

Rigorous bounds on the performance of a hybrid dynamical-decoupling quantum-computing scheme

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We study dynamical decoupling in a multiqubit setting, where it is combined with quantum logic gates. This is illustrated in terms of computation using Heisenberg interactions only, where global decoupling pulses commute with the computation. We derive a rigorous error bound on the trace distance or fidelity between the desired computational state and the actual time-evolved state, for a system subject to coupling to a bounded-strength bath. The bound is expressed in terms of the operator norm of the effective Hamiltonian generating the evolution in the presence of decoupling and logic operations. We apply the bound to the case of periodic pulse sequences and find that in order to maintain a constant trace distance or fidelity, the number of cycles—at fixed pulse interval and width—should scale in inverse proportion to the square of the number of qubits. This sets a scalability limit on the protection of quantum computation using periodic dynamical decoupling.

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I. INTRODUCTION

Quantum-information processing harbors enormous unleashed potential in the form of efficient algorithms for classically intractable tasks [1]. Perhaps the largest hurdle on the way to a realization of this potential is the problem of decoherence, which results when a quantum system, such as a quantum computer, interacts with an uncontrollable environment [2]. Decoherence reduces the information processing capabilities of quantum computers to the point where they can be efficiently simulated on a classical computer [3]. In spite of dramatic progress in the form of a theory of fault tolerant quantum error correction (e.g., [4]), finding methods for overcoming decoherence that are both efficient and practical remains an important challenge. An alternative to quantum error correction (QEC) that is substantially less resource intensive is dynamical decoupling (DD) [5]. This method does not require feedback or the exponential growth in the number of qubits typical of fault tolerant (concatenated) QEC. In DD one applies a succession of short pulses to the system, designed to decouple it from the environment. This can substantially slow down decoherence, though not halt it completely, in contrast to the promises of fault-tolerant QEC. While initially the general theory of DD was developed under the assumption of highly idealized (essentially infinitely fast and strong) pulses [6–8], subsequent work relaxed these assumptions, showing that DD can still be beneficial in the presence of bounded strength controls [9]. In the simplest possible DD protocol, known as “periodic DD” (PDD), one applies a certain predetermined sequence over and over again. While this protocol typically does not work as well as random [10–12], recursive-deterministic [13], or hybrid schemes [14] when finite pulse intervals and pulse width are accounted for, it has the advantage of simplicity. In this work

our purpose is to present a rigorous analysis of DD, and in particular to derive error bounds on its performance in the periodic (PDD) setting.

With a few exceptions that belong to the realm of idealized pulses [15–18] or to the paradigm of adiabatic quantum computing [19], DD studies have focused on preserving quantum information (memory), rather than processing it (computation). In order to combine computation with DD, Ref. [15] introduced three strategies: The first strategy requires applying the computational operations “stroboscopically,” i.e., at the end of each decoupling cycle, where the system is momentarily decoherence free. This is conceptually similar to computation over error-correcting codes, where a computational gate is applied at the end of an error-correction cycle [20]. The disadvantage of this “stroboscopic” approach is that, in reality, the computational operations take a finite time to implement, so that the system decoheres while a computational gate is being applied to it. The second strategy is to alternate and modulate the control Hamiltonian used to implement quantum computation, in which the net overall effect of the DD operations still allows a desired unitary operation on the system, along with the correction of errors. The third strategy proposed in Ref. [15] is to use DD pulses that commute with the computational operations, so that the two can be executed simultaneously. Here we address the problem of circuit-model quantum computation [1] using DD with realistic pulse assumptions. We combine DD with computation via the use of codes and universality results arising from the theory of decoherence-free subspaces and subsystems (DFSs) [21–23]. Our method is conceptually related to a hybrid version of the second and third strategies of Ref. [15], in that we impose the commutation condition between the DD pulses and the computational Hamiltonian, but we find that improved performance is

obtained if the DD and computational operations simply alternate. Thus, in our scheme the computational gate is “spread” over an entire DD cycle (or, conversely, the DD cycle is spread over the computational gate). We fully incorporate finite pulse intervals and pulse widths and assess the performance of our scheme in the PDD setting. We find a rigorous error bound, from which it follows that for a fixed error the number of DD cycles cannot scale faster than the inverse square of the system size (at fixed pulse width and pulse interval). This means that there is a tradeoff between the length of time over which decoherence errors can be suppressed using PDD, and the scalability of a quantum computation it is meant to protect.

The structure of this paper is as follows. We define the model in Sec. II. We provide background on dynamical decoupling in Sec. III, where we also derive the effective Hamiltonian describing the evolution under the action of decoupling and computation. This leads to the “error phase,” namely the effective Hamiltonian times time (a type of action), which is the quantity we wish to minimize. In Sec. IV we derive rigorous error bounds that relate the error between the desired and actual final state to the norm of the error phase. In Sec. V we estimate the error associated with the decoupled evolution (i.e., the evolution in the presence of a DD pulse sequence), relative to the decoherence-free evolution (no system-bath coupling). Section VI is where we derive our key result: We apply the idea of encoded operations and dynamical decoupling to PDD, and compute the error bound. In Sec. VII we illustrate our construction with encoded DD computation in a quantum dots setting, where computation is implemented via Heisenberg interactions. We conclude with a discussion of our results in Sec. VIII. Extensive background material is presented in the appendices.

II. MODEL

We express the total Hamiltonian for system plus bath in the form

$$H(t) = H_{\text{ctrl}}(t) \otimes I_B + H_{\text{err}} + I_S \otimes H_B, \quad (1)$$

where I is the identity operator, H_{ctrl} acts on the system only and serves to implement (encoded) control operations such as logic gates, H_{err} is the “error” Hamiltonian (system-bath couplings plus undesired interactions among system qubits that do not commute with H_{ctrl}), and H_B is the pure-bath Hamiltonian. Let U_{ctrl} be the (encoded) logic gate generated by switching on H_{ctrl} for duration T , in the absence of the bath and any undesired interactions within the system,

$$U_{\text{ctrl}}(T) = \mathcal{T} \exp\left(-i \int_0^T H_{\text{ctrl}}(t) dt\right) = \exp(-i\theta R), \quad (2)$$

where \mathcal{T} denotes time ordering, R is a dimensionless logic operator, and θ is the angle of rotation around this operator. However, due to the presence of the undesired H_{err} and H_B terms, we will in fact obtain the following unitary acting on the joint system and bath Hilbert space:

$$U_{\text{bare}}(T) = \mathcal{T} \exp\left(-i \int_0^T [H_{\text{ctrl}}(t) \otimes I_B + H_{\text{err}} + I_S \otimes H_B] dt\right), \quad (3)$$

This is the essence of the problem of any quantum control procedure, whether it be for quantum-information processing or other purposes: U_{bare} entangles system and bath and implements a transformation on the system that can be very different from the desired U_{ctrl} . Our goal in this work is to show how to modify U_{bare} so that the distance between a state evolving under it and a state evolving under U_{ctrl} can be made arbitrarily small. This will be done by adding another Hamiltonian to the system, which implements DD operations, and is designed to effectively cancel H_{err} without interfering with H_{ctrl} .

III. DYNAMICAL-DECOUPLING BACKGROUND AND THE ERROR PHASE

A. Dynamical decoupling defined

We assume that the decoupling operations are realized as pulses P_i by switching on (and off) a time-dependent Hamiltonian $H_{\text{DD}}(t)$. The essential condition that will ensure that the decoupling pulses interfere minimally with the control operations is

$$[H_{\text{DD}}(t), H_{\text{ctrl}}(t')] = 0 \quad \forall t, t'. \quad (4)$$

The total propagator is now generated by the time-dependent total Hamiltonian

$$H_{\text{tot}}(t) = H_{\text{DD}}(t) + H_{\text{ctrl}}(t) + H_{\text{err}} + H_B, \quad (5)$$

i.e.,

$$U(T) = \mathcal{T} \exp\left(-i \int_0^T H_{\text{tot}}(t) dt\right). \quad (6)$$

Notice that the total Hamiltonian includes the control, DD, and bare Hamiltonians. The pulses are applied at times $\{t_j + \tau_{j=0}^{N-1}\}$ given by

$$t_j = j(\tau + \delta), \quad (7)$$

where τ is the pulse interval and δ is the pulse width. From here on we assume for simplicity that $H_{\text{DD}}(t)$ is piecewise constant (thus we are performing a worst-case analysis, our conclusions can only be improved by pulse shaping [24,25]),

$$H_{\text{DD}}(t) = \begin{cases} 0, & t_j \leq t < t_{j+1} - \delta, \\ H_P^{(j+1)}, & t_{j+1} - \delta \leq t < t_{j+1}, \end{cases} \quad (8)$$

$$j \in \{0, \dots, N-1\}.$$

Let

$$T = t_N = N(\tau + \delta) \quad (9)$$

denote the time it takes to complete one DD cycle, consisting of N pulses generated by the H_P^j ,

$$P_j = \exp(-iH_P^j \delta), \quad j = 1, \dots, N. \quad (10)$$

The commutation condition (4) becomes

$$[H_P^{(j)}, H_{\text{ctrl}}(t)] = [P_j, H_{\text{ctrl}}(t)] = 0 \quad \forall j. \quad (11)$$

This will allow us to import many of the results of the control-free scenario, i.e., when $H_{\text{ctrl}}(t)=0$. For the remainder of this section we review this setting, and return to the question of how to ensure the commutation condition in Sec. VII.

