operators $B_{\vec\mu}$ that they are bounded,

$$J_{\vec\mu} := \|B_{\vec\mu}\| < \infty, \tag{17}$$

the Hamiltonian that gives rise to this general decoherence is

$$\widetilde{H} = \sum_{\vec\mu\in D_m} \widehat{\sigma}_{\vec\mu}\otimes B_{\vec\mu}, \tag{18}$$

where

$$D_m := \{(0,0),(1,0),(1,1),(0,1)\}^m, \tag{19a}$$

$$\widehat{\sigma}_{\vec\mu} := \sigma_{1,\mu_1}\otimes\cdots\otimes\sigma_{m,\mu_m}. \tag{19b}$$

Here the σ_{j,μ_j}'s are Pauli matrices or the identity and we use $j \in \{1,\ldots,m\}$ to index the qubits. For the jth qubit, we use the binary component $\mu_j \in \{(0,0),(1,0),(1,1),(0,1)\}$ of the vector $\vec\mu := (\mu_1,\mu_2,\ldots,\mu_m)$ to denote the Pauli matrix subscripts $\{0,x,y,z\}$, respectively.

The NUDD sequence for an m-qubit system consists of $2m$ nested levels (two per qubit). Let T be the total duration of the NUDD sequence and N_i' be the decoupling order of the ith-level UDD [Eq. (2)]. Then the pulses at the ith level are applied at the instants

$$\lambda_{l_{2m},l_{2m-1},\ldots,l_i} = \lambda_{l_{2m},l_{2m-1},\ldots,l_{i+1}} + (\lambda_{l_{2m},l_{2m-1},\ldots,l_{i+1}+1} - \lambda_{l_{2m},l_{2m-1},\ldots,l_{i+1}})\sin^2\frac{l_i\pi}{2N_i'+2}, \tag{20}$$

where $1 \leqslant i \leqslant 2m$ and $1 \leqslant l_i \leqslant N_i'$. Even values of i correspond to σ_x pulses applied to qubit number $j = i/2$, while odd values of i correspond to σ_z pulses applied to qubit number $j = (i+1)/2$. The control Hamiltonian is therefore

$$H_c(s) = \frac{\pi}{2}\sum_{\{i\geqslant 2,\text{even}\}}^{2m} \sigma_{i/2,x} \sum_{\{l_p=1\}_{p=i}^{2m}}^{N_p'} \delta\big(s - \lambda_{l_{2m},\ldots,l_i}\big) + \frac{\pi}{2}\sum_{\{i\geqslant 1,\text{odd}\}}^{2m-1} \sigma_{(i+1)/2,z} \sum_{\{l_p=1\}_{p=i}^{2m}}^{N_p'} \delta(s - \lambda_{l_{2m},\ldots,l_i}), \tag{21}$$

where the inner sums are multiple sums, one for each value of the index p labeling the nesting levels $i,i+1,\ldots,2m$. The control time-evolution operator is

$$U_c(s) = \mathcal{T}\exp\left(-i\int_0^s H_c(s')ds'\right). \tag{22}$$

The toggling-frame Hamiltonian is

$$H(s) = U_c(s)^\dagger \widetilde{H} U_c(s) \tag{23a}$$

$$= \sum_{\vec\mu\in D_m} f_{\vec\mu}(s)\,\widehat{\sigma}_{\vec\mu}\otimes B_{\vec\mu}, \tag{23b}$$

$$f_{\vec\mu}(s) = \prod_{j=1}^{m} f_{j,\mu_j}(s), \tag{23c}$$

where the $f_{j,\mu_j}(s)$'s are the switching functions. They can be obtained by the anticommutation relations of the Pauli matrices

$$f_{j,(0,0)}(s) = 1 \text{ for } s \in [0,1], \tag{24a}$$

$$f_{j,(1,0)}(s) = (-1)^{l_{2j-1}} \tag{24b}$$

$$\text{for } s \in \big[\lambda_{l_{2m},l_{2m-1},\ldots,l_{2j-1}-1}, \lambda_{l_{2m},l_{2m-1},\ldots,l_{2j-1}}\big),$$

$$f_{j,(0,1)}(s) = (-1)^{l_{2j}} \tag{24c}$$

$$\text{for } s \in \big[\lambda_{l_{2m},l_{2m-1},\ldots,l_{2j}-1}, \lambda_{l_{2m},l_{2m-1},\ldots,l_{2j}}\big),$$

$$f_{j,(1,1)}(s) = f_{j,(1,0)}(s)f_{j,(0,1)}(s) \text{ for } s \in [0,1]. \tag{24d}$$

In the last equation we used Eq. (11).

Now consider the total time evolution given by the unitary operator

$$U(T) = \mathcal{T}\exp\left(-iT\int_0^1 H(s)ds\right). \tag{25}$$

Standard time-dependent perturbation theory provides the following Dyson series for $U(T)$:

$$U(T) = \sum_{n=0}^{\infty}(-iT)^n \sum_{\{\vec\mu_k\in D_m\}_{k=1}^n} f_{\vec\mu_1,\ldots,\vec\mu_n}\,\widehat{Q}_{\vec\mu_1,\ldots,\vec\mu_n}, \tag{26a}$$

$$f_{\vec\mu_1,\ldots,\vec\mu_n} := \int_0^1 ds_n f_{\vec\mu_n}(s_n)\int_0^{s_n} ds_{n-1} f_{\vec\mu_{n-1}}(s_{n-1})\times\cdots \times\int_0^{s_3} ds_2 f_{\vec\mu_2}(s_2)\int_0^{s_2} ds_1 f_{\vec\mu_1}(s_1), \tag{26b}$$

$$\widehat{Q}_{\vec\mu_1,\ldots,\vec\mu_n} := \big(\widehat{\sigma}_{\vec\mu_n}\otimes B_{\vec\mu_n}\big)\cdots\big(\widehat{\sigma}_{\vec\mu_1}\otimes B_{\vec\mu_1}\big) \tag{26c}$$

$$= r\prod_{\vec\mu_k\in D_m} \widehat{\sigma}_{\vec\mu}^{n_{\vec\mu}}\otimes B_{\vec\mu_n}\cdots B_{\vec\mu_1}, \tag{26d}$$

TABLE I. Summary of single-axis error suppression from Ref. [18].

Single-axis error σ_α	N_1 mod 2	N_2 mod 2	Decoupling order d_α
$\alpha = x$	0 or 1	0 or 1	N_1
$\alpha = y$	0	0	$\max\{N_1,N_2\}$
	0	1	$\max\{N_1+1,N_2\}$
	1	0	N_1
	1	1	N_1+1
$\alpha = z$	0	0 or 1	N_2
	1	0 or 1	$\min\{N_1+1,N_2\}$

where $r = \prod_{j=1}^m r_j$ and each $r_j := (-1)^{v_j}$, where v_j counts how often two different σ_{j,μ_j} with the same j pass each other in order to obtain (26d) from (26c). Each $n_{\vec{\mu}}$ in Eq. (26d) indicates how many times $\widehat{\sigma}_{\vec{\mu}} \otimes B_{\vec{\mu}}$ appears in Eq. (26c) and the $n_{\vec{\mu}}$'s satisfy $\sum_{\vec{\mu}\in D_m} n_{\vec{\mu}} = n$.

