Frame-Based Filter-Function Formalism for Quantum Characterization and Control

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We introduce a theoretical framework for resource-efficient characterization and control of non-Markovian open quantum systems, which naturally allows for the integration of given, experimentally motivated, control capabilities and constraints. This is achieved by developing a transfer filter-function formalism based on the general notion of a frame and by appropriately tying the choice of frame to the available control. While recovering the standard frequency-based filter-function formalism as a special instance, this control-adapted generalization affords intrinsic flexibility and, crucially, it permits an efficient representation of the relevant control matrix elements and dynamical integrals if an appropriate finite-size frame condition is obeyed. Our frame-based formulation overcomes important limitations of existing approaches. In particular, we show how to implement quantum noise spectroscopy in the presence of non-stationary noise sources, and how to effectively achieve control-driven model reduction for noise-optimized prediction and quantum gate design.

I. INTRODUCTION

Accurate characterization and control (C&C) of open quantum systems coupled to realistic – temporally correlated (“non-Markovian”) – noise environments are vital for exploiting the full potential of quantum technologies. Open-loop control-engineering methods, based on tailored time-dependent modification of the open-system dynamics, offer a versatile and experimentally accessible approach to tackle this challenge. While techniques employing dynamical decoupling or dynamically-corrected gates [1–4] are beneficial under minimal knowledge about the noise-inducing degrees of freedom, extra knowledge is instrumental for optimizing their performance and efficiency in specific noise environments [4, 5]. Numerical quantum optimal control algorithms [6–8] represent an extreme example: although they can in principle deliver exceptionally high fidelities, their viability in non-Markovian settings requires detailed knowledge of the time-domain noise correlation functions (or the corresponding frequency-domain spectra) [9]. Beside permitting noise-optimized quantum storage and gate design, accurate noise characterization is key to counter the effect of non-Markovian noise in quantum sensing and metrology applications [10, 11].

This has motivated the development of “quantum noise spectroscopy” (QNS) protocols, in which noise spectral information is inferred from the system-only reduced dynamics, under the effects of the noise and user-defined control. Despite considerable progress [12–26], existing QNS protocols suffer from several disadvantages. First, they are not applicable to important types of noise that occur in practice – notably, non-stationary noise, for which a frequency-domain description need not be viable [27, 28]. Second, they do not easily lend themselves to the identification of simplified noise models which, while providing all the required detail for optimal control to be feasible, may permit C&C procedures to be extendible to increasingly larger qubit networks. Finally, to the best of our knowledge no formal analysis of the “universality” of QNS-inferred information for control purposes has been attempted, aimed at clarifying the extent to which such information may suffice to faithfully predict the dynamics of the system under an arbitrary control modulation, beyond what used in the QNS protocol itself.

In this paper, we overcome the above limitations by demonstrating how a “model-reduced” representation of the noisy dynamics of interest may be tied to the available, finite control resources. We achieve this by integrating the language of frames [29–33] – already a mainstay in signal processing – with the theory of open quantum systems. This leads to a novel transfer filter-function (FF) formalism [34–36], in which control capabilities and constraints (dubbed $\mathcal{C}$ henceforth) play the defining role. Crucially, our framework allows the identification of the noise components relative to $\mathcal{C}$ which are, at once, accessible to estimation by a QNS protocol and sufficient to optimally predict the behavior of the system. Moreover, it provides a rigorous way to determine (and quantify) if the information inferred via QNS is useful to predict the behavior of the system under a given control sequence.

The content is organized as follows. In Sec. [II] we introduce the relevant setting for controlled non-Markovian quantum dynamics, with special emphasis on highlighting the structure of the perturbative overlap integrals that enter any C&C protocol. Sec. [III] provides the conceptual foundation of our approach: after providing the essential mathematical background on frames, we show how the relationship between a frame $\mathcal{F}$ and its canonical dual $\tilde{\mathcal{F}}$ naturally suggests two complementary ways for separating the dynamical overlap integrals into control-dependent and noise-dependent contributions, resulting in what we call the standard picture vs. the control-adapted picture, relative to a chosen $(\mathcal{F}, \tilde{\mathcal{F}})$ pair. In particular, we recover the usual frequency-domain FF formalism as a special instance associated to the use of a Fourier frame in Sec. [III-B] whereas in Sec. [III-C] we make precise

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the sense in which control-driven model reduction may be achieved, provided that a suitable finite-size frame condition is obeyed. In essence, the latter ensures that arbitrary control sequences built out of $c$ may be well approximated by finite expansions over elements of $F$.

We then proceed to showcase the added generality and flexibility of our approach by focusing, in Sec. \[IV\] on multiqubit dynamics under simultaneous additive decoherence and multiplicative control noise. After providing a general frame construction for this setting, we specialize to the simplest paradigmatic case of single-qubit dynamics. In particular, in Sec. \[IV B\] we demonstrate how control-adapted QNS techniques that are designed to work directly in the time domain provide new capabilities over existing protocols, by allowing the characterization of non-stationary noise environments of both classical and genuinely quantum nature. A complete frame-based C&C protocol is exemplified in Sec. \[IV C\] where the information about the noise correlations acquired through a first stage of control-adapted QNS is subsequently incorporated in the optimal-control search for various target unitary gates. By comparing to the optimal-control solutions obtained under access to the full dynamics, we establish that our model-reduced representation incurs no significant loss of predictive power, insofar as arbitrary controlled evolutions built out of $c$ are considered. Finally, we present in Sec. \[IV D\] some important remarks on the extent to which QNS-inferred information may be universal for prediction and control, before concluding. Further technical detail is included in five separate Appendices, in order to make the presentation as self-contained as possible.

II. CONTROLLED OPEN QUANTUM DYNAMICS

We consider a controlled $d$-dimensional open quantum system $S$ evolving in the presence of an inaccessible environment (bath) $B$. In the interaction picture associated to the free bath evolution, the joint system-bath dynamics is governed by a Hamiltonian of the form $H(t) = H_S + H_{SB}(t) + H_{ct}(t)$, where the Hamiltonian $H_S$ describes the free evolution of $S$, $H_{SB}(t)$ couples $S$ and $B$, and $H_{ct}(t)$ describes open-loop control modulation acting on $S$ only. Let $\{\Lambda_0 \equiv I_S, \Lambda_u\}$ denote a generalized (Hermitian) Pauli basis for the operator space on $S$, with $\text{Tr}(\Lambda_u \Lambda_v) = \delta_{uv}$. We consider a broad class of Hamiltonians that simultaneously account for additive (control-independent) and multiplicative (control-dependent) noise, according to

$$H(t) = \sum_{u \neq 0} \Lambda_u \otimes B_u^{(a)}(t) + \sum_{v \neq 0} h_v(t)[1 + \beta_v^{(m)}(t)]\Lambda_v.$$

Here, the $B_u^{(a)}(t) \equiv B_u^{(a)}(t) + \beta_u^{(a)}(t)1_B$ describe the always-on additive ($a$) noise from quantum and classical sources, respectively, with $\beta_u^{(a)}(t)$ being bath operators (not necessarily traceless in order to account for evolution due to $H_S$) and $\beta_u^{(a)}(t)$ stochastic processes. Control is introduced via user-defined control profiles $\{h_v(t)\}$ which, subject to system-dependent constraints (e.g., maximum amplitude, finite time-bandwidth product), determine the control capabilities $c$ in the error-free scenario. More precisely, we define the control capabilities $c$ as the set of control Hamiltonians $\{h_v(t)\}_{v \neq 0}$ that can be implemented in a given experiment. There are two aspects to this: the allowed control "directions" $\Lambda_v$ and the "control profiles" $h_v(t)$, usually parametrically defined by a pulse shape and a range for the specifying parameters, e.g., $h_v(t) \sim \theta e^{-\gamma^2/2\sigma^2}$ for $\theta \in [\theta_{\text{min}}, \theta_{\text{max}}]$ and $\sigma \in [\sigma_{\text{min}}, \sigma_{\text{max}}]$. Furthermore, multiplicative ($m$) control noise, which often arises in realistic settings [16,20,37], is captured by the stochastic processes $\beta_v^{(m)}(t)$.

Our main objects of interest are the time-dependent expectation values of system observables $O = O^1$ given by

$$E[O(T)]_{\rho_{SB}} = \langle \text{Tr}_{SB}[U(T)\rho_{SB}U^{-1}(T)(O \otimes I_B)] \rangle_c,$$

where $\rho_{SB}$ is the initial state of the joint system and bath. To obtain useful expressions for them we proceed as follows. The unitary propagator for the evolution generated by $H(t)$ is given (in units $\hbar = 1$) by the time-ordered exponential $U(t) = T_u e^{-i \sum_s H(s)}$ and $\langle \cdot \rangle_c$ denotes the average over realizations of the stochastic processes. We may write $H(t) = H_0(t) + H_{ct}(t)$, with $H_0(t)$ representing the intended, error-free controlled dynamics and the error component $H_{ct}(t)$ accounting for unwanted evolution due to environmental and control noise, as well as possibly $H_{ct}(t)$ if $H_{ct}(t)$ is at zero and no control noise is present, $\beta_v^{(m)}(t) = 0$. The evolution due to $H_0(t)$ can then be isolated by moving to the interaction (toggling) frame associated to the error-free component $H_0(t)$. That is, we let $U(t) = U_0(t)\tilde{U}(t)$, where

$$U_0(t) = T_u e^{-i \sum_s H_0(s)}, \quad \tilde{U}(t) = T_u e^{-i \sum_s H_0(s)},$$

and $\tilde{H}(t) = U^\dagger_0(t)H(t)U_0(t)$ is the toggling-frame Hamiltonian. By construction, such Hamiltonian vanishes in the absence of noise, and can be compactly written as

$$\tilde{H}(t) = \sum_{\alpha=a,m} \sum_{u,v} y_{u,v}^{(a)}(t)\Lambda_v \otimes B_u^{(a)}(t),$$

where we have defined $B_u^{(m)}(t) = \beta_v^{(m)}(t)1_B$ and the elements $y_{u,v}^{(a)}(t)$ of the control matrix $Y^{(a)}$ capture the effect of the control modulation on the noise terms $H_0(t)$. Explicitly, we have

$$y_{u,v}^{(a)}(t) = \text{Tr}_B[U_0(t)\Lambda_v U_0(t)\Lambda_u]/d,$$

$$y_{u,v}^{(m)}(t) = h_u(t)y_{u,v}^{(a)}(t).$$

Finally, assuming that $\rho_{SB} = \rho_S \otimes \rho_B$ (see Ref. [38] for a more general treatment), and that $O$ is invertible, with $\tilde{O}(T) = U_0^\dagger(T)O U_0(T)$, we write the desired time-dependent expectation value, Eq. (4), as

$$E[O(T)]_{\rho_S \otimes \rho_B} = \text{Tr}_S[V_O(T)\rho_S \tilde{O}(T)],$$

where the system operator

$$V_O(T) = \text{Tr}_B[\tilde{O}^{-1}(T)\tilde{U}^{-1}(T)\tilde{O}(T)\tilde{U}(T)\rho_B].$$
contains all the unwanted effects due to $H_c(t)$ up to time $T$; that is, $V_0(T) = I_S$ represents ideal, noise-free dynamics.

The operator $V_0(T)$ may be computed perturbatively, for instance through a Dyson or cumulant expansion \cite{24,39}. Regardless of what technique is chosen it can be shown that, due to time ordering, the dynamics depends on certain linear combinations of $L_c(t)$, of the multi-time noise correlation functions \{\(\langle B_{\nu_1}^{(a_1)}(t_{\mu_1}) \cdots B_{\nu_k}^{(a_k)}(t_{\mu_k}) \rangle\)\}, with respect to the combined quantum and classical averages, \(\langle \cdot \rangle \equiv \langle \text{T}\{\rho B\} \rangle_c\), with $a_j \in \{a, m\}$ and $\mu$ being an arbitrary permutation of $k$ elements, $k \in \mathbb{N}$. While the specifics of the linear combinations which enter the expectations in Eq. (5) depends on both $O$ and the details of the system and control setting, the possible contributions are determined by overlap integrals of the form (see Appendix A)

\[
\mathcal{T}^{(k)}_{\vec{\alpha}, \vec{\alpha}, \vec{v}}(T) = \int_0^T d_\vec{\alpha} d_\vec{v} \prod_{j=1}^k \langle \delta \phi_{\alpha_j}^{(a_j)}(t_j) \rangle L_c(\vec{v}, \vec{\alpha}),
\]

with $\int_0^T d_\vec{\alpha} d_\vec{v} \equiv \int_0^T d t_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{k-1}} dt_k$.

These integrals are key to understanding the effect of the noise on the system. The conventional approach to their analysis involves rewriting them as multi-dimensional overlap integrals in frequency space via an appropriate Fourier transform. This leads to the standard FF formalism \cite{24,34,35}, where frequency-domain FFs and, for general non-Gaussian noise, higher-order (poly-)spectra capture the effect of the control and noise, respectively. On the one hand, one expects that, by (experimentally) obtaining the value of such an integral for various FFs, it may be in principle possible to deconvolve it, and thus infer relevant information about the noise correlation functions (or their Fourier transform). This is indeed how QNS protocols work. On the other hand, one also sees that mitigating the effect of the noise is akin to minimizing the value of such integrals, which is the working principle behind existing decoherence suppression and optimal control protocols. The frequency- (or time-)domain representations, however, are agnostic to the control capabilities or constraints $\mathcal{C}$, which are unavoidable in any realistic setting, since the $\{h_n(t)\}$ cannot be arbitrarily chosen. Indeed, these constraints translate into limitations to the information that can be inferred about the noise (e.g., in comb-based QNS protocols the frequency-domain spectra are sampled via a discrete grid), or superfluous information used for synthesizing optimal control (e.g., rather than full knowledge of the noise correlation functions, only knowledge the overlap between noise and the admissible controls should be necessary). This motivates the search for a space – or a mathematical language – in which the relevant overlap integrals can be more efficiently represented by incorporating information about $\mathcal{C}$ from the outset.

III. FRAME-BASED FILTER FUNCTIONS AND CONTROL-DRIVEN MODEL REDUCTION

In order to meet the challenge identified in the previous section, instead of moving to the frequency domain we use the more general language of frames \cite{29,33}. Frames have a long tradition in signal processing, thanks to the flexibility they afford as compared to bases (e.g., in generalizing time-to-frequency-domain transforms) as well as to various properties particularly advantageous to signal reconstruction (e.g., robustness to noise \cite{40}). Moreover, they are already successfully exploited in different quantum applications \cite{38,41,42}. Leveraging the frame language in our context will first and foremost afford extra flexibility, as a frame can be chosen in a way that matches – in a sense that will be made precise later – the available control. In turn, aided by a change in point of view, this will allow us to efficiently represent each of the overlap integrals $\mathcal{T}^{(k)}$ as a sum over a finite domain, thereby achieving control-driven model reduction.

