Universal dynamical decoupling of multiqubit states from environment
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Dynamical decoupling (DD) is a powerful tool to protect quantum systems from decoherence induced by the inevitable system-environment interaction [1]. The idea of DD is to dynamically control the system (or environment) evolution to suppress the decoherence caused by interaction. For example, a static magnetic field with unknown magnitude $B_z\sigma_z$ can induce dephasing of a qubit, but such dephasing can be fully eliminated by a spin flip $\sigma_z$ (i.e., Hahn echo) at half way of the evolution [2]. In practice, however, the Hahn echo only suppresses the dephasing to $O(T^2)$ for total evolution time $T$, because the magnetic field may have complicated time-dependence in both magnitude and orientation due to the evolution of the environment. Furthermore, if the environment consists of quantum degrees of freedom, it can become tangled with the system via the interaction. Hence it is a challenging task to design a universal DD scheme that can suppress decoherence to desired order independent of the details of system-environment interaction.

One particular interesting DD scheme is the concatenated DD (CDD), which has been shown to be universal for single qubits [3]. The limitation, however, is that the pulse number increases exponentially with the suppression order $N$ (approximately $4^N$ pulses to suppress both bit-flip and dephasing processes to $O(T^{N+1})$). It is the discovery of the universality of Uhrig DD (UDD) sequence [4–8] that makes the universal DD practically feasible. In contrast to CDD demanding exponentially many pulses [3], UDD uses only $O(N)$ spin-flip pulses to suppress the dephasing processes to $O(T^{N+1})$ [3, 6]. The discovery of UDD sequence has inspired many experimental efforts to further improve the coherence over a wide range of quantum systems, including trapped ions [9], electron spins [10], defect centers [10, 11], quantum dots [12, 13], and superconducting qubits [14]. However, UDD is restricted to pure dephasing errors of a single qubit. It is desirable to have an efficient DD scheme (with poly$(N)$ pulses) to suppress both bit-flip and dephasing processes for multiple qubits to $O(T^{N+1})$.

Recently, the quadratic DD (QDD) scheme has been proposed [15], which uses $(N + 1)^2$ pulses to suppress both bit-flip and dephasing errors of single qubits. As a generalization of QDD from 1-qubit system to $m$-qubit system, the nested UDD (NUDD) scheme has been proposed [16, 17], which uses $(N + 1)^{2m}$ pulses to suppress decoherence from the most general interaction between the $m$-qubit system and environment. Although there are numerical evidences [16, 18] and theoretical implications [7, 18, 19] that QDD/NUDD might be universal, it is still an open question whether QDD/NUDD are universal or not [15, 20].

In this Letter, we shall present a rigorous proof that the NUDD scheme with $2m$ nesting levels and $(N + 1)^{2m}$ pulses is a universal DD scheme for $m$-qubit system, which suppresses decoherence processes to $O(T^{N+1})$ for arbitrary system-environment interaction. We achieve...
this by providing a mapping between NUDD and a discrete “quantum walk” in 2m dimensional space. The rules that govern this quantum walk do not depend on 2m, which allows for an efficient proof for all nesting levels. Below we first introduce notations and explain the existing proof for UDD [8] using the language that can be naturally generalized for QDD/NUDD.

UDD.— Let us first consider the UDD sequence [4] for a qubit-environment interaction

\[ H(\tau) = \hat{S}_0 \otimes \hat{B}_0(\tau) + \hat{S}_1 \otimes \hat{B}_1(\tau) , \]

for \( \hat{S}_0 = I \) and \( \hat{S}_1 = \sigma_x \), and the time-dependent bath operators are analytic with series expansion \( \hat{B}_\alpha(t) = \sum_\alpha \hat{b}_{\alpha,\tau} t^\alpha \) for \( \alpha = 0, 1 \). The UDD sequence uses \( \pi \)-pulses (i.e., \( \sigma_x \) rotations) applied at times \( \tau = \Delta \lambda \), where

\[
\Delta \lambda = \sin^2 \frac{\lambda \pi}{2(N+1)}
\]

for \( \lambda = 1, 2, \cdots, N \). (An extra \( \sigma_x \) pulse is required at \( \tau_{N+1} = T \) for \( N \) odd [13].) It is convenient to consider the toggling frame associated with the qubit. In this frame the qubit-environment Hamiltonian is modulated in time as:

\[ \tilde{H}(\tau) = F_0(\tau/T) \hat{S}_0 \otimes \hat{B}_0(\tau) + F_1(\tau/T) \hat{S}_1 \otimes \hat{B}_1(\tau) , \]