Following steps analogous to the QDD case, we have

$$|f_{\vec{\mu}}| = 1, \tag{27a}$$

$$\|\widehat{Q}_{\vec{\mu}_1,\ldots,\vec{\mu}_n}\| \leqslant \prod_{\vec{\mu}\in D_m} J_{\vec{\mu}}^{n_{\vec{\mu}}}. \tag{27b}$$

This allows us to write

$$\|U(T)\| \leqslant \sum_{n=0}^{\infty} T^n F_n \sum_{\{\vec{\mu}_k\in D_m\}_{k=1}^n} \prod_{\vec{\mu}\in D_m} J_{\vec{\mu}}^{n_{\vec{\mu}}} \tag{28a}$$

$$=: S_{\rm N}(T), \tag{28b}$$

where F_n was defined in Eq. (16) and the right-hand side of (28a) is the Dyson series applied to

$$S_{\rm N}(T) = \exp\Big(T \sum_{\vec{\mu}\in D_m} J_{\vec{\mu}}\Big). \tag{29}$$

For an alternative derivation see Sec. III B.

III. BOUNDS FOR GENERAL DECOHERENCE

A. QDD

Very recently in Ref. [18] rigorous lower bounds were found on the decoupling orders of a QDD_{N_1,N_2} sequence. The result is summarized in Table I. We define the decoupling order of a single-axis error σ_α to be d_α for $\alpha \in \{x,y,z\}$. Thus, after applying the QDD_{N_1,N_2} sequence, the first nonvanishing term in the Dyson series (13a) that contributes to the σ_α-type error is of order $T^{d_\alpha+1}$ or higher.[1] We will use this result in deriving the bounds for decoherence.

Any operator acting on the qubit subspace can be expanded in terms of the Pauli matrices and the identity. Hence

$$U(T) = \sum_{\alpha\in\{0,x,y,z\}} \sigma_\alpha \otimes A_\alpha(T) \tag{30}$$

[1] In Ref. [17] the result for the decoupling order of σ_z when N_1 is odd was found numerically (using a spin-bath model) to be $\min\{2N_1+1,N_2\}$, which improves on the analytical bound $\min\{N_1+1,N_2\}$ from Ref. [18]. In all other cases Refs. [17,18] are in perfect agreement.

TABLE II. Classification of the error terms in the series Eq. (13a) according to the parities $p_\alpha := n_\alpha \mod 2$. Recall that n_α counts how many times the operator $\sigma_\alpha \otimes B_\alpha$ appears in $\widehat{Q}_{\vec{\alpha}}$. The "Channel" column gives the corresponding single-axis error term in Eq. (30). The last column gives the order to which the single-axis error is suppressed. For completeness, the identity channel σ_0 is also listed, although rather than being suppressed it increases in linear order.

Case j	p_x	p_y	p_z	Channel	Decoupling order
0	0	0	0	σ_0	1
1	0	0	1	σ_z	d_z
2	0	1	0	σ_y	d_y
3	0	1	1	σ_x	d_x
4	1	0	0	σ_x	d_x
5	1	0	1	σ_y	d_y
6	1	1	0	σ_z	d_z
7	1	1	1	σ_0	1

is another way to write Eq. (13a), which serves to define the bath operators $A_\alpha(T)$. We classify the decoherence error based on the parities

$$p_\alpha := n_\alpha \mod 2, \quad \alpha \in \{x,y,z\}. \tag{31}$$

Using

$$\sigma_\alpha\sigma_\beta = i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma + \delta_{\alpha\beta}\mathbb{1}, \quad \alpha,\beta \in \{x,y,z\}, \tag{32}$$

where $\varepsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol, we find the results gathered in Table II.

Similarly to the bounding series found in Ref. [14], we can straightforwardly deduce bounding series for the various cases in Table II from $S_{\rm Q}(T)$ in Eq. (15b). We first write $S_{\rm Q}(T)$ as a sum over the eight terms differing in at least one parity:

$$S_{\rm Q}(T) = \sum_{j=0}^{7} S_j(T), \quad j = 2^0 p_z + 2^1 p_y + 2^2 p_x. \tag{33}$$

The parity p_α of n_α is the parity of $S_{\rm Q}(T) = \exp[(J_0 + J_x + J_y + J_z)T]$ as a function of J_α. Since $\exp(J_\alpha T) = \cosh(J_\alpha T) + \sinh(J_\alpha T)$ nicely splits even and odd contributions, we can split $S_{\rm Q}(T)$ into separate bounding functions as listed in Table III.

TABLE III. Functions of the respective bounding series for the various contributions of parity combinations.

Case j	p_x	p_y	p_z	Bounding function S_j
0	0	0	0	$e^{J_0T}\cosh(J_xT)\cosh(J_yT)\cosh(J_zT)$
1	0	0	1	$e^{J_0T}\cosh(J_xT)\cosh(J_yT)\sinh(J_zT)$
2	0	1	0	$e^{J_0T}\cosh(J_xT)\sinh(J_yT)\cosh(J_zT)$
3	0	1	1	$e^{J_0T}\cosh(J_xT)\sinh(J_yT)\sinh(J_zT)$
4	1	0	0	$e^{J_0T}\sinh(J_xT)\cosh(J_yT)\cosh(J_zT)$
5	1	0	1	$e^{J_0T}\sinh(J_xT)\cosh(J_yT)\sinh(J_zT)$
6	1	1	0	$e^{J_0T}\sinh(J_xT)\sinh(J_yT)\cosh(J_zT)$
7	1	1	1	$e^{J_0T}\sinh(J_xT)\sinh(J_yT)\sinh(J_zT)$

TABLE IV. The eight cases implied by Eq. (37).

$p_x \oplus \delta_{\alpha,x}$	$p_y \oplus \delta_{\alpha,y}$	$p_z \oplus \delta_{\alpha,z}$	$\theta_{\alpha,\vec{p}}$
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	0
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

We would like to use the bounding functions S_j to upper-bound $\|A_\alpha\|$. To this end, note first that, using Eqs. (30) and (32), for $\alpha \in \{x,y,z\}$,

$$\frac{1}{2}\mathrm{tr}_{\mathrm{S}}[\sigma_\alpha U(T)] = \frac{1}{2}\sum_\beta \mathrm{tr}[\sigma_\alpha\sigma_\beta]A_\beta(T) = A_\alpha(T), \quad (34)$$

where tr_{S} denotes the partial trace over the system. On the other hand, using Eq. (13),

$$\mathrm{tr}_{\mathrm{S}}[\sigma_\alpha U(T)] = \sum_{n=0}^{\infty}(-iT)^n \sum_{\{\vec{\alpha};\dim(\vec{\alpha})=n\}} f_{\vec{\alpha}}\mathrm{tr}_{\mathrm{S}}[\sigma_\alpha \hat{Q}_{\vec{\alpha}}] \quad (35)$$

and

$$\mathrm{tr}_{\mathrm{S}}[\sigma_\alpha \hat{Q}_{\vec{\alpha}}] = r\,\mathrm{tr}\big[\sigma_\alpha\sigma_x^{n_x}\sigma_y^{n_y}\sigma_z^{n_z}\big]B_{\alpha_n}\cdots B_{\alpha_1}. \quad (36)$$

Using the fact that only the parity (31) of the exponents matters, we can rewrite the trace as

$$\theta_{\alpha,\vec{p}} := \frac{1}{2}\big|\mathrm{tr}\big[\sigma_\alpha\sigma_x^{n_x}\sigma_y^{n_y}\sigma_z^{n_z}\big]\big| \quad (37a)$$

$$= \frac{1}{2}\big|\mathrm{tr}\big[\sigma_x^{p_x\oplus\delta_{\alpha x}}\sigma_y^{p_y\oplus\delta_{\alpha y}}\sigma_z^{p_z\oplus\delta_{\alpha z}}\big]\big|, \quad (37b)$$

where $\vec{p} := (p_x,p_y,p_z)$ and $\oplus$ denotes addition modulo 2. The values of $\theta_{\alpha,\vec{p}}$ are given in Table IV. Combining Eqs. (34)–(37), we have

$$\|A_\alpha(T)\| \leqslant \sum_{n=0}^{\infty} T^n F_n \sum_{\{\vec{\alpha};\dim(\vec{\alpha})=n\}} \theta_{\alpha,\vec{p}} J_{\vec{\alpha}}, \quad (38)$$

where F_n was defined in Eq. (16).