A. Basics on frames

The mathematical theory of frames is quite sophisticated and an exhaustive review of the topic is beyond our scope. While we refer the interested reader to the extensive literature for a more complete and rigorous account \cite{30,31,33}, we summarize here the basic definitions needed for the exposition of our result. We further discuss in Appendix B illustrative examples directly relevant to the control scenarios we analyze.

Let $\mathcal{H}$ be a complex (finite-dimensional or separable) Hilbert space, consisting of functions $f(t)$, $t \in [0, T]$, with inner product and norm given, respectively, by

\[
(f, g) \equiv \frac{1}{T} \int_0^T dt f(t)g^*(t), \quad \|f\|^2 \equiv (f, f).
\]

A discrete frame for $\mathcal{H}$ is an (at most) countable sequence $\mathcal{F} = \{\phi_n\}_{n}^\infty$, with $\phi_n \in \mathcal{H}$ and $n \in \mathbb{Z}$, satisfying the frame condition, that is,

\[
A\|f\|^2 \leq \sum_n |(f, \phi_n)|^2 \leq B\|f\|^2, \quad \forall f \in \mathcal{H},
\]

with $0 < A \leq B < \infty$ being the lower and upper frame bounds, respectively. Of particular interest are tight frames, for which $A = B$, and Parseval frames, for which, in addition, $A = B = 1$. Notably, an orthonormal basis in $\mathcal{H}$ is a Parseval frame, and indeed one sees that in this case the frame condition is equivalent to Parseval’s identity.

Frames may be seen as redundant (linearly-dependent) spanning sets for $\mathcal{H}$, More precisely, any $f \in \mathcal{H}$ can be expanded as $f(t) = \sum_n c_n \phi_n(t)$, $t \in [0, T]$, where the coefficients are given by the reconstruction formula,

\[
f(t) = \sum_n (f, \phi_n) \phi_n(t) = \sum_n (f, \phi_n) \tilde{\phi}_n(t),
\]

and $\{\tilde{\phi}_n\}_n$ are elements of a frame dual to $\mathcal{F}$. While a frame $\mathcal{F}$ may in general admit infinitely many dual frames, there exists a canonical dual frame $\mathcal{F}^*$ which is special, in the sense that it minimizes the norm of the expansion

\[
\sum_n |(f, \phi_n)|^2 \leq \sum_n |c_n|^2,
\]
for any sequence \( \{c_n\}_n \in \ell_2(\mathbb{Z}) \) that satisfies \( f = \sum_n c_n \phi_n \), with equality holding if and only if \( c_n = (f, \phi_n) \) for all \( n \).

Such a dual frame is determined by \( \tilde{\mathcal{F}} = \{\tilde{\phi}_n\} = \{S^{-1}\phi_n\} \), in terms of the positive frame operator \( S: \mathcal{H} \rightarrow \mathcal{H} \), given by
\[
Sf \equiv \sum_n (f, \phi_n)\phi_n.
\]

Note that \( S \) is a multiple of the identity if the frame is tight and it coincides with the identity for a basis, that is, an orthonormal basis is self-dual. Of special relevance to this work will be finite frames, \( \{\phi_n\}_n, n = 1, \ldots, N_{\#} < \infty \).

More generally, continuous frames for which the labelling index \( n \mapsto x \in X \) changes continuously can also be constructed. Given a measure space \( (X, \mathcal{W}, \mu) \), a family \( \mathcal{F} \equiv \{\phi_x\}_x \) is a continuous frame if (i) for all \( f \in \mathcal{H} \), \( (f, \phi_x) \) is \( \mathcal{W}\)-measurable in \( X \); and (ii) there exist constants \( 0 < A \leq B < \infty \) such that
\[
A\|f\|^2 \leq \int_X \|(f, \phi_x)\|^2 d\mu(x) \leq B\|f\|^2, \quad \forall f \in \mathcal{H}. \tag{10}
\]

From the above it follows that \( \mathcal{F} = \{\phi_x\}_x \in X = \mathcal{H} \), and an appropriate notion of dual frame and the reconstruction formula can be introduced by essentially replacing sums – as in Eq. (9) – with integrals of the form \( \int_X d\mu(x) \). In this way, the special case of a discrete frame is recovered when \( \mu \) is a counting measure and \( X = \mathbb{Z} \) (or \( \mathbb{N} \)). Prominent examples of continuous frame expansions are expansions into canonical and generalized coherent states and the continuous short-time Fourier (or Gabor) transform [33], whereas Fourier series are a special case of expansions into discrete exponential (or Fourier) frames [30, 31].

B. Standard-picture vs. control-adapted filters and spectra

To apply the frame formalism to our problem, we start by noting that there are two ways of representing any of the time-ordered integrals of Eq. (7). On the one hand, we can write the noise correlation function in the chosen frame and rewrite the remaining factors as a FFT associated to that frame. We dub this the “standard picture” (SP). On the other hand, we may expand the control matrix elements in the frame and have the remaining factors be the equivalent of a noise spectra in the frame language – resulting in what we dub the “control adapted” (CA) picture. Mathematically, these two approaches lead, respectively, to
\[
\mathcal{I}^{(k)}_{\alpha,\beta,v}(T) = \sum_{\bar{n}} F^{(k)}_{\alpha,\beta,v}(\bar{n}, T) S^{(k)}_{\alpha,\beta,v}(\bar{n}) \tag{15a}
\]
and
\[
\mathcal{I}^{(k)}_{\alpha,\beta,v}(T) = \sum_{\bar{n}} \left[ \prod_{j=1}^k F^{(1)}_{\alpha_j;\alpha_j,v_j}(n_j, T) \right] \tilde{S}^{(k)}_{\alpha,\beta,v}(\bar{n}). \tag{15b}
\]

Eq. (15a) represents the direct generalization to the (discrete) frame language of the standard frequency-domain representation: the \( k \)-th order frame-based FFs and frame-based power spectra are given, respectively, by
\[
F^{(k)}_{\alpha,\beta,v}(\bar{n}, T) = \int d\bar{t} \prod_j y^{(\alpha_j)}_{n_j, v_j}(t_j) \tilde{\phi}^{(\alpha_j)}_{n_j}(t_j)^*, \tag{16a}
\]
\[
S^{(k)}_{\alpha,\beta,v}(\bar{n}) = \int d\bar{t} \mathcal{L}_{\alpha,\beta,v}(\bar{t}) \prod_{i=1}^k \phi^{(\alpha_i)}_{n_i}(t_i). \tag{16b}
\]

where we allow for different frames \( \mathcal{F}^{(a)} \) for \( a \in \{a, m\} \). Indeed, as shown explicitly in Appendix B 1, the standard frequency-domain FF formalism [34, 35] is recovered when one uses a Fourier frame [33]. In contrast, Eq. (15b) does not only represent a generalization to the frame language; but, importantly for our purposes, it also provides a change in viewpoint – a dual representation in which
\[
F^{(1)}_{\alpha_j;\alpha_j,v_j}(n_j, T) = (y^{(\alpha_j)}_{n_j, v_j}, \tilde{\phi}^{(\alpha_j)}_{n_j}(t_j))^*, \tag{17a}
\]
\[
S^{(1)}_{\alpha_j;\alpha_j,v_j}(n_j) = \int d\bar{t} \mathcal{L}_{\alpha_j;\alpha_j,v_j}(\bar{t}) \prod_{i=1}^k \phi^{(\alpha_i)}_{n_i}(t_i), \tag{17b}
\]
amable fundamental FFs and the frame-based CA-spectra, respectively. Note that, in the CA representation, the time-ordering is moved from the FFs to the CA-spectra, with a twofold implication: on the one hand, as in the SP setting, the CA-spectra encode all the information about noise correlations that influence the system dynamics, as we will explicitly demonstrate in Sec. IV. On the other hand, the fact that the CA-FFs are all one-dimensional integrals without any time ordering makes their use more advantageous to both theoretical analysis and numerical implementation of C&C.

We also note that there is a degree of arbitrariness in the above definitions since, given a frame \( \mathcal{F} = \{\phi_n\} \) and its dual \( \mathcal{F}^* = \{\tilde{\phi}_n\} \), their corresponding complex conjugates (say, \( \mathcal{F}^* \) and \( \mathcal{F}^{*\dagger} \)) are also frames. In order to maintain a certain symmetry in our expressions, in this paper we will choose to expand in \( \mathcal{F}^* \) and \( \mathcal{F} \) in order to generate, respectively, the SP- and CA-formalism. For completeness, we summarize the resulting expressions in Tab. I.

C. Frame-based control-driven model reduction

The next key step in our approach is to observe that, as far as the effect of the noise on the system is concerned (captured by the operator \( V_0 \) in Eq. (5)), what matters are not the control inputs \( \{h_u(t)\} \) themselves, but rather their control matrix elements \( \{y^{(\alpha)}_{u,v}(t)\} \), which are related to the \( \{h_u(t)\} \) via conjugation under the known map \( U_0(t) \). Moreover, any constraints on \( h_u(t) \) (say, limited bandwidth, a minimum time between two consecutive pulses, or a finite time resolution) necessarily translate into limitations on the possible form that the \( y^{(\alpha)}_{u,v}(t) \) can take.

These observations, the flexibility of frames, and the CA representation of \( \mathcal{I}^{(k)}_{\alpha,\beta,v} \) come together as follows: (i) for given
control capabilities $\mathcal{C}$, the possible $\{y_{u,v}(t)\}$ are known; (ii) it is in principle possible to tailor the choice of frame $\mathcal{F}^{(\alpha)}$ so that it “efficiently” represents such $\{y_{u,v}(t)\}$; (iii) this, in turn, leads to an “efficient” representation of the integrals in $T^{(k)}_{\alpha;u,v}$. More formally, we introduce the following condition:

**Definition [Finite-size frame (FSF) condition].** Let $\mathcal{C}$ specify fixed control capabilities, which determine a (possibly infinite) set of control matrix elements, $y_{u,v}^{(\alpha)}(t) \in L^2([0,T[)$, $\alpha \in \{a,m\}$. We say that the FSF condition holds if one can build finite-size frames $\mathcal{F}^{(\alpha)} \equiv \{f_n^{(\alpha)}\}$, $n = 1, \ldots, N^{(\alpha)}$, and dual frame $\tilde{\mathcal{F}}^{(\alpha)}$, such that for all $y_{u,v}^{(\alpha)}(t)$ allowed by $\mathcal{C}$,

$$y_{u,v}^{(\alpha)}(t) = \sum_{n=1}^{N^{(\alpha)}} F_{\alpha;u,v}^{(1)}(n,t) f_n^{(\alpha)}(t).$$

We say that the FSF condition is satisfied to tolerance $\varepsilon \geq 0$ over $[0,T]$ if the above equality can be approximately obeyed with error no larger than $\varepsilon$ (in the $L^2$ norm).

If the FSF condition holds, the $\{y_{u,v}^{(\alpha)}(t)\}$ are represented efficiently in the sense that they are well approximated by a finite expansion over the elements of $\mathcal{F}^{(\alpha)}$. It then follows that

$$T^{(k)}_{\alpha;u,v}(T) \simeq \sum_{n_1=1}^{N^{(\alpha)}} \left( \prod_j F_{\alpha;u,v}^{(1)}(n_j) \right) \tilde{S}^{(k)}_{\alpha;u,v}(\tilde{n}).$$

That is, each integral can be efficiently represented by a finite sum up to an error which scales as $O(\varepsilon k)$. A key consequence of the above is that it allows us to identify the components of the noise that are relevant to the dynamics allowed by $\mathcal{C}$, namely, the finite set of CA-spectra,

$$\mathcal{S}|_{\mathcal{C}} = \{ \tilde{S}^{(k)}_{\alpha;u,v}(\tilde{n}) \}, \quad n_j \in [1, N^{(\alpha)}],$$

(20)

(or specific combinations thereof) that contribute to the expectations of observables as in Eq. [5]. Thus, $\mathcal{S}|_{\mathcal{C}}$ represents both the information that can be extracted from the reduced system dynamics, and what suffices to optimally control it, under the resource constraints $\mathcal{C}$, i.e., a model-reduced description of the noisy dynamics. Generally, there will be a trade-off between the model-reduction properties of the frame and the accuracy: a larger frame will lead to a smaller $\varepsilon$, which however necessarily implies that each $T^{(k)}_{\alpha;u,v}(T)$ is represented by a sum over a larger domain.

It is clear then why there is a need for a flexible language: one must design $\mathcal{F}$ according to $\mathcal{C}$. The frame language provides a constructive and relatively straightforward mechanism to do so. For instance, one can choose as frame elements a subset of the possible $y_{u,v}^{(\alpha)}(t)$, say $\mathcal{C}_0$, and expand every control matrix element in terms of this subset via Eq. [9]. If $\mathcal{C}_0$ is chosen adequately, the error $\varepsilon$ in the reconstruction can be made small, and an accurate model reduction is achieved. This ($\mathcal{F} = \{y(t)|_{\mathcal{C}_0}\}$) will be essentially how we build our

| (i) Standard-Picture (SP) | (ii) Control-Adapted (CA) |
|--------------------------|--------------------------|
| $L_{\alpha;u,v}(\tilde{t}) = \sum_{\alpha} \left( L_{\alpha;u,v}(\tilde{t}), \prod_i \phi_{\alpha_i}^{(\alpha)}(s_i) \right) \prod_j \phi_{\alpha_j}^{(\alpha)}(t_j)$ | $\prod_j y_{u,v}^{(\alpha)}(t_j) = \prod_j \sum_{\alpha} \left( y_{u,v}^{(\alpha)}(s_j), \phi_{\alpha_i}^{(\alpha)}(s_j) \right) \phi_{\alpha_j}^{(\alpha)}(t_j)$ |
| $= \sum_{\alpha} S_{\alpha;u,v}^{(k)}(\tilde{n}) \prod_j \phi_{\alpha_j}^{(\alpha)}(t_j)$ | $= \prod_j \sum_{\alpha} F_{\alpha;u,v}^{(1)}(n_j) \phi_{\alpha_j}^{(\alpha)}(t_j)$ |
| $F_{\alpha;u,v}^{(k)}(\tilde{n}) = \int d\tilde{t}_k \prod_j y_{u,v}^{(\alpha)}(t_j) \phi_{\alpha_j}^{(\alpha)}(t_j)$ | $F_{\alpha;u,v}^{(1)}(n_j) = \int dt y_{u,v}^{(\alpha)}(t) \phi_{\alpha_j}^{(\alpha)}(t)$ |
| $\tilde{T}^{(k)}_{\alpha;u,v} = \sum_{\alpha} F_{\alpha;u,v}^{(k)}(\tilde{n}) S_{\alpha;u,v}^{(k)}(\tilde{n})$ | $\tilde{S}_{\alpha;u,v}^{(k)}(\tilde{n}) = \int d\tilde{t}_k L_{\alpha;u,v}(\tilde{t}) \prod_j \phi_{\alpha_j}^{(\alpha)}(t_j)$ |
| Table I. Summary of the defining relationships for standard (i) vs. control-adapted (ii) pictures. The corresponding frequency-domain SP and CA representations are also included in (iii) and (iv) for comparison.
frames in this paper, as it greatly simplifies the CA-QNS problem: if one chooses as control for a QNS protocol an element of $C_0$, the sum in Eq. 19 can reduce to a single term. Now, while a full CA-QNS protocol is not as simplistic as that, this observation gives a glimpse into how much the “correct” language can simplify the task. Notice that such a simplification could not be achievable in general if one insists on considering only expansions in orthonormal bases, as the $y_{u,v}^{(a)}(t)$ are typically not orthogonal to each other.

