Supplemental Information: Noise-Assisted Feedback Control of Open Quantum Systems for Ground State Properties

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I. BOUND FOR $\beta(t)$

For a closed system under unitary dynamics, we have

$$\beta(t) = -A(t) = -\langle |i[H_d, H_p]| \rangle . \tag{1}$$

According to the Cauchy-Schwarz inequality,

$$\frac{1}{2} | \langle |i[H_d, H_p]| \rangle | \le \Delta H_d \Delta H_p, \tag{2}$$

where $\Delta H = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$ for an operator H. The variance is upper-bounded by the semi-norm $||H||$ of a Hermitian operator H as $\Delta^2 H \le ||H||/4$. The semi-norm is defined as, $||H|| = M_H - m_H$, where $M_H(m_H)$ is the maximum (minimum) eigenvalue of H. Defining $n_p = \sqrt{||H_p||}$ and $n_d = \sqrt{||H_d||}$ and combining with Eq. (2) we find

$$\frac{n_p n_d}{4} \ge \Delta H_d \Delta H_p \ge \frac{1}{2} | \langle |i[H_d, H_p]| \rangle | = -\frac{1}{2}\beta(t), \tag{3}$$

which introduces a lower bound for $\beta(t)$ as $\beta(t) \ge -\frac{n_p n_d}{2}$.

II. BOUND FOR $\Gamma_k(t)$

Consider the non-Markovian master equation, where we define

$$\Gamma_k(t) = -\left(\langle P_k^\dagger H_p P_k \rangle - \langle H_p \rangle\right)_t = \mathrm{Tr}[\rho(t)(P_k^\dagger H_p P_k - H_p)], \tag{4}$$

and $\Gamma_k(0) = \lambda_k$. The fidelity between the initial and the final reduced density matrices can be defined as

$$F(t) = \mathrm{Tr}[\rho(0)\rho(t)], \tag{5}$$

as the initial state is a known pure state, i.e., $\mathrm{Tr}[\rho(0)^2] = 1$. Defining $O_k = P_k^\dagger H_p P_k - H_p$ leads to

$$|\Gamma_k(t) - \Gamma_k(0)| \approx \mathrm{Tr}[(\rho(t) - \rho(0))O_k] \le ||O_k|| \cdot ||\rho(t) - \rho(0)||_1, \tag{6}$$

where $|| \cdot ||$ is the operator norm (largest singular value), and $|| \cdot ||_1$ is the trace-norm. The trace distance is bounded by

$$||\rho(t) - \rho(0)||_1 \le 2\sqrt{1 - F(t)}. \tag{7}$$

Combining the two equations, we get a bound for the decay operators as

$$|\Gamma_k(t) - \Gamma_k(0)| = |\Gamma_k(t) - \lambda_k| \le 2\, ||O_k|| \cdot \sqrt{1 - F(t)}, \tag{8}$$

where the fidelity at short times can be calculated asymptotically (see Appendix. III).

However, a weaker but easily obtained bound can also be found using the Cauchy-Schwarz inequality for operators $|\mathrm{Tr}(A^\dagger B)|^2 \le \mathrm{Tr}(A^\dagger A)\mathrm{Tr}(B^\dagger B)$. This leads to

$$|\mathrm{Tr}[\rho(t)(P_k^\dagger H_p P_k)]| \le \sqrt{\mathrm{Tr}[\rho(t)^2]}\, ||H_p||_2, \tag{9}$$

which gives us the final inequality as

$$\begin{aligned} |\Gamma_k(t)| &\le |\mathrm{Tr}[\rho(t)(P_k^\dagger H_p P_k)]| + ||H_p|| \\ &\le \sqrt{\mathcal{P}(t)}\, ||H_p||_2 + ||H_p|| \\ &\le 2\, ||H_p||_2, \end{aligned} \tag{10}$$

where $\mathcal{P}(t) = \mathrm{Tr}[\rho(t)^2]$ is the purity of the final state.

III. FIDELITY FOR THE SHORT-TIME QUANTUM DECAY

The bound defined in Eq. (8) requires knowledge of the fidelity $F(t)$, and here we obtain an analytic expression for $F(t)$ in the short-time limit [1]. Its first derivative reads

$$\begin{aligned} \frac{d}{dt}F(t) &= \mathrm{Tr}[\rho(0)\dot{\rho}(t)] \\ &= -i\mathrm{Tr}\{\rho(0)[H(t), \rho(t)]\} \\ &+ \sum_{k\in\mathcal{K}} \Gamma_k(t)\{\mathrm{Tr}[\rho(0)P_k\rho(t)P_k^\dagger] - \mathrm{Tr}[\rho(0)\rho(t)]\}. \end{aligned} \tag{11}$$

At $t = 0$, $F'(t)$ reduces to

$$\begin{aligned} F'(0) &= \lim_{t\to 0} \frac{d}{dt}F(t) \\ &= -\sum_{k\in\mathcal{K}} \Gamma_k(0)\{\mathrm{Tr}[\rho(0)^2] - \mathrm{Tr}[\rho(0)P_k\rho(0)P_k^\dagger]\} \\ &= -\sum_{k\in\mathcal{K}} \Gamma_k(0)\Delta P_k^2, \end{aligned} \tag{12}$$

with the variance of the operator $\Delta P_k^2 = \langle P_k^2 \rangle - \langle P_k \rangle^2$ and $\Gamma_k(0) = \lambda_k$. Hence, in a short-time asymptotic expansion, the