In view of Table IV, Eq. (38) provides the decomposition by parity of Eq. (15). Consider, e.g., the case $\alpha = x$. Then Table IV tells us that $\theta_{x,\vec{p}} = 1$ only when $\{p_x = 1, p_y = 0, p_z = 0\}$ (second row) or $\{p_x = 0, p_y = 1, p_z = 1\}$ (bottom row). In all other cases $\theta_{x,\vec{p}} = 0$. Comparing with Table III, we see that these two nonzero cases correspond to $j = 4$ and $j = 3$, respectively. A similar argument informs us that $\theta_{y,\vec{p}} = 1$ only when $\{p_x = 0, p_y = 1, p_z = 0\}$ or $\{p_x = 1, p_y = 0, p_z = 1\}$, which corresponds to $j = 2$ and $j = 5$ in Table III, and $\theta_{z,\vec{p}} = 1$ only when $\{p_x = 0, p_y = 0, p_z = 1\}$ or $\{p_x = 1, p_y = 1, p_z = 0\}$, which corresponds to $j = 1$ and $j = 6$ in Table III.

Now, note that the right-hand side of Eq. (38) without the θ_α factor is just $S_{\mathrm{Q}}(T)$ as defined in Eq. (15b). We can thus conclude from Eq. (38) that, due to the θ_α prefactor, its right-hand side consists of only two nonvanishing terms for each value of θ_α, which acts like a Kronecker δ function for the parity triple (p_x,p_y,p_z) of the bounding functions S_j, namely, $\alpha = x \Rightarrow j = 3,4$, $\alpha = y \Rightarrow j = 2,5$, $\alpha = z \Rightarrow j = 1,6$. Thus,

$$\|A_x(T)\| \leqslant S_3(T) + S_4(T), \quad (39a)$$

$$\|A_y(T)\| \leqslant S_2(T) + S_5(T), \quad (39b)$$

$$\|A_z(T)\| \leqslant S_1(T) + S_6(T). \quad (39c)$$

Next, to account for the suppression of decoherence by QDD we define

$$p_k^{(j)} := \frac{1}{k!}\frac{\partial^k}{\partial T^k}S_j\Big|_{T=0}, \quad (40)$$

so that

$$S_j = \sum_{k=0}^{\infty} p_k^{(j)}T^k. \quad (41)$$

We consider the partial Taylor series $\Delta_d^{(j)}$ of the analytic bounding functions S_j which leave out the contributions up to and including T^d:

$$\Delta_d^{(j)} := \sum_{k=d+1}^{\infty} p_k^{(j)}T^k. \quad (42)$$

According to Tables II and III, the contributions of case j are bounded by the corresponding partial Taylor series $\Delta_d^{(j)}$, where d is the decoupling order of the channel. This is a manifestation of the fact that the QDD sequence causes the first d_α powers in T of A_α to vanish, i.e., $A_\alpha(T) = O(T^{d_\alpha+1})$ [18]. Using Eq. (39) we deduce that

$$L_x := \Delta_{d_x}^{(3)} + \Delta_{d_x}^{(4)} \geqslant \|A_x(T)\|, \quad (43a)$$

$$L_y := \Delta_{d_y}^{(2)} + \Delta_{d_y}^{(5)} \geqslant \|A_y(T)\|, \quad (43b)$$

$$L_z := \Delta_{d_z}^{(1)} + \Delta_{d_z}^{(6)} \geqslant \|A_z(T)\|. \quad (43c)$$

This is our first key result for QDD.

Due to the analyticity in the variable T of S_j for each j, we know that the residual term vanishes for $d \to \infty$, that is,

$$\lim_{d\to\infty}\Delta_d^{(j)} = 0. \quad (44)$$

We define the dimensionless parameters ($\hbar$ is set to unity)

$$\varepsilon := J_0 T, \quad \eta_\alpha := J_\alpha/J_0, \quad (45)$$

where $\alpha \in \{x,y,z\}$. Thus, we can write the bounding functions S_j as $S_j(\varepsilon,\vec{\eta})$, where $\vec{\eta} = (\eta_x,\eta_y,\eta_z)$. By Taylor-expanding $S_j(\varepsilon,\eta_x,\eta_y,\eta_z)$, we can express the bounding functions in terms of ε and functions $\{g_l^{(n)}(\vec{\eta})\}_{n=1}^6$ given in Appendix A:

$$\Delta_{d_\alpha}^{(j)} = \sum_{n=d_\alpha+1}^{\infty} g_n^{(j)}(\vec{\eta})\varepsilon^n \quad (46a)$$

$$= g_{d_\alpha+1}^{(j)}(\vec{\eta})\varepsilon^{d_\alpha+1} + O(\varepsilon^{d_\alpha+2}). \quad (46b)$$

The behaviors of the bounding functions L_x, L_y, and L_z are shown in Fig. 2 for different $\vec{\eta}$. Here we assume that the decoherence is isotropic, i.e., $\eta := \eta_x = \eta_y = \eta_z$. Given this assumption, it makes sense to choose $N_1 = N_2$ so that the decoupling orders for different types of error are close. To simplify the computation, we choose both N_1 and N_2 to be

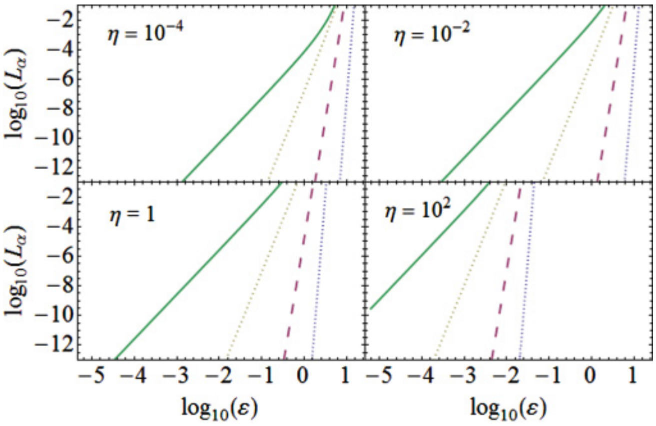

FIG. 2. (Color online) The upper bound L_α for $\|A_x\| = \|A_y\| = \|A_z\|$ according to Eqs. (43) in the isotropic case, i.e., $\eta_x = \eta_y = \eta_z$, as a function of ε for various numbers of pulses $N_1 = N_2 = N \in \{2,6,16,34\}$, at fixed values of η_α. In each panel the curves become steeper as N increases.

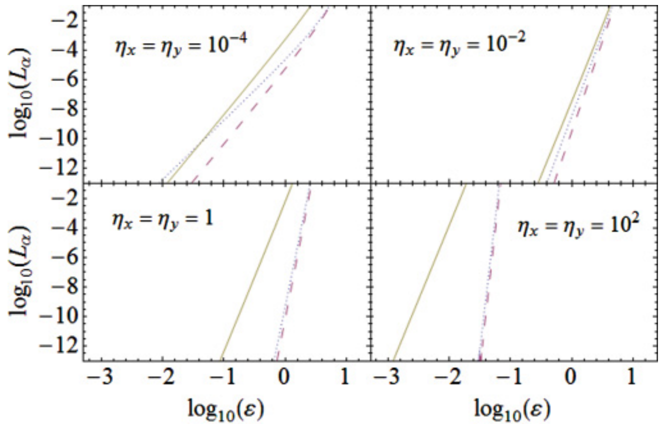

FIG. 4. (Color online) The upper bounds for $\|A_x\|$ (dotted lines), $\|A_y\|$ (dashed lines) and $\|A_z\|$ (filled lines) according to Eqs. (43). We take N_2 to be 9 in this case. The values of N_1 in the four panels going from left to right and top to bottom are 3, 10, 19, and 34. The value of $\eta_z = 10^{-2}$ as in the previous case.

even and thus, according to Table I, $d_x = d_y = d_z$. Note that in this situation L_x, L_y, and L_z are identical.