Clearly, our choice for $f$ is not unique and other ways of building a convenient frame may be possible, depending on the task at hand. In general, this problem is related to that of building a parsimonious model — in the language of the model-reduction literature [44] — which in our context characterizes the ability of the chosen frame to approximate the elements of the control matrix. We leave it to future work to explore what frame, for fixed control capabilities $C$, allows for maximum parsimony while retaining sufficient predictive power. We stress, however, that the key is tying the choice of $f$ to the available $C$ and the tolerance $e$. This follows the reasoning that if $C$ changes, then the components of the noise that affect the quantum system also change. Indeed, given a change $C \rightarrow C'$ the first step should be verifying that $f$ still satisfies the FSF condition to an acceptable $e$. Now, the change in $f$ can take many forms depending on the change in $C$. It can be as radical as completely changing the functional form of the frame elements or as simple as adding more elements to the original frame. The former is necessary when, for example, the accessible control profiles change from $h_u(t) \sim e^{-(t-\tau)^2/2\sigma^2}$ to $h_u'(t) \sim e^{-(t-\tau)^2/2\sigma^2}$ in the case of additive noise, described as before by $\sigma\mathcal{N}(0, \mathcal{N})$. In contrast, the latter type of change would be sufficient, for example, when the shape of the profiles $h_u(t)$ remains the same but the range of the defining parameters changes, e.g., to $\sigma \in [\sigma_{\min}', \sigma_{\max}']$.

IV. FRAME-BASED APPROACH TO CHARACTERIZATION AND CONTROL

A. From noise and control assumptions to frame construction

We are now ready to deploy our tools. To do so, we first introduce a multiqubit system control problem and show that the same frame can be used irrespective of the number of qubits, as long as the control constraints are homogeneous. We will exemplify the frame construction for both instantaneous and non-instantaneous control settings and use these in the two key applications we anticipated: QNS beyond the standard frequency domain and noise-tailored optimized gate design.

1. The multiqubit model system

To demonstrate the usefulness of our formalism, we now specialize our system to $N$-qubits, and correspondingly take $\{\Lambda_u\} \equiv \{\Sigma_u\}$ to be the usual Pauli product-operator basis, with $u \in \{0, \ldots, 4^N - 1\}$ and $\Sigma_0 = I^{\otimes N}$. The qubits are exposed to additive noise, described as before by $B_u^{(a)}(t) = B_u^{(a)}(t) + \beta_u^{(a)}(t) I_B$, along with multiplicative control noise which, for simplicity, we assume to be isotropic, $B_u^{(m)}(t) \equiv \beta_u^{(m)}(t) I_B$, for all $u$. We focus on the paradigmatic scenario in which $C$ comprises $M$ non-overlapping pulses of duration $\tau \equiv T/M$ applied over $[0, T]$, implemented by

$$H_{\text{ctrl}}(t) = \left(1 + \beta^{(m)}(t)\right) \sum_{j=1}^M \theta_j h(t_j, t) \mathcal{N}(j). \Sigma/2,$$  \hspace{1cm} (21)

where $\Sigma$ excludes $\Sigma_0$, $\mathcal{N}(j) \in \mathbb{R}^{4^N-1}$, $\|\mathcal{N}(j)\| = 1$ and $\theta_j \in [0, 2\pi]$ specifies the $j$th pulse, described by a fixed (normalized) control profile $h(t_j, t)$ and proportional to a window function $W_{j,\tau}(t)$ defined via

$$W_{j,\tau}(t) \equiv \begin{cases} 1 & (j-1)\tau \leq t < j\tau, \\ 0 & \text{otherwise}. \end{cases}$$  \hspace{1cm} (22)

The above form of $H_{\text{ctrl}}(t)$ is general enough to support single- or multi-body Hamiltonian controls, although in a realistic system one would typically be limited to at most two-body Hamiltonians. To simplify our calculations, however, we demand that the possible control inputs $h_u(t)$ are the same regardless of $\Sigma_u$, that is, the same control constraints apply to any of the possible $H_{\text{ctrl}}(t)$.

Under the above assumptions, one realizes that the form of the frame is independent of the number of qubits, as we will show. Mathematically, the finite support of $h(t_j, t)$ implies that one can write $U_0(t)$ as a piece-wise function given by

$$U_0(t) = U_j \prod_{\ell=1}^{j-1} U_\ell, \quad t \in [(j-1)\tau, j\tau],$$

where

$$U_j = e^{-it \int_{(j-1)\tau}^t ds h(t_j, s)},$$

$$\psi_j^{(j)} = \int_{(j-1)\tau}^t ds \mathcal{N}(t),$$

with $\mathcal{N}(t) = U_j U_0(t) U_j^{\dagger}$. In turn, this leads to a toggling-frame Hamiltonian (Eq. 3) of the form

$$\bar{H}(t) = \sum_{u,v} [y_{u,v}^{(a)}(t) \Sigma_u \otimes B_u^{(a)}(t) + y_{v}^{(m)}(t) \beta^{(m)}(t) \Sigma_v].$$  \hspace{1cm} (24)

Here, the additive control matrix elements are given by

$$y_{u,v}^{(a)}(t) = \frac{1}{2^N} \text{Tr}[U_0(t) \Sigma_u U_0(t) \Sigma_v] = \frac{1}{2^N} \sum_{u=0}^{4^N-1} \sum_{w=0}^{4^N-1} c_{u,w}^{(j-1)} \text{Tr} [U_j^{\dagger} \Sigma_u U_j \Sigma_w].$$  \hspace{1cm} (25)

for $t \in [(j-1)\tau, j\tau]$, where we have used that

$$(\prod_{\ell=1}^{j-1} U_\ell) \Sigma_u (\prod_{\ell=1}^{j-1} U_\ell) = \sum_{w} \text{Tr} [(\prod_{\ell=1}^{j-1} U_\ell) \Sigma_u (\prod_{\ell=1}^{j-1} U_\ell) \Sigma_w] \Sigma_w/2^N = \sum_{w} c_{u,w}^{(j-1)} \Sigma_w/2^N.$$ 

In this approach, we have considered that $W_{j,\tau}(t)$ is a step function, which allows for a straightforward implementation of the control pulses. However, in a more practical scenario, $W_{j,\tau}(t)$ could be a more continuous function, such as a Gaussian pulse, which would require the evaluation of integrals instead of products. In any case, the key advantage of this approach is that it allows for the design of optimized control pulses that are tailored to the specific noise environment of the quantum system.
This ultimately leads to

$$y_{u,v}^{(a)}(t) = \sum_{w=0}^{m-1} c^{(j-1)}_{v,v,w} \left( k_{j,\tau,v,w}^{(0)} \cos[\theta_j \psi_t^{(j)}] p_t(\vec{n}(j)) \right)$$

$$+ k_{j,\tau,v,w}^{(1)} \sin[\theta_j \psi_t^{(j)}] p_t(\vec{n}(j)) + k_{j,\tau,v,w}^{(2)},$$

(26)

where \( k_{j,\tau,v,w}^{(s)} \) and \( p_t(\vec{n}(j)) \) are polynomials of the elements of \( \vec{n}(j) \), whose values can be numerically calculated (from Eq. \( (25) \)) given a fixed number of qubits \( N \).

The multiplicative control matrix elements can be similarly calculated, by noting that \( h(t_j, t) \) is assumed to be compactly supported in \([j-1], j, \tau \]. Thus,

$$U_0(t)^\dagger (h(t_j, t) \vec{n}(j) \cdot \vec{\Sigma}) U_0(t) =$$

$$h(t_j, t) \left( \prod_{\ell=1}^{j-1} U_\ell \right) \vec{n}(j) \cdot \vec{\Sigma} \left( \prod_{\ell=1}^{j-1} U_\ell \right),$$

for \( t \in [j-1], j, \tau \), since \( U_j(\vec{n}(j) \cdot \vec{\Sigma}) U_j^\dagger = \vec{n}(j) \cdot \vec{\Sigma} \). It follows that

$$y_v^{(m)}(t) = \left( \sum_{w} \eta_w^{(j)} u_{v,w}^{(j-1)} \right) h(t_j, t) \theta_j / 2. \quad (27)$$

2. The frame

The important consequence of the above calculations is that \( y_{u,v}^{(a)}(t) \) is spanned by the functions \( \{ W_j, \tau(t) \sin[\eta \psi_t^{(j)}], W_j, \tau(t) \cos[\eta \psi_t^{(j)}] \} \), for some \( \eta \) and \( W_j, \tau \), while the \( y_v^{(m)}(t) \) are spanned by the \( h(t_j, t) \). Given this, it is then natural to use as frames

$$\mathcal{F}_{(a)}^{(\eta)} \equiv \{ W_j, \tau \cos[\eta \psi_t^{(j)}], W_j, \tau \sin[\eta \psi_t^{(j)}] \},$$

$$\mathcal{F}_{(m)}^{(\eta)} \equiv \{ h(t_j, t) \},$$

$$j \in [1, M], \quad \eta = 2\pi k / N_\#, \quad k \in [0, N_\#],$$

(28)

where \( N_\# \) is a free parameter which determines the size of the frame and the tolerance \( \varepsilon \), i.e., how well the FSF condition is satisfied. We note that while a finite \( N_\# \) implies a non-zero \( \varepsilon \), the latter decreases as \( N_\# \) grows: if \( \mathcal{F}_{(a)}^{(\eta)} \) contains all admissible \( y_{u,v}^{(a)}(t) \), the FSF is exactly satisfied (\( \varepsilon = 0 \)). Moreover, the non-overlapping nature of the pulses implies that the error \( \varepsilon |_{M} \) for an \( M \)-pulse control matrix grows only linearly with \( M \), i.e., \( \varepsilon |_{M} \sim O(M, \varepsilon |_{1}) \) for a frame with \( N_\# = M(2N_\# + 1) \) elements. A larger \( N_\# \) can thus be chosen so that \( \varepsilon |_{M} \) is below a user-defined tolerance \( \varepsilon \) as \( M \) increases.

The remaining missing element in our description of the model is the control capabilities \( \mathcal{S} \). This is where the frame construction shows its flexibility in dealing with various types of control. For illustration, we will consider two scenarios:

- First, we address the important limiting case in which control is enacted via perfect, instantaneous pulses. In this case, \( \beta^{(m)}(t) = 0 \) and \( h(t_j, t) = \delta(t - j \tau) \), leading to piecewise-constant “switching functions” \( \{ y_{u,v}^{(a)}(t) \} \). Given this, \( \mathcal{F}_{(a)}^{(\eta)} \) reduces to a collection of window functions \( \{ W_j, \tau \}_{j=1}^{M} \), for which the FSF holds exactly, with \( N_\# = M \).

Thus, in this case, any digital basis suffices as a finite \( \mathcal{F}_{(a)}^{(\eta)} \), and an especially compelling choice is provided by the Walsh functions, thanks to their potential for minimizing sequencing complexity [45-47].

- Second, we consider a windowed Gaussian control profile, \( h(t_j, t) = W_j, \tau e^{-(t-t_j)^2/2\sigma^2} \), with \( \sigma = 1 \mu s, \tau = 10 \mu s \), although other possibilities, such as square or Slepian pulses [20], can be easily accommodated. With \( M = 1 \) and \( \mathcal{F}_{(a,m)}^{(\eta,\tau)} \) as above, one finds that \( \varepsilon |_{N_\# = 2} = 2.4 \cdot 10^{-5} \) i.e., a 1.1% relative error [48], whereas \( \varepsilon |_{N_\# = 4} = 2.8 \cdot 10^{-8} \), i.e., a 0.0014% relative error. That is, a modest-size frame ensures the FSF condition is basically satisfied. Exemplifying the \( M \) and \( N_\# \) interplay, for \( M = 100 \) pulses, a value of \( N_\# = 4 \), i.e., an \( N_\# = 900 \) elements frame, ensures an overall error \( \sim 0.15\% \).

The above highlights the aforementioned trade-off between model-reduction and accuracy, highlighting the importance of building a (maximally) parsimonious frame – our choice here need not be optimal as is only meant as a proof-of-principle. Moreover, we note that the dynamics of the system generally depends on linear combinations of the \( \mathcal{F}_{(a,m)}^{(\eta,\tau)} (k \leq k_{\text{max}}) \), where the number of terms is typically a function of the range of the values the indices \( \{ u, v, \alpha \} \) can take. Accordingly, one must ensure that the error in each \( \mathcal{F}_{(a,m)}^{(\eta,\tau)} \) and also in the relevant linear combinations is small. Ultimately, this implies that while the form of the frame is the same regardless of the dimension of the system \( d \), the number of non-overlapping pulses \( M \), or the largest order of perturbation being considered \( k_{\text{max}} \), the tolerance \( \varepsilon \) must be small enough – and thus \( N_\# \) must be large enough – so that the overall error is below a user-defined tolerance for a given \( d, M \), and \( k_{\text{max}} \).

