Sensitivity Bounds for Quantum Control and Time-Domain Performance Guarantees

S. P. O'Neil[1,*], E. A. Jonckheere[1], S. Schirmer[2]

***Abstract*— Control of quantum systems via time-varying external fields optimized to maximize a fidelity measure at a given time is a mainstay in modern quantum control. However, current analysis techniques for such quantum controllers provide no analytical robustness guarantees. In this letter we provide analytical bounds on the differential sensitivity of the gate fidelity error to structured uncertainties for a closed quantum system controlled by piecewise-constant, optimal control fields. We additionally determine those uncertainty structures that result in this worst-case maximal sensitivity. We then use these differential sensitivity bounds to provide conditions that guarantee performance, quantified by the fidelity error, in the face of parameter uncertainty.**

I. Introduction

Control based on the optimal tuning of time-varying external fields forms the backbone of effective control for current quantum technology [1]. Such open-loop techniques have been successfully applied in areas from the implementation of quantum gates based on superconducting qubits [2], to quantum metrology [3], and temperature and magnetic field sensing via large defect ensembles of Nitrogen-Vacancy Centers in diamond [4]. Despite these successes of quantum optimal control, robustness issues remain. Even with the best modeling, uncertainty in the underlying Hamiltonian persists [1], and is aggravated for artificial atoms and manufactured systems such as superconducting qubits comprised of Josephson junctions [5]. Such issues generate the potential for sub-optimal performance of an optimized controller as the true plant diverges from the model system.

Closed-loop or robust control techniques provide options to improve robust performance. It terms of the latter, inclusion of a sensitivity-type penalty function in the optimal control synthesis algorithm is a popular method for implementing robustness to internal uncertainty or external perturbations. For example in [4], inclusion of a penalty based on the differential sensitivity resulted in controllers with good robustness to small deviations in detuning frequency as measured for the gate fidelity of a superconducting fluxonium qubit-based gate. Despite these successes, robustness properties are generally only apparent through testing via Monte-Carlo simulations or in experiments over a range of conditions. Additionally, current techniques lack an analytic basis for determining bounds that quantify the worst-case robustness and fundamental limitations on performance associated with such worst-case scenarios.

This touches on the need for a formal theory of robust quantum control. The survey [6] highlights the issues with robust control of quantum systems via open-loop and feedback approaches while revealing the nascent stage of development of robustness considerations in quantum control. In [7], Horowitz makes the point that a good theory of sensitivity should guarantee tolerances on performance over a range of parameter uncertainty, while in [8] Safonov outlines the performance and robustness trade-offs inherent in the application of frequency-domain robust control. This letter is a step in the direction of such a theory for quantum control aimed at providing reliable analytic bounds on the differential sensitivity for controllers optimized for high fidelity of quantum gates. We then use these sensitivity bounds to provide guarantees on the gate fidelity in the face of the uncertainty. Further, since coherent quantum systems must remain oscillatory, and hence marginally stable, to retain their quantum properties, time-domain techniques are the natural choice to approach control at the edge of stability. This is the approach taken here, departing from the established frequency-domain techniques of classical robust control [9].

The nominal system model and performance metrics are defined in Section II, followed by the uncertainty model in Section III. The differential sensitivity of the controlled system for a given uncertainty model is derived in Section IV, followed by bounds on the differential sensitivity and the uncertainty structures that maximize the sensitivity in Section V. In Section VI we leverage these bounds to provide performance guarantees in terms of the structure and size of the uncertainty. The results are illustrated for a gate fidelity optimization problem in Section VII.

II. Preliminaries

Consider a closed quantum system of Q qubits with underlying Hilbert space of dimension $N = 2^Q$. The state is characterized by the wavefunction $\psi(t) \in \mathbb{C}^N$ with nominal drift Hamiltonian $H_0 \in \mathbb{C}^{N\times N}$. To control the evolution of $\psi(t)$, introduce M control fields that optimally steer the trajectory of the wavefunction from an initial state ψ_0 to a final state ψ_f at a readout time t_f. The control fields take on constant values at κ uniform time intervals of length Δ so that $t_f = \kappa\Delta = \Delta_k$ where the initial time is $\Delta_0 = 0$ and any intermediate time is given as $\Delta_k = k\Delta$, $k \leq \kappa$. Each control

[1] Dept of Electrical & Computer Engineering, University of Southern California, CA, USA. jonckhee@usc.edu, seanonei@usc.edu

[2] Faculty of Science & Engineering, Physics, Swansea University, UK. s.m.shermer@gmail.com

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pulse $f_{mk} \in \mathbb{R}$ enters the dynamics through an interaction Hamiltonian H_m so that in the interval $1 \leq k \leq \kappa$

$$H_k = H_0 + \sum_{m=1}^{M} H_m f_{mk}. \tag{1}$$

Here f_{mk} is the strength of the mth control field in the time interval $\Delta_{k-1} \leq t < \Delta_k$. Let u_k be a pulse of unit magnitude that is only non-zero for the interval $\Delta_{k-1} \leq t_k \leq \Delta_k$ (if $u(t)$ is the standard unit step then $u_k = u(\Delta_{k-1}) - u(\Delta_k)$). Then the total Hamiltonian is the sum of H_k over time

$$H(t) = \sum_{k=1}^{\kappa} H_k u_k = H_0 + \sum_{k=1}^{\kappa}\sum_{m=1}^{M} H_m f_{mk} u_k. \tag{2}$$