We also investigated the case where $\eta_x = \eta_y \neq \eta_z$ and how the parities of N_1 and N_2 affect the bounds. In Figs. 3 and 4, we plotted two cases. The first is where both N_1 and N_2 are even, which is represented by the thick lines. The second is where N_1 and N_2 are either even or odd, which is represented by the thin lines. We pick η_z to be 10^{-2} for all the plots and $\eta_x = \eta_y \in \{10^{-4}, 10^{-2}, 1, 10^2\}$. Since η_z is fixed, we also fix the values of N_2 for the two cases. We picked N_2 to be 10 in the first case and 9 in the second case to explore the effect of parity. We varied the value of N_1 based on the values η_x and η_y. We can see from the figures that, in the majority of cases, the parities of N_1 and N_2 change the decoupling order only by 1 or do not change it at all, so the bounds do not vary much. However, when N_1 is small compared to N_2, the parities can change the bounds nontrivially as seen in the top left panels of Figs. 3 and 4. We can also see this from Table I. When N_1 is small compared to N_2, the decoupling orders of σ_y and σ_z can decrease considerably when N_1 switches between even and odd values.

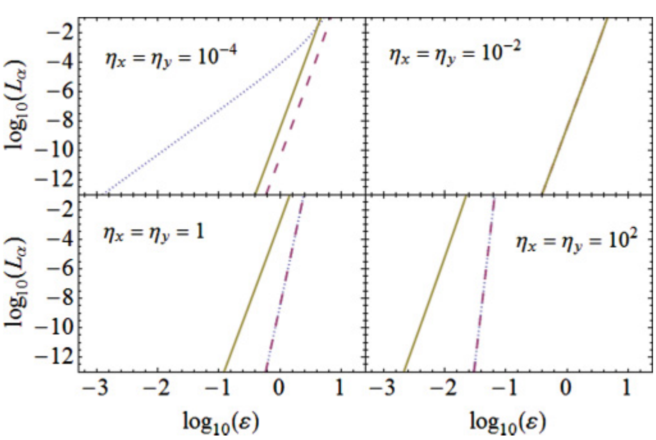

FIG. 3. (Color online) The upper bounds for $\|A_x\|$ (dotted lines), $\|A_y\|$ (dashed lines) and $\|A_z\|$ (filled lines) according to Eq. (43). Here N_2 is 10. The values of N_1 in the four panels going from left to right and top to bottom are 2, 10, 18, and 34. The value of $\eta_z = 10^{-2}$.

Equation (43) allows us to establish tight bounds on the representation of the unitary time evolution as given in Eq. (30). In Sec. IV A we use this fact to establish a bound on the trace-norm distance between the unperturbed qubit state and the protected qubit state.

B. NUDD

If we were to use the same method for NUDD for m qubits as we did in the QDD case for one qubit, we would need to consider $2^{(3^m)}$ cases based on the parities of $n_{\vec{\mu}}$. Recall that $n_{\vec{\mu}}$ indicates how many times $\widehat{\sigma}_{\vec{\mu}} \otimes B_{\vec{\mu}}$ appears in $(\widehat{\sigma}_{\vec{\mu}_n} \otimes B_{\vec{\mu}_n}) \cdots (\widehat{\sigma}_{\vec{\mu}_1} \otimes B_{\vec{\mu}_1})$; Eq. (26d). To simplify the analysis, unlike in the QDD case, we do not address each error term separately.

Any operator acting on the space of m qubits can be expanded in the $\{\sigma_{\vec{\mu}}\}$ basis. Generalizing the QDD case [Eq. (30)], we can thus write

$$U(T) = \sum_{\vec{\mu} \in D_m} \widehat{\sigma}_{\vec{\mu}} \otimes A_{\vec{\mu}}(T), \tag{47}$$

where $\widehat{\sigma}_{\vec{\mu}}$ and D_m were defined in Eqs. (19). Equation (47) provides another way to organize the terms in Eq. (26a). We introduce the upper-bounding series $S_{\vec{\mu}}$ for each $A_{\vec{\mu}}$ such that

$$\|A_{\vec{\mu}}(T)\| \leqslant S_{\vec{\mu}}(T), \tag{48a}$$

$$S_{\rm N}(T) = \sum_{\vec{\mu} \in D_m} S_{\vec{\mu}}(T) \tag{48b}$$

holds. Below we construct this series explicitly. Let

$$\vec{0} := \{0, \ldots, 0\}, \tag{49a}$$

$$\mathcal{K} := D_m \backslash \vec{0}. \tag{49b}$$

Since $\widehat{\sigma}_{\vec{0}}$ is the all-identity term, it is the term that causes no errors; its corresponding bounding series is $S_{\vec{0}}(T)$. On the other hand, every $\widehat{\sigma}_{\vec{\mu}}$ with $\vec{\mu} \in \mathcal{K}$ is an error term with corresponding bounding series $S_{\vec{\mu}}(T)$. For later use, we note that $S_{\vec{0}}(0) = 1$ and $S_{\vec{\mu}}(0) = 0$ for all $\vec{\mu} \in \mathcal{K}$.

In order to derive bounds we first recall that $U(T)$ from Eq. (25) is the solution of the Schrödinger equation

$$\partial_T U(T) = -iH(T)U(T) \tag{50a}$$

$$= -i\left[\sum_{\vec{\mu}\in D_m} f_{\vec{\mu}}(t/T)\widehat{\sigma}_{\vec{\mu}} B_{\vec{\mu}}\right] U(T) \tag{50b}$$

with $U(0) = \mathbb{1}$. Equation (50b) generates exactly all terms of the series of $U(T)$. Thus, in order to obtain the series for $S_{\rm N}(T)$ all we need to do is to replace $-i \to |-i| = 1$, $f_{\vec{\mu}} \to |f_{\vec{\mu}}| = 1$, $\widehat{\sigma}_{\vec{\mu}} \to \|\widehat{\sigma}_{\vec{\mu}}\| = 1$, and $B_{\vec{\mu}} \to \|B_{\vec{\mu}}\| = J_{\vec{\mu}}$ on the right-hand side. This provides us with the generating differential equation for the bounding series:

$$\partial_T S_{\rm N}(T) = \left[\sum_{\vec{\mu}\in D_m} J_{\vec{\mu}}\right] S_{\rm N}(T). \tag{51}$$

Its integration from $S_{\rm N}(0) = 1$ recovers the previous result (29) precisely.