Denoting a free evolution period (when $H_{\text{DD}}=0$) of duration τ by

$$f_\tau = \exp[-i\tau(H_{\text{err}} + H_B)], \quad (12)$$

a single cycle can be written as

$$\begin{aligned} & P_N f_\tau P_{N-1} f_\tau P_{N-2} \cdots P_1 f_\tau \\ &= P_N f_\tau (P_N^\dagger P_N) P_{N-1} f_\tau [(P_N P_{N-1})^\dagger (P_N P_{N-1})] P_{N-2} \cdots P_1 f_\tau \\ &= (D_N f_\tau D_N^\dagger) (D_{N-1} f_\tau D_{N-1}^\dagger) D_{N-2} \cdots D_1 f_\tau D_1^\dagger \\ &\equiv e^{-iT H_{\text{eff}}(T)}, \end{aligned} \quad (13)$$

where the unitary ‘‘decoupling group’’ [6] $\mathcal{G} = \{D_j\}_{j=1}^N$ has elements defined as

$$D_j \equiv P_N \cdots P_j, \quad D_1 \equiv I_S, \quad (14)$$

where the condition $D_1 \equiv I_S$ is imposed because of the appearance of D_1^\dagger in Eq. (13); this imposes a relation among the pulse Hamiltonians $H_P^{(j)}$ via Eq. (10). Note that this is only possible in the zero width limit, since such a relation cannot be satisfied when the system-bath and bath Hamiltonians are present during the pulse.

The effective Hamiltonian $H_{\text{eff}}(T)$ can be approximated using the Magnus expansion [26] (see also Appendix A). To first order in the Magnus expansion

$$\begin{aligned} H_{\text{eff}}(T) &\equiv H_{\text{eff}}^{[1]}(T) + H_{\text{eff}}^{[2+]}, \\ H_{\text{eff}}^{[1]}(T) &\equiv \sum_{j=1}^N D_j (H_{\text{err}} + H_B) D_j^\dagger = \Pi_{\mathcal{G}}(H_{\text{err}}) + N H_B, \\ \|H_{\text{eff}}^{[2+]}\| &= O(T \|H_{\text{err}} + H_B\|^2). \end{aligned} \quad (15)$$

This can be viewed as a projection

$$\Pi_{\mathcal{G}}(H_{\text{err}}) \equiv \sum_{j=1}^N D_j H_{\text{err}} D_j^\dagger \quad (16)$$

into the centralizer $Z(\mathcal{G}) \equiv \{V | [V, D_j] = 0, \forall D_j \in \mathcal{G}\}$. Indeed, since $[H_B, D_j] = 0$ for all j ,

$$\begin{aligned} D_k^\dagger [H_{\text{eff}}^{[1]}, D_k] &= D_k^\dagger \sum_{j=1}^N (D_j H_{\text{err}} D_j^\dagger + H_B, D_k) \\ &= \sum_{j=1}^N (D_k^\dagger D_j) H_{\text{err}} (D_k^\dagger D_j)^\dagger - D_j H_{\text{err}} D_j^\dagger = 0 \\ &\Rightarrow [H_{\text{eff}}^{[1]}, D_k] = 0 \quad \forall k, \end{aligned} \quad (17)$$

where in the last equality we used the group closure property, $\forall k, j \exists i$ such that $D_k^\dagger D_j = D_i$. For a unitary irreducible representation of \mathcal{G} this immediately implies, by Schur’s lemma,

that $H_{\text{eff}}^{[1]} = c I_S \otimes H_B$ where c is a constant, i.e., $H_{\text{eff}}^{[1]}$ acts harmlessly on the system. The second- and higher-order terms in the Magnus expansion of the effective Hamiltonian, $H_{\text{eff}}^{[2+]}$ include terms due to the finite width of pulses and the remaining undecoupled terms, as the projection into the centralizer is only approximate. We will include these terms in our detailed efficiency estimates.

If the algebraic structure of H_{err} is known, we can choose the decoupling group such that it satisfies the ‘‘decoupling condition’’ for any Hamiltonian H_{err} [6,7],

$$\Pi_{\mathcal{G}}(H_{\text{err}}) = \sum_{j=1}^N D_j H_{\text{err}} D_j^\dagger = 0. \quad (18)$$

In the limit $\tau, \delta \rightarrow 0$, and in the absence of control, the first-order Magnus expansion is exact and condition (18) guarantees the stroboscopic elimination of H_{err} , in the sense that $H_{\text{eff}}^{[1]}(T) = N H_B$, and this would be true at the end of every DD cycle. Another way to understand condition (18) is to recall that $D_1 = I_S$, which means that $\sum_{j=2}^N D_j H_{\text{err}} D_j^\dagger = -H_{\text{err}}$: The negative sign in front of H_{err} means that the role of the decoupling group is to effectively time reverse the error Hamiltonian at the end of the cycle.

B. Interaction picture

In a setting where decoupling works perfectly the system evolves independently from the bath, purely under the action of the control Hamiltonian. Therefore, we use the interaction picture of

$$H_{\text{sec}} \equiv H_{\text{ctrl}} + H_B \quad (19)$$

(the sum of the secular terms) to calculate the full propagator [Eq. (6)],

$$U(t) = U_{\text{sec}} U_{\text{err}}(t, 0), \quad (20)$$

where

$$U_{\text{sec}} \equiv U_{\text{ctrl}}(t) \otimes U_B(t), \quad (21)$$

$$U_{\text{ctrl}}(t) = \mathcal{T} \exp\left(-i \int_0^t H_{\text{ctrl}}(s) ds\right), \quad (22)$$

$$U_B(t) = \exp(-it H_B). \quad (23)$$

If $|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$ (Schrödinger picture) then $|\tilde{\Psi}(t)\rangle = U_{\text{sec}}^\dagger |\Psi(t)\rangle = U_{\text{err}}(t) |\Psi(0)\rangle$ is the corresponding state in the interaction picture. Similarly, for mixed states, $\tilde{\rho}(t) = U_{\text{sec}}^\dagger \rho(t) U_{\text{sec}} = U_{\text{err}}(t, 0) \rho(0) U_{\text{err}}^\dagger(t, 0)$. The interaction picture propagator U_{err} contains all the ‘‘errors,’’ in the sense that if it becomes the identity operator then decoupling is perfect. For then, $U(t) = U_{\text{ctrl}}(t) \otimes U_B(t)$ and the desired system dynamics is completely decoupled from the bath. In this sense the interaction picture is naturally suited to our analysis: by moving the ‘‘ideal’’ evolution $U_{\text{ctrl}}(t) \otimes U_B(t)$ to the left, we have isolated the ‘‘error propagator’’ U_{err} . In this setting quantum

computation (or any quantum control procedure) is implemented with the control Hamiltonian (corresponding to “no system evolution” in the interaction picture) while the DD Hamiltonian is used to reduce decoherence in the interaction picture. U_{err} satisfies the Schrödinger equation

$$\frac{dU_{\text{err}}(t,0)}{dt} = -i\tilde{H}_{\text{err}}(t)U_{\text{err}}(t,0), \quad U_{\text{err}}(0,0) = I, \quad (24)$$

with

$$\begin{aligned} \tilde{H}_{\text{err}}(t) &= (U_B^\dagger \otimes U_{\text{ctrl}}^\dagger)[H_{\text{DD}}(t) \otimes I_B + H_{\text{err}}](U_B \otimes U_{\text{ctrl}}) \\ &= H_{\text{DD}}(t) + \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}], \end{aligned} \quad (25)$$

where the linear adjoint map $\text{Ad}_A[B]$ has the Baker-Campbell-Hausdorff formula [27]

$$\text{Ad}_A[B] \equiv e^{iA} B e^{-iA} = \sum_{n=0}^{\infty} \frac{i^n}{n!} [{}_n A, B], \quad (26)$$

where $[{}_n A, B]$ denotes a nested commutator term $[A, [\dots [A, B]]]$ in which A appears n times. Note that—thanks to the commutation condition (4)— $H_{\text{DD}}(t)$ remains invariant under the interaction picture transformation in Eq. (25). This is where the commutation condition shows up explicitly in our analysis.

Let us define an effective (dimensionless) “error phase” Φ_E via [28]

$$\exp[-i\Phi_E(T)] \equiv U_{\text{err}}(T,0). \quad (27)$$

Thus $\Phi_E(T)$ is the final effective Hamiltonian times the total time, and it measures the deviation from ideal dynamics. In other words, the goal of the decoupling procedure is to minimize $\Phi_E(T)$. In Sec. IV we relate Φ_E to conventional fidelity measures. Throughout this work we repeatedly use the technique of expressing unitaries in terms of the “final effective Hamiltonian.” In fact, this was already done in our review of DD above, when we used the effective Hamiltonian $H_{\text{eff}}^{(1)}(T)$ in Eq. (13).

C. Error phase

We now wish to calculate the total propagator U [Eq. (6)] in the presence of both decoupling and control. The evolution generated by $\tilde{H}_{\text{err}}(t)$ [Eq. (25)] can be decomposed into “free” and pulse periods as follows:

$$\tilde{H}_{\text{err}}(t) = \begin{cases} \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}], & t_{i-1} < t < t_{i-1} + \tau, \\ H_P^{(i)} + \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}], & t_{i-1} + \tau < t < t_i. \end{cases} \quad (28)$$

[These time limits are equivalent to the ones in Eq. (8).] In Appendix B we prove the following “switching lemma.”