The wavevector dynamics are governed by

$$\dot{\psi}(t) = H(t)\psi(t)\ ,\ \psi(0) = \psi_0 \tag{3}$$

with solution at the readout time t_f

$$\begin{gathered}\psi(t) = \Phi_{(\kappa,0)}\psi_0 = \prod_{k=1}^{\kappa} \Phi_{(k,k-1)}\psi_0 = \\ \Phi_{(\kappa,\kappa-1)}\Phi_{(\kappa-1,\kappa-2)}\ldots\Phi_{(1,0)}\psi_0\end{gathered} \tag{4}$$

where $\prod_{k=1}^{\kappa}$ indicates an ordered product. Here

$$\Phi_{(k,k-1)} = e^{-iH_k(\Delta_k - \Delta_{k-1})} \tag{5}$$

is the solution to the Schrödinger equation on the interval $[\Delta_{k-1}, \Delta_k]$ and $\Phi_{(\kappa,0)}$ is the concatenation of the state transition matrices from $k = 1$ through $k = \kappa$ covering the evolution from $t = 0$ to $t = t_f$.

Equivalently, we can optimize to produce a unitary operator $U(t_f) = \Phi_{(\kappa,0)} \in \mathbb{U}(N)$ with target $U_f \in \mathbb{U}(N)$ where $\psi(t_f) = U(t_f)\psi(0)$. In this case the dynamics are governed by $\dot{U}(t) = -iH(t)U(t)$ with $U(0) = I$, where I is the identity on $\mathbb{C}^N$, and the solution is

$$U(t_f) = \Phi_{(\kappa,0)}U_0 = \prod_{k=1}^{\kappa} \Phi_{(k,k-1)}U_0. \tag{6}$$

The figure of merit is the normalized gate fidelity at t_f,

$$\mathcal{F}(t_f) = \frac{1}{N}\left|\mathrm{Tr}\left[U_f^\dagger \Phi_{(\kappa,0)}\right]\right| \tag{7}$$

and the corresponding fidelity error is $e(t_f) = 1 - \mathcal{F}(t_f)$.

III. Uncertainty Model

Consider an uncertain parameter in $H(t)$ modeled as $\delta\hat{H}_\mu$ where $\delta \in [\delta_1, \delta_2]$ is the scalar deviation of the uncertain parameter from its nominal value, structured as $\hat{H}_\mu \in \mathbb{C}^{N\times N}$ and normalized such that $\left\|\hat{H}_\mu\right\|_F = 1$. $\hat{H}_\mu$ must be Hermitian as the Hamiltonian of a closed system must remain Hermitian under the uncertainty. The uncertain Hamiltonian is

$$\tilde{H}(t) = \sum_{k=1}^{\kappa} \tilde{H}_k u_k, \tag{8a}$$

$$\tilde{H}_k = H_0 + \sum_{m=1}^{M} H_m f_{mk} + \delta\hat{H}_\mu\alpha_{\mu k}. \tag{8b}$$

We consider the following uncertainty cases:

- Collective uncertainty in H_0: In this case $\tilde{H}_0 = H_0 + \delta\hat{H}_0$ so that $\hat{H}_\mu = \hat{H}_0$, $\alpha_{\mu k} = 1$ for all k, and $\hat{H}_0 = H_0/\left\|H_0\right\|_F$ is the normalized structure matrix for H_0.
- Collective uncertainty in interaction Hamiltonian H_m: In this case $f_{mk}\tilde{H}_m = f_{mk}(H_m + \delta\hat{H}_m)$ so that the final term in (8) is $\delta f_{mk}\hat{H}_m$ and $\alpha_{\mu k} = \alpha_{mk} = f_{mk}$. Here $\hat{H}_\mu = \hat{H}_m$ which is the normalized structure matrix for H_m.

The perturbed solution to Eq (6) at t_f is given by

$$\tilde{U}(t_f) = \tilde{\Phi}_{(\kappa,0)} = \prod_{k=1}^{\kappa} \tilde{\Phi}_{(k,k-1)}, \tag{9a}$$

$$\tilde{\Phi}_{(k,k-1)} = e^{-i\tilde{H}_k(\Delta_k - \Delta_{k-1})}. \tag{9b}$$

and the perturbed fidelity error due to the uncertainty $\hat{H}_\mu$

$$\tilde{e}_\mu(t_f) = 1 - \tilde{\mathcal{F}}_\mu(t_f) = 1 - \frac{1}{N}\left|\mathrm{Tr}\left[U_f^\dagger \tilde{\Phi}_{(\kappa,0)}\right]\right|. \tag{10}$$

IV. Differential Sensitivity

Taking the derivative of $\tilde{e}_\mu(t_f)$ with respect to the uncertain parameter δ structured as H_μ yields the following from Eq. (11) of [10] and Eq. (28) of [11] when evaluated at $\delta = 0$

$$\left.\frac{\partial\tilde{e}_\mu(t_f)}{\partial\delta}\right|_{\delta=0} = -\frac{\Re\left\{\mathrm{Tr}\left[U_f\Phi_{(\kappa,0)}^\dagger\right]\mathrm{Tr}\left[U_f^\dagger\sum_{k=1}^{\kappa}\Lambda_{(\kappa,k)}\right]\right\}}{N\left|\mathrm{Tr}\left[U_f^\dagger\Phi_{(\kappa,0)}\right]\right|}. \tag{11}$$