In analogy, the differential equation for each $A_{\vec{\mu}}(T)$ reads

$$\partial_T A_{\vec{\mu}}(T) = -i\left[\sum_{\vec{\nu}\in D_m} f_{\vec{\mu}\oplus\vec{\nu}}(t/T) R_{\vec{\mu}\oplus\vec{\nu};\vec{\nu}} B_{\vec{\mu}\oplus\vec{\nu}}\right] A_{\vec{\nu}}(T), \tag{52}$$

where, as before, $\oplus$ stands for sums modulo 2. Note that addition and subtraction are equivalent modulo 2: $\vec{\mu} \oplus \vec{\nu} = \vec{\mu} \ominus \vec{\nu}$. It is essential that the sums modulo 2 in $\{(0,0),(1,0),(1,1),(0,1)\}$ faithfully reproduce the spin algebra of the identity and the Pauli matrices except for factors of $\pm i$, which are collected in $R_{\vec{\mu}\oplus\vec{\nu};\vec{\nu}}$. Replacement of operators by their norms and complex numbers by their moduli on the right-hand side yields the generating differential equation for the bounding series $S_{\vec{\mu}}$ satisfying Eq. (48a),

$$\partial_T S_{\vec{\mu}}(T) = \left[\sum_{\vec{\nu}\in D_m} J_{\vec{\mu}\oplus\vec{\nu}}\right] S_{\vec{\nu}}(T). \tag{53}$$

Unfortunately, the set of differential equations (53) is still too difficult to be solved generally. Hence we aim at a looser bound by defining

$$J_1 := \max_{\vec{\mu}\in\mathcal{K}} J_{\vec{\mu}}, \tag{54a}$$

$$\eta := \frac{J_1}{J_{\vec{0}}}, \tag{54b}$$

$$\varepsilon := J_{\vec{0}} T. \tag{54c}$$

If we substitute J_1 for each $J_{\vec{\mu}}$ with $\vec{\mu} \in \mathcal{K}$ we obtain one bounding series $S_1(T)$ for all $S_{\vec{\mu}}(T) = S_1(T)$. To see this we insert $S_1(T) = S_{\vec{\mu}}(T)$ on the right-hand side of Eq. (53), yielding

$$\partial_T S_{\vec{0}}(T) = J_{\vec{0}} S_{\vec{0}}(T) + \gamma J_1 S_1(T), \tag{55a}$$

$$\partial_T S_{\vec{\mu}}(T) = J_{\vec{0}} S_1(T) + J_1 S_{\vec{0}}(T) + (\gamma - 1) J_1 S_1(T), \tag{55b}$$

where $\vec{\mu} \in \mathcal{K}$ and $\gamma := 4^m - 1 = |\mathcal{K}|$ is the number of nonidentity terms. The first term on the right-hand side of (55a) results from $\vec{0} = \vec{0} \oplus \vec{0}$, the second from $\vec{\nu} = \vec{0} \oplus \vec{\nu}$ for $\vec{\nu} \in \mathcal{K}$. The first term on the right-hand side of (55b) results from $\vec{0} = \vec{\mu} \oplus \vec{\mu}$, the second from $\vec{\mu} = \vec{\mu} \oplus \vec{0}$, and the third from $\vec{\mu} \oplus \vec{\nu}$ where $\vec{\nu} \in \mathcal{K}\backslash\vec{\mu}$. There are $\gamma - 1$ terms of the latter kind, independent of $\vec{\mu}$. This independence implies the equality of all $S_{\vec{\mu}}(T)$ for $\vec{\mu} \in \mathcal{K}$ because they all start at the same value $S_{\vec{\mu}}(0) = 0$. Thus, replacing Eq. (55b), we have

$$\partial_T S_1(T) = J_{\vec{0}} S_1(T) + J_1 S_{\vec{0}}(T) + (\gamma - 1) J_1 S_1(T), \tag{56}$$

which, together with Eq. (55a), constitutes a two-dimensional set of linear differential equations. The two eigenvalues of the corresponding matrix are $\lambda_+ = J_{\vec{0}} + \gamma J_1$ and $\lambda_- = J_{\vec{0}} - J_1$ so that the general solution reads $S_1(T) := A\exp(\lambda_+ T) + B\exp(\lambda_- T)$ with coefficients A and B. The initial conditions $S_{\vec{0}}(0) = 1$ and $S_1(0) = 0$ imply $\partial_T S_1(0) = J_1$ from which A and B are determined, to yield

$$S_1(T) = \frac{\exp(J_{\vec{0}} T)}{\gamma + 1}[\exp(\gamma J_1 T) - \exp(-J_1 T)]. \tag{57}$$

The bounding series of the sum of all error terms is given by $S_{\mathcal{K}}(T) := \gamma S_1(T)$, which reads

$$S_{\mathcal{K}}(T) = \frac{\gamma \exp(J_{\vec{0}} T)}{\gamma + 1}[\exp(\gamma J_1 T) - \exp(-J_1 T)]. \tag{58}$$

This result is the bounding series for all error terms in NUDD.

We define

$$p_k := \frac{1}{k!}\frac{\partial^k}{\partial T^k} S_{\mathcal{K}}\bigg|_{T=0}, \tag{59a}$$

$$\Delta_N := \sum_{k=N+1}^{\infty} p_k T^k, \tag{59b}$$

and

$$d_{\min} := \min_{1\leqslant i\leqslant 2m}\{N_i'\} \tag{60}$$

is the decoupling order of the NUDD sequence [19]. Since $\|A_{\vec{\mu}}\| \leqslant S_{\vec{\mu}}(T)$, we have

$$\sum_{\vec{\mu}\in\mathcal{K}} \|A_{\vec{\mu}}\| \leqslant \sum_{\vec{\mu}\in\mathcal{K}} S_{\vec{\mu}}(T) \leqslant S_{\mathcal{K}}(T), \tag{61}$$

and hence

$$\sum_{\vec{\mu}\in\mathcal{K}} \|A_{\vec{\mu}}\| \leqslant \Delta_{d_{\min}}. \tag{62}$$

By Taylor-expanding Eq. (58) we can write $S_{\mathcal{K}}(T)$ and thus Δ_d as an infinite series in terms of ε and η of Eqs. (54c) and (54b). We do not write the result explicitly, but the formula (58) for $S_{\mathcal{K}}(T)$ is simple enough to allow the bounds to be computed easily with any computer algebra program. This is our first key result for the NUDD sequence.

To leading order in ε, we find

$$\Delta_d = g_{d+1}(\eta,m)\varepsilon^{d+1} + O(\varepsilon^{d+2}), \tag{63}$$

where

$$g_l(\eta,m) := (1 - 4^{-m})\frac{(1 - \eta + 4^m\eta)^l - (1-\eta)^l}{l!}. \tag{64}$$

In Fig. 5 we include plots of $\Delta_{d_{\min}}$ as a function of ε for various values of $d_{\min}$ and η. We can see that, as expected, the behavior of $\Delta_{d_{\min}}$ is similar to that of L_α in the QDD case.

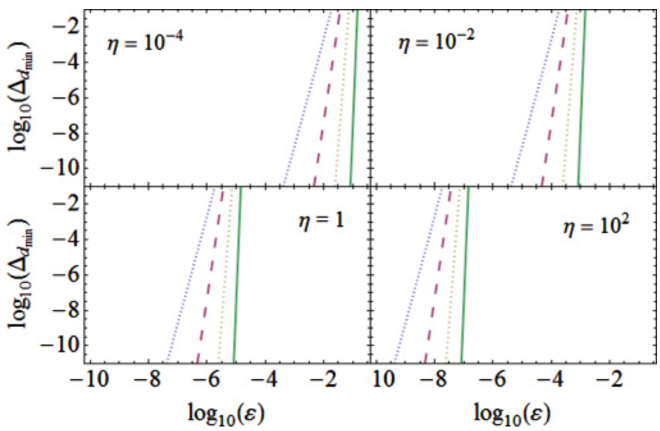

FIG. 5. (Color online) The upper bound $\Delta_{d_{\min}}$ for $\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\|$ as a function of ε for various pulse numbers $d_{\min}\in\{5,10,20,40\}$, at fixed values of η, and for $m=10$. In each panel the curves become steeper as $d_{\min}$ increases.