Lemma 1. The propagator generated by a “switched Hamiltonian,”

$$H(t) = H_i(t) \quad t_{i-1} < t < t_i, \quad i = 1, \dots, N, \quad (29)$$

can be decomposed into corresponding segments,

$$U(t_N, t_0) = U(t_N, t_{N-1}) \cdots U(t_1, t_0), \quad (30)$$

where $U(t_{i+1}, t_i)$, with $t_i \leq t \leq t_{i+1}$, satisfies the Schrödinger equation

$$\frac{dU(t, t_i)}{dt} = -iH(t)U(t, t_i), \quad U(t_i, t_i) = I. \quad (31)$$

We can thus write

$$U_{\text{err}}(T, 0) = U_{\text{err}}(t_N, t_{N-1}) \cdots U_{\text{err}}(t_1, t_0), \quad (32)$$

where $U_{\text{err}}(t_i, t_{i-1})$, with $t_{i-1} \leq t \leq t_i$, satisfies the Schrödinger equation

$$\frac{dU_{\text{err}}(t, t_{i-1})}{dt} = -i\tilde{H}_{\text{err}}(t)U_{\text{err}}(t, t_{i-1}),$$

$$U_{\text{err}}(t_{i-1}, t_{i-1}) = I, \quad (33)$$

whose formal solution is

$$U_{\text{err}}(t, t_{i-1}) = \mathcal{T} \exp\left(-i \int_{t_{i-1}}^t \tilde{H}_{\text{err}}(t) dt\right). \quad (34)$$

Analogously, we can further decompose each segment into a pulse and a free evolution, each with an effective Hamiltonian. The pulse part is

$$\begin{aligned} U_{\text{err}}(t_i, t_{i-1}) &= U_{\text{err}}(t_i, t_i - \delta) U_{\text{err}}(t_i - \delta, t_{i-1}) \\ &= \mathcal{T} e^{-i \int_{t_i - \delta}^{t_i} \tilde{H}_{\text{err}}(t) dt} U_{\text{err}}(t_i - \delta, t_{i-1}) \\ &= P_i e^{-i \delta H_{\text{err}}^P} U_{\text{err}}(t_i - \delta, t_{i-1}), \end{aligned} \quad (35)$$

which, using Eq. (28), serves to define the effective error

$$\exp[-i\delta H_{\text{err}}^P(\delta)] \equiv P_i^\dagger \mathcal{T} e^{-i \int_{t_i - \delta}^{t_i} (H_P^{(i)} + \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}]) dt} \quad (36)$$

associated with the width of the ideal pulse $P_i = \exp(-i\delta H_P^{(i)})$.

The i th free segment $(t_{i-1}, t_i - \delta)$ is similarly generated by an effective Hamiltonian $H_{\text{err}}^{(i)}$ defined via

$$\exp(-i\tau H_{\text{err}}^{(i)}) \equiv U_{\text{err}}(t_{i-1} + \tau, t_{i-1}) = \mathcal{T} e^{-i \int_0^\tau \text{Ad}_{(s+t_{i-1})H_{\text{sec}}}[H_{\text{err}}] ds}. \quad (37)$$

The overall error unitary $U_{\text{err}}(T, 0)$ can thus be written as

$$\begin{aligned} U_{\text{err}}(T, 0) &= P_N \exp(-i\delta H_{\text{err}}^{P_N}) \exp(-i\tau H_{\text{err}}^{(N)}) \times \cdots \\ &\quad \times P_1 \exp(-i\delta H_{\text{err}}^{P_1}) \exp(-i\tau H_{\text{err}}^{(1)}). \end{aligned} \quad (38)$$

To incorporate the effect of the DD operations we recall the definition of the decoupling group in terms of the pulse unitaries [Eq. (14)] and rewrite Eq. (38) as

$$\begin{aligned} U_{\text{err}}(T, 0) &= D_N e^{-i\delta H_{\text{err}}^{P_N}} D_N^\dagger D_N e^{-i\tau H_{\text{err}}^{(N)}} D_N^\dagger \times \cdots \\ &\quad \times D_1 e^{-i\delta H_{\text{err}}^{P_1}} D_1^\dagger D_1 e^{-i\tau H_{\text{err}}^{(1)}} D_1^\dagger \\ &= \prod_{j=0}^{N-1} \exp(-i\delta D_{N-j} H_{\text{err}}^{P_{N-j}} D_{N-j}^\dagger) \\ &\quad \times \exp(i\tau D_{N-j} H_{\text{err}}^{(N-j)} D_{N-j}^\dagger). \end{aligned} \quad (39)$$

By Lemma 1, the following time-dependent Hamiltonian generates $U_{\text{err}}(T, 0)$:

$$H_m(t) \equiv \begin{cases} D_i H_{\text{err}}^{(i)} D_i^\dagger & \text{for } t_i < t < t_i + \tau, \\ D_i H_{\text{err}}^{P_i} D_i^\dagger & \text{for } t_i + \tau < t < t_{i+1}. \end{cases} \quad (40)$$

The “free evolution error-Hamiltonian” $H_{\text{err}}^{(i)}$ and “pulse error-Hamiltonian” $H_{\text{err}}^{P_i}$ are defined, respectively, in Eqs. (37) and (36). Gathering our results we can write

$$\exp[-i\Phi_E(T)] = U_{\text{err}}(T, 0) = \mathcal{T} \exp\left(-i \int_0^T H_m(t) dt\right). \quad (41)$$

IV. ERROR BOUNDS

In this section we derive rigorous error bounds that relate the error between the desired and actual final state to the norm of the error phase $\Phi_E(T)$. Throughout this work we use the trace distance

$$D(\rho_1, \rho_2) \equiv \frac{1}{2} \|\rho_1 - \rho_2\|_1, \quad (42)$$

where

$$\|A\|_1 \equiv \text{tr}(\sqrt{A^\dagger A}), \quad (43)$$

as the distance measure between state, and the quantum fidelity, defined for any pair of positive operators A and B ,

$$F_Q(A, B) \equiv \|\sqrt{A} \sqrt{B}\|_1 \stackrel{A^\dagger=A, B^\dagger=B}{=} \text{tr} \sqrt{\sqrt{BA} \sqrt{B}}. \quad (44)$$

There is a useful relation between the trace distance and the quantum fidelity [1],

$$1 - D(\rho_1, \rho_2) \leq F_Q(\rho_1, \rho_2) \leq \sqrt{1 - D(\rho_1, \rho_2)^2}, \quad (45)$$

which means that the trace distance and fidelity can be used to bound one another from below and above.

When one or more of the states is pure ($|\psi_1\rangle, |\psi_2\rangle$), we shall write $D(\psi_1, \psi_2)$ and $F(\psi_1, \psi_2)$, or use a mixed notation $D(\psi_1, \rho_2)$ and $F(\psi_1, \rho_2)$, etc.

We also make repeated use of the operator norm

$$\|A\|_\infty \equiv \sup_{\|\psi\|=1} \|A|\psi\rangle\|. \quad (46)$$

For a review of these measures along with key properties see Appendix C.

In the absence of the bath the control Hamiltonian $H_{\text{ctrl}}(t)$ would implement a quantum computation via the propagator U_{ctrl} [Eq. (2)]. Equivalently, the state of the quantum computer at the final time T would be described by the solution $|\psi(T)\rangle$ of the Schrödinger equation $|\dot{\psi}\rangle = -iH_{\text{ctrl}}|\psi\rangle$. Imperfect control of $H_{\text{ctrl}}(t)$ means that even in the absence of the bath, $|\psi(T)\rangle$ is not the ideal final state, which would be obtained if one could implement a completely accurate and noise-free

Hamiltonian $H_{\text{ctrl}}^{\text{ideal}}(t)$, with corresponding final state $|\phi(T)\rangle$. Minimization of the corresponding closed-system control error

$$\delta_{\text{id}} \equiv D[|\psi(T)\rangle, |\phi(T)\rangle] \quad (47)$$

belongs to the realm of fault-tolerant quantum computation [29] and composite pulse techniques [30], and will not be addressed here.

The initial bath state is $\rho_B(0)$ and in the absence of coupling to the system it evolves under the pure-bath Hamiltonian to $\rho_B^0(t; \theta) = U_B(t) \rho_B^0(\theta) U_B(t)^\dagger$ (the superscript 0 denotes no system-bath coupling).

In the general mixed-state setting we distinguish between “ideal” system evolution described by a pure state $\rho_S^{\text{ideal}}(t) = |\phi(t)\rangle\langle\phi(t)|$, with $|\phi(t)\rangle = U_{\text{ctrl}}^{\text{ideal}}(t)|\phi(0)\rangle$ and $U_{\text{ctrl}}^{\text{ideal}}$ generated by $H_{\text{ctrl}}^{\text{ideal}}$, and bath-free nonideal system evolution (due to control errors), described by a mixed state $\rho_S^0(t)$ (the mixed nature can be due to, e.g., the need to average over stochastic realizations of unitary evolutions). In the absence of any coupling between system and bath the joint initial states $\rho_S^{\text{ideal}}(0) \otimes \rho_B^0(0)$ or $\rho_S^0(0) \otimes \rho_B^0(0)$ evolve in the two scenarios to $\rho^{\text{ideal}}(t) \equiv \rho_S^{\text{ideal}}(t) \otimes \rho_B^0(t)$ or $\rho^0(t) \equiv \rho_S^0(t) \otimes \rho_B^0(t)$, respectively.

Then the final error due to imperfect control in the uncoupled setting is

$$D_{\text{id}} \equiv D[\rho^0(T), \rho^{\text{ideal}}(T)] = D[\rho_S^0(T), \rho_S^{\text{ideal}}(T)], \quad (48)$$

where we have used the multiplicativity property (C7) and unitary invariance. Minimization of the pure-system control error D_{id} [generalization of Eq. (47)] once again lies in the domain of fault tolerant quantum error correction [29] and composite pulse techniques [30].

