Platform tailored co-design of gate-based quantum simulation

Kushal Seetharam,1,2 Dries Sels,3,4 and Eugene Demler5

1Department of Electrical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
2Department of Physics, Harvard University, Cambridge, MA, 02138, USA
3Department of Physics, New York University, New York, NY, 10003, USA
4Center for Computational Quantum Physics, Flatiron Institute, New York, NY, 10010, USA
5Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland

(Dated: September 4, 2024)

The utility of near-term quantum computers and simulators is likely to rely upon software-hardware co-design, with error-aware algorithms and protocols optimized for the platforms they are run on. Here, we show how knowledge of noise in a system can be exploited to improve the design of gate-based quantum simulation algorithms. We demonstrate this co-design in the context of a trapped ion quantum simulation of the dynamics of a Heisenberg spin model. Specifically, we derive a theoretical noise model describing unitary gate errors due to heating of the ions’ collective motion, finding that the temporal correlations in the noise induce an optimal gate depth. We then illustrate how tailored feedforward control, best applied at this optimum, can be used to partially mitigate unitary gate errors and improve the simulation outcome. Our results provide a practical guide to the co-design of gate-based quantum simulation algorithms.

I. INTRODUCTION

Large-scale fault-tolerant quantum computers have the potential to catalyze progress in physics and material science, chemistry and drug development, as well as optimization and machine learning [1, 2]. In the near-term, noisy intermediate-scale quantum (NISQ) technology may still demonstrate a quantum advantage over classical computers for certain tasks. The first useful task of NISQ computers likely to demonstrate a quantum advantage is the simulation of quantum dynamics [1, 3, 4]. Digital quantum simulation, accomplished by discretizing the dynamics into several gates, is a flexible approach with controllable error that can improve our understanding of spin systems [5, 6], quantum chemistry [7, 8], biochemistry [9], and high energy physics [10, 11]. A common challenge in all such gate-based quantum simulation is to optimize the quantum circuit implementing the algorithm for a particular NISQ platform. Specifically, the discretization error in the algorithm is reduced by increasing the number of gates, while hardware noise in the system causing decoherence leads to error that typically worsens as the number of gates increases. To achieve the best performance of the algorithm, we must therefore determine both the optimal number of gates and the optimal parameters for these gates in order to account for noise. The focus of this work is to provide insight into these questions which lie at the heart of software-hardware co-design of gate-based quantum simulation.

More generally, understanding the principles of co-design and error-mitigation is essential to realize the potential of quantum computers, as hardware noise usually wipes out the effects responsible for quantum advantages [12]. Even fault-tolerant quantum computers of the future will rely on the characterization and mitigation of noise. The existence of a fault tolerance threshold is only rigorously defined when errors are assumed to be independent; this Markovian idealization is only true when spatial and temporal correlations in the noise die off quickly [13–15]. The magnitude of independent errors, in turn, affects the resource cost of the system, with noisier systems requiring a larger overhead of physical qubits per logical qubit. For near-term noisy, intermediate-scale platforms, characterizing the noise in a system is even more critical. Practical applications will require the co-design of protocols optimized to different hardwares. Indeed, understanding the nature of noise in a system can enable tailored quantum-control and error mitigation that improves desired performance metrics [16, 17]. In some cases, noise can even be exploited as a feature of the system to simulate the dynamics of complicated many-body models [18].

The three categories of error in quantum computations and simulations are measurement errors, incoherent errors, and coherent errors. The first, measurement error, arises as quantum observables have inherent uncertainty and hence their expectation value can only be determined with a certainty set by the number of measurement samples. The second, incoherent error, arises from coupling between the qubits and their environment, with these interactions causing the internal state of the qubit to
change. The last, coherent error, occurs when a desired unitary transformation of the system imparts an angle different than intended. These unitary errors are the focus of this work and arise due to limitations of the platform’s analog control hardware or the dynamics of the physical qubits [19]. Over the course of a quantum computation or simulation, such unitary errors accumulate and dephase the system state, killing the coherent effects responsible for a quantum advantage and degrading the fidelity of any simulation. In trapped ions, for example, one dominant source of decoherence is the ions’ collective motion, which is thermally excited due to electric field fluctuations from trap electrodes. While the internal qubit states of the ions are not directly affected by this motion, any quantum gate applied via individually addressed lasers imparts an erroneous phase to the qubit states, as depicted in Fig. 1. We can understand the source of this noise as the phonon mode associated with the center of mass of the chain having an energy that undergoes diffusion due to heating from electric field fluctuations. This slow diffusion of the phonon in energy space causes the unitary error to be non-Markovian, with correlations arising between gates applied at different times during an experiment.