IV. DISTANCE BOUND

A. QDD

Next, we shall use the bounds on the bath operators A_x, A_y, and A_z to derive a bound on the trace-norm distance

$$D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big]=\frac{1}{2}\big\|\rho_{\rm S}(T)-\rho_{\rm S}^0(T)\big\|_1 \qquad (65)$$

between the actual qubit state

$$\rho_{\rm S}(T):={\rm tr}_{\rm B}[\rho_{\rm SB}(T)] \qquad (66)$$

and the "error-free" qubit state

$$\rho_{\rm S}^0(T):={\rm tr}_{\rm B}\big[\rho_{\rm SB}^0(T)\big], \qquad (67)$$

where $\rho_{\rm SB}^0(T)$ is the time-evolved state of the whole qubit-bath system without coupling between the qubit and the bath, and ${\rm tr}_{\rm B}$ denotes the partial trace over the bath degrees of freedom. The trace norm $\|A\|_1$ is the trace of $(A^\dagger A)^{1/2}$. The trace-norm distance D is the standard distance measure between density matrices [1]. The method we employ here is similar to the one in Ref. [14]. We consider an initial state

$$\rho_{\rm SB}^0(0)=|\psi\rangle\langle\psi|\otimes\rho_{\rm B} \qquad (68)$$

in which the qubit is in a pure state $|\psi\rangle$ and the bath is in an arbitrary state $\rho_{\rm B}$ (e.g., a mixed thermal equilibrium state). The initial state evolves to $\rho_{\rm SB}(T)=U(T)\rho_{\rm SB}^0(0)U^\dagger(T)$ when the qubit and the bath are coupled, or to $\rho_{\rm SB}^0(T)=[\mathbb{1}_{\rm S}\otimes U_{\rm B}(T)]\rho_{\rm SB}^0(0)[\mathbb{1}_{\rm S}\otimes U_{\rm B}^\dagger(T)]$ when the qubit is isolated from its environment. The unitary bath time-evolution operator without coupling reads

$$U_{\rm B}(T):=\exp(-iTB_0) \qquad (69)$$

where B_0 is the bath term in Eq. (5).

Let us first define the bath correlation functions

$$b_{\alpha\beta}(T):={\rm tr}[A_\alpha(T)\rho_{\rm B}A_\beta^\dagger(T)], \qquad (70)$$

where $\alpha,\beta\in\{0,x,y,z\}$. To simplify the notation, we will omit the time dependence T in $b_{\alpha\beta}(T)$ and $A_\alpha(T)$ from now on. Computation yields (see Appendix B 1)

$$D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big]\leqslant\frac{1}{2}|b_{xx}+b_{yy}+b_{zz}| +\frac{1}{2}\left(\sum_{\alpha,\beta\in\{0,x,y,z\}}|b_{\alpha\beta}|-|b_{00}|\right). \qquad (71)$$

We know from the unitarity of U and Eq. (30) that

$$\begin{aligned}\mathbb{1}&=U^\dagger(T)U(T)\\&=\mathbb{1}_{\rm S}\otimes\sum_{\alpha\in\{0,x,y,z\}}A_\alpha^\dagger A_\alpha\\&\quad+\sum_{\alpha\in\{x,y,z\}}\sigma_\alpha\otimes(A_\alpha^\dagger A_0+A_0^\dagger A_\alpha+i[A_\beta^\dagger,A_\gamma]),\end{aligned} \qquad (72)$$

where in the last sum $\{\beta,\gamma\}$ are adjusted to α so that $\{\alpha,\beta,\gamma\}$ is a cyclic permutation of $\{x,y,z\}$. Therefore we have

$$\mathbb{1}=A_0^\dagger A_0+A_x^\dagger A_x+A_y^\dagger A_y+A_z^\dagger A_z, \qquad (73a)$$
$$0=A_x^\dagger A_0+A_0^\dagger A_x+iA_y^\dagger A_z-iA_z^\dagger A_y, \qquad (73b)$$
$$0=A_y^\dagger A_0+A_0^\dagger A_y+iA_z^\dagger A_x-iA_x^\dagger A_z, \qquad (73c)$$
$$0=A_z^\dagger A_0+A_0^\dagger A_z+iA_x^\dagger A_y-iA_y^\dagger A_x. \qquad (73d)$$

It follows from Eq. (73a) that $\langle i|\sum_{\alpha\in\{0,x,y,z\}}A_\alpha^\dagger A_\alpha|i\rangle=1$ for all normalized states $|i\rangle$, and thus

$$\langle i|A_0^\dagger A_0|i\rangle=\|A_0|i\rangle\|^2\leqslant 1 \qquad (74)$$

because $\langle i|\sum_{\alpha\in\{x,y,z\}}A_\alpha^\dagger A_\alpha|i\rangle=\sum_{\alpha\in\{x,y,z\}}\|A_\alpha|i\rangle\|^2$ is nonnegative. In particular, we know that

$$\|A_0\|\leqslant 1. \qquad (75)$$

To obtain a bound on the functions $b_{\alpha\beta}$ we use the following general correlation function inequality (see Ref. [14] for a proof):

$$|{\rm tr}[Q\rho_{\rm B}Q']|\leqslant\|Q\|\|Q'\|, \qquad (76)$$

which holds for arbitrary bounded bath operators Q,Q'. Use of Eq. (75), Eq. (76), and the bounds (43) in Eq. (71) yields

$$\begin{aligned}&D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big]\\&\leqslant\|A_x\|+\|A_y\|+\|A_z\|+\|A_x\|^2+\|A_y\|^2+\|A_z\|^2\\&\quad+\|A_x\|\|A_y\|+\|A_y\|\|A_z\|+\|A_x\|\|A_z\| &(77a)\\&\leqslant L_x+L_y+L_z+L_x^2+L_y^2+L_z^2+L_xL_y+L_yL_z\\&\quad+L_xL_z &(77b)\\&=\Delta_{d_x}^{(3)}+\Delta_{d_x}^{(4)}+\Delta_{d_y}^{(2)}+\Delta_{d_y}^{(5)}+\Delta_{d_z}^{(1)}+\Delta_{d_z}^{(6)}\\&\quad+\big(\Delta_{d_x}^{(3)}\big)^2+\big(\Delta_{d_x}^{(4)}\big)^2+\big(\Delta_{d_y}^{(2)}\big)^2+\big(\Delta_{d_y}^{(5)}\big)^2+\big(\Delta_{d_z}^{(1)}\big)^2\\&\quad+\big(\Delta_{d_z}^{(6)}\big)^2+2\Delta_{d_x}^{(3)}\Delta_{d_x}^{(4)}+2\Delta_{d_y}^{(2)}\Delta_{d_y}^{(5)}+2\Delta_{d_z}^{(1)}\Delta_{d_z}^{(6)}\\&\quad+\Delta_{d_x}^{(3)}\Delta_{d_y}^{(2)}+\Delta_{d_x}^{(3)}\Delta_{d_y}^{(5)}+\Delta_{d_x}^{(4)}\Delta_{d_y}^{(2)}+\Delta_{d_x}^{(4)}\Delta_{d_y}^{(5)}\\&\quad+\Delta_{d_y}^{(2)}\Delta_{d_z}^{(1)}+\Delta_{d_y}^{(2)}\Delta_{d_z}^{(6)}+\Delta_{d_y}^{(5)}\Delta_{d_z}^{(1)}+\Delta_{d_y}^{(5)}\Delta_{d_z}^{(6)}\\&\quad+\Delta_{d_x}^{(3)}\Delta_{d_z}^{(1)}+\Delta_{d_x}^{(3)}\Delta_{d_z}^{(6)}+\Delta_{d_x}^{(4)}\Delta_{d_z}^{(1)}+\Delta_{d_x}^{(4)}\Delta_{d_z}^{(6)}. &(77c)\end{aligned}$$

This is the rigorous bound on the trace-norm distance and hence our second key result for QDD.

Using Eq. (46b), one can rewrite this bound in terms of ε and $\vec{\eta}$; we do not write this out here for brevity.