The actual system-bath state obtained by time evolution under the full propagator $U(t)$ [Eq. (6)] is $\rho(t) = U(t)[\rho_S(0) \otimes \rho_B(0)]U(t)^\dagger$, and the actual system state is $\rho_S(t) = \text{tr}_B \rho(t)$. The distance we wish to minimize is the distance between the actual final system state $\rho(t)$ and the ideal final system state (no control errors, no coupling to the bath),

$$D_S \equiv D[\rho_S(T), \rho_S^{\text{ideal}}(T)]. \quad (49)$$

Define

$$D_{\text{tot}} \equiv D[\rho(T), \rho^{\text{ideal}}(T)]. \quad (50)$$

By virtue of Eq. (C11) we know that removing the partial trace can only increase the distance between states, i.e.,

$$D_S \leq D_{\text{tot}}. \quad (51)$$

Let

$$D_{\text{DD}} \equiv D[\rho(T), \rho^0(T)] = D[\tilde{\rho}(T), \tilde{\rho}^0(0)], \quad (52)$$

where we have used the fact that in the interaction picture $\tilde{\rho}^0(t) = \tilde{\rho}^0(0) = \rho_S(0) \otimes \rho_B(0)$. D_{DD} is the distance due to coupling between system and bath, and the role of the decoupling procedure is to minimize this distance.

Using the triangle inequality on $\|\rho(T) - \rho^0(T) + \rho^0(T) - \rho^{\text{ideal}}(T)\|_1$ we have

$$D_{\text{tot}} \leq D_{\text{DD}} + D_{\text{id}}, \quad (53)$$

which shows that minimizing the total error can be done by separately minimizing the open-system decoupling error and the closed-system control error.

In Appendix D (see also [31] for a more general treatment) we prove the following lemma:

Lemma 2. Let $U = \exp(-iA)$ where A is Hermitian. Then for any submultiplicative norm

$$\begin{aligned} \|UBU^\dagger - B\| &\leq \|B\| \min[2, e^{2\|A\|_\infty} - 1] \\ &\stackrel{2\|A\|_\infty \leq 1}{\leq} 2\|B\| \min[1, (e-1)\|A\|_\infty]. \end{aligned} \quad (54)$$

By identifying A with the error phase $\Phi_E(T)$ and B with $\tilde{\rho}_0(0)$ this allows us to write

$$\begin{aligned} D_{\text{DD}} &= \frac{1}{2} \|U_{\text{err}}(T,0) \tilde{\rho}(0) U_{\text{err}}^\dagger(T,0) - \tilde{\rho}_0(0)\|_1 \\ &\leq \frac{1}{2} \|\rho_0(0)\|_1 \min[2, (e^{2\|\Phi_E(T)\|_\infty} - 1)] \\ &= \min \left[1, \frac{1}{2} (e^{2\|\Phi_E(T)\|_\infty} - 1) \right] \stackrel{2\|\Phi_E(T)\|_\infty \leq 1}{\leq} 2\|\Phi_E(T)\|_\infty. \end{aligned} \quad (55)$$

Inequality (55) shows that minimization of the error phase $\Phi_E(T)$ is sufficient for minimizing the decoherence error D_{DD} . Combining our bounds [Eqs. (48), (53), and (55)] we have the quantum fidelity lower bound between the actual and ideal system state,

$$F_Q[\rho_S(T), \rho_S^{\text{ideal}}(T)] \geq 1 - D[\rho_S^0(T), \rho_S^{\text{ideal}}(T)] - \min \left[1, \frac{1}{2} (e^{2\|\Phi_E(T)\|_\infty} - 1) \right]. \quad (56)$$

In other words, minimization of the pure-system control distance together with minimization of the error phase $\Phi_E(T)$ is sufficient for minimization of the total distance D_S . Note that the bound we have derived is not necessarily tight: It is possible to minimize D_{DD} and D_{id} simultaneously, rather than separately, as is done in fault tolerant quantum error correction [29].

V. ERROR ESTIMATES FOR DYNAMICALLY DECOUPLED LOGIC GATES

Our goal in this section is to estimate the error associated with the decoupled evolution (i.e., the evolution in the presence of a DD pulse sequence), relative to the decoherence-free evolution (no system-bath coupling). The decoupled evolution at the end of a DD cycle is described by the propagator $U_{\text{err}}(T,0)$ of Eq. (39). The appropriate dimensionless error parameter is the norm of the total error phase $\|\Phi_E\|_\infty$ [Eq. (27)]. Our strategy for estimating Φ_E will be to calculate approximations to the final effective Hamiltonian and then to bound its norm. As we showed in Sec. IV, in the limit that Φ_E vanishes the final state is free of decoherence errors.

Our main technical tool is the following lemma. For a proof see [31].

Lemma 3. Consider a quantum evolution generated by a time-dependent Hamiltonian $H(s) = H_0(s) + V(s)$, $0 \leq s \leq t$, with propagators satisfying $dU(s,0)/ds = -iH(s)U(s,0)$ and $dU_0(s,0) = -iH_0(s)U_0(s,0)$. Then there exists a time-dependent Hamiltonian $H_{\text{eff}}(t)$ such that

$$\exp[-itH_{\text{eff}}(t)] \equiv U_0^\dagger(t,0)U(t,0) \quad (57)$$

and the following inequality holds for any unitarily invariant norm:

$$\|H_{\text{eff}}\| \leq \frac{1}{t} \int_0^t ds \|V(s)\| \equiv \langle \|V\| \rangle_t \quad (58)$$

$$\leq \sup_{0 < s < t} \|V(s)\|. \quad (59)$$

This lemma allows us to relate the strength of the effective interaction picture Hamiltonian at the end of the evolution $H_{\text{eff}}(t)$ to the strength of the (time-dependent) perturbation V .

As a first application, let us relate $\|H_{\text{err}}^{P_i}\|_\infty$ to $\|H_{\text{err}}\|_\infty$. Comparing Lemma 3 with Eq. (36) and identifying H_0 with $H_P^{(i)}$ [and thus $U_0(t,0)$ with the ideal pulse P_i], $V(t)$ with $\text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}]$ (and thus $H(t)$ with $H_P^{(i)} + \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}]$), and $\delta H_{\text{eff}}(\delta)$ with $\delta H_{\text{err}}^{P_i}(\delta)$, we have

$$\|H_{\text{err}}^{P_i}(\delta)\|_\infty \leq \langle \|H_{\text{err}}\|_\infty \rangle_\delta \leq \sup_{t_{i+1}-\delta < t < t_{i+1}} \|H_{\text{err}}(t)\|_\infty. \quad (60)$$

This means that the application of a pulse, with inclusion of the system-bath coupling during the pulse as in Eq. (36), does not cause a growth in the error rate. This is rather remarkable and can be summarized as ‘‘pulses cannot hurt.’’¹

Similarly, by setting $H_0 = 0$ and $V(t) = \text{Ad}_{tH_{\text{sec}}}[H_{\text{err}}]$ in Lemma 3, we obtain for the free evolution

$$\|H_{\text{err}}^{(i)}\|_\infty \leq \langle \|H_{\text{err}}\|_\infty \rangle_\tau \leq \sup_{t_i < t < t_i + \tau} \|H_{\text{err}}(t)\|_\infty. \quad (61)$$

Now let us return to H_m [Eq. (40)], i.e., the Hamiltonian describing the total evolution over a DD cycle. From now on we simply denote $\langle \|H_{\text{err}}\|_\infty \rangle_\delta$ and $\langle \|H_{\text{err}}\|_\infty \rangle_\tau$ by $\|H_{\text{err}}\|_\infty$. Then the last two inequalities yield $\|D_i H_{\text{err}}^{P_i} D_i^\dagger\|_\infty \leq \|H_{\text{err}}\|_\infty$ and $\|D_i H_{\text{err}}^{(i)} D_i^\dagger\|_\infty \leq \|H_{\text{err}}\|_\infty$, so that

$$\|H_m(t)\|_\infty \leq \|H_{\text{err}}\|_\infty. \quad (62)$$

At this point we are ready to use the Magnus expansion to estimate the error phase $\Phi_E(T)$. Recalling Eq. (41), the Magnus expansion for the error phase is given by

$$\begin{aligned} \Phi_E(T) &= \int_0^T ds_1 H_m(s_1) + \frac{i}{2} \int_0^T ds_1 \int_0^{s_1} ds_2 [H_m(s_2), H_m(s_1)] \\ &\quad + \dots, \end{aligned} \quad (63)$$

and converges as long as $\int_0^T ds_1 \|H_m(s_1)\|_\infty < \pi$ [Eq. (A7)], i.e., a sufficient condition for convergence is

¹Of course by other measures pulses can hurt. For example, broadband pulses can cause unwanted transitions. But for the purposes of our error estimates the absence of growth of the error norm is the crucial aspect.

$$T\|H_{\text{err}}\|_{\infty} < \pi. \quad (64)$$

We assume that our decoupling sequence $\{P_{ij}\}$ is designed for cancelling error terms up to the first order in the Magnus expansion, as in Sec. III. Accordingly we rewrite Φ_E as a sum of the first-order terms and a second-order correction, which we can in principle improve upon by designing a pulse sequence that cancels error terms up to a higher order,

$$\Phi_E(T) = \int_0^T H_m(s)ds + \Phi_{2\text{nd}}(T). \quad (65)$$

In Appendix E we prove the following lemma.

Lemma 4. Consider a time-dependent Hamiltonian $H(t)$, $0 \leq t \leq T$, and the partial sum of k th- and higher-order terms in the corresponding Magnus expansion:

$$\Phi_k = \sum_{i=k}^{\infty} \Omega_i. \quad (66)$$

Assume the Magnus expansion converges. Then,

$$\|\Phi_k\|_{\infty} \leq c_k(T \sup_{0 < t < T} \|H(t)\|_{\infty})^k, \quad (67)$$

where $c_k = O(1)$ is a constant.