In this work, we demonstrate how to exploit knowledge of the noise underlying a system to optimize gate-based quantum simulations. To provide an example, we do so in the context of simulating the dynamics of a Heisenberg spin model in a system of trapped ions. We first introduce the quantum simulation task and associated gate-based algorithm. Then, we derive a theoretical noise model describing unitary errors from thermal ion motion in trapped ion systems and provide a protocol to experimentally extract the latent variable underlying the model. We discuss how temporal correlations in the noise induce an optimal gate depth of the quantum simulation circuit. These correlations cause the error in the simulation arising from motional noise to accumulate as the gate depth is increased, while the Trotter error associated with discretization of the time-evolution decreases as the gate depth is increased. The competition of these two errors induces an optimal gate depth.

Next, we provide a platform-independent framework for optimal feedforward control of unitary gate errors, which involves applying gates with angles that are modified to compensate for the predicted noise in the system. We illustrate the utility of feedforward control in the trapped ion implementation of simulating the Heisenberg Hamiltonian, showing that feedforward control partially mitigates both discretization error and decoherence error in the simulation output.

Our work provides three results that are generally applicable to the co-design of gate-based quantum algorithms beyond the discussed simulation task: (i) the understanding that non-Markovian correlations are the root cause of decoherence and the subsequent limitation on gate depth in any platform where unitary errors are the dominant noise, (ii) a method to optimally leverage noise characterization to mitigate unitary gate errors via feedforward control, and (iii) an accurate model of unitary gate errors arising from thermally-excited ion motion in trapped ion systems.

II. HAMILTONIAN SIMULATION

Simulating the quantum dynamics of a system is a natural application of digital quantum computers and analog quantum simulators, and is likely to be the first problem of practical interest where a quantum advantage over classical computers is demonstrated on near-term quantum platforms [3]. The goal is to simulate the time-evolution, \[ \hat{U}(t) = \exp \left( -i \hat{H} t / \hbar \right) \], of a system whose dynamics are generated by a Hamiltonian \( \hat{H} \). Here, we focus on the Heisenberg Hamiltonian,

\[
\hat{H} = \sum_{i,j} J_{ij} \hat{S}_i \cdot \hat{S}_j + \sum_i h_i \hat{S}_i^z
\]

which is a paradigmatic spin model that describes the magnetic properties of many insulating crystals [20], appears in the study of thermalization in quantum systems [21–23], and describes the essential physics underlying nuclear magnetic resonance (NMR) spectroscopy [9].

Many near-term quantum algorithms and simulations focus on the task of estimating the expectation value of some observable after time-evolution, with the value of such observables often being less susceptible to noise than the full system state [23]. In this vein, we benchmark the quality of gate-based quantum simulation of Eq. (1) with the spectrum simulation task discussed in Ref. [9] and experimentally demonstrated in Ref. [25]. This algorithm uses time-evolution under the Heisenberg Hamiltonian, Eq. (1), to compute the NMR spectrum

\[
A(\omega) = \text{Re} \int_0^\infty dt \cdot e^{i\omega t - \gamma t} \langle S(t) \rangle
\]

where

\[
S(t) = \langle \hat{S}_{\text{tot}}^z(t) \hat{S}_{\text{tot}}^z \rangle = \text{Tr} \left[ e^{i\hat{H}t} \hat{S}_{\text{tot}}^z e^{-i\hat{H}t} \hat{S}_{\text{tot}}^z \rho_0 \right]
\]

is the total magnetization response function and \( \rho_0 \) is the initial state of the spin system. For typical NMR experiments, it is a good approximation to assume that the system starts in an infinite temperature state \( \rho_0 = \frac{I}{\text{Tr}[I]} \), where \( I \) is the identity operator.