We may equivalently write this as

$$\left.\frac{\partial\tilde{e}_\mu(t_f)}{\partial\delta}\right|_{\delta=0} = \Re\left\{-\frac{e^{-i\phi}}{N}\mathrm{Tr}\left[U_f^\dagger\sum_{k=1}^{\kappa}\Lambda_{(\kappa,k)}\right]\right\} \tag{12}$$

where $\phi = \angle\,\mathrm{Tr}\left[U_f^\dagger\Phi_{(\kappa,0)}\right]$ and $\Lambda_{(\kappa,k)}$ is defined as

$$\Lambda_{(\kappa,k)} = \Phi_{(\kappa,k)}\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\Phi_{(k-1,0)} \tag{13}$$

where $\frac{\partial}{\partial\delta}\tilde{\Phi}_{(k,k-1)}$ is given by Eq. (28) of [11]

$$\int_{\Delta_{k-1}}^{\Delta_k} e^{-iH_k(\Delta_k-\tau)}\left(-i\hat{H}_\mu\alpha_{\mu k}\right)e^{-iH_k(\tau-\Delta_{k-1})}d\tau \tag{14}$$

and $\alpha_{\mu k}$ takes values in $\{1, f_{mk}\}$ based on the type of uncertainty as described in Section III. For brevity in what follows, we define $\frac{\partial}{\partial\delta}\tilde{e}_\mu(t_f) = \zeta_\mu(t_f)$ as the derivative of fidelity error in the direction $\hat{H}_\mu$ evaluated at $\delta = 0$.

V. Differential Sensitivity Bounds

We now consider bounds on the size of the differential sensitivity. To provide an initial bound on the differential sensitivity, we directly bound the absolute value of Eq. (12):

$$|\zeta_\mu(t_f)| \le \left|\frac{e^{-i\phi}}{N}\right| \cdot \left|\mathrm{Tr}\left[U_f^\dagger \sum_{k=1}^{\kappa} \Lambda_{(\kappa,k)}\right]\right| \le \frac{1}{N}\sum_{k=1}^{\kappa}\left|\mathrm{Tr}\left[U_f^\dagger \Lambda_{(\kappa,k)}\right]\right|. \tag{15}$$

Invoking the von Neumann trace inequality, and noting that all singular values $\sigma_\ell(U_f^\dagger)$ of $U_f^\dagger$ are 1, gives the bound

$$|\zeta_\mu(t_f)| \le \frac{1}{N}\sum_{k=1}^{\kappa}\sum_{\ell=1}^{N}\sigma_\ell\left(\Lambda_{(\kappa,k)}\right) = B_1. \tag{16}$$

As all $\Phi_{(\kappa,k)}$ are unitary we can bound the singular values

$$\sigma_\ell(\Lambda_{(\kappa,k)}) = \sigma_\ell\left(\Phi_{(\kappa,k)}\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\Phi_{(k-1,0)}\right) = \sigma_\ell\left(\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\right) \le \left\|\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\right\|_2 = \bar{\sigma}\left(\Lambda_{(\kappa,k)}\right)$$

where $\bar{\sigma}(A)$ is the maximum singular value of A. Further

$$\left\|\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\right\|_2 \le \int_{\Delta_{k-1}}^{\Delta_k}\left\|e^{-iH_k(\Delta_k-\tau)}\right\|_2 \times \left\|\alpha_{\mu k}\hat{H}_\mu\right\|_2 \times \left\|e^{-iH_k(\tau-\Delta_{k-1})}\right\|_2 d\tau = \Delta\,|\alpha_{\mu k}|\,\left\|\hat{H}_\mu\right\|_2 \tag{17}$$

now yields the bound

$$\|\zeta_\mu(t_f)\| \le \Delta\left\|\hat{H}_\mu\right\|_2\sum_{k=1}^{\kappa}|\alpha_{\mu k}| = B_2. \tag{18}$$

This bound is conservative and only relevant to a specific perturbation structure $\hat{H}_\mu$. However, being based solely on the parameters that define the control scheme, it is independent of the size of the perturbation δ.

To obtain tighter bounds locally about $\delta = 0$, applicable to a more general uncertainty structure, we unpack the latter from the differential sensitivity to make the reliance on the uncertainty structure more transparent. Employing the cyclic property and linearity of the trace, we rewrite the last term of Eq. (12) as

$$\mathrm{Tr}\left[U_f^\dagger\sum_{k=1}^{\kappa}\Lambda_{(\kappa,k)}\right] = \sum_{k=1}^{\kappa}\mathrm{Tr}\left[\Phi_{(k-1,0)}U_f^\dagger\Phi_{(\kappa,k)}\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}\right]$$

where $\hat{H}_\mu$ is restricted to a subset of the $N\times N$ Hermitian matrices, which is justified as the perturbations are necessarily Hermitian and constrained to the drift and interaction Hamiltonian matrices by the assumptions of Section III. Define a basis for this subset of the Hermitian matrices as $\{H_m\}_{m=0}^{M}$ for $M < N^2$. An arbitrary, normalized uncertainty structure is represented as