Thus, subject to Eq. (64),

$$\|\Phi_{2\text{nd}}(T)\|_{\infty} \leq c(T\|H_{\text{err}}\|_{\infty})^2 \quad (68)$$

for some constant c . The fact that starting from arbitrary k th order the error phase is upper bounded by $(T\|H_{\text{err}}\|_{\infty})^k$ means that the design of higher-order pulse sequences can be very advantageous in achieving improved convergence of the DD procedure (see also [25,32,37]), but we will not pursue this here.

To calculate the first-order integral in Eq. (65) we separate the pulse and free parts,

$$\begin{aligned} \int_0^T H_m(s)ds &= \Phi_{\text{pulse}} + \Phi_{\text{free}}, \\ \Phi_{\text{pulse}} &\equiv \sum_{i=1}^N \int_{t_i-\delta}^{t_i} H_m(s)ds, \\ \Phi_{\text{free}} &\equiv \sum_{i=0}^{N-1} \int_{t_i}^{t_i+\tau} H_m(s)ds. \end{aligned} \quad (69)$$

Using Eq. (62), the error phase due to the pulses Φ_{pulse} is bounded by

$$\|\Phi_{\text{pulse}}\|_{\infty} \leq \Delta\|H_{\text{err}}\|_{\infty}, \quad (70)$$

where

$$\Delta \equiv N\delta \quad (71)$$

is the total length of the pulse durations. Without use of additional techniques such as pulse shaping [25,32] or composite pulse sequences [30], the only means at our disposal to minimize this error is to make the pulse duration δ small. Taking stock, we have, so far

$$\begin{aligned} \|\Phi_E(T)\|_{\infty} &\leq \left\| \int_0^T H_m(s)ds \right\|_{\infty} + \|\Phi_{2\text{nd}}(T)\|_{\infty} \\ &\leq \Delta\|H_{\text{err}}\|_{\infty} + \|\Phi_{\text{free}}\|_{\infty} + c(T\|H_{\text{err}}\|_{\infty})^2. \end{aligned} \quad (72)$$

The ‘‘free error’’ $\|\Phi_{\text{free}}\|_{\infty}$ is the target of the DD pulses. Explicitly, we have, using Eq. (40),

$$\Phi_{\text{free}} = \tau \sum_{i=1}^N D_i H_{\text{err}}^{(i)} D_i^{\dagger}. \quad (73)$$

The effective error Hamiltonians $H_{\text{err}}^{(i)}$ can be Magnus expanded to first order in $\tilde{H}_{\text{err}}(t) = \text{Ad}_{H_{\text{sec}}}[H_{\text{err}}]$ [recall Eq. (28)], so that the higher-order commutators arising from the time ordering in the definition of $H_{\text{err}}^{(i)}$ are included in a new term C that will be absorbed into $\Phi_{2\text{nd}}$. First,

$$\begin{aligned} \exp(-i\tau H_{\text{err}}^{(i)}) &= \mathcal{T} \exp\left(-i \int_{t_{i-1}}^{t_{i-1}+\tau} \tilde{H}_{\text{err}}(t)dt\right) \\ &= \exp\left(-i \int_{t_{i-1}}^{t_{i-1}+\tau} \tilde{H}_{\text{err}}(t)dt + C^{(i)}\right) \\ &= \exp\left(-i \int_{t_{i-1}}^{t_{i-1}+\tau} \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \right. \\ &\quad \left. \times [{}_n H_{\text{sec}}, H_{\text{err}}] dt + C^{(i)}\right), \end{aligned} \quad (74)$$

where by Lemma 4,

$$\|C^{(i)}\|_{\infty} \leq d(\tau \sup_{t_{i-1} \leq t \leq t_{i-1}+\tau} \|\tilde{H}_{\text{err}}(t)\|_{\infty})^2 = d(\tau\|H_{\text{err}}\|_{\infty})^2, \quad (75)$$

and where d is a constant. The integrals yield

$$f_{n,j} \equiv \int_{t_{j-1}}^{t_{j-1}+\tau} \frac{(-it)^n}{n!} dt = \frac{(-i)^n}{(n+1)!} [(t_{j-1} + \tau)^{n+1} - t_{j-1}^{n+1}]t. \quad (76)$$

Therefore, we can define $H_{\text{err}}^{(i)}$ via the expansion

$$\tau H_{\text{err}}^{(i)} = \tau H_{\text{err}} + \sum_{n=1}^{\infty} f_{n,i} [{}_n H_{\text{sec}}, H_{\text{err}}] + C^{(i)}. \quad (77)$$

Returning now to Φ_{free} [Eq. (73)], notice that the first term (H_{err}) in Eq. (77) does not depend on t_i and is singled out, so that we may write

$$\Phi_{\text{free}} = \Phi_{\text{dec}} + \Phi_{\text{undec}} + C,$$

$$\Phi_{\text{dec}} \equiv \tau \sum_{i=1}^N D_i H_{\text{err}} D_i^{\dagger},$$

$$\Phi_{\text{undec}} \equiv \sum_{i=1}^N \sum_{n=1}^{\infty} f_{n,i} [{}_n H_{\text{sec}}, D_i H_{\text{err}} D_i^{\dagger}],$$

$$C \equiv \sum_{i=1}^N D_i C^{(i)} D_i^\dagger, \quad (78)$$

where

$$\|C\|_\infty \leq Nd(\tau\|H_{\text{err}}\|_\infty)^2 = \frac{d}{N}[(T-\Delta)\|H_{\text{err}}\|_\infty]^2. \quad (79)$$

The purpose of the DD procedure is, of course, to cancel Φ_{dec} [recall Eq. (18)]. Pulse sequences that cancel higher-order terms ($n \geq 1$ in Φ_{undec}) can be found, but this will not be pursued here. Thus in our case the undecoupled terms will be given by Φ_{undec} . Define

$$\beta \equiv \|H_{\text{sec}}\|_\infty, \quad J \equiv \|H_{\text{err}}\|_\infty. \quad (80)$$

Let us first note that, using the triangle inequality on $\Phi_{\text{undec}} = \Phi_{\text{free}} - \Phi_{\text{dec}}$ and Eqs. (73) and (77),

$$\begin{aligned} \|\Phi_{\text{undec}}\|_\infty &\leq \|\Phi_{\text{free}}\|_\infty \leq \tau \sum_{i=1}^N \|D_i H_{\text{err}}^{(i)} D_i^\dagger\|_\infty \\ &= \tau \sum_{i=1}^N \|H_{\text{err}}^{(i)}\|_\infty \leq T \|H_{\text{err}}\|_\infty = JT. \end{aligned} \quad (81)$$

This trivial upper bound simply means that the undecoupled error is bounded above by “do nothing.” Another upper bound for Φ_{undec} can be found by making use of norm submultiplicativity,

$$\|[A, B]\|_\infty \leq 2\|A\|_\infty \|B\|_\infty, \quad (82)$$

for any pair of operators A and B in the combined system-bath Hilbert space. Then,

$$\begin{aligned} \|\Phi_{\text{undec}}\|_\infty &\leq \sum_{i=1}^N \sum_{n=1}^{\infty} \|f_{n,i}\| \| [n, H_{\text{sec}}, D_i H_{\text{err}} D_i^\dagger] \|_\infty \\ &\leq \sum_{i=1}^N \sum_{n=1}^{\infty} |f_{n,i}| (2\beta)^n J \\ &= J \sum_{i=1}^N \sum_{n=1}^{\infty} \frac{(t_{i-1} + \tau)^{n+1} - t_{i-1}^{n+1}}{(n+1)!} (2\beta)^n \\ &\leq J \sum_{i=1}^N \sum_{n=1}^{\infty} \frac{(\tau + \delta + t_{i-1})^{n+1} - t_{i-1}^{n+1}}{(n+1)!} (2\beta)^n \\ &= J \sum_{n=1}^{\infty} \frac{(2\beta)^n}{(n+1)!} \sum_{i=1}^N t_i^{n+1} - t_{i-1}^{n+1} \\ &= \frac{J}{2\beta} \sum_{n=1}^{\infty} \frac{T^{n+1}}{(n+1)!} (2\beta)^{n+1} = JT \frac{(e^{2\beta T} - 1 - 2\beta T)}{2\beta T}, \end{aligned} \quad (83)$$

where in the penultimate equality we used $T = t_N$ and $t_0 = 0$.

Combining the bounds in Eqs. (81) and (83) we obtain the following bound on the strength of the undecoupled terms:

$$\|\Phi_{\text{undec}}\|_\infty \leq JT \min \left[1, \frac{\exp(2\beta T) - 1}{2\beta T} - 1 \right]. \quad (84)$$

Combining the expressions for various parts of the total error phase Φ_E , we obtain the following upper bound:

$$\begin{aligned} \|\Phi_E\|_\infty &\leq \|\Phi_{2\text{nd}}\|_\infty + \|\Phi_{\text{pulse}}\|_\infty + \|\Phi_{\text{dec}}\|_\infty + \|\Phi_{\text{undec}}\|_\infty + \|C\|_\infty \\ &\leq c(JT)^2 + J\Delta + 0 + JT \min \left[1, \frac{\exp(2\beta T) - 1}{2\beta T} - 1 \right] \\ &\quad + \frac{d}{N} [J(T-\Delta)]^2. \end{aligned} \quad (85)$$

Now note that for fixed N and Δ we can always write $d(T-\Delta)/\sqrt{N}$ as $c'T$, where c' accounts for the shift and rescaling of T . This allows us to absorb $\frac{d}{N}[(T-\Delta)J]^2$ into $c(TJ)^2$ (redefining c in the process), so that

$$\|\Phi_E\|_\infty \leq c(JT)^2 + J\Delta + JT \min \left[1, \frac{\exp(2\beta T) - 1}{2\beta T} - 1 \right]. \quad (86)$$

This, in conjunction with Eq. (56), finally gives us the desired lower bound on the quantum fidelity of one period of DD.