3. Case study: Single-qubit reduced dynamics

The final step is to obtain the expectation values of system’s observables, \( E[O(t)]_{\rho_0 \otimes \rho_{P_{\psi}}} \). To simplify our expressions and the analysis in the illustrative applications, we shall specialize in what follows to the simplest paradigmatic setting of a single-qubit dephasing model. Thus, we consider additive noise only along one direction, \( B_{u}(t) \equiv B_z(t) \), whereas the multiplicative noise will be present, as in Eq. \( (24) \), whenever the control is assumed to be imperfect. Noting that in this scenario the \( \Sigma_{u} \) reduce to the single-qubit Pauli operators \( \sigma_u \), \( u \in \{ x, y, z \} \), Eq. \( (26) \) simplifies to

$$y_v^{(a)}(t) \equiv y_v^{(a)}(t) =$$

$$\sum_{u} c_{u,v}^{(j-1)} \left( k_{j,v}^{(0)} \cos[\theta_j \psi_t^{(j)}] + k_{j,v}^{(1)} \sin[\theta_j \psi_t^{(j)}] + k_{j,v}^{(2)} \right). \quad (29)$$

Further, we enforce in our model that the multiplicative and additive noise sources are uncorrelated, i.e.,
(B^{(m)}(t_1)B^{(a)}(t_2)) = (B^{(m)}(t_1))(B^{(a)}(t_2)) = 0. We do not, however, require stationarity nor Gaussianity.

In a suitable weak-coupling regime where, formally, max \{t_1, \ldots, t_k \} \langle B^{(\alpha)}(t_1) \cdots B^{(\alpha)}(t_k) \rangle T^2 \ll 1, Eq. (5) becomes

\[ E[O(T)]_{\rho_S \otimes \rho_B} \approx \langle \operatorname{Tr}_S \left( (I_S - D^{(2)}_\alpha(T)) \rho_S O(T) \right) \rangle, \]

where the second-order Dyson term \( D^{(2)}_\alpha(T) \) can be written as a functional of a reduced set of CA-spectra. Specifically, the components of the spectra relevant to \( C \) are found to be (see Appendix C for full detail)

\[ \tilde{S}_\alpha \in \{ \tilde{S}_\alpha^+(n,n'), (\tilde{S}_\alpha^-(n,n') - \tilde{S}_\alpha^-(n',n)) \}, \]

for \( n \in [1,N_y] \) and \( \alpha \in \{ a, m \} \), where \( \tilde{S}_\alpha^{\pm} \) are associated to the “classical” \((+)\) and “quantum” \((-)\) two-point bath correlation functions [13],

\[ C^{(\alpha)}_\pm(t_1,t_2) = \langle [B^{(\alpha)}(t_1),B^{(\alpha)}(t_2)]_\pm \rangle, \]

with \( [A,A']_\pm \equiv AA' \pm A'A \). Since only FFs \( \{ F_{\alpha,u}^{(1)}(n,T) \} \) allowed by \( \mathcal{C} \) can be generated, only the above noise parameters can be inferred from the reduced dynamics via CA-QNS. Still, such finite information suffices for the prediction - and eventual optimization - of the qubit dynamics at time \( T \) under any of the (infinite) control sequences allowed by \( \mathcal{C} \).

### B. QNS beyond frequency domain

Regardless of whether multi-pulse or continuous control modulation is employed (such as, respectively, in comb-based [19] or Slepian- [20] and spin-locking-based [15, 21] protocols), existing QNS methods largely rely on the possibility to describe the noise properties in the frequency domain. This prevents applicability to non-stationary noise [27, 28] as well as noise with singular correlation functions [49], which must be described in the time domain.

To illustrate how such limitations are overcome in our frame-based approach, in this section we implement CA-QNS via instantaneous perfect pulses applied at separate uniform intervals over a total time \( T \). We thus specialize the control Hamiltonian in Eqs. (21)-(22) to

\[ H_{\text{ctrl}}(t) = \sum_{j=1}^M \delta(t - j\tau)\theta_j \tilde{n}^{(j)} \cdot \vec{\sigma}/2, \]

where \( M \) is now the number of intervals and \( \tau = T/M \) is the minimum separation time between pulses (that is, each pulse is applied at a non-zero multiple of the minimum "switching-time" \( \tau > 0 \) [50]). A direct specialization of Eq. (29) reveals that the control matrix elements \((i)\) are necessarily linear combinations of \( \{ W_{t_1,\tau} \cos[\theta_{j} \tilde{n}_j^{(j)}], W_{t_1,\tau} \sin[\theta_{j} \tilde{n}_j^{(j)}] \} \); and \((ii)\) satisfy the constraints \( \langle y_{u}^{(a)}(t) \rangle \in [-1,1] \); and \( \sum_j |y_{u}^{(a)}(t)|^2=1 \). As discussed in Sec. IV A, a suitable (self-dual) frame in this case is the Walsh basis, which obeys the FSF condition exactly \( (\varepsilon = 0) \). In our CA-QNS protocol, we chose \( \theta_j \in \{ 0, \pi/2, \pi \} \) and \( \tilde{n}^{(j)} = (0,1,0) \), for all \( j \). In contrast with previous Walsh-based characterization methods [47], the use of non-\( \pi \) pulses now makes it possible to generate control matrix elements \( \{ y_{u}^{(a)}(t) \} \) that are linear combinations of Walsh functions with \( M \) switches over the time range \( [0,T] \). This leads to the ability to infer the Walsh-basis CA-spectra \( \tilde{S}_\alpha^\pm(n,n') \) for all \( n,n' \), not only generalizing the approach of [47] beyond reconstruction of signals with a finite number of frequency components, but allowing reconstruction of non-stationary noise.

In particular, we apply the CA-QNS protocol to two distinct settings: (i) a classical non-stationary Wiener process; and (ii) a genuinely quantum (bosonic) non-stationary environment. Our task will be to show that the protocol provides sufficient information about the correlation functions, which in turns allows one to infer the parameters describing the noise model under consideration. Full detail about the sequences we used is included in Appendix C2.
Example 1. Non-stationary noise from a classical time-dependent diffusion process

Motivated by the physical setting described in [27], we consider noise induced by a random walk of molecules in solution, resulting in translational diffusion in the presence of an external magnetic field – a process ubiquitously encountered in liquid-state NMR and beyond. The relevant dephasing Hamiltonian may be written as

\[ H(t) = \sigma_z \cdot h \gamma_M G \beta(t) \equiv \sigma_z B(t), \]

where \( \gamma_M = 2.67 \cdot 10^8 \text{ rad s}^{-1} \text{T}^{-1} \) is the gyromagnetic ratio of protons, \( G = 0.0214 \text{ T m}^{-1} \) is a constant magnetic gradient along \( z \), and \( \beta(t) \) is a Gaussian stochastic process representing the Brownian excursions of the molecule. That is,

\[ \langle \beta(t) \rangle = 0, \quad C(t_1, t_2) \equiv \langle \beta(t_1) \beta(t_2) \rangle = D \min(t_1, t_2), \]

with \( D \) being the molecular diffusion constant. While the non-stationary nature of the process is evident – \( C(t_1, t_2) \) is not invariant under an arbitrary shift in time – we further assume here that the diffusion constant varies periodically in time according to \( D \rightarrow D \cos(\nu t_1) \cos(\nu t_2) \), where \( \nu \) is an unknown angular frequency (see Fig. 1a). This renders the modified process \( \beta(t) \) second-order cyclostationary [51], with

\[ C(t_1 + 2\pi n/\nu, t_2 + 2\pi n/\nu) = C(t_1, t_2), \quad \forall t_1, t_2, n \in \mathbb{Z}. \]

We further assume that, for each of the control experiments required by a QNS protocol, the system is re-initialized, i.e., the diffusion process is also effectively reset.

Applying the CA-QNS protocol, we estimate the CA-spectra, \( \mathcal{S}^{(+)}(n, n') \) (notice that in this case \( \mathcal{S}^{(-)}(n, n') = 0 \)) and, from there, the digitized correlation function \( \langle |B(t_1), B(t_2)|_\pm \rangle \) by using the general relation

\[ \langle |B(t_1), B(t_2)|_\pm \rangle \equiv \sum_{n,n'} (\mathcal{S}^{(\pm)}(n, n') \pm \mathcal{S}^{(\pm)}(n', n)) \tilde{\phi}_n(t_1) \tilde{\phi}_{n'}(t_2). \]
The result of the digital reconstruction is shown in Fig. 1. In addition, by leveraging the knowledge of the physical origin of the noise, we infer the parameters in the model Hamiltonian, $P \equiv \{D, \nu\}$ (see Tab. I), by following an approach we outline in more detail in Example 2 below. It should be noted that the accuracy in the estimation of the parameters relies on the control capabilities. While in our example the given $T = 40 \text{ ms}$ and $M = 16$ suffice to achieve a good estimation, this need not be the case in general, as we exemplify next.

**Example 2. Non-stationary noise from a quantum time-dependent bosonic environment**

Consider now a scenario where the qubit couples to a two-mode bosonic environment via a periodically varying coupling operator, that is,

$$B(t) = \sum_{\ell=1}^{2} g_{\ell}(t)(e^{i\Omega_{\ell} t} a_{\ell}^\dagger + \text{H.c.}), \quad g_{\ell}(t) = \bar{g}_{\ell} \cos(w_{\ell} t).$$

Again, the time dependence in the couplings makes the noise non-stationary, as $\langle B(t_1) B(t_2) \rangle$ is manifestly a function of both $t_1 + t_2$ and $t_1 - t_2$, although periodic in the former. Also, we assume that the initial state of the bath is thermal, $\rho_B \propto e^{-\sum_{\ell=1}^{2} \beta_{T_{\ell}} (a_{\ell}^\dagger a_{\ell})}$, with $\beta_{T_{\ell}} \equiv 1/k_B T_{\ell}$, so that $\langle B(t) \rangle_c = 0$, and the symmetric and anti-symmetric part of the correlation function can be written, respectively, as

$$\langle [B(t_1), B(t_2)]_+ \rangle_c = \sum_{\ell} |\bar{g}_{\ell}|^2 \left( \cos(w_{\ell}(t_1 + t_2)) + \cos(w_{\ell}(t_1 - t_2)) \right) \cos(\Omega_{\ell}(t_1 - t_2)) \text{coth}(\hbar \beta_{\ell} \Omega_{\ell}/2),$$

$$\langle [B(t_1), B(t_2)]_- \rangle_c = -i \sum_{\ell} |\bar{g}_{\ell}|^2 \left( \cos(w_{\ell}(t_1 + t_2)) + \cos(w_{\ell}(t_1 - t_2)) \right) \sin(\Omega_{\ell}(t_1 - t_2)).$$

Applying the CA-QNS protocol described earlier, one can infer $S(\pm)(n, n')$, $S(\pm)(n, n') - \tilde{S}(\pm)(n, n')$, and, from there, obtain a digital reconstruction (by using Eq. (30)) of both the classical and quantum components of the correlation function. While this information is also crucial for control, in this section we focus only on the open-system characterization aspect of our problem, i.e., leveraging the information CA-QNS provides and knowledge of the noise model to estimate the relevant parameters. We execute the protocol for two resolutions $\tau = T/M$, namely, for $T = 1536 \text{ ps}$, $M = 16$ and $T = 16 \text{ ps}$, $M = 16$. The resulting reconstructions are presented in Fig. 2 and Fig. 3 respectively, which reveal the impact of the time resolution. As Fig. 2 demonstrates, the coarse resolution reconstruction does not detect the effect of the fast oscillations. Equipped only with this information, it is not possible to infer the value of comparatively large frequencies with high accuracy. In contrast, the high-resolution reconstruction – consistent with a minimum inter-pulse timing of 1 ps (see Fig. 3) – can detect the fast oscillations in our model, and allows us to accurately estimate all the model parameters. By using both the low and high resolution, we infer the physical parameters as follows. The parameters of interest are the set

$$P \equiv \{w_1, w_2, \Omega_1, \Omega_2, \bar{g}_1, \bar{g}_2, T_1, T_2\}.$$

Assuming knowledge of the model, we estimate them by minimizing a cost function

$$C_{\delta}(P) \equiv \sum_{\mu=\pm} \sum_{n,n'=1}^{N_\delta} \left( S^{(\mu)}(n, n')|_P - \tilde{S}^{(\mu)}(n, n') \right)^2,$$

where the $S^{(\pm)}(n, n')|_P$ is calculated from the assumed model for a given set of parameters $P$, and $\tilde{S}^{(\pm)}(n, n')$ is estimated as $\tilde{S}^{(\pm)}(n, n') = \tilde{S}^{(\pm)}(n, n') \pm \tilde{S}^{(\pm)}(n', n)$, with the input spectra calculated from the $\mathbb{R}[\xi]$. We perform the optimization, $\arg\min_{P} C_{\delta}(P)$, in two settings: (i) with only the low (or coarse) resolution $\mathbb{R}[\xi]$; and (ii) combining both the low- and high-resolution information. As expected, the optimization in the first approach only accurately estimates the parameters corresponding to the slow frequencies, but not the high frequency generating the fast oscillations in the correlation functions. In contrast, in the second more powerful approach, we estimate all the parameters of interest with high accuracy (assuming no other source of error but the digitization of the reconstruction induced by the available control). We summarize our estimation results in Tab. II. We highlight that the example above shows that it is possible to perform “local bath thermometry” using a single qubit probe in a “short-time” regime, in contrast with existing approaches for stationary noise, which require either a steady-state regime [52] or multiple probes [18].

### C. Control-adapted noise-tailored optimized gate design

Beyond the task of bath characterization, and perhaps more relevant to the implementation of quantum technologies, one can leverage the information QNS provides to achieve high-fidelity operations, by tailoring the control to the noise affecting the qubit, via numerical optimal control algorithms [8] or geometric techniques [53]. While the details are method-dependent, and the underlying non-Markovian dynamics may be modeled in different forms (i.e., via a master equation or
Table III. Actual and estimated physical parameters in two-mode bosonic model described by Eq. (31a) and Eq. (31b). The second row shows the actual parameters of the model. The third and the fourth row show the estimated parameter using CA-spectra from coarse reconstruction only and both coarse and fine reconstruction, respectively.

|                | $\tilde{g}_1/\hbar$ (MHz) | $\tilde{g}_2/\hbar$ (MHz) | $\Omega_1$ (GHz) | $\Omega_2$ (GHz) | $w_1$(GHz) | $w_2$(GHz) | $\frac{\hbar}{e}\tau_1$ (ps) | $\frac{\hbar}{e}\tau_2$ (ps) |
|----------------|-----------------------------|-----------------------------|------------------|------------------|------------|------------|-----------------------------|-----------------------------|
| Actual         | 976.56                      | 345.27                      | 3.07             | 184.08           | 4.09       | 30.68      | 61.44                       | 2.05                        |
| Coarse         | 976.55                      | 317.80                      | 3.07             | 179.63           | 4.09       | 25.93      | 61.44                       | 2.03                        |
| Coarse and Fine| 976.56                      | 345.27                      | 3.07             | 184.08           | 4.09       | 30.68      | 61.44                       | 2.05                        |

Figure 3. (Color online) (a) Actual anti-symmetric (quantum), component of the correlation function, and (b) their corresponding digital reconstruction, in units of (10^3 GHz)^2 for $T = 16$ ps and $M = 16$. While the resolution is $\tau = 1$ ps = $\frac{16}{1536} = 0.1036$ ps, equivalent to performing a digital reconstruction on a total time of 1536 ps with a $1536 \times 1536$ grid, notice that in the reconstruction with $T = 16$ ps, the slow oscillations cannot be appreciated.