where \( F_\alpha(t) = (-1)^{\alpha \lambda} \) for \( t \in (\Delta \lambda, \Delta \lambda+1) \). The unitary evolution operator of the toggling frame Hamiltonian is \( \tilde{U}(T) = T \exp \left[-i \int_0^T \tilde{H}(\tau) \, d\tau \right] \), where \( T \) is the time-ordering operator. \( \tilde{U}(T) \) has Dyson expansion

\[
\sum_{s=0}^\infty \sum_{\{\alpha_j, p_j\}} (-i)^s \hat{S}_{(\oplus \alpha_j)} \prod_{j=1}^s \hat{b}_{\alpha_j, p_j} F_{\alpha_1, \cdots, \alpha_s} T^{s+p_1+\cdots+p_s},
\]

where \( \hat{S}_{(\oplus \alpha_j)} = \hat{S}_{\alpha_1} \cdots \hat{S}_{\alpha_s} \) and the coefficient \( F_{\alpha_1, \cdots, \alpha_s} \) can be obtained by the following integral

\[
\int_0^1 dt_1 \cdots \int_0^{t_2} \prod_{j=1}^s F_{\alpha_j}(t_j) t_j^{p_j}.
\]

When \( \oplus^{s+1}_j \alpha_j = 0 \), the operator \( \hat{S}_{(\oplus \alpha_j)} = I \) is the identity operator that acts trivially on the qubit. Hence we only need to consider the terms with \( \oplus^{s+1}_j \alpha_j \neq 0 \) that act non-trivially on the qubit. To show the universality of the UDD sequence, we just need to prove \( \tilde{U}(T) = I \otimes \hat{U}_B(T) + O(T^{N+1}) \), which can be reduced to verifying

\[
F_{\alpha_1, \cdots, \alpha_s} = 0
\]

for \( \oplus^{s+1}_j \alpha_j \neq 0 \) and \( s + \sum_{j=1}^s p_j \leq N \). Eq.(4) resembles the proof of Ref.[7] for universality of UDD. The key difference is that here additional indices \( \{\alpha_j\} \) are introduced to label different possible qubit operators (I and \( \sigma_x \)) which will be necessary for the proof of universality of QDD and NUDD.

QDD.— Let us now consider the QDD sequence [15] for generic interaction between a single qubit and environment,

\[
H(\tau) = \sum_{\alpha} \hat{S}_\alpha \otimes \hat{B}_\alpha(\tau),
\]

where \( \hat{S}_\alpha = I, \sigma_x, \sigma_y, \sigma_z \) for binary vector labels \( \alpha = (a_2, a_1) = (0, 0), (1, 0), (1, 1), (0, 1) \), respectively. For Pauli matrices, one can verify that \( \hat{S}_\alpha \hat{S}_{\alpha'} = \pm \hat{S}_{\alpha \oplus \alpha'} \), which represents pairwise binary addition without carry (e.g., \( (0, 1) \oplus (0, 1) = (0, 0) \)). The QDD sequence consists of two nesting levels of UDD with a total of \( Q = (N+1)^2 \) pulses [15]. The pulses \( \sigma_x \) and \( \sigma_z \) are associated with the first and second levels, respectively. To label these \( Q \) pulses, we introduce the vector label \( \lambda = (l_2, l_1) \in \{0, \cdots, N\} \otimes \{1, \cdots, N+1\} \) with \( l_2(N+1)+l_1 \in \{1, \cdots, Q\} \) [21]. The \( \lambda \)th pulse is applied at time \( \tau_\lambda = T\Delta_{(l_2, l_1)} \) with

\[
\Delta_{(l_2, l_1)} = \Delta_{l_2} + (\Delta_{l_2+1} - \Delta_{l_2}) \Delta_{l_1}.
\]
for \( r = 2, \ldots, 2m \). As illustrated in Fig. 4, the timing for the pulses has a self-similar structure [25]. The toggling frame Hamiltonian for the NUDD sequence is the same as Eq. (5), with \( \alpha \) summed over all \( 4^r \) generators. Similar to UDD and QDD, to show universality of the NUDD sequence, we just need to prove Eq. (6) for \( \otimes_{j=1}^{s} \alpha_j \neq 0 \) and \( s + \sum_{j=1}^{s} p_j \leq N \). We can view UDD and QDD as special cases of NUDD with one and two nesting levels, respectively. Since the universality of UDD, QDD, and NUDD all relies on verifying Eq. (6), we will give a general proof of Eq. (6) in the rest of the paper.