VI. PERIODIC DYNAMICAL DECOUPLING

Note that in principle the bound (86) is appropriate for any DD sequence, since the time T is arbitrary (subject to the convergence of the Magnus expansion) and the decoupling group can have arbitrarily many elements. However, in practice DD pulse sequences have some deterministic structure, such as periodicity or self-similarity, or are random. Structure generally results in improved performance under appropriate circumstances [13,33–38], and hence the bound (86) may be too weak.

In this section we apply the idea of encoded operations and dynamical decoupling to the periodic case (PDD) [7] and derive the final-time error bound. The encoded operation consists of the switching of a physical Hamiltonian corresponding to a logical Hamiltonian for a duration of T_m . This switching period T_m is punctuated at various points by the action of dynamical-decoupling operations. In the preceding section, the analysis was performed for a basic cycle of N pulses. In this section we consider what happens when this sequence is applied m times.

Consider a basic decoupling sequence p designed to cancel all terms in H_{err} , as in Eq. (13),

$$p(f_\tau) = P_N f_\tau P_{N-1} f_\tau P_{N-2} \cdots P_1 f_\tau, \quad (87)$$

where $\{P_i\}$ is the sequence of N decoupling pulses and f_τ denotes a “pause” of duration $\tau = \frac{T}{N}$ in decoupling, during which the control Hamiltonian $H_{\text{ctrl}}(t)$ generating the encoded logic gate is operative. Consider now the longer periodic sequence PDD_m formed by repeating $p(f_\tau)$ m times to obtain a sequence of length $T_m = mT$ with $N_m = mN$ pulses,

$$\text{PDD}_m = \prod_{j=1}^m p(f_\tau). \quad (88)$$

In the absence of encoded operations the sequence $p(f_\tau)$ is designed to cancel dynamics up to the first order. The longer sequence PDD_m has the same canceling properties as the sequence p in the limit of $\tau \rightarrow 0$.

So far we have not been specific about how we implement the encoded operation. Namely, we have considered general time-dependent control Hamiltonians. For simplicity, from now on we consider the following simple method for realizing encoded operations. First, we only implement one logic gate during each PDD sequence. In other words, a new logic gate requires a new PDD sequence. Second, each logic gate is implemented in terms of a constant control Hamiltonian. Thus, if ideally we wish to implement $U_{\text{ctrl}}(T_m) = \exp(-iT_m H_{\text{ctrl}}) = \exp(-i\theta R)$ [Eq. (2)], where $H_{\text{ctrl}} = \lambda R$ with λ the magnitude of H_{ctrl} and $\theta = \lambda T_m$ the phase, then in practice we will implement the decoupling-free intervals as

$$f_\tau = \exp\left(-i\tau(H_{\text{err}} + H_B) - i\frac{\theta}{N_m}R\right). \quad (89)$$

That is, the encoded operation is implemented little by little, using N equal N_m th root segments.

Let us now find a bound on the fidelity of PDD_m in this setting. Since we implement the encoded operations using the fixed step f_τ , the propagator for each cycle in the periodic sequence is the same, and hence so is the error phase at the end of each DD cycle. Formally, the total propagator in the interaction picture is simply [recall Eq. (41)]

$$\begin{aligned} U_{\text{err}}(T_m, 0) &= U_{\text{err}}(T_m, (m-1)T) \cdots U_{\text{err}}(2T, T) U_{\text{err}}(T, 0) \\ &= \prod_{j=1}^m e^{-i\Phi_E(jT)} = (e^{-i\Phi_E(T)})^m = e^{-im\Phi_E(T)} \equiv e^{-i\Phi_{\text{PDD}_m}}. \end{aligned} \quad (90)$$

Recalling our fidelity bound equation (56), our task is to estimate the norm of the error phase associated with the periodic sequence after time T_m , i.e., $\Phi_{\text{PDD}_m} \equiv m\Phi_E(T)$. It thus follows immediately from Eq. (86) that

$$\begin{aligned} \|\Phi_{\text{PDD}_m}\|_\infty &\leq c(JT_m)^2/m + N_m J \delta \\ &\quad + JT_m \min\left[1, \frac{\exp(2\beta T_m/m) - 1}{2\beta(T_m/m)} - 1\right]. \end{aligned} \quad (91)$$

In the limit of $\delta=0$ and $\beta T_m \ll 1$, we have (second-order Taylor expansion)

$$\|\Phi_{\text{PDD}_m}\|_\infty \leq m(cJ^2 + J\beta)T^2. \quad (92)$$

We postpone an analysis of this result until Sec. VIII.

VII. EXAMPLE: QUANTUM COMPUTATION USING THE HEISENBERG INTERACTION

The commutation condition (4) is crucial to our results. At first sight it appears that one cannot satisfy it while having

nontrivial decoupling operations. However, as pointed out in Ref. [19], it can be satisfied using the double commutant construction, which we now explain.

The decoupling group \mathcal{G} induces a decomposition of the system Hilbert space \mathcal{H}_S via its group algebra $\mathbb{C}\mathcal{G}$ and its commutant $\mathbb{C}\mathcal{G}'$, as follows [39,40]:

$$\mathcal{H}_S \cong \bigoplus_J \mathbb{C}^{n_J} \otimes \mathbb{C}^{d_J}, \quad (93)$$

$$\mathbb{C}\mathcal{G} \cong \bigoplus_J I_{n_J} \otimes M_{d_J}, \quad \mathbb{C}\mathcal{G}' \cong \bigoplus_J M_{n_J} \otimes I_{d_J}. \quad (94)$$

Here n_J and d_J are, respectively, the multiplicity and dimension of the J th irrep of the unitary representation chosen for \mathcal{G} , while I_N and M_N are, respectively, the $N \times N$ identity matrix and unspecified complex-valued $N \times N$ matrices. We encode the computational state into (one of) the left-hand factors $C_J \equiv \mathbb{C}^{n_J}$, i.e., each such factor (with J fixed) represents an n_J -dimensional code C_J storing $\log_d n_J$ qudits. Our DD pulses act on the right-hand factors. As shown in [39], the dynamically decoupled evolution on each factor (code) C_J will be noiseless in the ideal limit $w, \tau \rightarrow 0$ if and only if $\Pi_{\mathcal{G}}(S_\alpha) = \bigoplus_J \lambda_{J,\alpha} I_{n_J} \otimes I_{d_J}$ [the projection $\Pi_{\mathcal{G}}$ was defined in Eq. (16)] for all system operators S_α in H_{SB} , whence $H_{\text{eff}}^{[1]} = \bigoplus_J [(I_{n_J} \otimes I_{d_J})_S \otimes (\sum_\alpha \lambda_{J,\alpha} B_\alpha)_B]$. Thus, assuming the latter condition is met, under the action of ideal DD the action of $H_{\text{eff}}^{[1]}$ on the code C_J is proportional to I_{n_J} , i.e., is harmless. Quantum logic is enacted by the elements of $\mathbb{C}\mathcal{G}'$. Dynamical-decoupling operations are enacted via the elements of $\mathbb{C}\mathcal{G}$. We satisfy condition (4) because $[\mathbb{C}\mathcal{G}, \mathbb{C}\mathcal{G}'] = 0$.

As an example, consider quantum computation with the Heisenberg interaction [23,41,42]. For the purposes of quantum computing with electron spins in quantum dots, where a linear system-bath interaction of the form

$$H_{SB}^{\text{lin}} = \sum_{\alpha=x,y,z} \sum_j \sigma_j^\alpha \otimes B_j^\alpha, \quad (95)$$

is the dominant source of decoherence due to hyperfine coupling to impurity nuclear spins, it is convenient to use only Heisenberg interactions $H_{\text{Heis}} = \sum_{i<j} J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j$, without physical-level single-qubit gates [42]. Here $\vec{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ are the Pauli matrices on the j th system qubit and B_j^α are arbitrary bath operators. To beat H_{SB}^{lin} we use the Abelian ‘‘universal decoupling group’’ [7] $\mathcal{G}_{\text{uni}} = \{I, X, Y, Z\}$, where $X = \otimes_j \sigma_j^x$, $Y = \otimes_j \sigma_j^y$, $Z = \otimes_j \sigma_j^z$. It is simple to verify that $\Pi_{\mathcal{G}_{\text{uni}}}(H_{SB}^{\text{lin}}) = 0$. This is compatible with using \mathcal{G}_{uni} to eliminate H_{SB}^{lin} , since the global X , Y , and Z pulses commute with the Heisenberg interaction. That is, this is an explicit example of Eq. (4), where we identify H_{ctrl} with H_{Heis} , and H_{DD} with the Hamiltonian generating the global pulses X , Y , and Z , namely, $\sum_j \sigma_j^\alpha$, $\alpha=x,y,z$. As is well known [23,41,42], universal quantum computation is possible using only the Heisenberg interaction provided qubits are encoded into appropriate decoherence-free subspaces or subsystems.