Letting \( |z_j\rangle \) be the eigenstates of \( \hat{S}_{\text{tot}}^z \) corresponding to eigenvalues \( n_j \), the response function is computed as

\[
S(t) = 2 \sum_{j: n_j > 0} \frac{m_j}{2N_s} \langle z_j(t) | \hat{S}_{\text{tot}}^z | z_j(t) \rangle
\]

where \( |z_j(t)\rangle = e^{-i\hat{H}t} |z_j\rangle \) and \( N_s \) is the number of spins in the system. The quantum algorithm is thus prepartion of the desired computational basis states \{ |z_j\rangle \},
Hamiltonian simulation of $\hat{H}$ through implementation of the time-evolution operator $\hat{U}(t) = e^{-iHt}$, and projective measurements in the computational basis. These measurements yield the response function, $S(t)$, whose Fourier transform gives the desired spectrum, $A(\omega)$.

We implement this time-evolution using a first-order Trotter decomposition into gates commonly used in trapped ion platforms. Specifically, we split the total time-evolution into $r$ Trotter steps yielding $\hat{U}(t) = \left[ \hat{U}(\Delta t) \right]^r$ where $\Delta t = \frac{t}{r}$. The unitary $\hat{U}(\Delta t) = e^{-iH\Delta t}$ is then approximated with the Suzuki-Trotter product formula

$$\hat{U}_1(\Delta t) = e^{-i(\sum_n h_n \hat{S}_n^z)\Delta t} \left( \Pi_{(ij)} e^{-i\hat{S}^y_i \hat{S}^y_j (2J_{ij}\Delta t)} \right) \times$$

$$\times \left( \Pi_{(ij)} e^{-i\hat{S}^x_i \hat{S}^x_j (2J_{ij}\Delta t)} \right) \left( \Pi_{(ij)} e^{-i\hat{S}^y_i \hat{S}^y_j (2J_{ij}\Delta t)} \right) \tag{6}$$

where $(ij)$ corresponds to all unique pairs of spins as $J_{ij} = J_{ji}$ in the Hamiltonian. Furthermore, we only include pairs of spins where $J_{ij} \neq 0$. The total time-evolution is then given by $\hat{U}_1(t) = \left[ \hat{U}_1(\Delta t) \right]^r$. Defining the two-qubit gates $\hat{U}^{\alpha\alpha}(\phi_{ij}) = \exp \{-i\hat{S}^y_i \hat{S}^y_j \phi_{ij}\}$ where $\phi_{ij} = 2J_{ij} \Delta t$, single-qubit rotation gates $\hat{R}^{\alpha}_i(\phi) = e^{-i\hat{S}_i^\alpha \phi}$, and angles $\phi_i = 2\hbar_i \Delta t$, the quantum circuit for time evolution is given by

$$\hat{U}_1(t) = \Pi_{r=1} \left\{ \left( \Pi \hat{R}^{y}_i \left( -\frac{\pi}{2} \right) \right) \left( \Pi \hat{R}^{z}_i \left( -\phi_i \right) \right) \times$$

$$\times \left( \Pi_{(ij)} \hat{U}^{xx}(\phi_{ij}) \right) \left( \Pi_{(ij)} \hat{U}^{yy}(\phi_{ij}) \right) \times$$

$$\times \left( \Pi \hat{R}^{z}_i \left( \frac{\pi}{2} \right) \right) \left( \Pi_{(ij)} \hat{U}^{xx}(\phi_{ij}) \right) \right\} \tag{7}$$

where we apply gates from right to left. The Trotter decomposition, Eq. (7), is expressed in terms of the Molmer-Sorensen gates, $\hat{U}^{xx}(\phi_{ij})$, and single qubit rotations that are commonly used in trapped ion computations.