**Universality Proof.**—To prove Eq. (6), we represent each integration over \( t_j \) as a linear operator acting on functions of \( t_j \), which generates a function of \( t_{j+1} \). Thus, the process of multiple integrations can be thought of as a discrete quantum walk in a functional space. We choose the basis of this functional space according to the following consideration — the functional basis should be complete with respect to the operation \( \int_0^t \frac{d t'}{t} F_{\alpha} (t') t^p \) for all relevant orders up to \( O (T^{N+1}) \). Since \( F_{\alpha} (t) \) is a piece-wise analytic function with at most \( Q = (N + 1)^{2m} \) discontinuities, it will be convenient to use piece-wise analytic functions as our functional basis. In addition, we only need to consider all polynomials up to power \( N + 1 \) to characterize all the effects up to \( O (T^{N+1}) \). Therefore, we choose basis that consists of \( (N + 1) \cdot Q \) functions

\[
\eta_{q, \lambda} (t) = t^q \eta_{\lambda} (t)
\]

with \( \eta_{\lambda} (t) = 1 \) for \( t \in (\Delta_\lambda, \Delta_{\lambda+1}) \) and \( \eta_{\lambda} (t) = 0 \) otherwise. Here \( q \in \{0, 1, \ldots, N\} \) is the polynomial label and \( \lambda \in \{0, 1, \ldots, N\} \otimes 2^m \) is the pulse label.

Then, we use Eq. (7) to rewrite the integral

\[
\mathcal{F}_{\lambda, q, \alpha} = \int_0^{t_0} dt_s \sum_{p_s \leq N \lambda} \int_0^{t_s} dt_{s-1} \sum_{p_{s-1} \leq N \lambda} \cdots \int_0^{t_2} dt_1 t_1^{p_1} F_{\beta_0} (t_1) \times 1,
\]

where \( \int_0^{t_0} dt' = F_{\beta_0} (t_0) \int_0^{t_0} dt' F_{\beta_0} (t') \) and \( \beta_j = \otimes_{j'=1}^{j} \alpha_{j'} \). For \( s + \sum_{j=1}^{s} p_j \leq N \), we can compute the integral \( \mathcal{F}_{\lambda, q, \alpha} \) using functional basis \( \{ \eta_{\lambda} (t) \} \). For each operation \( O \), let us define the matrix form \( \mathbf{W}_{q, \lambda} \) as \( \mathbf{A} \cdot \eta_{\lambda} = \mathbf{W}_{q, \lambda} \), where summation over repeating indices is implied. For example, the multiplication \( \mathbf{t} \cdot \eta_{\lambda} = \eta_{\lambda+1} \) has the matrix form \( \mathbf{W}_{q, \lambda} = \delta_{q, \lambda} I \), with Kronecker delta function \( \delta_{q, \lambda} \). The other operations are listed in Table [I].

Using block diagonal properties of matrices involved, \( \mathcal{F}_{\lambda, q, \alpha} \) can be further reduced as multiplication of \( Q \times Q \) sub-matrices \( B_{\beta} \) and \( D_{\beta} \).

\[
\mathbf{v}_L \cdot M^p_1 \cdot G_{\beta_{s-1}} \cdot M^p_{s-1} \cdots G_{\beta_1} \cdot M^p_1 \cdot F_{\beta_0} \cdot \mathbf{v}_R = \sum_{(i_1 \geq 0)} \mathbf{v}_{\beta_{s-1}} \otimes \mathbf{v}_{\beta_{s-1}} \otimes \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}} \mathbf{v}_{\beta_{s-1}}
\]

where the operations are defined in Eq. (13).
for the initial state, ‘|κ⟩’ for unexplored functional basis states. At least $N = 4$ steps are necessary to reach the target states, which is an illustration of Eq. (14). (a) For UDD, a discrete quantum walk occurs in a one-dimensional functional basis, with initial state $|\kappa⟩$, target state $|\kappa^*⟩$, and a quantum walk matrix $D_{(01)}$. (b) For QDD, a discrete quantum walk occurs in a two-dimensional functional basis, with initial state $|\kappa⟩$, target state $|\kappa^*⟩$, and a quantum walk matrix $D_{(01)}$.

$k_{nl} = 1$ to $k_{nl}^* = N + 1$. Therefore, there is zero amplitude in the target states when the number of steps $\sum_{j=1}^{N} i_j \leq N - 1$. This completes the proof of Eq. (14) and implies the universality of NUDD. We emphasize that after the basis in Eq. (11) is introduced, all operations are matrix multiplications, and all our analytical statements have been explicitly checked numerically.