$$\hat{H}_\mu = \sum_{m=0}^{M} s_m\hat{H}_m. \tag{19}$$

If $\mathbf{s}_\mu \in \mathbb{R}^{M+1}$ is a column vector of the scalars s_m and $\left\|\hat{H}_m\right\|_F = 1$, i.e., the uncertainty structure matrices are normalized as per Section III, then retaining normalization requires $\left\|\hat{H}_\mu\right\|_F = \sqrt{\mathrm{Tr}\left[\hat{H}_\mu^\dagger\hat{H}_\mu\right]} = 1$, which holds if $\|\mathbf{s}_\mu\|_2 = 1$. With this expansion for $\hat{H}_\mu$ Eq. (14) gives

$$\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta} = \sum_{m=0}^{M}\mathbf{X}_m^{(k)}s_m = \mathbf{X}^{(k)}\mathbf{s}_\mu \tag{20}$$

where $\mathbf{X}^{(k)} \in \mathbb{C}^{N\times N(M+1)}$ is a row of $N\times N$ matrices

$$\mathbf{X}_m^{(k)} = -i\int_{\Delta_{k-1}}^{\Delta_k} e^{-iH_k(\Delta_k-\tau)}\hat{H}_m\alpha_{mk}e^{-iH_k(\tau-\Delta_{k-1})}d\tau. \tag{21}$$

Defining

$$\Re\left\{-\frac{e^{-i\phi}}{N}\mathrm{Tr}\left[\Phi_{(k-1,0)}U_f^\dagger\Phi_{\kappa,k}\mathbf{X}_m^{(k)}\right]\right\} = Z_{km} \tag{22}$$

the differential sensitivity has the compact expression

$$\left.\frac{\partial\tilde{e}_\mu(t_f)}{\partial\delta}\right|_{\delta=0} = \mathbf{1}^T\mathbf{Z}(t_f,\mathbf{f})\mathbf{s}_\mu = \mathbf{\Gamma}(t_f,\mathbf{f})\mathbf{s}_\mu \tag{23}$$

where $\mathbf{1} \in \mathbb{R}^{1\times\kappa}$ is the row vector of κ 1s that sum the vectorized components of $\frac{\partial\tilde{\Phi}_{(k,k-1)}}{\partial\delta}$. The t_f and $\mathbf{f}$ in $\mathbf{Z}$ and $\mathbf{\Gamma}$ indicate the dependence of these matrices on the read-out time and control fields.

Before deriving the improved upper bound on the sensitivity, note that (23) facilitates two interpretations of the differential sensitivity based on the constraints of the uncertainty. Specifically, if the uncertainty is constrained to be constant for the entire evolution, then $\mathbf{s}_\mu$ is a constant vector so that $\mathbf{\Gamma}(t_f,\mathbf{f})(\cdot)$ can be viewed as a function that accepts as input a single uncertainty structure, $\mathbf{s}_\mu$ and provides as output, the sensitivity in that direction. This interpretation lends itself to an uncertainty in the Hamiltonian that does not vary with time. In this case, we provide the following maximum bound on the differential sensitivity at $\delta = 0$:

Theorem 1: The maximum of $\left.\frac{\partial}{\partial\delta}\tilde{e}_\mu(t_f)\right|_{\delta=0} = \left.\zeta_\mu(t_f)\right|_{\delta=0}$ in Eq. (23) with constant $\mathbf{s}_\mu$ is $B_3 := \|\mathbf{\Gamma}\|_2$. Further, the uncertainty that maximizes $\left.|\zeta_\mu(t_f)|\right|_{\delta=0}$ is given by $\bar{H}_\mu = \sum_{m=0}^{M}v_m\hat{H}_m$ where $\{v_m\}$ are the components of the normalized vector $\hat{\mathbf{v}} = \mathbf{\Gamma}/B_3$.

Proof: Following directly from (23) and for a normalized uncertainty structure $\|\mathbf{s}_\mu\|_2 = 1$, $|\zeta_\mu(t_f)| = \|\mathbf{\Gamma}\mathbf{s}_\mu\|_2 \le \|\mathbf{\Gamma}\|_2\cdot\|\mathbf{s}_\mu\|_2 = \|\mathbf{\Gamma}\|_2 = B_3$. Noting that $\mathbf{\Gamma}$ is simply a real $M+1$-dimensional row vector, the $\mathbf{s}_\mu$ that maximizes the inner product $\mathbf{\Gamma}\mathbf{s}_\mu$ with $\|\mathbf{s}_\mu\|_2 = 1$ is $\hat{\mathbf{v}} = \mathbf{\Gamma}^T/B_3$. The maximum uncertainty direction $\bar{H}_\mu$ in terms of the Hamiltonian uncertainty basis $\{\hat{H}_m\}$ directly follows. ■

Alternatively, consider an uncertainty that is constant over each time step but varies over the evolution. Then we have for each time step k, $\hat{H}_\mu^{(k)} = \sum_{m=0}^{M}s_m^{(k)}\hat{H}_m$ with a corresponding $\mathbf{s}_\mu^{(k)}$ in the vectorized representation, and the following differential sensitivity

$$\zeta_{\{\mu\}}(t_f) = \left.\frac{\partial \tilde{e}_{\{\mu\}}(t_f)}{\partial \delta}\right|_{\delta=0}$$
$$= \sum_{k=1}^{\kappa}\left(\sum_{m=0}^{M} Z_{km} s_m{}^{(k)}\right) = \sum_{k=1}^{\kappa} \mathbf{Z}_k \mathbf{s}_\mu^{(k)} = \sum_{k=1}^{\kappa} \varsigma_k \quad (24)$$

where $\mathbf{Z}_k$ is the kth row of $\mathbf{Z}(t_f, \mathbf{f})$ in (23) and $\tilde{e}_{\{\mu\}}$ indicates that H_μ is not fixed over all time steps but given by the sequence $\{H_\mu^{(k)}\}_{k=1}^{\kappa}$. This leads to the following alternative bound to the differential sensitivity.