Assuming that enough measurements are made during a computation to ignore measurement errors in the expectation values, $(z_j(t) | \hat{S}^z_{tot} | z_j(t))$, the computed spectrum will still include discretization errors from Trotterization and unitary gate errors from the ion motion described in Sec. III. The feedforward control discussed in Sec. IV can help mitigate the latter. Figure 2 shows an example spectrum (black), the same spectrum with both Trotter and unitary noise (orange), and the noisy spectrum with feedforward control (green).

III. TRAPPED ION NOISE MODEL

Trapped ions have emerged as a leading platform for quantum computation and simulation due to their long coherence times, identical nature, and negligible idle errors [12, 20]. The ions in these systems crystallize into a chain after being tightly confined in two directions via an oscillating electric field. Entanglement between the qubits is generated by a laser-induced interaction between states that is mediated by the collective motion of ions. Usually, the motional modes along the tightly confined transverse direction are used for these operations as they are less sensitive to electric field fluctuations arising from the electrodes generating the trap. These fluctuations do, however, excite the weakly confined longitudinal modes of the chain. The deviation of the ions from their lattice positions causes them to experience erroneous intensities from the individually addressed laser beams used to implement different operations. As the longitudinal motion of the ions heats up, these errors build into a dominant form of noise that limits the operational time window of the system [20]. Here, we develop a noise model for errors arising from this longitudinal heating, ignoring other possible sources of error in trapped ion systems that may be more prevalent in different operational regimes of the device.

We first characterize the gate error in the system due to longitudinal movement of the ions in the $x$-direction, depicted in Fig. 1. The individually addressed single- and two-qubit gates in trapped ion systems are enacted by shining a narrowly focused laser on a single or pair of ion lattice sites respectively. The gates take the form $\hat{U}(\phi) = \exp \left(-i\phi \hat{A}\right)$, where $\hat{A}$ is either a single spin oper-
ator, $\hat{S}_j^\gamma$, acting on a site $j$, or the bilinear, $\hat{S}_j^+ \hat{S}_j^-$, acting on a pair of sites. These gates form a sufficient set for universal quantum computation. Letting $\hat{S}_i^+$ and $\hat{S}_i^-$ be the creation and annihilation operators of the ion momentum operator, we define the usual bosonic creation annihilation operator.

The phase of the gate is initiated at time $t_g$, where $t_g$ is the duration of the laser pulse, and $\Omega$ is the Rabi frequency set by the electric field amplitude of the laser. This amplitude typically has a Gaussian distribution of the erroneous phase $\phi$, making it difficult to compute the Bose-Einstein distribution of the electric field occupation. We assume that the background electric field is at infinite temperature so both these rates are equal and redefine $\gamma$ such that $\gamma_+ = \gamma - \gamma$. Given that the relevant phonon frequencies are of the order of a few hundreds of kHz, this approximation is satisfied down to very low temperatures.

In trapped ion experiments, it is possible to cool the chain close to its motional ground state during preparation of the system. We therefore assume that the initial motional state of the system is the phonon vacuum $\rho(0) = \{0\} \langle 0 |$. Dynamics under Eq. (9) will then evolve the system into a harmonically oscillating coherent state undergoing a diffusive random walk in its amplitude. It therefore makes sense to describe the system state in terms of its Glauber-Sudarshan P-function representation:

$$\rho = \int d^2 \alpha \mathcal{P}(\alpha, \alpha^*, t) |\alpha\rangle \langle \alpha|$$

where $\{\langle \alpha |\}$ are coherent states that form a basis for the system. The dynamics of the system is then captured by a Fokker-Planck equation for the P-function, $P(\alpha, \alpha^*, t)$,

$$\frac{d}{dt} P = \left\{ -\omega_0 \left( \frac{\partial}{\partial \alpha} \alpha - \frac{\partial}{\partial \alpha^*} \alpha^* \right) + \gamma \frac{\partial^2}{\partial \alpha \partial \alpha^*} \right\} P.$$  \hspace{0.5cm} (11)