In explicit calculations the leading order in ε will dominate for $\varepsilon \to 0$. Then only the first line in Eq. (77c) plays a role, since all other terms are of higher order. Hence we have

$$\begin{aligned} D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \leqslant{}& \big[g^{(3)}_{d_x+1}(\vec{\eta}) + g^{(4)}_{d_x+1}(\vec{\eta})\big]\varepsilon^{d_x+1} \\ &+\big[g^{(2)}_{d_y+1}(\vec{\eta}) + g^{(5)}_{d_y+1}(\vec{\eta})\big]\varepsilon^{d_y+1} \\ &+\big[g^{(1)}_{d_z+1}(\vec{\eta}) + g^{(6)}_{d_z+1}(\vec{\eta})\big]\varepsilon^{d_z+1} \\ &+O\big(\varepsilon^{\min_{\alpha\in\{x,y,z\}}\{d_\alpha\}+2}\big). \end{aligned} \tag{78}$$

Equation (78) is our third key QDD result. It shows that the QDD bound is dominated by the channel with the smallest decoupling order d_α, as was expected intuitively.

B. NUDD

We consider an initial state

$$\rho_{\rm SB}^0(0) = |\psi\rangle\langle\psi| \otimes \rho_{\rm B}, \tag{79}$$

where $|\psi\rangle$ is the state of the m-qubit system. The initial state evolves to $\rho_{\rm SB}(T) = U(T)\rho_{\rm SB}^0(0)U^\dagger(T)$ when the qubit and the bath are coupled, or to $\rho_{\rm SB}^0(T) = [\mathbb{1}_{\rm S} \otimes U_{\rm B}(T)]\rho_{\rm SB}^0(0)[\mathbb{1}_{\rm S} \otimes U_{\rm B}^\dagger(T)]$ when the qubit is isolated from its environment. The unitary bath time-evolution operator without coupling reads

$$U_{\rm B}(T) := \exp(-iTB_{\vec{0}}), \tag{80}$$

where $B_{\vec{0}}$ is the bath operator that corresponds to the identity system operator. We know from the unitarity of $U(T)$ and Eq. (47) that

$$\sum_{\vec{\mu}\in D_m} A_{\vec{\mu}}^\dagger A_{\vec{\mu}} = \mathbb{1}. \tag{81}$$

Following the same steps as in the QDD case yields

$$\|A_{\vec{0}}\| \leqslant 1. \tag{82}$$

Explicit computation (see Appendix B2) as in the QDD case shows that

$$D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \leqslant \Bigg(\sum_{\vec{\mu}\in\mathcal{K}} \|A_{\vec{\mu}}\|\Bigg)^2 + \|A_{\vec{0}}\| \sum_{\vec{\mu}\in\mathcal{K}} \|A_{\vec{\mu}}\|. \tag{83}$$

We use the bounds on the operators $A_{\vec{\mu}}$ to derive a bound on the trace-norm distance between $\rho_{\rm SB}(T)$ and $\rho_{\rm SB}^0(T)$. Substituting Eqs. (62) and (82) into Eq. (83), we conclude that

$$D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \leqslant \Delta_{d_{\min}}^2 + \Delta_{d_{\min}}, \tag{84}$$

where $\Delta_{d_{\min}}$ is the bound presented in Eq. (59b). The bound is dominated by $\Delta_{d_{\min}}$ which is the leading-order term for $\varepsilon \to 0$. By expanding $\Delta_{d_{\min}}$ we find for the leading-order term

$$D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \leqslant g_{d_{\min}+1}(\eta,m)\varepsilon^{d_{\min}+1} + O\big(\varepsilon^{d_{\min}+2}\big). \tag{85}$$

Equation (85) is our second key result for NUDD.

V. CONCLUSIONS

We have derived and presented rigorous performance bounds for the QDD and NUDD sequences, respectively. These sequences, which build on the UDD sequence, protect a qubit or system of qubits from general decoherence, under the assumptions that the pulses are instantaneous and the bath operators are bounded in operator norm. Our key bounds are given in Eq. (77c) for QDD and in Eq. (84) for NUDD. The leading-order terms are identified in Eq. (78) (for QDD) and Eq. (85) (for NUDD). These results show that, if the total sequence time is fixed, we can make the error $D[\rho_{\rm S}(T),\rho_{\rm S}^0(T)]$ arbitrarily small by increasing the number of pulses at each UDD level comprising the QDD or NUDD sequences.

When instead the minimum pulse interval is fixed, we expect that, just as in the case of UDD [14], there will be an optimal sequence order, beyond which performance starts to decrease. A rigorous study of this aspect of QDD and NUDD is an interesting topic for a future investigation. We hope that the results presented here will inspire experimental tests of the QDD and NUDD sequences in physical systems with bath spectral densities exhibiting relatively hard high-frequency cutoffs, a condition which corresponds to our key assumptions [Eqs. (6) and (17)] of bounded bath operators.

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APPENDIX A: BOUNDING POLYNOMIALS

The polynomials that appear in the Taylor expansions of the bounding functions $S_j(\varepsilon,\vec{\eta})$ are

$$\begin{aligned} g_l^{(1)}(\vec{\eta}) = \frac{1}{8l!}&[(1+\eta_x+\eta_y+\eta_z)^l + (1-\eta_x+\eta_y+\eta_z)^l \\ &+(1+\eta_x-\eta_y+\eta_z)^l + (1-\eta_x-\eta_y+\eta_z)^l \\ &-(1+\eta_x+\eta_y-\eta_z)^l - (1-\eta_x+\eta_y-\eta_z)^l \\ &-(1+\eta_x-\eta_y-\eta_z)^l - (1-\eta_x-\eta_y-\eta_z)^l], \end{aligned} \tag{A1}$$

$$\begin{aligned} g_l^{(2)}(\vec{\eta}) = \frac{1}{8l!}&[(1+\eta_x+\eta_y+\eta_z)^l + (1-\eta_x+\eta_y+\eta_z)^l \\ &-(1+\eta_x-\eta_y+\eta_z)^l - (1-\eta_x-\eta_y+\eta_z)^l \\ &+(1+\eta_x+\eta_y-\eta_z)^l + (1-\eta_x+\eta_y-\eta_z)^l \\ &-(1+\eta_x-\eta_y-\eta_z)^l - (1-\eta_x-\eta_y-\eta_z)^l], \end{aligned} \tag{A2}$$

$$g_l^{(3)}(\vec{\eta}) = \frac{1}{8l!}[(1+\eta_x+\eta_y+\eta_z)^l + (1-\eta_x+\eta_y+\eta_z)^l - (1+\eta_x-\eta_y+\eta_z)^l - (1-\eta_x-\eta_y+\eta_z)^l - (1+\eta_x+\eta_y-\eta_z)^l - (1-\eta_x+\eta_y-\eta_z)^l + (1+\eta_x-\eta_y-\eta_z)^l + (1-\eta_x-\eta_y-\eta_z)^l], \tag{A3}$$

$$g_l^{(4)}(\vec{\eta}) = \frac{1}{8l!}[(1+\eta_x+\eta_y+\eta_z)^l - (1-\eta_x+\eta_y+\eta_z)^l + (1+\eta_x-\eta_y+\eta_z)^l - (1-\eta_x-\eta_y+\eta_z)^l + (1+\eta_x+\eta_y-\eta_z)^l - (1-\eta_x+\eta_y-\eta_z)^l + (1+\eta_x-\eta_y-\eta_z)^l - (1-\eta_x-\eta_y-\eta_z)^l], \tag{A4}$$

$$g_l^{(5)}(\vec{\eta}) = \frac{1}{8l!}[(1+\eta_x+\eta_y+\eta_z)^l - (1-\eta_x+\eta_y+\eta_z)^l + (1+\eta_x-\eta_y+\eta_z)^l - (1-\eta_x-\eta_y+\eta_z)^l - (1+\eta_x+\eta_y-\eta_z)^l + (1-\eta_x+\eta_y-\eta_z)^l - (1+\eta_x-\eta_y-\eta_z)^l + (1-\eta_x-\eta_y-\eta_z)^l], \tag{A5}$$

$$g_l^{(6)}(\vec{\eta}) = \frac{1}{8l!}[(1+\eta_x+\eta_y+\eta_z)^l - (1-\eta_x+\eta_y+\eta_z)^l - (1+\eta_x-\eta_y+\eta_z)^l + (1-\eta_x-\eta_y+\eta_z)^l + (1+\eta_x+\eta_y-\eta_z)^l - (1-\eta_x+\eta_y-\eta_z)^l - (1+\eta_x-\eta_y-\eta_z)^l + (1-\eta_x-\eta_y-\eta_z)^l]. \tag{A6}$$