Theorem 2: The maximum size of $\left|\zeta_{\{\mu\}}(t_f)\right|_{\delta=0}$ for the formulation of (24) with uncertainty defined by the sequence $\{\mathbf{s}_\mu^{(k)}\}$ and $\left\|\mathbf{s}_\mu^{(k)}\right\| = 1$ for all k is $\|\{\bar{\varsigma}_k\}\|_{\ell^1} =: B_4$ where $\bar{\varsigma}_k = \|\mathbf{Z}_k\|_2$. Further the sequence $\{\bar{\mathbf{s}}_\mu^{(k)}\}$ that achieves the bound B_4 is given by $\bar{\mathbf{s}}_\mu^{(k)} = \mathbf{Z}_k^T/\bar{\varsigma}_k$ for $1 \le k \le \kappa$.

Proof: Suppose $\mathbf{s}_\mu^{(k)}$ is normalized for all k and the differential sensitivity is given by (24). Then $\left|\zeta_{\{\mu\}}(t_f)\right| = \left|\sum_{k=1}^{\kappa} \mathbf{Z}_k \mathbf{s}_\mu^{(k)}\right| \le \sum_{k=1}^{\kappa}\left|\mathbf{Z}_k \mathbf{s}_\mu^{(k)}\right| = \|\varsigma_k\|_{\ell^1}$. It follows that this sum is maximized if each term ς_k is of the same sign and takes on the maximum $\bar{\varsigma}_k = |\max_{\mathbf{s}_\mu^{(k)}} \mathbf{Z}_k \mathbf{s}_\mu^{(k)}|$ for each $k \in \{1, 2, \ldots, \kappa\}$. Since $\mathbf{s}_\mu^{(k)}$ is normalized, we have that $\bar{\varsigma}_k = \|\mathbf{Z}_k\|_2$. As such the maximum sensitivity is given by $B_4 := \sum_{k=1}^{\kappa} |\bar{\varsigma}_k| = \|\bar{\varsigma}_k\|_{\ell^1}$. Turning to the sequence of uncertainty structures $\mathbf{s}_\mu^{(k)}$, we have that for each k, the inner product $\mathbf{Z}_k \mathbf{s}_\mu^{(k)}$ is maximized by $\mathbf{s}_\mu^{(k)} = \mathbf{Z}_k^T / \|\mathbf{Z}_k\| = \mathbf{Z}_k^T/\bar{\varsigma}_k$. The sequence $\{\bar{\mathbf{s}}_\mu^{(k)}\} = \{\mathbf{Z}_k/\bar{\varsigma}_k\}$ that maximizes the sensitivity directly follows. ■

VI. Guaranteed Performance

We now seek to leverage the sensitivity bound B_2 of (18) to guarantee performance in the face of uncertainty structured as H_μ with strength δ. For a given controller, characterized by the set of control fields $\{f_{mk}\}$ and read-out time t_f, we view the perturbed error in the direction H_μ as a function of the uncertain parameter δ, $\tilde{e}_\mu(\delta)$. We likewise consider the differential sensitivity as a function of δ so that

$$\zeta_\mu(\delta) = \frac{\partial \tilde{e}_\mu(\delta)}{\partial \delta} = \lim_{\Delta\delta \to 0} \frac{\tilde{e}_\mu(\delta + \Delta\delta) - \tilde{e}_\mu(\delta)}{\Delta\delta}.$$

We consider the case where H_μ is one of the matrices from the set $\{\hat{H}_m\}$. Our goal is to determine a bound on $\delta \in [\delta_1, \delta_2]$ such that $\tilde{e}_\mu(\delta) \le \epsilon$ for the error threshold ϵ. Here δ_1 and δ_2 determine the endpoints of the uncertainty set for the parameter δ admitted by the physical model. Before providing the main result, we establish a pair of lemmas.

Lemma 1: On any interval $[\delta_1, \delta_2] \subset \mathbb{R}$ such that the fidelity $\tilde{\mathcal{F}}_\mu(\delta) \neq 0$, the function $\tilde{e}_\mu(\delta)$ is locally Lipschitz.

Proof: To establish that $\tilde{e}_\mu(\delta)$ is locally Lipschitz it suffices to show that $\tilde{e}_\mu(\delta)$ is real analytic in δ. We rewrite $-i\tilde{H}_k$ as $-i(A_k + \delta B_k)$ with

$$A_k = H_0 + \sum_{m=1}^{M} H_m f_{mk}, \quad B_k = \hat{H}_\mu \alpha_{\mu k}.$$

Allowing a non-vanishing, complex perturbation $\eta = x + iy$ and considering deviations Δx and Δy we have $F(\eta) = \exp[-i(\Delta_k - \Delta_{k-1})(A_k + \eta B_k)]$ is complex analytic as

$$\left.\frac{\partial F(\eta)}{\partial x}\right|_{\eta\neq 0} = \left.\frac{\partial F(\eta)}{i\partial y}\right|_{\eta\neq 0} =$$
$$\int_{\Delta_{k-1}}^{\Delta_k} e^{-i(\Delta_k-\tau)(A_k+\eta B_k)}\left(-iB_k\right) e^{-i(\tau-\Delta_{k-1})(A_k+\eta B_k)} d\tau.$$