The Green’s function of the Fokker-Planck equation, expressed in the rotating frame of the phonon mode with frequency $\omega_0$, is

$$K(\alpha', t' | \alpha, t) = \frac{1}{\pi \gamma (t' - t)} \exp \left\{ -\frac{|\alpha' - \alpha|}{\gamma (t' - t)} \right\},$$

where $\gamma$ is the increase in the oscillation amplitude at rate $\gamma_+$, and the third term represents a decrease in the oscillation amplitude at rate $\gamma_-$. These latter two terms describe the incoherent dynamics of the ions resulting from background electric field fluctuations.
it suffices to consider the $T = 0$ limit in which case the P-function is simply $P(\alpha, \alpha^*) = \delta(\alpha)\delta(\alpha^*)$. This Green’s function can be used to compute the probability distribution and correlations of observables expressed in the coherent state basis. Letting $\phi(\tau) = \Pi(\tau) t_g$ be the angle imparted by a unitary gate applied at time $\tau$ in the experiment, when the phonon mode is in state $|\alpha(\tau)\rangle$, the Rabi phase of the qubit will advance by an angle

$$\phi(\tau) = \phi_{in} \exp \left\{ - \left( \frac{a_{osc}}{a_{laser}} \right)^2 |\alpha(\tau)|^2 \right\}, \quad (13)$$

where $a_{osc} = \sqrt{\hbar/(m\omega_0)}$ and $a_{laser} = \sqrt{2\sigma}$ are the characteristic length scales of the harmonic oscillator and Gaussian laser respectively. The probability distribution of the angle can then be computed as

$$p_\phi(\phi; c_2) = \frac{1}{c_2 \tau} \frac{1}{\phi_{in}} \Theta(\phi_{in} - \phi), \quad (14)$$

where we have defined the heating rate constant

$$c_2 = \gamma \left( \frac{a_{osc}}{a_{laser}} \right)^2 \quad (15)$$

and the Heaviside step function, $\Theta(\phi_{in} - \phi)$, encodes the fact that the time-averaged Rabi frequency felt by the ion cannot be more than spending all its time at the center of the laser where its intensity is strongest. The distribution of angles, Eq. (14), is the noise model we need for feedforward control. Note that it only depends on a single latent variable, $\lambda = c_2 \tau$, representing the amount of diffusion the ions’ motion has undergone.

We can gain insight into the angle distribution by examining the average and typical angles that are applied by the gate,

$$\phi_{avg} = \mathbb{E}_\phi[\phi] = \frac{\phi_{in}}{1 + \lambda} \quad (16)$$

$$\phi_{typ} = \exp(\mathbb{E}_\phi[\log \phi]) = \phi_{in} e^{-\lambda}. \quad (17)$$

We see that at late experimental times compared to the rate $c_2$ such that $\lambda \to \infty$, both the average and typical angles go to zero. Physically, the amplitude of the ions’ oscillation becomes so large that the ion never spends time inside the laser beam and hence its internal qubit state is not changed. While the average angle algebraically decays to zero at late times, the typical angle becomes very small as $\tau$ crosses $1/c_2$, thus showing that $c_2$ sets the timescale where we can coherently manipulate the qubits in an experiment.

We can further understand the effects of noise on a quantum computation or simulation by examining the correlation between two gates applied at a time $\Delta \tau$ apart,

$$\text{Corr}(\phi(\tau + \Delta \tau) \phi(\tau)) = \frac{\text{Cov}(\phi(\tau + \Delta \tau) \phi(\tau))}{\sqrt{\text{Var}(\phi(\tau)) \text{Var}(\phi(\tau))}}$$

$$= \frac{\tau}{\tau + \Delta \tau} \sqrt{\frac{1 + 2c_2 \tau}{1 + 2c_2(\tau + \Delta \tau)}} \quad (18)$$

Taking the limit at late times, we have

$$\lim_{\tau \to \infty} \text{Corr}(\phi(\tau + \Delta \tau) \phi(\tau)) = \frac{1}{1 + \frac{2}{\tau} \Delta \tau} + \mathcal{O} \left( \frac{1}{\tau} \right), \quad (19)$$
which shows that $c_2$ also sets the temporal correlation length between different gates. Given that the gate application time, $t_g$, is small compared to typical values of $c_2$ in trapped ion experiments, the unitary gate errors will be temporally correlated.