VIII. DISCUSSION AND CONCLUSIONS

It was our goal in this work to evaluate the effectiveness of combining a periodic DD sequence on an appropriately

chosen subspace with quantum logic gates implemented on that subspace. We wish to characterize the conditions under which such a scheme leads to higher fidelity quantum computation compared to the alternative of not applying DD operations. To do so, we now combine our two main results, Eqs. (56) and (91), for m PDD cycles, each of duration T , i.e., of total duration T_m , involving N_m pulses each of width δ and interval τ ,

$$F_Q[\rho_S(T_m), \rho_S^{\text{ideal}}(T_m)] \geq 1 - D[\rho_S^0(T_m), \rho_S^{\text{ideal}}(T_m)] - \min \left[1, \frac{1}{2} (e^{2\|\Phi_{\text{PDD}_m}\|_\infty} - 1) \right], \quad (96)$$

$$\|\Phi_{\text{PDD}_m}\|_\infty \leq c(JT_m)^2/m + N_m J \delta + JT_m \min \left[1, \frac{\exp(2\beta T_m/m) - 1}{2\beta(T_m/m)} - 1 \right], \quad (97)$$

or, in simplified form (assuming $\beta T_m \ll 1$, $\|\Phi_{\text{PDD}_m}\|_\infty \leq 1/2$, and zero-width pulses)

$$F_Q[\rho_S(T_m), \rho_S^{\text{ideal}}(T_m)] \geq 1 - D[\rho_S^0(T_m), \rho_S^{\text{ideal}}(T_m)] - 2m(cJ^2 + J\beta)T^2. \quad (98)$$

We remind the reader that the term $D[\rho_S^0(T_m), \rho_S^{\text{ideal}}(T_m)]$ is the error due to control imperfections in the uncoupled setting, and must be dealt with using methods such as fault tolerant quantum error correction, composite pulses, or pulse shaping.

The term $c(JT_m)^2/m = mcJ^2T^2$ in Eq. (97) is a bound on the error due to the fact that we have terminated the Magnus expansion at second order. It can in principle be improved by performing a more careful higher-order perturbation theory analysis. The term $NJ\delta$ is the error due to finite pulse width. This error can be improved by using pulse shaping techniques [24,25]. The last term in Eq. (97) is a bound on the undecoupled errors, i.e., errors due to imperfect decoupling. Considering the zero-width pulse limit, Eq. (98), we see that provided the number of cycles m scales more slowly than $[2(cJ^2 + J\beta)T^2]^{-1}$, i.e., if

$$m = o\{[2(cJ^2 + J\beta)T^2]^{-1}\}, \quad (99)$$

the fidelity is guaranteed to be dominated by the error $D[\rho_S^0(T_m), \rho_S^{\text{ideal}}(T_m)]$ due to control imperfections (the “little- o ” notation means that the right-hand side dominates the left-hand side asymptotically).

We also recall that $\beta \equiv \|H_{\text{sec}}\|_\infty = \|H_{\text{ctrl}} \otimes I_B + I_S \otimes H_B\|_\infty \leq \|H_{\text{ctrl}}\|_\infty + \|H_B\|_\infty$ and $J \equiv \|H_{\text{err}}\|_\infty = \|H_{SB} + H_{S,\text{res}}\|_\infty$, where H_{SB} is the system-bath interaction Hamiltonian and $H_{S,\text{res}}$ are residual undesired pure-system terms that do not commute with H_{ctrl} . Expressing the system-bath interaction as $H_{SB} = \sum_\alpha S_\alpha \otimes B_\alpha$ (sum over system times bath operators), we have $J \leq \sum_\alpha \|S_\alpha\|_\infty \|B_\alpha\|_\infty + \|H_{S,\text{res}}\|_\infty$. For local Hamiltonians involving n system qubits we can reasonably expect $J \propto n$ (e.g., for electron spin qubits, each of which is coupled to a local bath of nuclear spin impurities). Similarly, we have $\|H_{\text{ctrl}}\|_\infty \propto n$ (assuming full parallelism in the operation of the quan-

tum computer). The norm of the pure-bath Hamiltonian ($\|H_B\|_\infty$) may be very large, though in practice it is always finite due to a high-energy cutoff or spatial cutoff determining the relevant bath degrees of freedom. Assuming that we are dealing with a bath for which $\|H_B\|_\infty \propto Mn$ (appropriate spatial cutoff, such that the n qubits couple to a bath with M degrees of freedom, where M can be very large), we also have $\beta \propto n$. Thus, we have from Eq. (99) that for fixed T ,

$$m \sim c'n^{-2+\varepsilon}, \quad (100)$$

where c' is a dimensionless constant involving the various energy scales of the problem and $\varepsilon > 0$. This last result establishes that using PDD with fixed cycle time, there is a tradeoff between the number of cycles and the size of the quantum register, i.e., there is a limit on scalability. On the other hand, the complete inequality suggested by Eq. (99) is

$$\sqrt{m}T \ll [2(cJ^2 + J\beta)]^{-1/2} \sim n^{-1}, \quad (101)$$

so that a better strategy might be to invest resources in shrinking the cycle duration T with n , so as to increase the number of cycles m .

Ultimately, based on various comparative studies [11,33–35], we expect that there are strategies that will outperform PDD altogether and will lead to much improved scalability. Such strategies are concatenated DD [13,33–36], randomized DD [10–12], and specially tailored DD such as the sequence proposed in [37] for the diagonal spin-boson model. We expect that the rigorous analysis we have presented here will prove useful in the analysis of these more elaborate pulse sequences.

In the appendixes we provide background and prove the various lemmas found in the main text. For convenience we restate all of the lemmas.

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APPENDIX A: MAGNUS EXPANSION

This appendix is a brief summary of [26,43]. The Magnus expansion is a method for solving first-order operator-valued linear differential equations,

$$\frac{dU(t,0)}{dt} = -iH(t)U, \quad t \geq 0,$$

$$U(0) = I. \quad (A1)$$

Here $H(t)$ can be any bounded linear operator. When $H(t)$ is Hermitian (the only case we consider), Eq. (A1) is the time-dependent Schrödinger equation and the Magnus expansion provides a unitary perturbation theory, in contrast to the Dyson series. The unitary nature of the Magnus expansion is one of its most appealing features.

The formal solution of Eq. (A1) is the time-ordered integral

$$U(t) = \lim_{N \rightarrow \infty} \prod_{j=0}^N \exp \left[-i \frac{t}{N} H \left(\frac{j t}{N} \right) \right] \equiv \mathcal{T} \exp \left(-i \int_0^t H(s) ds \right). \quad (\text{A2})$$

The Magnus expansion represent the solution in the form $U(t) = \exp[-i\Omega(t)]$ and expresses $\Omega(t)$ in a series expansion. When $H(t)$ commutes with $\int_0^t H(s) ds$ the solution is $U(t) = \exp[-i\int_0^t H(s) ds]$, $t \geq 0$ (no time ordering). Otherwise the solution is an infinite series,

$$U(t,0) = \lim_{n \rightarrow \infty} e^{iM_n(t)}, \quad (\text{A3})$$

where $M_n(t)$ is the Hermitian operator

$$M_n = \sum_{i=1}^n \Omega_i, \quad (\text{A4})$$

where

$$\begin{aligned} \Omega_i[H(t)]_0^i &= \sum_j c_{j,i} \int_{t_1} \int_{t_2} \cdots \int_{\substack{t_n \\ 0 < t_1 < \cdots < t_n < t}} [[H(t_1), \dots, H(t_n)]] dt_n \cdots dt_1, \end{aligned} \quad (\text{A5})$$

where $[[H(t_1), \dots, H(t_n)]]$ denotes an n th level nested time-ordered commutator expression between $H(t_i)$, and the coefficients $c_{j,i}$ are recursively defined and can be computed to any order. The first few terms are

$$\begin{aligned} \Omega_1 &= \int_0^t H(t_1) dt_1, \\ \Omega_2 &= \frac{i}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)], \\ \Omega_3 &= \frac{1}{12} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 [H(t_3), [H(t_2), H(t_1)]] \\ &\quad + \frac{1}{4} \int_0^t dt_1 \int_0^{t_1} ds' \int_0^{t_2} dt_3 [[H(t_3), H(t_2)], H(t_1)]. \end{aligned} \quad (\text{A6})$$

A sufficient (but not necessary) condition for absolute convergence of the Magnus series $M_n(t)$ in the interval $[0, t)$ is [43]

$$\int_0^t \|H(s)\|_{\infty} ds < \pi. \quad (\text{A7})$$

APPENDIX B: EVOLUTION LEMMA FOR A SWITCHED HAMILTONIAN

We prove Lemma 1.

The propagator generated by a “switched Hamiltonian,”

$$H(t) = H_i(t) \quad t_{i-1} < t < t_i, \quad i = 1, \dots, N,$$

can be decomposed into corresponding segments

$$U(t_N, t_0) = U(t_N, t_{N-1}) \cdots U(t_1, t_0), \quad (\text{B1})$$

where $U(t_{i+1}, t_i)$, with $t_i \leq t \leq t_{i+1}$, satisfies the Schrödinger equation

$$\frac{dU(t, t_i)}{dt} = -iH(t)U(t, t_i), \quad U(t_i, t_i) = I. \quad (\text{B2})$$

Proof. Denote the propagator generated by a time-dependent Hamiltonian $H(t)$ starting from an initial time t_0 by $U(t, t_0)$. Evolving backward in time from t_i to t_0 , followed by a forward in time evolution from t_0 to t yields a net evolution from t_i to t ,

$$U(t, t_i) = U(t, t_0)U(t_i, t_0)^\dagger. \quad (\text{B3})$$

Letting $t = t_N$ and $t_i = t_{N-1}$ we thus have

$$U(t_N, t_0) = U(t_N, t_{N-1})U(t_{N-1}, t_0). \quad (\text{B4})$$

Repeating this via $U(t_{N-1}, t_0) = U(t_{N-1}, t_{N-2})U(t_{N-2}, t_0)$, etc., we arrive at Eq. (B1). To prove that $U(t, t_i)$ satisfies Eq. (B2) we differentiate Eq. (B3) with respect to t ,

$$\begin{aligned} \frac{dU(t, t_i)}{dt} &= \frac{dU(t, t_0)}{dt} U(t_i, t_0)^\dagger \\ &= -iH(t)U(t, t_0)U(t_i, t_0)^\dagger = -iH(t)U(t, t_i). \end{aligned} \quad (\text{B5})$$

■

APPENDIX C: NORMS AND DISTANCES

Throughout this work we use unitarily invariant norms on bounded operators A [44] (Chap. 4),

$$\|A\| = \|UAV\| \quad U, V \text{ unitary}. \quad (\text{C1})$$

A norm is weakly unitarily invariant if $\|A\| = \|UAU^\dagger\|$ for every unitary U . Obviously, if a norm is unitarily invariant then it is also weakly unitarily invariant. In addition to being subadditive, i.e., satisfying the triangle inequality (by definition of a norm) $\|A+B\| \leq \|A\| + \|B\|$, unitarily invariant norms are also submultiplicative [44]:

$$\|AB\| \leq \|A\| \|B\|. \quad (\text{C2})$$

Define

$$|A| \equiv \sqrt{A^\dagger A}. \quad (\text{C3})$$

The set of all square matrices, together with a submultiplicative norm, is an example of a Banach algebra, and every C^* algebra is a Banach algebra. Note that not all matrix norms are submultiplicative. For example, if we define $\|A\|_{\Delta} = \max_{ij} |a_{ij}|$ then for the matrices $A=B = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ we have $\|A\|_{\Delta} = \|B\|_{\Delta} = 1$ but $\|AB\|_{\Delta} = 2$.