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fidelity can be written as

$$F(t) = 1 + F'(0)t + \mathcal{O}(t^2) \approx 1 - t\sum_{k\in\mathcal{K}} \lambda_k \Delta P_k^2. \quad (13)$$

IV. LYAPUNOV CONTROLLED DECOHERENCE-FREE SUBSPACE

The decoherence-free subspace (DFS) method was introduced as an alternative method for error-free quantum computation [2]. This is an important concept, as the states in DFS evolve unitarily, even in the presence of decoherence. The Markovian dynamics representing the noise in the NISQ hardware is governed by Eq. (4) of the main text with the learned positive error rates, $\{\lambda\}$. Here, we add an extra Lyapunov control field $\gamma(t)$ and a control Hamiltonian H_n to cancel out the dissipative part of the master equation. With the additional controls, the master equation becomes

$$\frac{d\rho}{dt} = -i[H_p + \beta(t)H_d + \gamma(t)H_n, \rho] + \mathcal{D}_{\text{int}}[\rho], \quad (14)$$

where $\mathcal{D}_{\text{int}}[\rho]$ is the stochastic Pauli noise channel of the NISQ device. For the new controlled Hamiltonian, Eq. 5 (main text) reduces to

$$\langle \dot{H}_p \rangle = \beta(t)\langle i[H_d, H_p]\rangle + \gamma(t)\langle i[H_n, H_p]\rangle + \text{Tr}(\mathcal{D}_{\text{int}}[\rho]H_p). \quad (15)$$

Making a connection with [3], we choose

$$\gamma(t) = -\frac{\text{Tr}(\mathcal{D}_{\text{int}}[\rho]H_p)}{\langle i[H_n, H_p]\rangle}, \quad \beta(t) = -\langle i[H_d, H_p]\rangle, \quad (16)$$

such that $\langle \dot{H}_p\rangle \leq 0$. There should always exist a $\gamma(t)$ unless $\langle i[H_n, H_p]\rangle = 0$.This approach can be called the Lyapunov-controlled decoherence-free subspace (LC-DFS).

Here we discuss the limitations of the LC-DFS compared to those of NAFQA. First, the choice of additional Lyapunov control Hamiltonians is restricted due to the condition $\langle i[H_n, H_p]\rangle \neq 0$. Second, the commutator $[H_n, H_p]$ may contain higher-order terms, which will be difficult to implement on quantum computers. For example, for the spin glass Hamiltonian considered in the main text, $H_p = \sum_{m<n} J_{mn}Z_m Z_n + \sum_l h_l Z_l$, and a two-body control Hamiltonian $H_n = \sum_{i<j}(Y_i Z_j + Z_i Y_j)$, the commutator $[H_n, H_p]$ contains one-body X, two-body XZ, ZX, and three-body XZZ, ZZX operators. In this case, implementing the three-body operators on quantum computers is not straightforward, which further restricts the choice of control Hamiltonians and the application of the LC-DFS approach.

V. AMPLITUDE AND PHASE DAMPING NOISE CHANNELS

In the main text, we have considered the implementation of NAFQA with the stochastic Pauli noise (unital) channels. However, one can also study the behavior of the NAFQA algorithm beyond the stochastic Pauli noise channel, for instance, with the amplitude and phase damping channels, which are widely considered in OQS dynamics [4]. The GKSL equation corresponding to the local amplitude and phase damping is given by

$$\frac{d\rho}{dt} = -i[H, \rho] + \mathcal{D}_{\text{r}}[\rho]. \quad (17)$$

The Lindblad dissipator takes the form

$$\mathcal{D}_{\text{r}}[\rho] = \sum_{k=1}^{N} \lambda_k \left(s_k^{(-)}\rho s_k^{(+)} - \frac{1}{2}\{s_k^{(+)}s_k^{(-)}, \rho\}\right) + \sum_{k=1}^{N} \frac{\lambda_k}{4}\left(Z_k \rho Z_k - \rho\right), \quad (18)$$

which is a combination of the amplitude damping noise with decay rates λ_k and the phase damping noise with rates $\lambda_k/4$. Here, $s_k^{(\pm)} = \frac{1}{2}(X_k \pm iY_k)$, and $s_k^{(+)}s_k^{(-)} = |1\rangle\langle 1|_k$ corresponds to the k^{th} qubit. The condition for the single-qubit dephasing channel follows a procedure similar to that of the stochastic Pauli noise (Eq. (7) of the main text). However, the Lyapunov condition for the amplitude-damping channel takes the form

$$\frac{d}{dt}\langle H_p\rangle = \beta(t)\langle i[H_d, H_p]\rangle + \sum_{k\in\mathcal{K}} \Gamma_k(t)\left(\langle s_k^{(+)} H_p s_k^{(-)}\rangle - \frac{1}{2}\langle\{H_p, s_k^{(+)}s_k^{(-)}\}\rangle\right) \leq 0. \quad (19)$$

The amplitude and phase damping channels can be implemented on quantum circuits with or without the help of ancilla qubits [5, 6]. Similarly to the feedback-based noise-assisted approach discussed in the Results, one can engineer the time-dependent decay rates based on the feedback law to use the amplitude and phase damping channels as a resource to assist quantum simulations.

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