The key point, however, is that while given limited control capabilities $\mathcal{C}$, one cannot characterize such correlation functions in full, but rather only the portion of them which is relevant to $\mathcal{C}$. While the intuition rings true, namely, one can only infer what is needed as an input.

To demonstrate this, we consider the task of executing a target quantum gate $G$ with the highest possible fidelity. Importantly, we will assume no a priori knowledge of the noise correlation functions and, in contrast to the previous subsection, we will consider the realistic setting of noisy bounded-strength (non-instantaneous) control. Specifically, we will restrict our control capabilities $\mathcal{C}$ to the scenario where $h_{\alpha}(t)$ in each of the $M = 2$ pulses has a Gaussian shape, and a total execution time $T = 10 \mu s$. In the non-Markovian setting, achieving a high-quality operation implies minimizing an appropriate cost function, which is a functional of the overlap integrals $I_{\mathcal{G},\mathcal{C}}(T)$ and whose explicit form depends on the perturbative expansion of choice. While many choices are possible, we define our as follows. Noting that a single-qubit gate $G$ can be specified by the expectations

$$E[\sigma_u]_{\sigma_v} = \text{Tr}_S[G\sigma_vG^\dagger\sigma_u] \equiv E_{u,v;G}, \quad u, v \in \{0, x, y, z\},$$

we define the cost function for executing $G$ over time $T$ as

$$\mathcal{E}_G^G(P; T) \equiv \sum_{u,v} |E_{u,v;G} - e_{u,v}(P; T)|^2,$$  \hspace{2cm} (33)

where $e_{u,v}(P; T)$ is a fixed-order (here, $k = 2$) perturbative expansion of $E[\sigma_u(T)]_{\sigma_v \otimes \sigma_B}$ corresponding to a control parameter set $P = \{\theta_1, \bar{n}^{(k)}\}$, calculated using full knowledge of $\langle [B(t_1), B(t_2)]_\pm \rangle$ (as would be the case in numerical optimal control routines). In contrast, when we specialize our equations to the model-reduced representation associated to $\mathcal{F}$ of the integrals $I_{\mathcal{G},\mathcal{C}}(T)$ (such as e.g., Eq. (19)), we will write the cost function as

$$\mathcal{E}_G^G(P; T)_{|\mathcal{F}} \equiv \sum_{u,v} |E_{u,v;G} - e_{u,v}(P; T)|_{|\mathcal{F}}|^2.$$  \hspace{2cm} (34)

In each case the optimization, given $\mathcal{C}$, consists in finding the set $P$ such that the corresponding cost function is minimized. Our objective will be to show that the model-reduced and full-knowledge optimal solutions, namely,

$$P^\star_{|\mathcal{F}} \equiv \text{argmin}_P \mathcal{E}_G^G(P; T)_{|\mathcal{F}}, \quad \text{vs.} \quad P^\star \equiv \text{argmin}_P \mathcal{E}_G^G(P; T),$$

yield similar performances, in the sense that $\mathcal{E}_G^G(P^\star_{|\mathcal{F}},T) \approx \mathcal{E}_G^G(P^\star;T)$. If this indeed happens, it follows that there is no
significant loss of information and effective model reduction has been achieved, and we will show this is the case below.

### 1. Noise characterization

Since we stipulated that no knowledge of the noise correlation functions is available, we first need to characterize the open quantum system to the best of our ability, i.e., within the limits allowed by $\mathcal{C}$. As in Sec. IV A 3, we assume that the qubit is evolving in the presence of uncorrelated additive and multiplicative noise sources (both zero-mean), which we take here to be stationary and characterized by correlation functions $C_{\alpha}(t_1-t_2)$, $\alpha = a, m$. While unknown to the experimenter, for demonstration we choose the latter to be the in-vacuum noise case, centered at

$$\phi(a,m) = \{0, 0, \sqrt{2} \},$$

inferred in the above characterization stage; or (i) the cost function brings to the problem of optimally executing a desired gate $G$ given $\mathcal{C}$. Using standard Nelder-Mead numerical routines, for several representative choices of $G$, we search for the optimal parameters $P^* = \{\theta^*_1, \theta^*_2, \vec{\phi}^{(1)}, \vec{\phi}^{(2)}\}$ that minimize: (i) the cost function $E^G(P; T)$, by using the information $\mathcal{S} |\mathcal{C}$ inferred in the above characterization stage; or (ii) the cost function $E^G(P; T)$, by assuming full knowledge of the noise model, with access to the full model time-domain equations. The scenario (ii) is a drastic idealization as such a knowledge is never available in practice, and no QNS protocol can provide such information unless one assumes arbitrary control capabilities. Nevertheless, it is a useful benchmark, as our objective is to show that our model-reduced representation of the dynamics captures all the relevant information, as dictated by $\mathcal{C}$, to a very good approximation.

The results are presented in Tab. IV. They demonstrate the model reduction capabilities of the formalism, as there is little to no predictive power lost. Note that $E^G(P^*; T) \sim E_S^G(P^*; T)$, as desired. Finally, for completeness and to highlight the benefits of control, we calculate the value of the cost function $E^G(P_0; t)$ for $G = I$ using full information and in the absence of control, i.e., the effect of the natural decoherence of the system. One finds that in the absence of control $E^G_S(P_0; T/2) = 9.77 \cdot 10^{-3}$ and

$$\theta_1, \theta_2 \in \{0, \pi, \frac{64\pi}{35}, \frac{17\pi}{10}, 2\pi\}.$$
For control purposes, however, one is interested in overlap integrals of the form given in Tab.\ref{tab:comparison} (panel (iii)), hence the information provided by the sampling is necessarily incomplete. Therefore, it is necessary to complement it with additional assumptions, by interpolating between the sampled points. The assumptions that are more or less implicitly made in this completion step – e.g., in choosing a particular interpolation method – can be highly arbitrary and user-defined, and yet they can decisively influence our ability to predict the dynamics accurately. For instance, given a sampling set, there are in principle infinitely many possible interpolations consistent with it, and it is easy to build a control sequence for which the details of the interpolation are crucial: a simple example demonstrating how the latter can directly impact observable expectation values is given in Fig.\ref{fig:interpolation}. That is, $\mathcal{S}\mid \mathcal{C}_0$ is not universal in general. Consequently, obtaining rigorous criteria to characterize the control sequences whose effect on the system can be accurately predicted given such information is not only desirable but also imperative. Of course, this is not a problem exclusive to spectral estimation in either the classical \cite{54,55} or quantum settings, and indeed the task of picking a good interpolation given sampled data is a mainstay in applied mathematics, with various possible criteria available \cite{57}.

The frame-based approach we proposed in Sec. \ref{sec:frame} and


| Gate | Model-reduced, \( P^* \) | Full knowledge, \( P^* \) |
|------|-------------------|-------------------|
|      | \( (\theta_*, \tilde{\eta}^{(1)*}) \) | \( (\theta_*, \tilde{\eta}^{(1)*}) \) |
|      | \( (\theta_*, \tilde{\eta}^{(2)*}) \) | \( (\theta_*, \tilde{\eta}^{(2)*}) \) |
|      | \( \varepsilon_F^G(P; T) \) | \( \varepsilon_F^G(P; T) \) |
|      | \( (10^{-3}) \) | \( (10^{-3}) \) |
| \( I \) | \( (1.56, \{1, 0, 0\}) \) | \( (1.56, \{1, 0, 0\}) \) |
|      | \( (1.56, \{1, 0, 0\}) \) | \( (1.56, \{1, 0, 0\}) \) |
|      | \( 10.8 \) | \( 11.1 \) |
| \( X \) | \( (3.14, \{1, 0, 0\}) \) | \( (3.14, \{1, 0, 0\}) \) |
|      | \( 3.48 \) | \( 3.51 \) |
| \( Z \) | \( \{0.80, 0.57, -0.19\} \) | \( \{0.69, 0.70, -0.19\} \) |
|      | \( 6.99 \) | \( 7.13 \) |
| \( e^{ix_{1/8}} \) | \( \{0.95, 0.26, -0.16\} \) | \( \{0.91, 0.38, -0.16\} \) |
|      | \( 2.22 \) | \( 2.25 \) |
| \( H \) | \( \{0.82, 0.58, 0.02\} \) | \( \{0.82, 0.57, 0.01\} \) |
|      | \( 6.69 \) | \( 6.82 \) |

Table IV. Optimal control parameters \( P^* = \{\theta_*, \tilde{\eta}^{(1)*}\} \) (all rounded to two decimals) found by minimizing the model-reduced and full knowledge cost functions, respectively. A fair and experimentally relevant comparison is made by evaluating \( \varepsilon_F^G(P; T) \) at the corresponding optimal values \( P = P^* \) (fifth column) and comparing them with the minimal values of the full-knowledge cost function (rightmost column). We find that there is virtually little difference in doing so, indicating that there is no significant loss of information due to model reduction so long as the controls are in \( \mathcal{C} \). Notably, across multiple examples our numerical routine was less likely to be trapped in a local minimum when optimizing \( \varepsilon_F^G \) as compared to optimizing \( \varepsilon_F^G \), suggesting a potential additional benefit of model reduction. Optimal gate-design results for the same noise model with different noise parameters are also included in Appendix E, similar to dynamically corrected gates or composite pulses [3].

In closing, we note that the question of universality is vital when model-reduced representations of complex systems are introduced (not necessarily related to control). For example, recent work [60] has addressed similar questions but related to the “objectivity” of classical noise representations of quantum baths. In our setting, if one thinks of the context [60] to be defined by \( \mathcal{C} \), then universality of the QNS-inferred information based on \( \mathcal{C}_0 \) may be taken to signify a degree of objectivity of the noise representation for control purposes. Moving forward, it would be interesting to better understand how different model simplifications interact and can lead to more comprehensive model-reduced representations (relative to the combined contexts, for example).

\[ \varepsilon = \frac{\sum_{i=1}^{N} |\hat{F}(\omega_i)|^2}{\sum_{i=1}^{N} |\hat{F}(\omega_i)|^2} \]

\[ \text{V. CONCLUSION AND OUTLOOK} \]

We have introduced a framework for constructing a model-reduced representation of open quantum dynamics relative to given control capabilities, which both mathematically formalizes and substantially simplifies the problem of C&C for general non-Markovian noise environments. While we have exemplified our analysis in two paradigmatic applications – QNS of non-stationary noise and model-reduced C&C of a single qubit – our results also formally justify the success of the machine-learning enhanced approach for noise discrimination proposed in [58].

Our framework lends itself to several generalizations. On the one hand, a natural and important next step is to develop explicit frame-based protocols applicable to multiqubit C&C tasks in the presence of more general noise models, including multiaxis and non-Gaussian noise. As we mentioned, of special significance in this context will be to understand how, for fixed control capabilities \( \mathcal{C} \), a model-reduced description with maximum parsimony may be obtained without sacrificing accuracy [44]. On the other hand, the use of frame-based optimization need not be restricted to the synthesis of unitary target gates; one could imagine leveraging the natural decoherence of the system in the presence of applied control to optimally implement a reachable completely positive trace-
preserving map, possibly in connection with ideas from [59]. Ultimately, we believe that the use of frames will ease the integration of signal processing tools into quantum control and prove instrumental to develop efficient model-reduced approaches to C&C of realistic open quantum systems of growing complexity, as needed by both realistic NISQ-era devices and full-fledged fault-tolerant architectures.

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Appendix A: Time-dependent expectation values

As discussed in the main text, in order to capture the system dynamics under the simultaneous effect of the noise and the applied time-dependent, open-loop control we consider the expectation value of a system-only (invertible) observable $O$, given in the physical frame by $E[O(T)]_{\rho_S \otimes \rho_B} = \langle \text{Tr} \left[ U(T)(\rho_S \otimes \rho_B) U^\dagger(T)O \right] \rangle_c$. The latter may be rewritten in the form

$$E[O(T)]_{\rho_S \otimes \rho_B} = \left\langle \text{Tr} \left[ \tilde{U}(T)(\rho_S \otimes \rho_B) \tilde{U}^\dagger(T)\tilde{O}(T) \right] \right\rangle_c = \text{Tr}_{\tilde{S}} \left[ \tilde{O}(T)^{-1}\tilde{U}(T)\tilde{O}(T)\tilde{U}(T) \right] \rho_S \tilde{O}(T),$$

where $\langle \cdot \rangle_c$ represents averaging over realizations of the stochastic process, $\langle \cdot \rangle = \langle \text{Tr}_B[\cdot \rho_B] \rangle_c$ is the joint classical-quantum average, and $\tilde{O}(T) = U_0^\dagger(T)OU_0(T)$. Following a similar line of reasoning as in [61], we write $V_O(T)$ as a time-ordered exponential, $V_O(T) = (T+e^{-i\int_T^{T}dt\tilde{H_O}(s)})$, with

$$\tilde{H_O}(t) = \begin{cases} \overline{H}(T-t) & t \in [0,T], \\ \overline{H}(T+t) & t \in [-T,0], \end{cases}$$

where $\overline{H}(t) = -\tilde{O}(T)^{-1}\tilde{H}(t)\tilde{O}(T)$, and $\tilde{H}(t)$ being the toggling-frame Hamiltonian given in Eq. (3) of the main text. In turn, this allows us to expand $V_O(T)$ via a cumulant or Dyson expansion,

$$\left\langle T+e^{-i\int_T^{T}dt\tilde{H_O}(s)} \right\rangle = e^{\sum_{k=1}^{\infty}(-i)^k C_O^{(k)}(T)/k!} = 1 + \sum_{k=1}^{\infty} \frac{D_O^{(k)}(T)}{k!},$$

where $C_O^{(k)}$ is the generalized cumulant defined implicitly as a function of the Dyson-like terms

$$\frac{D_O^{(k)}(T)}{k!} = (-i)^k \int_{-T}^{T} d\tau \tilde{\ell}_k \langle H_O(t_1) \cdots H_O(t_k) \rangle ,$$

with correlators

$$C_{\ell;k} \equiv \left\langle \prod_{j=1}^{\ell} \Pi(t_{\pi(j)}) \prod_{j'=\ell+1}^{k} \tilde{H}(t_{\pi(j')}) \right\rangle,$$