We can illustrate the quantum walk for special cases: (1) For UDD, the orthogonal transformation $c_{\kappa,\lambda} = c_{(k_1), (l_1)} = \sin \left[ \frac{k_1 2\pi i + 1}{N+1}\right]$ is simply the Fourier transformation as in Ref. [6]. The functional basis $\{ |\kappa⟩ \}$ with $\kappa = (k_1) \in \{1, \cdots, N+1\}$ forms a one-dimensional array. As illustrated in Fig. 2a, it will take at least $N$ steps to walk from $\kappa = (1)$ to $\kappa^* = (N + 1)$. (2) For QDD, the orthogonal transformation is a little more complicated $c_{\kappa,\lambda} = c_{(k_2, k_1), (l_2, l_1)} = (-1)^{(k_1-1)/2} \sin \left[ \frac{k_2 2\pi i + 1}{N+1}\right] \sin \left[ \frac{k_1 2\pi i + 1}{N+1}\right]$ for odd $k_1$ and $(-1)^{k_1/2} \cos \left[ \frac{k_2 2\pi i + 1}{N+1}\right] \sin \left[ \frac{k_1 2\pi i + 1}{N+1}\right]$ for even $k_1$. The functional basis $\{ |\kappa⟩ \}$ with $\kappa = (k_2, k_1)$ forms a two-dimensional array. As illustrated in Fig. 2b, it will also take at least $N$ steps to walk from $\kappa = (1,1)$ to $\kappa^* = (N + 1,1)$ or $(k_2, N+1)$. (3) For NUDD, the functional basis forms a $2m$-dimensional array. Similar to UDD and QDD, it will take at least $N$ steps to walk from $\kappa = (1, \cdots, 1)$ to $\kappa^* = (N + 1)$.

When the suppression order is $N_r$ for the $r$th nesting level of NUDD, the overall suppression of decoherence is $O \left( T^{N_r+1} \right)$ limited by the lowest suppression order $N^* = \min \{N_1, \cdots, N_2m\}$.

Summary & Outlook.— We have proved the universality of the NUDD sequence, which can restore an unknown initial state of $m$-qubit system to $O \left( T^{N+1} \right)$ using $2m$ nesting levels and $(N + 1)^{2m}$ pulses, independent of the details of the system-environment interaction. The NUDD sequence is experimentally feasible, because it requires only $\text{poly}(N)$ pulses acting on individual qubits. Our work illustrates a general connection between DD problems and discrete quantum walks. The techniques developed can be used to address a variety of questions, such as investigation of environment correlations using DD, schemes of efficient DD for particular system-environment interaction, and the combination of multi-qubit DD schemes with quantum error correcting codes and quantum algorithms.

Note added.— After submission of this work, a preprint of closely related work by Kuo and Lidar became available, with a different proof of the universality of QDD.

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[24] We use the Greek letters $\alpha, \beta, \lambda, \kappa$ to represent vector labels, and use the Latin letters $a_r, b_r, l_r, k_r$ to represent the $r$-th element of the corresponding vectors.
[25] For $N$ odd, pulses at different levels may coincide and form one pulse. Hence the unitary evolution of the $\lambda$th instantaneous pulse is: 
\[ \hat{\Omega}(l_2 m, \ldots, l_1 \neq N+1) = \Omega_1, \]
\[ \hat{\Omega}(l_2 m, \ldots, l_r \neq N, N, \ldots, N, N+1) = \Omega_r \hat{\Omega}_{r-1} \cdots \hat{\Omega}_1 \]
for $r \geq 2$, and 
\[ \hat{\Omega}(N, \ldots, N, N+1) = \Omega_N \cdots \hat{\Omega}_1 \]
where $\Omega_{2j-1} = \sigma_2^{(j)}$ and $\Omega_{2j} = \sigma_2^{(j)}$.
[26] Note that exactly $(N+1)^2$ of $(N+2)^2$ possible $\chi_\kappa$’s are non-zero functions, which form a new complete orthogonal basis. Other functions are simply zeros (e.g., $\chi(k_{2m, \ldots, k_2, 0}) = \chi(k_{2m, \ldots, k_{r+2}, N+1, 2h, \ldots}) = \chi(k_{2m, \ldots, k_{r+2}, 0, 2h_r+1, \ldots}) = 0$), which are kept for notational convenience.