Then $F(\eta)$ restricted to $\delta = \Re\{\eta\}$ is real analytic and has a convergent power series in $\delta \in [\delta_1, \delta_2]$. Given the product of real analytic functions is real analytic and, by the Faà di Bruno formula, the composition of real analytic functions is real analytic [12], $\mathrm{Tr}\left[U_f^\dagger \tilde{\Phi}_{(\kappa,0)}(\delta)\right] = g(\delta) \in \mathbb{C}$ is real analytic. Employing the same argument for $|g(\delta)| = \sqrt{g(\delta)g^*(\delta)}$, we have that $\left|\mathrm{Tr}\left[U_f^\dagger \tilde{\Phi}_{(\kappa,0)}(\delta)\right]\right|$ is real analytic except for when $g(\delta) = 0$, where $\tilde{\mathcal{F}}_\mu(\delta) = 0$. It then follows that $\tilde{e}_\mu(\delta) = 1 - \tilde{\mathcal{F}}_\mu(\delta)$ is locally Lipschitz on an arbitrary interval $[\delta_1, \delta_2]$ if $\tilde{\mathcal{F}}_\mu(\delta) \neq 0$. ■

Lemma 2: On the interval $[\delta_1, \delta_2]$ and given that $\tilde{H}_k$ remains Hermitian, $|\zeta_\mu(\delta)|$ is uniformly bounded with Lipschitz constant B_2 established by (18).

Proof: Given that B_2 is an upper bound at $\delta = 0$, it suffices to show that if B_2 is independent of δ, the bound holds on an arbitrary interval $[\delta_1, \delta_2]$. To establish the independence, consider evaluation of $\zeta_\mu(\delta)$ at some $\delta_0 \neq 0$. Then we have from (14)

$$\left.\frac{\partial \tilde{\Phi}_{(k,k-1)}}{\partial \delta}\right|_{\delta=\delta_0} = \int_{\Delta_{k-1}}^{\Delta_k} e^{-i\tilde{H}_k(\delta_0)(\Delta_k-\tau)} \times$$
$$\left(-i\alpha_{\mu k}\hat{H}_\mu\right) e^{-i\tilde{H}_k(\delta_0)(\tau-\Delta_{k-1})} d\tau \quad (25)$$

where the perturbed Hamiltonians are

$$\tilde{H}_k(\delta_0) = H_0 + \sum_{m=1}^{M} H_m f_{mk} + \alpha_{\mu k}\hat{H}_\mu \delta_0. \quad (26)$$

Given that $\hat{H}_\mu$ is still Hermitian, it follows that the terms $\left\|e^{-iH_k(\Delta_k-\tau)}\right\|_2$ and $\left\|e^{-iH_k(\tau-\Delta_{k-1})}\right\|_2$ in (25) are still unitary, and the bounds in (17) and (18) remain unchanged. As such we have $|\zeta_\mu(\delta)| \le B_2$ on $[\delta_1, \delta_2]$. ■

We now state the main result and provide a bound on δ to guarantee a given performance requirement.

Theorem 3: Given a maximum allowable error ϵ and uncertainty structure $\hat{H}_\mu$, the perturbed fidelity error $\tilde{e}_\mu(\delta) < \epsilon$ for all $|\delta| < \bar{\delta} = \frac{\epsilon - e(0)}{B_2}$.

Proof: From Lemma 1, $\tilde{e}_\mu(\delta)$ is locally Lipschitz on $[\delta_1, \delta_2]$. It follows that $|\tilde{e}_\mu(\delta_a) - \tilde{e}_\mu(\delta_b)| \le L_{ab}|\delta_a - \delta_b|$

on each open interval $(\delta_a, \delta_b) \subset [\delta_1, \delta_2]$ with Lipschitz constant L_{ab}. From Lemma 2, the bound B_2 for a given $\hat{H}_\mu$ for a given controller provides a uniform upper bound on L_{ab} over the interval $[\delta_1, \delta_2]$ so that $\tilde{e}_\mu(\delta)$ is Lipschitz on $[\delta_1, \delta_2]$ with Lipschitz constant B_2. Then, since $\delta = 0$ (the "nominal" uncertainty) necessarily lies in the interval $[\delta_1, \delta_2]$ of allowable uncertainty, $|\tilde{e}_\mu(\delta) - e(0)| \leq B_2 |\delta - 0|$. Since the fidelity error is always non-negative, the perturbed error is bounded by $\tilde{e}_\mu(\delta) \leq e(0) + B_2|\delta|$ where $e(0)$ is the nominal error. We now have the performance condition $\tilde{e}_\mu(\delta) \leq e(0) + B_2|\delta| \leq \epsilon$ from which the bound $|\delta| \leq \frac{\epsilon - e(0)}{B_2}$ guarantees $\tilde{e}_\mu(\delta) \leq \epsilon$. ■