and $d_\tau \tilde{\ell}_k$ represents time-ordered integration, i.e., such that $t_1 \geq \cdots \geq t_k$. In Eq. (A3), we have performed a change of variables, allowing us to change the integration domain, which leads to the sum over the set $\Pi_{\ell;k}$, containing the permutations of $\{1, \ldots, k\}$ such that $t_{\pi(1)} \leq \cdots \leq t_{\pi(\ell)}$ and $t_{\pi(\ell+1)} \geq$...
\[ \cdots \geq t_{\pi(k)}. \] Expanding each of the correlators, we find
\[
C_{k;\ell} = (-1)^{\ell} \sum_{\vec{a},\vec{u},\vec{v}} f^{O}_{\vec{v}_{\ell}} \left( \prod_{j=1}^{k} y^{(\alpha_j)}_{u_{j},v_{j}}(t_{\pi(j)}) \Lambda_{u_{j}} \otimes B^{(\alpha_j)}_{u_{j}}(t_{\pi(j)}) \right) = (-1)^{\ell} \sum_{\vec{a},\vec{u},\vec{v}} f^{O}_{\vec{v}_{\ell}} \kappa_{\pi} \hat{\Lambda}_{\vec{v}} \left( \prod_{j=1}^{k} y^{(\alpha_j)}_{u_{j},v_{j}}(t_{\pi(j)}) \right) \left( \prod_{j=1}^{k} B^{(\alpha_j)}_{u_{j}}(t_{\pi(j)}) \right),
\]
where \( f^{O}_{\vec{v}_{\ell}} \equiv \frac{1}{\bar{d}} \text{Tr}[O^{-1} \Lambda_{v_{\ell}} \cdots \Lambda_{v_{1}} O(\Lambda_{v_{1}} \cdots \Lambda_{v_{\ell}})^{-1} \Lambda_{t}] \) and we have assumed for simplicity that the chosen operator basis is such that \( \prod_{j=1}^{k} \Lambda_{v_{j}} \equiv \kappa_{\sigma} \hat{\Lambda}_{\vec{v}} \), for \( \kappa_{\sigma} \in \mathbb{C} \) and \( \hat{\Lambda}_{\vec{v}} \) invariant under permutations of \( \vec{v} \). Finally, this implies that we can write
\[
D^{(k)}_{\vec{v}_{\ell}}(T) = k!(-i)^{\ell} \sum_{\vec{a},\vec{u},\vec{v}} (-1)^{\ell} f^{O}_{\vec{v}_{\ell}} \kappa_{\pi} \hat{\Lambda}_{\vec{v}} \int_{0}^{T} d_{\vec{r}} \left[ \prod_{j=1}^{k} y^{(\alpha_j)}_{u_{j},v_{j}}(t_{\pi(j)}) \left( \hat{B}^{(\pi(\vec{a}))}_{\vec{u}}(\pi(t)) \right) \right],
\]
\[
= k!(-i)^{\ell} \sum_{\vec{a},\vec{u},\vec{v}} (-1)^{\ell} \sum_{\pi} \kappa_{\pi} \hat{\Lambda}_{\vec{v}} \int_{0}^{T} d_{\vec{r}} \left[ \prod_{j=1}^{k} y^{(\alpha_j)}_{u_{j},v_{j}}(t_{\pi(j)}) \left( f^{O}_{\vec{v}_{\ell}} \left( \hat{B}^{(\pi(\vec{a}))}_{\vec{u}}(\pi(t)) \right) \right) \right],
\]
\[
= k!(-i)^{\ell} \sum_{\vec{a},\vec{u},\vec{v}} (-1)^{\ell} \sum_{\pi} \hat{\Lambda}_{\vec{v}} \int_{0}^{T} d_{\vec{r}} \left[ \prod_{j=1}^{k} y^{(\alpha_j)}_{u_{j},v_{j}}(t_{\pi(j)}) \left( \kappa_{\pi(\vec{u})} f^{O}_{\vec{v}_{\ell}} \left( \hat{B}^{(\pi(\vec{a}))}_{\vec{u}}(\pi(t)) \right) \right) \right]. \tag{A4}
\]

From Eq. (A4), obtained by an adequate relabeling of the indices and observing that the sum is over all \( \vec{u}, \vec{v}, \vec{a} \), one deduces that for each configuration of \( \alpha_j, u_j, v_j \) in \( \{x, y, z\} \), the term \( \hat{\Lambda}_{\vec{a}} \prod y^{(\alpha_j)}_{u_j,v_j}(t_{\pi(j)}) \) appearing modulates a linear combination of bath correlation functions, \( \left\langle \hat{B}^{(\pi(\vec{a}))}_{\vec{u}}(\pi(t)) \right\rangle \), i.e., a linear combination \( L_{\vec{a};\vec{u},\vec{v}}(\vec{r}) \). That is, each of the relevant overlap integrals \( I_{\vec{a};\vec{u},\vec{v}}^{(k)}(T) \) appearing in the sum have the structure claimed in Eq. (7) of the main text. We also highlight that any other perturbative expansion, e.g., a cumulant expansion, can be written in terms of structurally similar overlap integrals. Moreover, any function of the reduced dynamics, e.g., the fidelity, can be expanded in terms of the above integrals and resulting filter function representation. Which function is chosen is then a matter of convenience given a task at hand.

**Appendix B: Illustrative frame examples**

1. Fourier frames and frequency-domain FFs revisited

The frame formalism encompasses both the Fourier series and the short-time Fourier transform, by relating them to expansions in terms of appropriate discrete Fourier frames \([43]\) or, respectively, discrete and continuous Gabor frames \([35][62]\). Specifically, the frame of complex exponentials,
\[
\mathcal{F}_{FS} = \left\{ \phi_n(t) = e^{-in \frac{2\pi}{T} t}, \ n \in \mathbb{Z} \right\},
\]
is a discrete, self-dual frame for functions \( f \in L^2(\Lambda) \), where \( \Lambda \) is a closed interval on \( \mathbb{R} \) (e.g., \( \Lambda = [0, 1] \)) and the inner product \( (a, b) = \int_{\Lambda} \frac{dt}{|\Lambda|} a(t)b(t)^* \). The resulting frame expansion corresponds to the usual Fourier series on \( \Lambda \), namely, \( f(t) = \sum f_n \phi_n e^{-in \frac{2\pi}{T} t}, \) for \( t \in \Lambda \).

Likewise, given \( f \in L^2(\mathbb{R}) \), recall that the short-time Fourier transform (STFT, also known as the “windowed” FT or the Weyl-Heisenberg transform) with respect to a window function \( g \in L^2(\mathbb{R}) \) is given by
\[
F_g(\omega, \tau) \equiv \int_{-\infty}^{\infty} dt f(t) \phi_{\omega,\tau}(t), \ \phi_{\omega,\tau}(t) = g(t - \tau) e^{-i\omega t},
\]
where \( \phi_{\omega,\tau}(t), \omega, \tau \in \mathbb{R}, \) are elements of a (continuous) Gabor frame \([62][63]\). That is, a two-dimensional representation of the signal is obtained by taking the FT of \( f \) as the window function (e.g., a Gaussian or Hanh function centered around zero) is slid along the time axis. Conversely, the inverse STFT is given by \( f(t) = \int_{-\infty}^{\infty} \int d\omega F_g(\omega, \tau) \phi_{\omega,\tau}^*(t) \), where the functions \( \{ \phi_{\omega,\tau}(t) \} \) dual to \( \{ \phi_{\omega,\tau}(t) \} \).

Given the above formalism, one can now see how the standard frequency-domain FF formalism \([34][50]\) constitutes a particular limit of our construction. At an intuitive level, this is possible by considering the FT as an appropriate limit of the Fourier series, in the context of eigenfunction expansions (see e.g. Sec. 5.7 in \([64]\)). More formally in our context, the key observation is that any function corresponding to a physically admissible control (including free evolution) is necessarily time-limited, i.e., \( f_i \leq T \) for some finite \( T \) in our overlap integrals. Further, one has for the SP that
\[
I_{\vec{a};\vec{u},\vec{v}}^{(k)}(T) = \int_{-\infty}^{\infty} d\vec{r} \int_{-\infty}^{\infty} d\vec{\omega} \left[ \int_{-\infty}^{\infty} d\vec{\tau} \right] S_{\vec{a};\vec{u},\vec{v}}^{(k)}(\vec{\omega}, \vec{\tau}) \right] S_{\vec{a};\vec{u},\vec{v}}^{(k)}(\vec{\omega}, \vec{\tau}) \right] g(\vec{r} - \vec{\tau}) e^{-i\vec{\omega} \cdot \vec{r}} \right] \]
the FTFT associated to a sliding-window function \( g(\vec{t}) \) \([62]\). By
effectively an expansion on the frame given by (iii)-(iv) of the main text. The two representations are summarized in Tab. I (provided a compelling choice [46, 47]. As it turns out, any ε defined in Eq. (22) in the main text. As it turns out, noticing that for any \( T \), there is a \( \bar{r} \) such that \( g(\bar{r} - r) \) and \( \prod_{j=1}^{k} y_{w_j}(t_j) \) have negligible overlap when \( |\bar{r}| > \bar{r} \), one finds that

\[
T_{\alpha,\beta,\gamma,\delta}^{(k)} \simeq \int_{|r| \leq \bar{r}} d\bar{r} |k| \int_{-\infty}^{\infty} d\tilde{\omega} |k| F_{\alpha,\beta,\gamma,\delta}^{(k)}(\tilde{\omega}) \phi_{\gamma,\delta}(\tilde{\omega}, \bar{r}).
\]

In other words, the standard frequency FF formalism is effectively an expansion on the frame given by \( \{ \phi_{\gamma,\delta} \} \), for \( |\bar{r}| < \bar{r} \). A similar reasoning can be applied to the CA representation. The two representations are summarized in Tab. I (iii)-(iv) of the main text.

### 2. Digital frames for instantaneous pulses

Beyond Fourier and Gabor frames, the frame formalism allows for considerable flexibility. Consider the scenario in which the control matrix elements, \( y_{u,v}(t) \), are piece-wise constant in time. As we show in Appendix C, this is relevant, for instance, when one considers \( M \) (equidistant) instantaneous pulses over a time \( T \), implemented by control profiles \( h(t_j, t) = \delta(t - (t_j + \tau/2)) \), for \( j \in [1, M] \) and \( \tau = T/M \). Such control matrix elements are naturally spanned by the sequence \( \mathcal{T}_W = \{ W_{j,\tau} \} \), where the window function \( W_{j,\tau} \) is defined in Eq. (22) in the main text. As it turns out, \( \mathcal{T}_W \) is not only a frame but also a basis, and for the above scenario the FSF condition is exactly satisfied (\( \varepsilon = 0 \)). What is more, any digital basis suffices, among which the Walsh functions provide a compelling choice [46, 47].

Walsh functions [45] \( w_n(t) \) are a complete set of orthogonal functions in an interval \([0, T]\) with the inner product

\[
(a, b) = \int_{0}^{T} a(t)b(t) dt^*,
\]

which form a basis for piece-wise constant functions in \([0, T]\) with \( 2^N \) intervals \((N \in \mathbb{N})\). They are digital, taking values in \([-1, 1]\), and can be defined via the rows of the Hadamard matrix \( H_{2^N} \). We choose the so-called sequency ordering [45, 47] for their labeling for convenience, such that the sequence \( \mathcal{F}_{\text{Walsh},N} = \{ w_j(t) \}_{j=1}^{2^N} \) is a basis for \( 2^N \)-interval piecewise constant functions. The first eight Walsh functions are illustrated in Fig. 6.

### 3. Custom-built frames for arbitrary pulse profiles

For general non-instantaneous pulses, corresponding to arbitrary control profiles, one often encounters the situation where the allowed control matrix \( \mathcal{Y} \) has a particular structure, e.g., its components are linear combinations of specific functions of the available control profile, and its elements belong to a particular Hilbert space \( \mathcal{H} \). Two notable examples, typical of the unitary control scenario resulting from \( M \) non-overlapping pulses in time \( T \) we describe in the main text (and in detail in Appendix C), are

\[
\mathcal{Y}^{(a)} \in \mathcal{H}_{\mathcal{Y}^{(a)}} = \text{span}\left\{ W_{j,\tau} \cos[\theta_j \psi^{(j)}], W_{j,\tau} \sin[\theta_j \psi^{(j)}] \right\},
\]

with \( \psi^{(j)} = \int_{(j-1)\tau}^{j \tau} h(t_j, s) ds \) \( (B1) \)

\[
\mathcal{Y}^{(m)} \in \mathcal{H}_{\mathcal{Y}^{(m)}} = \text{span}\left\{ \theta_j h(t_j, t) \right\}. \quad \text{(B2)}
\]

Consider a generic case where

\[
\mathcal{H} = \text{span}_\mathbb{T}\left\{ f_\ell(\{ \theta_j \}, \{ b_j(t) \}) \mid \ell \in [1, L], j \in [1, M] \right\},
\]

for some set of functions \( \{ b_j(t) \} \), e.g., \( b_j(t) = h(t_j, t) \) as above or where each \( b_j(t) \) is an element of a convenient (truncated) basis in which control profiles can be expanded. One can build a frame/dual-frame pair as follows. Imagine that each \( \theta_j \in [0, 2\pi] \) takes values among integer multiples of \( 2\pi/N_{\text{ctrl}} \), for certain \( N_{\text{ctrl}} \in \mathbb{Z} \). Then, the \( N_{\text{ctrl}} = \)
$N_\#(L, M, \tilde{N}_\#)$-element sequence

$$\mathcal{F}_\# = \{\phi_n\} \equiv \{f_\ell(\{\eta_j\}, \{b_j(t)\})\}, \ell \in [1, L], j \in [1, M],$$

with $\eta_j = 2\pi k_i / \tilde{N}_\#$, $k_i \in [0, \tilde{N}_\#]$, spans $\mathcal{H}$ when $\tilde{N}_\# = N_{\mathrm{ctrl}}$ and is indeed (trivially) a frame. For a different choice of parameter $\tilde{N}_\#$, e.g., if $\tilde{N}_\# < N_{\mathrm{ctrl}}$, the frame property is lost as $\mathcal{F}_\#$ no longer spans $\mathcal{H}$. One can nevertheless proceed to build a dual sequence $\tilde{\mathcal{F}}_\# = \{\tilde{\phi}_n(t)\}_{n=1}^{N_{\#}}$ via the Moore-Penrose pseudo-inverse method (see below), such that by construction the orthogonality condition $(\phi_n, \tilde{\phi}_{n'}) = \delta_{n, n'}$ is satisfied. With this one can write

$$\tilde{y}(t) = \sum_{n=1}^{N_{\#}} (y, \tilde{\phi}_n) \phi_n(t), \quad \text{(B3)}$$

and calculate the error bound

$$\max_{y(t)} ||y(t) - \tilde{y}(t)||_2 = \max_{y(t)} \sqrt{\int_0^T |y(t) - \tilde{y}(t)|^2 dt} \leq \varepsilon,$$

for the candidate $\mathcal{F}_\#$ and $\tilde{\mathcal{F}}_\#$, as necessary to verify the FSF condition. That is, one can assess the ability of a candidate frame/dual-frame pair to approximate every $y(t) \in \mathcal{H}$ via Eq. (B3), thereby verifying the parsimony of $\mathcal{F}_\#$.