We now give three important examples [44].

The trace norm is

$$\|A\|_1 \equiv \text{tr}(|A|) \stackrel{A^\dagger=A}{=} \text{tr} A. \quad (\text{C4})$$

Note that if ρ is a density matrix then $\|\rho\|_1 = \text{tr} \rho = 1$. The trace distance $D(\rho_1, \rho_2) \equiv \frac{1}{2} \|\rho_1 - \rho_2\|_1$, plays a special role since it captures the measurable distance between different density matrices ρ_1 and ρ_2 [45]. Namely, $D(\rho_1, \rho_2)$ is an achievable upper bound on the trace distance between probability distributions arising from measurements P performed on ρ_1 and ρ_2 [1] (Theorem 9.1), in the sense that $D(\rho_1, \rho_2) = \max_P (\langle P \rangle_1 - \langle P \rangle_2)$, where $P \leq I$ is a positive operator, and $\langle P \rangle_i = \text{tr}(P\rho_i)$.

The Frobenius (or Hilbert-Schmidt) norm

$$\|A\|_2 \equiv \sqrt{\langle A, A \rangle} = \sqrt{\text{tr}(A^\dagger A)} = \left(\sum_{ij} |a_{ij}|^2 \right)^{1/2} \quad (\text{C5})$$

(where A has matrix elements a_{ij}) is the norm induced by the Hilbert-Schmidt inner product

$$\langle A, B \rangle \equiv \text{tr} A^\dagger B. \quad (\text{C6})$$

Finally, the operator norm is

$$\|A\|_\infty \equiv s_1(A) = \sup_{\|\psi\|=1} \|A|\psi\rangle\|,$$

where $s_1(A)$ is the first (largest) singular value of A , i.e., the largest eigenvalue of $|A|$.

All three norms are multiplicative with respect to the tensor product [46] (Chap. 2)

$$\|A \otimes B\|_i = \|A\|_i \|B\|_i, \quad i = 1, 2, \infty. \quad (\text{C7})$$

They satisfy the ordering

$$\|A\|_\infty \leq \|A\|_2 \leq \|A\|_1. \quad (\text{C8})$$

Another useful inequality is [46] (Chap. 2)

$$\|ABC\| \leq \|A\|_\infty \|B\| \|C\|_\infty, \quad (\text{C9})$$

where $\|\cdot\|$ denotes any unitarily invariant norm. A special case of this is obtained by setting A , B or $C=I$,

$$\|AB\| \leq \|A\|_\infty \|B\|, \|A\|_\infty \|B\|_\infty, \|B\|_\infty \|A\|. \quad (\text{C10})$$

An important inequality we need relates the norm of the partial trace and the norm of the operator being traced over (for a proof see [31]),

$$\|\text{tr}_B X\|_i \leq d_i \|X\|_i \quad (i = 1, 2, \infty),$$

$$d_1 = 1,$$

$$d_2 = \sqrt{\dim(\mathcal{H}_B)},$$

$$d_\infty = \dim(\mathcal{H}_B), \quad (\text{C11})$$

where X is a linear operator over the tensor product Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$. For the trace norm this is a special case of the well-known result that trace-preserving maps (in this case the partial trace) are contractive [1].

APPENDIX D: NORM TO ERROR PHASE INEQUALITY FOR MIXED STATES

We prove Lemma 2.

Let $U = \exp(-iA)$ where A is Hermitian. Then for any sub-multiplicative norm

$$\begin{aligned} \|UBU^\dagger - B\| &\leq \|B\| \min[2, e^{2\|A\|_\infty} - 1] \\ &\stackrel{2\|A\|_\infty \leq 1}{\leq} 2\|B\| \min[1, (e-1)\|A\|_\infty]. \end{aligned}$$

Proof. First note that

$$e^x - 1 = x \left(1 + \sum_{n=2}^{\infty} \frac{x^{n-1}}{n!} \right)^{x \leq 1} \leq x \left(1 + \sum_{n=2}^{\infty} \frac{1}{n!} \right) = (e-1)x. \quad (\text{D1})$$

By a similar calculation we also get $\frac{e^x-1}{x} - 1 \leq (e-2)x$.

By the triangle inequality

$$\|UBU^\dagger - B\| \leq \|UBU^\dagger\| + \|B\| \leq 2\|B\|. \quad (\text{D2})$$

On the other hand, using the Taylor expansion of $\exp(-i[A, \cdot])$ we have

$$\begin{aligned} \|UBU^\dagger - B\| &= \left\| \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} [{}_n A, B] - B \right\| \\ &= \left\| \sum_{n=1}^{\infty} \frac{i^n}{n!} [{}_n A, B] \right\| \leq \sum_{n=1}^{\infty} \frac{1}{n!} \| [{}_n A, B] \| \\ &\leq \sum_{n=1}^{\infty} \frac{2^n \|A\|_\infty^n}{n!} \|B\| \\ &= (e^{2\|A\|_\infty} - 1) \|B\| \\ &\stackrel{2\|A\|_\infty \leq 1}{\leq} 2(e-1)\|A\|_\infty \|B\|, \end{aligned} \quad (\text{D3})$$

where in the penultimate inequality we iterated

$$\|[A, B]\| \leq 2\|AB\| \leq 2\|A\|_\infty \|B\| \quad (\text{D4})$$

[where we used submultiplicativity together with Eq. (C10)] to obtain

$$\|[{}_n A, B]\| \leq \|A\|_\infty \|[{}_{n-1} A, B]\| \leq \dots \leq \|A\|_\infty^n \|B\|. \quad (\text{D5})$$

APPENDIX E: MAGNUS EXPANSION TRUNCATION BOUND

We prove Lemma 4.

Consider a time-dependent Hamiltonian $H(t)$, $0 \leq t \leq T$, and the partial sum of k th- and higher-order terms in the corresponding Magnus expansion,

$$\Phi_k = \sum_{i=k}^{\infty} \Omega_i.$$

Assume the Magnus expansion converges in the trace norm. Then

$$\|\Phi_k\| \leq c_k [T \sup_{0 < t < T} \|H(t)\|_\infty]^k,$$

where $c_k = O(1)$ is a constant.

Proof. Define $h \equiv \sup_{0 < t < T} \|H(t)\|_\infty$ and rescale $H(t)$ by hT ,

$$H'(t) = \frac{H(t)}{hT}. \quad (\text{E1})$$

We can rewrite Ω_i as

$$\begin{aligned} \Omega_i[H(t)]_0^T &= (hT)^i \sum_j c_{j,i} \int_0^T \cdots \int_0^T [[H'(t_1), \dots, H'(t_n)]] dt_n \cdots dt_1 \\ &= (hT)^i \Omega_i[H'(t)]_0^T. \end{aligned} \quad (\text{E2})$$

Recall the condition for absolute convergence of the Magnus expansion, Eq. (A7). Since $\int_0^T \|H(t)\| dt \leq T \sup_{0 < t < T} \|H(t)\|$ a sufficient condition is

$$hT < 1. \quad (\text{E3})$$

Absolute convergence (convergence of the sum of absolute values) means that if we define, for $k \geq 1$, the partial sum

$$B_{n,k} \equiv \sum_{i=k}^n \|\Omega_i[H(t)]_0^T\| \quad (\text{E4})$$

then

$$\lim_{n \rightarrow \infty} B_{n,k} = \beta_k [H(t)]_0^T < \infty, \quad (\text{E5})$$

where β_k is some functional of $H(t)$. Similarly for $H'(t)$,

$$\lim_{n \rightarrow \infty} \sum_{i=k}^n \|\Omega_i[H'(t)]_0^T\| = \beta_k [H'(t)]_0^T \equiv A_k = O(1). \quad (\text{E6})$$

Let us now focus on the partial sum of k th- and higher-order terms in the Magnus expansion, $\Phi_k = \sum_{i=k}^\infty \Omega_i$. We can bound Φ_k in the following manner:

$$\begin{aligned} \|\Phi_k\| &\leq \sum_{i=k}^\infty \|\Omega_i[H(t)]_0^T\| \stackrel{\text{Eq. (E2)}}{=} (hT)^k \sum_{i=k}^\infty (hT)^{i-k} \|\Omega_i[H'(t)]_0^T\| \\ &\stackrel{\text{Eq. (E3)}}{\leq} (hT)^k \sum_{i=k}^\infty \|\Omega_i[H'(t)]_0^T\| \stackrel{\text{Eq. (E6)}}{=} (hT)^k A_k = O[(hT)^k]. \end{aligned} \quad (\text{E7})$$

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