Although the bound $\bar{\delta} = \frac{\epsilon - e(0)}{B_2}$ above guarantees that $\tilde{e}_\mu(\delta)$ does not exceed the threshold ϵ, the conservative bound B_2 yields a highly conservative performance bound on δ. Further, evaluation of a minimum δ that violates the performance criteria by this procedure is valid only for a specific uncertainty structure $\hat{H}_\mu = \hat{H}_m$. However, we can apply an iterative process based on the local bounds established by Theorem 2 to determine a bound on δ that guarantees a given performance criterion. Specifically, quantizing the uncertainty size δ into uniform steps of a given magnitude δ_0, we compute the directions of the maximum sensitivity of the fidelity error over every piecewise interval at uniform perturbation strength $n\delta_0 = \delta_n$. These maximum sensitivity directions computed from Theorem 2 take the form $\mathbf{s}_\mu^{(k)}(\delta_n) = \left[s_0^{(k)}(\delta_n), s_1^{(k)}(\delta_n), \ldots, s_M^{(k)}(\delta_n)\right]^T$ generated by the Hamiltonian $\tilde{H}_k(\delta_n)$ at strength δ_n (and associated $\mathbf{Z}(\delta_n)$ as per (24)). Computing the Hamiltonian for a perturbation of size δ_0 in direction $\mathbf{s}_\mu^{(k)}$ yields the recursive definition

$$\tilde{H}_k(\delta_1) = H_0 + \sum_{m=1}^{M} H_m f_{mk} + \delta_0 \sum_{m=0}^{M} \alpha_{mk} \hat{H}_m s_m^{(k)}(\delta_0),$$

$$\tilde{H}_k(\delta_n) = \tilde{H}_k(\delta_{n-1}) + \delta_0 \sum_{m=0}^{M} \alpha_{mk} \hat{H}_m s_m^{(k)}(\delta_{n-1}).$$

The perturbed error at this δ_n, $\tilde{e}_\mu(\delta_n)$ is then calculated from Eq. (9b) and (10) using the sequence of Hamiltonian matrices $\{\,\tilde{H}_k(\delta_n)\,\}$. If $\epsilon - \tilde{e}_\mu(\delta_n) > 0$, increment n by one, compute the gradient from Theorem 2, evaluate $\tilde{e}_\mu(\delta_{n+1})$. For some $\bar{n}$ we have $\epsilon - \tilde{e}_\mu(\delta_{\bar{n}}) \geq 0$. We then have the minimum perturbation that guarantees performance in any direction as $\bar{\delta} = \delta_{\bar{n}}$. We demonstrate this process in the following section.

VII. Case Study: Gate Optimization

To illustrate the results of the previous sections, we consider dynamic controllers optimized for maximum gate fidelity for a three-spin chain with Heisenberg coupling [10]. As opposed to full spin addressability, we consider the case of control only applied to the initial spin of the chain, a more challenging optimization problem. For brevity, we refer to this system as an $A00$-chain indicating control only on the first qubit. The

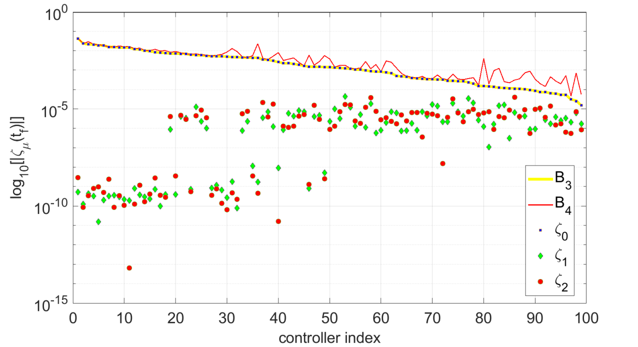

Fig. 1: Semilog plot of $\left|\frac{\partial \tilde{e}_\mu}{\partial \delta}\right|_{\delta=0} = |\zeta_\mu(t_f)|$ versus controller index for the $A00$-chain gate problem. The red line indicates the upper bound B_4 for a variable uncertainty structure while the yellow line indicates the upper bound B_3 for a static structure. Controllers are ordered in decreasing value of B_3

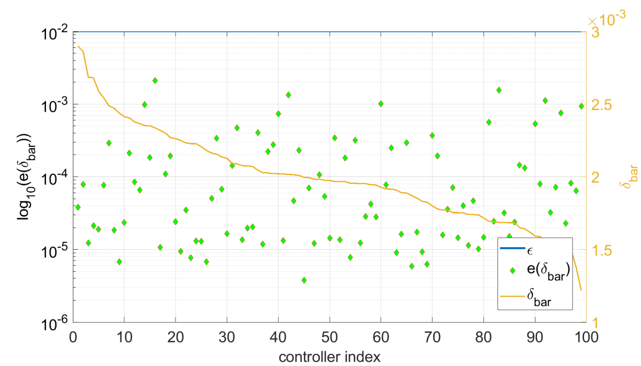

Fig. 2: Semilog plot of $\tilde{e}_1(\bar{\delta})$ and $\bar{\delta}$ versus controller index with $\epsilon = 0.01$. Here $\bar{\delta}$ is calculated directly from Theorem 3. Controllers are sorted in decreasing value of $\bar{\delta}$.

drift and interaction Hamiltonian matrices are:

$$H_0 = \frac{1}{2} \sum_{\ell=1}^{2} \left(\sigma_x^{(\ell)} \sigma_x^{(\ell+1)} + \sigma_y^{(\ell)} \sigma_y^{(\ell+1)} + \sigma_z^{(\ell)} \sigma_z^{(\ell+1)}\right), \quad (27)$$

$$H_1 = \frac{1}{2}\sigma_x^1, \quad H_2 = \frac{1}{2}\sigma_y^1, \quad (28)$$

where $\sigma_{\{x,y,z\}}$ are the Pauli spin operators. Here $\sigma_{\{x,y,x\}}^{(\ell)}$ is given by $\sigma_{\{x,y,z\}} \otimes I_2 \otimes I_2$ for $\ell = 1$, $I_2 \otimes \sigma_{\{x,y,z\}} \otimes I_2$ for $\ell = 2$, and $I_2 \otimes I_2 \otimes \sigma_{\{x,y,z\}}$ for $\ell = 3$. The target gate U_f is a randomly generated unitary gate, and the initial gate is taken as the identify matrix I_8. The choice of a randomly-generated unitary gate as the target is justified in the desire to make the optimization target as challenging as possible. The read-out time is $t_f = 15$ with $\kappa = 32$ time steps.