### a. Single-qubit addtive and multiplicative noise

For the additive dephasing noise we study in the main text (see also Appendix C below), the five dual frame functions built for $\tilde{N}_\# = 2$ and $M = 1$ are depicted in Fig. 7(a). Here, the associated frame is given by $\mathcal{F}_\#(a) = \{\phi_n(a)(t)\} = \{1, \cos[\pi \psi_1(t)], \cos[2\pi \psi_1(t)], \sin[\pi \psi_1(t)], \sin[2\pi \psi_1(t)]\}$, and its dual can be calculated as outlined below. It is worth highlighting that when the $b_j(t)$ are non-overlapping, as in the $b_j(t) = h(t_j, t)$ case considered here, one has $N_\# = ML(\tilde{N}_\# + 1)$, that is, the size of the frame grows linearly with the number of pulses $M$ (Note that the $\phi_n(a) = \sin[0 \psi_1(t)] = 0$ is trivial and thus excluded from the frame definition, leading to $N_\# = 5$). For any $y(t)$ one can calculate an upper bound $\varepsilon$ to the $L^2$-distance $||y(t) - \tilde{y}(t)||_2$ by evaluating these quantities for any $\theta_1 = \frac{\pi}{100} \cdot 2\pi$, for $k \in [0, 100]$. We find that $\varepsilon|_{\tilde{N}_\#=2} = 2.4 \cdot 10^{-5}$ and $\varepsilon|_{\tilde{N}_\#=4} = 2.8 \cdot 10^{-8}$. In Fig. 7(b), we plot seven such $y(t)$...
its dual is also a frame. The starting point is a reference or-

tion. When the sequence under consideration is a frame, then

An orthonormal basis for

\( \phi \)

Gram-Schmidt process to

\( \sum \)

inverse. One has then that

The dual frame can then be built via Moore-Penrose pseudo-

inverse. One has then that

where we have used that \( \tilde{\phi}_j = \sum_{j'}(\phi_{j'}, g_{j'}) g_{j'} \), or, equival-

ently, \( \tilde{\phi} = T \tilde{g} \), and that the \( \{g_{j'}\} \) are a basis. The above

implies that \( T^T T = I \), which, noting that \( T^T T \) is invertible,

has the solution \( T = T(T^T T)^{-1} \). Thus, the elements of \( F \)

are given by

\( \tilde{\phi} = T(T^T T)^{-1} \tilde{g} \).

Appendix C: Single-qubit frame-based protocols

1. Single-qubit reduced dynamics and determination of \( S^c \)

We are interested in obtaining explicit expressions for ex-

pectation values of an invertible observable \( O \) at a time \( T \).

As mentioned in the text, this can be accomplished in a weak-

coupling regime via a truncated Dyson expansion given by

\[ E[O(T)]_{\rho_S \otimes \rho_H} \approx \langle \text{Tr}[(I_S - D_O^{(2)}(T))\rho_S \tilde{O}(T)] \rangle \]

\[ = \text{Tr}[\rho_S \tilde{O}(T)] - \langle \text{Tr}[D_O^{(2)}(T)\rho_S \tilde{O}(T)] \rangle, \]

where the Dyson term is given by (see Eq. (A4))

\[ D_O^{(2)}(T) = 2 ! \int_0^T d_T \tilde{\gamma} \left( \tilde{H}(t_1) \tilde{H}(t_2) - \tilde{H}(t_2) \tilde{H}(t_1) \right) \]

\[ - \tilde{H}(t_1) \tilde{H}(t_2) + \tilde{H}(t_2) \tilde{H}(t_1) \right) c, \]

and \( \tilde{H}(t) \equiv \sum_u y_u(t) \sum_{c} f_c^u \sigma_c \otimes B^{(v)}(t) \), with \( f_c^u = T \text{Tr}[\tilde{O}(T)\sigma_a \tilde{O}(T)\sigma_a]. \) Assuming that there are no cor-

relations between additive and multiplicative noise, i.e.

\( \langle B^{(v)}(t_1) B^{(v)}(t_2) \rangle = 0 \), for all \( t_1, t_2 \), we have

\[ \frac{D_O^{(2)}(T)}{2} = \sum_{\alpha, \mu, \nu} \int_0^T d_T \tilde{\gamma} \left( y_\alpha(t_1) y_\nu(t_2) \sigma_u \sigma_v \left< B^{(v)}(t_1) B^{(v)}(t_2) \right> _c \right. \]

\[ - y_\alpha(t_1) y_\nu(t_2) \left( \sum_c f_c^u \sigma_c \right) \sigma_v \left< B^{(v)}(t_1) B^{(v)}(t_2) \right> _c \]

\[ - y_\alpha(t_1) y_\nu(t_2) \left( \sum_c f_c^u \sigma_c \right) \sigma_v \left< B^{(v)}(t_1) B^{(v)}(t_1) \right> _c \]

\[ + y_\alpha(t_1) y_\nu(t_2) \sum_{c, c'} f_c^u f_{c'}^\nu \sigma_c \sigma_c \left< B^{(c)}(t_2) B^{(c)}(t_1) \right> _c \]

which, in the frame language, reads

\[ \frac{D_O^{(2)}(T)}{2} = \frac{\sigma_0}{4} \sum_{\alpha, \mu, \nu} S_\alpha^{(u)}(n, n') F_{\alpha;u}^{(+)}(n, T) F_{\alpha;u}^{(-)}(n', T) + \sum_{\alpha, \mu, \nu} \left( \sigma_u \sigma_v \right) S_\alpha^{(v)}(n, n') F_{\alpha;u}^{(+)}(n, T) F_{\alpha;v}^{(-)}(n', T). \]

The last equation follows after change of variables \( c \leftrightarrow u, c' \leftrightarrow v \) and using \( F_{\alpha;u}^{(+)}(n, T) \) to denote the frame \( F^{(\alpha)} \)

representation of \( Y^{(\pm)}(t) \equiv y_\alpha(t) \pm \sum_c f_c^u y_c(t) \), with the definition for \( S_\alpha^{(u)}(n, n') \) used in the main text. Therefore,

the second term in Eq. (C1) contains the effect of the noise that we are interested in. In the following, we isolate the quantities

\( \text{Tr}[D_O^{(2)}(T)\sigma_l], l \in \{x, y, z\} \), for a given control sequence, initial system state, and measured observable, so that we can build
our CA-QNS protocol by cycling over a sufficiently large set of controls and observables. First we note that

\[
E[O(T)] \left[ \frac{1}{2} (I_s + \sigma_k) \otimes \rho_B \right] + E[O(T)] \left[ \frac{1}{2} (I_s - \sigma_k) \otimes \rho_B \right] = \left\langle \text{Tr} \left[ D_O^{(2)}(T) \bar{O}(T) \right] \right\rangle ,
\]
(C3a)

\[
E[O(T)] \left[ \frac{1}{2} (I_s + \sigma_k) \otimes \rho_B \right] - E[O(T)] \left[ \frac{1}{2} (I_s - \sigma_k) \otimes \rho_B \right] = \text{Tr} \left[ \sigma_k \bar{O}(T) \right] - \left\langle \text{Tr} \left[ D_O^{(2)}(T) \sigma_k \bar{O}(T) \right] \right\rangle ,
\]
(C3b)

which implies that from the (measured) expectation values we can infer the value of \( \left\langle \text{Tr} [ D_O^{(2)}(T) \sigma_r \bar{O}(T) ] \right\rangle \), for \( r \in \{0, x, y, z\} \).

Then, we note that for a choice of control and observable, the operator \( \bar{O}(T) = \sum_k \frac{\text{Tr}[\sigma_k \bar{O}(T)]}{2} \sigma_k \equiv \sum_k \sigma_k \) is known and fixed, which allows us to write the system of equations

\[
\left\{ \text{Tr} [ D_O^{(2)}(T) \sigma_r \bar{O}(T) ] \right\} = \sum_{l=0,x,y,z} \sum_{k=x,y,z} \text{Tr} [ D_O^{(2)}(T) \sigma_l ] \sigma_k \sum_{r \in \{0,x,y,z\}} \frac{\text{Tr}[\sigma_l \sigma_k]}{2},
\]
(C4)

from which the \( \left\{ \text{Tr} [ D_O^{(2)}(T) \sigma_l ] \right\} \) can be inferred, as desired.

We then combine these values – for a fixed \( U_0(T) \) – to construct \( \text{Tr} [ D_O^{(2)}(T) \sigma_r \bar{O}(T) ] \), for \( \bar{O}(T) = \sigma_r \), for all \( r, \gamma \), which simplifies the \( \bar{O}(T) \)-dependent expression for \( F^{(1,\pm)}_{\alpha,u}(n, T) \). A direct calculation for \( r = 0 \) shows that

\[
\left\langle \text{Tr} [ D_O^{(2)}(T) \sigma_0 \bar{O}(T) ] \right\rangle_c = \sum_{\alpha,n,n'} \sum_{u \neq v} \sum_{\mu = \pm} i \epsilon_{uv\gamma} S^{(n)}_{\alpha}(n,n') F^{(1,-)}_{\alpha,u}(n,T) F^{(1,\mu)}_{\alpha,v}(n',T),
\]

\[
= \sum_{\alpha,n,n'} \sum_{u \neq v} \sum_{\mu = \pm} i \epsilon_{uv\gamma} (1 + \mu g_{\alpha}^u) (1 - g_{\alpha}^v) F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T) S^{(\mu)}_{\alpha}(n,n'),
\]

\[
= 4 i \sum_{\alpha,n,n'} \sum_{u \neq v} \epsilon_{uv\gamma} F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T) S^{(-)}_{\alpha}(n,n'),
\]

\[
= 4 i \sum_{\alpha,n,n'} \epsilon_{uv\gamma} T^{(2,-)}_{\alpha,u,v}(T),
\]

where \( \epsilon_{uv\gamma} \) is the Levi-Civita symbol, \( g_{\alpha}^u = \frac{1}{2} \text{Tr}[\sigma_u \sigma_v \sigma_u \sigma_v] \), and

\[
T^{(2,-)}_{\alpha,u,v}(T) \equiv \sum_{n,n'} \left( S^{(-)}_{\alpha}(n,n') - S^{(-)}_{\alpha}(n',n) \right) F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T).
\]

Similarly, for \( r \neq 0 \) we find

\[
\left\langle \text{Tr} [ D_O^{(2)}(T) \sigma_r \bar{O}(T) ] \right\rangle_c = \sum_{\alpha,n,n'} \sum_{u \neq v} \sum_{\mu = \pm} \delta_{u,\gamma} (1 - g_{\alpha}^u) (1 - \mu g_{\alpha}^v) F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T) S^{(\mu)}_{\alpha}(n,n')
\]

\[
+ \sum_{\alpha,n,n'} \sum_{u \neq v} \sum_{\mu = \pm} \delta_{r,\gamma} (1 - g_{\alpha}^u) (1 + \mu g_{\alpha}^v) F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T) S^{(\mu)}_{\alpha}(n,n')
\]

\[
= \sum_{\alpha,n,n'} \sum_{u \neq v} \left( \delta_{r,\gamma} F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T) S^{(+)}_{\alpha}(n,n') - \delta_{r,u} F^{(1)}_{\alpha,v}(n,T) F^{(1)}_{\alpha,u}(n',T) S^{(+)}_{\alpha}(n,n') \right),
\]

\[
= \sum_{\alpha,n,n'} \left( \delta_{r,\gamma} T^{(2,+,\gamma)}_{\alpha,u,v}(T) - \delta_{r,u} T^{(2,+,\gamma)}_{\alpha,v,u}(T) \right),
\]

where the index structure forbids the contribution from \( \tilde{S}^{(-)}_{\alpha}(n,n') \), and we have defined

\[
T^{(2,+)}_{\alpha,u,v}(T) \equiv \sum_{n,n'} S^{(+)}_{\alpha}(n,n') F^{(1)}_{\alpha,u}(n,T) F^{(1)}_{\alpha,v}(n',T).
\]

Therefore, from the possible \( r, \gamma \) configurations, and

\[
\left\langle \text{Tr} [ D_O^{(2)}(T) \sigma_r \bar{O}(T) ] \right\rangle_c = \begin{cases} 
4 \sum_{\alpha,n,n'} \epsilon_{uv\gamma} T^{(2,-)}_{\alpha,u,v}(T) & r = 0, \\
4 \sum_{\alpha,n,n'} T^{(2,+,\gamma)}_{\alpha,u,v} & r = \gamma, \\
-4 \sum_{\alpha,n,n'} \delta_{u,r} T^{(2,+,\gamma)}_{\alpha,v,u} & r \neq \gamma, r \neq 0,
\end{cases}
\]
we conclude that only the integrals $\mathcal{I}^{(2,+)}_{\alpha;u,v}$, for all $u, v$, and $\mathcal{I}^{(2,-)}_{\alpha;u,v}$, for all $u \neq v$, influence the reduced qubit dynamics. In turn, this implies that only the quantities $\bar{S}_{\alpha} = \left\{ S^{(+)}_{\alpha}(n,n'), \bar{S}^{(-)}_{\alpha}(n,n') - \bar{S}^{(-)}_{\alpha}(n',n) \right\}$ are relevant to the dynamics given $\mathcal{C}$. The objective of QNS is to precisely extract all the spectra in $[\bar{S}]_e$.