APPENDIX B: DISTANCE BOUND CALCULATION

1. QDD

In this appendix we prove the bound on the trace-norm distance in Eq. (71). To simplify the notation, we let

$$P_0 := |\psi\rangle\langle\psi|. \tag{B1}$$

Then

$$\begin{aligned} &2D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \\ &= \big\|{\rm tr}_{\rm B}\big[\rho_{\rm SB}(T)-\rho_{\rm SB}^0(T)\big]\big\|_1 \\ &= \big\|{\rm tr}_{\rm B}\big[U(T)\rho_{\rm SB}^0(0)U^\dagger(T)\big]-{\rm tr}_{\rm B}\big[\rho_{\rm SB}^0(0)\big]\big\|_1 \\ &= \left\|{\rm tr}_{\rm B}\left\{\left[\sum_{\alpha\in\{0,x,y,z\}}\sigma_\alpha\otimes A_\alpha\right](P_0\otimes\rho_{\rm B})\left[\sum_{\alpha\in\{0,x,y,z\}}\sigma_\alpha\otimes A_\alpha^\dagger\right]\right\}-P_0\right\|_1 \\ &= \|(b_{00}-1)P_0+b_{0x}P_0\sigma_x+b_{0y}P_0\sigma_y \\ &\quad +b_{0z}P_0\sigma_z+b_{x0}\sigma_xP_0+b_{xx}\sigma_xP_0\sigma_x \\ &\quad +b_{xy}\sigma_xP_0\sigma_y+b_{xz}\sigma_xP_0\sigma_z+b_{y0}\sigma_yP_0 \\ &\quad +b_{yx}\sigma_yP_0\sigma_x+b_{yy}\sigma_yP_0\sigma_y+b_{yz}\sigma_yP_0\sigma_z \\ &\quad +b_{z0}\sigma_zP_0+b_{zx}\sigma_zP_0\sigma_x+b_{zy}\sigma_zP_0\sigma_y \\ &\quad +b_{zz}\sigma_zP_0\sigma_z\|_1 \end{aligned} \tag{B2a}$$

$$\begin{aligned} &\leqslant |b_{00}-1|+|b_{0x}|+|b_{0y}|+|b_{0z}| \\ &\quad +|b_{x0}|+|b_{xx}|+|b_{xy}|+|b_{xz}| \\ &\quad +|b_{y0}|+|b_{yx}|+|b_{yy}|+|b_{yz}| \\ &\quad +|b_{z0}|+|b_{zx}|+|b_{zy}|+|b_{zz}|. \end{aligned} \tag{B2b}$$

In going from Eq. (B2a) to Eq. (B2b), we used the triangle inequality, the unitary invariance of the trace norm, and the normalization of $|\psi\rangle$.

We require one last result:

$$\begin{aligned} &|b_{00}-1| \\ &= |{\rm tr}[A_0\rho_{\rm B}A_0^\dagger]-1| \\ &= |{\rm tr}[A_0^\dagger A_0\rho_{\rm B}]-1| \\ &= |{\rm tr}\{[\mathbb{1}-A_x^\dagger A_x-A_y^\dagger A_y-A_z^\dagger A_z]\rho_{\rm B}\}-1| \\ &= |{\rm tr}[\rho_{\rm B}]-{\rm tr}[A_x\rho_{\rm B}A_x^\dagger]-{\rm tr}[A_y\rho_{\rm B}A_y^\dagger]-{\rm tr}[A_z\rho_{\rm B}A_z^\dagger]-1| \\ &= |b_{xx}+b_{yy}+b_{zz}|, \end{aligned} \tag{B3}$$

where we used cyclic invariance of the trace in $b_{\alpha\beta}$ together with Eq. (73a) and the normalization ${\rm tr}[\rho_{\rm B}]=1$. Equation (71) now follows immediately from the triangle inequality.

2. NUDD

Here we prove Eq. (83) following the same steps as in the QDD case:

$$\begin{aligned} &2D\big[\rho_{\rm S}(T),\rho_{\rm S}^0(T)\big] \\ &= \big\|{\rm tr}_{\rm B}\big[\rho_{\rm SB}(T)-\rho_{\rm SB}^0(T)\big]\big\|_1 \\ &= \big\|{\rm tr}_{\rm B}\big[U(T)\rho_{\rm SB}^0(0)U^\dagger(T)\big]-{\rm tr}_{\rm B}\big[\rho_{\rm SB}^0(0)\big]\big\|_1 \\ &= \left\|{\rm tr}_{\rm B}\left\{\left[\sum_{\vec{\mu}\in\{0,1\}^{2m}}\sigma_{\vec{\mu}}A_{\vec{\mu}}\right](P_0\otimes\rho_{\rm B})\left[\sum_{\vec{\mu}\in\{0,1\}^{2m}}\sigma_{\vec{\mu}}A_{\vec{\mu}}^\dagger\right]\right\}-P_0\right\|_1 \\ &= \left\|\sum_{\vec{\mu}\in\{0,1\}^{2m}}\sum_{\vec{\nu}\in\{0,1\}^{2m}}{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{\nu}})\sigma_{\vec{\mu}}P_0\sigma_{\vec{\nu}}-P_0\right\|_1 \\ &\leqslant |{\rm tr}(A_{\vec{0}}^\dagger\rho_{\rm B}A_{\vec{0}})-1|+\sum_{\vec{\mu}\in\mathcal{K}}\sum_{\vec{\nu}\in\mathcal{K}}|{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{\nu}})| \\ &\quad +\sum_{\vec{\mu}\in\mathcal{K}}|{\rm tr}(A_{\vec{0}}^\dagger\rho_{\rm B}A_{\vec{\mu}})|+\sum_{\vec{\mu}\in\mathcal{K}}|{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{0}})| \\ &\leqslant \sum_{\vec{\mu}\in\mathcal{K}}|{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{\mu}})|+\sum_{\vec{\mu}\in\mathcal{K}}\sum_{\vec{\nu}\in\mathcal{K}}|{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{\nu}})| \\ &\quad +\sum_{\vec{\mu}\in\mathcal{K}}|{\rm tr}(A_{\vec{0}}^\dagger\rho_{\rm B}A_{\vec{\mu}})|+\sum_{\vec{\mu}\in\mathcal{K}}|{\rm tr}(A_{\vec{\mu}}^\dagger\rho_{\rm B}A_{\vec{0}})| \end{aligned}$$

$$\leqslant \left(\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\|\right)^2+\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\|^2+2\|A_{\vec{0}}\|\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\| \tag{B4a}$$

$$\leqslant 2\left(\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\|\right)^2+2\|A_{\vec{0}}\|\sum_{\vec{\mu}\in\mathcal{K}}\|A_{\vec{\mu}}\|. \tag{B4b}$$

In the derivation we used the unitary invariance of the trace norm, triangle inequality, the normalization of $|\psi\rangle$, Eq. (76), and Eq. (81). The step from inequality (B4a) to (B4b) is not necessary, but loosens the bound for the sake of simplicity of the result.

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