As discussed in Sections III and V we choose as a basis for the perturbation structure $\{\hat{H}_\mu\}$ for $\mu = 0$ to 2. We first examine the bound on all perturbations at $\delta = 0$. Figure 1 shows the tightness of the bounds B_3 and B_4 obtained from Theorems 1 and 2 for $\zeta_\mu(t_f)$ localized around $\delta = 0$, nearly matching the sensitivity generated by the uncertainty structure $\hat{H}_0$. As expected, the bound for a non-static uncertainty structure is

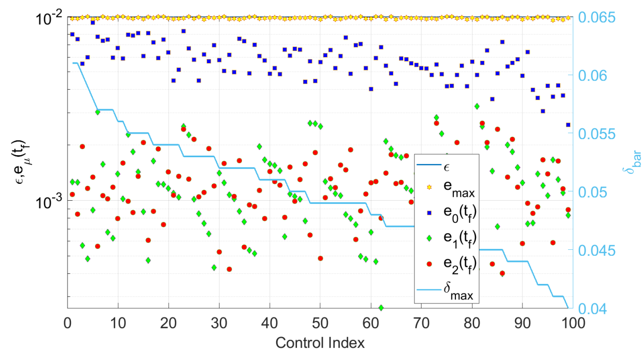

Fig. 3: Semilog plot of $\tilde{e}_\mu(\bar{\delta})$ versus $\bar{\delta}$ versus controller index with $\epsilon = 0.01$. Here $\bar{\delta}$ computed by iterating on B_4 based on Theorem 2. Controllers are ordered in decreasing value of $\bar{\delta}$. A perturbation of size $\bar{\delta}$ in any of the principal directions $\hat{H}_\mu$ does not produce an error that exceeds ϵ.

slightly larger than B_3, but not significantly greater.

Turning to performance, we examine the closeness of the performance guarantees of Theorem 3 to the actual perturbed error based on the predicted value of $\bar{\delta}$. We set the value of ϵ at 0.01, so that a gate fidelity of 99% is the minimum performance threshold. As shown in Figure 2, perturbing the system in the direction $\hat{H}_1$ at the value of $\bar{\delta}$ given by Theorem 3 does not violate the performance criteria $\tilde{e}_1(\bar{\delta}) < \epsilon$. However, the plot reveals the conservativeness of $\bar{\delta}$ calculated this way. Specifically, the predicted value of $\bar{\delta}$ results in a fidelity error $e_1(\bar{\delta})$ with a margin of $\approx 10^2$ before exceeding the performance criteria $\epsilon = 10^{-2}$ in roughly half of the controllers. Surprisingly, for seven controllers, the conservative $\bar{\delta}$ pushes $\tilde{e}_1(\bar{\delta})$ to within an order of magnitude of the limiting error ϵ, providing some utility to the first order, differential-based performance bound. Still, the overall result indicates the limitation of differential sensitivity techniques to guarantee performance for non-vanishing perturbations. However, as noted in Section VI, we can use Theorem 2 to iterate a computational search for the minimum value of δ that exceeds the performance bounds in any uncertainty direction $\hat{H}_\mu$. Figure 3 shows the results of iterating on δ to find the smallest δ such that a violation $\tilde{e}_\mu(\delta) \geq \epsilon$ of the performance criteria occurs. Values of $\bar{\delta}$ average two magnitudes greater than those predicted by Theorem 3. As seen in the figure, the iterative procedure results in a $\bar{\delta}$ such that the sequence of perturbations $\{\, \delta_0 \mathbf{s}_\mu^{(n)} \,\}$ pushes the fidelity error to the limit of the performance criteria ϵ indicated by $\tilde{e}_{max}$. Additionally, we note that in the perturbative regime around $\delta = 0$, perturbations structured as $\hat{H}_0$ show the greatest sensitivity. As seen in Figure 3, perturbations of this same structure lead to those values of $\tilde{e}_\mu(\delta)$ that most closely approach the ϵ-threshold. This suggests that the sensitivity properties gleaned form the differential sensitivity at $\delta = 0$ are indicative of sensitivity to the error at non-vanishing values of δ, at least for this controller set.

VIII. Conclusion

We have shown that the calculation of the differential sensitivity as in [13] is easily extended to the case of piecewise constant controls generated by quantum optimal control algorithms. Further, the differential sensitivity can be reliably bounded for small perturbations about the nominal operating point and those uncertainty structures that generate this maximum sensitivity can be deduced. However such differential sensitivity techniques have limited applicability beyond the realm of vanishing perturbations, suggesting the need for a coherent theory to accommodate performance guarantees for larger perturbations.

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