2. Control-adapted QNS protocol with instantaneous control

In the case of instantaneous control, notice that each switching function is exactly expanded by appropriate digital basis as mentioned in Sec. [IVA.2] We thus use Walsh functions (see Appendix [B2]) as our frame. To perform CA-QNS for such a frame, it is enough to use rotations around the $y$-axis. In this situation, the toggling-frame Hamiltonian specializes to

$$\bar{H}(t) = y_{z,z}(t)\sigma_z \otimes B(t) + y_{z,x}(t)\sigma_x \otimes B(t),$$

where the control matrix elements are such that in the $j$-th time interval they are given by

$$y_{z,z}(t) = \cos(\tilde{\theta}_j) = \frac{1}{2} \text{Tr}\left[ e^{i\frac{\pi}{2}\sigma_y \epsilon_j} e^{-i\frac{\pi}{2}\sigma_y \epsilon_j} \right],$$

$$y_{z,x}(t) = -\sin(\tilde{\theta}_j) = \frac{1}{2} \text{Tr}\left[ e^{i\frac{\pi}{2}\sigma_y \epsilon_j} e^{-i\frac{\pi}{2}\sigma_y \epsilon_j} \right],$$

where the relation between the $\tilde{\theta}_j$ and $\theta_j$ set by the equations

$$\begin{align*}
0 &= \tilde{\theta}_1, \\
\theta_k &= \tilde{\theta}_{k+1} - \tilde{\theta}_k, \quad 1 \leq k \leq M - 1, \\
\theta_M &= -\tilde{\theta}_M.
\end{align*}$$

The above considerations suggest that:

(1) Using only $\tilde{\theta} = \pi$ pulses, one can ensure that $y_{z}(t)$ and $y_{x}(t)$ take values in $\{-1, 1\}$, and equal (up to a sign) to any desired Walsh function $w_{n}(t)$ for $t \in [0, T]$ and $n \in [1, M]$. This implies, for example, that

$$F^{(1)}_z(n, T) = \int_0^T dt \ w_m(t) w_n(t) = T \delta_{mn},$$

and thus

$$\mathcal{I}^{(+)}_{\alpha}(T) = \mathcal{I}^{(-)}_{\alpha}(T) = T^2 \sum_{n,n'} \bar{S}^{(+)}(n,n') \delta_{nm} \delta_{n'm} = T^2 \bar{S}^{(+)}(m, m).$$

That is, we can directly sample diagonal elements $\bar{S}^{(+)}(m, m)$.

(2) Using $\tilde{\theta} \in \{\pi, \pi/2\}$, we ensure that $y_{z}(t)$ and $y_{x}(t)$ take values in $\{-1, 0, 1\}$, with the constraint $|y_{z}(t)|^2 + |y_{x}(t)|^2 = 1$. In particular, one can choose angles such that $y_{z}(t) = w_m(t) + w_{m'}(t)$, while $y_{x}(t) = w_m(t) - w_{m'}(t)$ and thus

$$F^{(1)}_z(n, T) = \int_0^T dt \ \frac{1}{2} \left( w_m(t) + w_{m'}(t) \right) w_n(t) = \frac{T}{2} (\delta_{nm} + \delta_{n'm}),$$

$$F^{(1)}_x(n, T) = \int_0^T dt \ \frac{1}{2} \left( w_m(t) - w_{m'}(t) \right) w_n(t) = \frac{T}{2} (\delta_{nm} - \delta_{n'm}).$$

When applied to our dynamical equations, the above implies that

$$\mathcal{I}^{(+)}_{\alpha}(T) = \mathcal{I}^{(-)}_{\alpha}(T) = T^2 \left( \bar{S}^{(+)}(m,m) + \bar{S}^{(+)}(m',m) + \bar{S}^{(+)}(m',m') - \bar{S}^{(+)}(m,m') - \bar{S}^{(+)}(m,m') - \bar{S}^{(+)}(m',m') \right).$$

and thus we can infer the elements $\bar{S}^{(+)}(n,n')$ and $\bar{S}^{(-)}(n,n') - \bar{S}^{(-)}(n',n)$, as desired.

Given access to the corresponding $\bar{S}_e$ and noting that the SP and the CA pictures are related via $S^{(\pm)}(n,n') = S^{(\pm)}_{\alpha}(n,n') \pm \bar{S}^{(\pm)}(n',n)$, one can then obtain Walsh reconstructions $C^{(\alpha)}_{\pm}(t_1, t_2)$ of $C^{(\alpha)}_{\pm}(t_1, t_2)$ given by

$$C^{(\alpha)}_{\pm}(t_1, t_2) = \sum_{n,n'=1}^{N_\pm} \left( \bar{S}^{(\pm)}(n,n') \pm \bar{S}^{(\pm)}(n',n) \right) w_n(t_1) w_{n'}(t_2).$$

The reconstruction resolution will depend on the free parameters in the above protocol, namely, the total time $T$ and the
minimum switching time $\tau$, which upper-bounds the value of $N_\#$. In general, a smaller $\tau$ leads to higher resolution.

Appendix D: Symmetry analysis for control-adapted spectra

Given the frame of choice as plotted in Fig. 8 there are symmetries in the CA-spectra. We systematically classify any symmetries present in $S^+_a(n, n')$ by a kernel analysis method (which also works for more general noise models) as follows.

(1) The relevant set of parameters, $S^+_a(n, n')$, are not linearly independent. To prove this, we decompose each of them by dividing the integration region $0 \leq t_2 \leq t_1 \leq T$ into three distinct subregions, namely $I_1 = \{0 \leq t_2 \leq t_1 \leq T/2\}$, $I_2 = \{T/2 \leq t_2 \leq t_1 \leq T\}$ and $I_3 = \{0 \leq t_2 \leq T/2, T/2 \leq t_1 \leq T\}$, and thus, letting $S^+_a(n, n')|_1$ be the component of $S^+_a(n, n')$ in the $I_1$ integration subregion, such that

$$S^+_a(n, n') = S^+_a(n, n')|_1 + S^+_a(n, n')|_2 + S^+_a(n, n')|_3.$$ 

The key point is that this division allows the systematic study of the symmetries in the frame elements within each as well as between different integration subregions, e.g., the stationary assumption implies that $S^+_a(n, n')|_1 = S^+_a(m, m')|_2$ when $\phi_{\alpha}(n, t_2 - T/2) = \phi_{\alpha}(m, t_2)$ and $\phi_{\alpha}(n, t_2 - T) = \phi_{\alpha}(m, t_2)$. Moreover, parity symmetries lead to further reduction in the free parameters, e.g., $S^+_a(n, n')|_1 = -S^+_a(n', n)|_1$ when $\phi_{\alpha}(n, t_1)$ is an odd function in $0 \leq t_1 \leq T/2$ (anti-symmetric about $t_1 = T/4$) and $\phi_{\alpha}(n, t_2)$ is an even function in $0 \leq t_2 \leq T/2$ (symmetric about $t_2 = T/4$). We then associate a vector $s(n, n')$ to each $S^+_a(n, n')$ such that the $l$-th entry, $s(n, n')_l$, is non-zero if $S^+_a(n, n')$ has a non-zero projection on the $l$-th element of the set of independent elements $\{S^+_a(n, n')|_l\}$ (after considering all the symmetries above), and zero otherwise. Furthermore, we use all elements of the vectors $s(n, n')$ to construct the matrix

$$S_K = \begin{pmatrix} s(1, 1) & s(1, 2) & \cdots \\ s(1, 2) & s(1, 2) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$ 

Since the kernel of $S_K$ represents the vanishing linear combinations of its columns, calculating it provides exactly the linear dependencies among $\{S^+_a(n, n')\}$ we seek. For our choice of frame, we find 70 such symmetries (see Tab. [V]), and thus the number of free parameters which describe the additive noise is now reduced from 100 to 30.

(2) Recalling that for multiplicative noise, the $j$-th frame element is supported on the $j$-th interval, one then has $S^+_a(n, n') = 0$ for $j < j'$ and $S^+_a(n, j, j') = S^+_a(n, j', j')$.

(3) Finally, we point out that the additive and multiplicative noise components can be separately inferred by first fixing $\{\theta_i\}$ and cycling over a sufficiently large set of directions $\vec{n}$, and then repeating these steps for several choices of $\{\theta_i\}$.

Appendix E: Faster gates need not be more accurate

Here we showcase another noise example where two-interval control can, somewhat surprisingly, lead to better performance in some gate design tasks than single-interval control. This noise model is the same as Sec. [V C T] except that the parameter values are changed as $b_0^{(a)}/\hbar = 2000$ kHz, $c_0^{(a)} = 0.08 \text{ ms}^2$, $b_1^{(a)}/\hbar = 5 \cdot 10^4$ kHz, $c_1^{(a)} = 0.64 \text{ s}^2$, $\omega_1^{(a)} = 400$ kHz, $b_0^{(m)}/\hbar = 0.1 \text{ mHz}$, $c_0^{(m)}/\hbar = 6\sqrt{2}\pi$ Hz and $\omega_0^{(m)} = 60$ Hz. The optimal gate design results are summarized in Tab. [VI]. In comparison, the shortest implementation of the $\pi/8$ gate around $X$ allowed by $C$, yields the larger error $E_x^G(\{\pi/4\}; T/2) = 7.75 \cdot 10^{-3}$. As in dynamically corrected gates [2] and composite pulses [3], multiple segments of evolution may be crucial to enable error cancellation, despite the gate taking longer.
Table V. Symmetry equation list. Number 1 to 45 list all the combinations of \((j_1, k_1)\) and \((j_2, k_2)\) such that 
\[ S_m^u (j_1, k_1) \pm S_m^u (j_2, k_2) = 0. \]
Number 46 to 70 list all the \((j_3, k_3)\) such that 
\[ S_m^u (j_3, k_3) = 0. \]

| \# | \((j_1, k_1)\)          | \((j_2, k_2)\)          | \((j_3, k_3)\)          |
|----|-------------------------|-------------------------|-------------------------|
| 1  | (1, 1)                  | (6, 6)                  |                          |
| 2  | (1, 2)                  | (7, 6)                  |                          |
| 3  | (1, 3)                  | (8, 6)                  |                          |
| 4  | (1, 4)                  | (9, 6)                  |                          |
| 5  | (1, 5)                  | (10, 6)                 |                          |
| 6  | (6, 7)                  | (7, 6)                  |                          |
| 7  | (6, 8)                  | (8, 6)                  |                          |
| 8  | (6, 9)                  | (9, 6)                  |                          |
| 9  | (6, 10)                 | (10, 6)                 |                          |
| 10 | (2, 1)                  | (7, 6)                  |                          |
| 11 | (2, 2)                  | (7, 7)                  |                          |
| 12 | (2, 3)                  | (8, 7)                  |                          |
| 13 | (2, 4)                  | (9, 7)                  |                          |
| 14 | (2, 5)                  | (10, 7)                 |                          |
| 15 | (7, 8)                  | (8, 7)                  |                          |
| 16 | (7, 9)                  | (9, 7)                  |                          |
| 17 | (7, 10)                 | (10, 7)                 |                          |
| 18 | (3, 1)                  | (8, 6)                  |                          |
| 19 | (3, 2)                  | (8, 7)                  |                          |
| 20 | (3, 3)                  | (8, 8)                  |                          |
| 21 | (3, 4)                  | (9, 8)                  |                          |
| 22 | (3, 5)                  | (10, 8)                 |                          |
| 23 | (8, 9)                  | (9, 8)                  |                          |
| 24 | (8, 10)                 | (10, 8)                 |                          |
| 25 | (4, 1)                  | (9, 6)                  |                          |
| 26 | (4, 2)                  | (9, 7)                  |                          |
| 27 | (4, 3)                  | (9, 8)                  |                          |
| 28 | (4, 4)                  | (9, 9)                  |                          |
| 29 | (4, 5)                  | (10, 9)                 |                          |
| 30 | (9, 10)                 | (10, 9)                 |                          |
| 31 | (5, 1)                  | (10, 6)                 |                          |
| 32 | (5, 2)                  | (10, 7)                 |                          |
| 33 | (5, 3)                  | (10, 8)                 |                          |
| 34 | (5, 4)                  | (10, 9)                 |                          |
| 35 | (5, 5)                  | (10, 10)                |                          |

Figure 8. Frame elements in \(\mathcal{F}_\phi^{(a)}\) for \(M = 2\) and \(\bar{N}_\phi = 2\). Horizontal axes are time, \(t(\mu s)\).
| Gate | Model reduced, $P^*|\gamma = \arg\min_P \mathcal{E}^C(|P;T)|\gamma$ | Full knowledge, $P^* = \arg\min_P \mathcal{E}^C(|P;T)$ |
|------|-----------------------------------------------|-----------------------------------------------|
| $G$  | $(\theta_1, n^{(1)})$                         | $(\theta_1, n^{(1)})$                         |
| $I$  | $(2.22, \{1, 0, 0\})$                        | $(2.22, \{1, 0, 0\})$                        |
|      | $(2.13, \{-1, 0, 0\})$                      | $(2.13, \{-1, 0, 0\})$                      |
|      | $1.64 \times 10^{-6}$                        | $1.64 \times 10^{-6}$                        |
| $X$  | $(1.56, \{1, 0, 0\})$                        | $(1.56, \{1, 0, 0\})$                        |
|      | $(3.14, \{0, 1, 0\})$                        | $(3.14, \{0, 1, 0\})$                        |
|      | $3.14 \times 10^{-3}$                        | $3.14 \times 10^{-3}$                        |
| $Z$  | $(1.71, \{0, -0.16\})$                       | $(1.71, \{0, -0.16\})$                       |
|      | $(0.01, 0.99, -0.16)$                        | $(0.01, 0.99, -0.16)$                        |
|      | $5.26 \times 10^{-3}$                        | $5.26 \times 10^{-3}$                        |
| $e^{\pi/8}$ | $(2.03, \{1, 0, 0\})$              | $(2.03, \{1, 0, 0\})$              |
|      | $(2.42, \{1, 0, 0\})$                        | $(2.42, \{1, 0, 0\})$                        |
|      | $8.63 \times 10^{-6}$                        | $8.63 \times 10^{-6}$                        |
| $e^{\pi/8}$ | $(1.57, \{0, -0.16\})$              | $(1.57, \{0, -0.16\})$              |
|      | $(1.57, \{0.01, 0.99, -0.16\})$           | $(1.57, \{0.01, 0.99, -0.16\})$           |
|      | $1.11 \times 10^{-3}$                        | $1.11 \times 10^{-3}$                        |
| $H$  | $(1.35, \{0.82, 0.58, 0.02\})$              | $(1.35, \{0.82, 0.58, 0.02\})$              |
|      | $(0.66, 0.68, 0.31)$                        | $(0.66, 0.68, 0.31)$                        |
|      | $3.97 \times 10^{-3}$                        | $3.97 \times 10^{-3}$                        |

Table VI. Optimal gate design results for the noise model in Appendix E.
Throughout the manuscript we calculate the relative error between an approximated/estimated quantity $\hat{A}$ and the actual one $A$, by $E_{\text{relative}} = \|\hat{A} - A\|/\|A\|$. 

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