As a limiting case, we can examine how the noisy gate angles are distributed at short times when the ions are very close to the center of the laser beam. By simultaneously taking the limits $\phi \to \phi_0$ and $c_2 \tau \to 0$ in Eq. (14), we get the short time distribution

$$p_{\theta}^{\text{short}}(\theta; \tau, c_2) = \frac{1}{c_2 \tau \phi_0} e^{-\left(\frac{\phi_0 - \theta}{c_2 \tau \phi_0}\right)} \Theta(\phi_0 - \theta).$$

(20)

This expression can equivalently be derived by Taylor expanding Eq. (13) as $\phi(\tau) = \phi_0 \left(1 - \frac{\alpha(\tau)}{\Delta_{\text{man}}}ight)^2$ and computing the probability distribution of gate angles using the Green’s function given in Eq. (12). The exponential distribution of gate angles described in Eq. (20), valid at short times, is in agreement with the ion noise model discussed in Ref. [26].

We now give a protocol to experimentally extract the value of $c_2$ which characterizes the noise in a particular trapped ion set-up. Prepare a system of two qubits in the computational basis state $\ket{\downarrow \downarrow}$, wait a time $\tau$, and apply a gate $\hat{U}_{xx}(\phi) = \exp(-i\phi S_x^i S_x^j)$ with an input angle $\phi_0$. Then, do a projective measurement in the computational basis state to extract the return probability of the system being in the $\ket{\downarrow \downarrow}$ state. If there was no noise in the system, this probability would be

$$P_{\downarrow \downarrow} = \bra{\downarrow \downarrow} \hat{U}_{xx}(\phi_0) \ket{\downarrow \downarrow} = \cos^2\left(\frac{\phi_0}{4}\right)$$

(21)

for all $\tau$. With unitary gate error due to the ions’ motion, the probability becomes

$$T_{\downarrow \downarrow}(\phi_0, c_2 \tau) = \mathbb{E}_\phi \left[ \cos^2\left(\frac{\phi}{4}\right) \right]$$

$$= \cos^2\left(\frac{\phi_0}{4}\right) + \frac{\phi_0^2 c_2 \tau}{8 + 16 c_2^2 \tau} \times$$

$$\times \ _2F_2\left(1 + \frac{1}{2c_2^2 \tau}, \frac{3}{2}, \frac{2}{2} + \frac{1}{2c_2^2 \tau}, -\phi_0^2 / 16\right).$$

(22)

where $\ _2F_2$ is the generalized hypergeometric function. This average return probability is directly related to the moment generating function of Eq. (14). Measuring Eq. (22) for different input angles, $\phi_0$, and wait times, $\tau$, yield curves that can be used to fit the value $c_2$. We give examples of these curves in Fig. 3(a). In Fig. 3(b), we show the return probability to differentiate between the noise model derived here and typical phase damping. The latter leads to a return probability characterized by an exponentially decaying oscillations with a constant phase shift dependent on the input angle. Armed with knowledge of the noise model, Eq (14), and a method to experimentally determine the latent variable, $c_2$, we now illustrate how non-Markovian correlations in the noise induce an optimal gate depth when implementing a quantum algorithm.

## IV. OPTIMAL GATE DEPTH

We can gain insight into how non-Markovian correlations amongst gates induce an optimal gate depth in a quantum algorithm by first considering a single one- or two-qubit gate $\hat{U}(\phi_{\text{tot}}) = \exp(-i\phi_{\text{tot}} \hat{A})$ of the form discussed in Sec III. Let us discretize this gate into $r$ Trotter steps: $\hat{U}(\phi_{\text{tot}}) = \left[\hat{U}(\phi)\right]^r$ where $\phi = \phi_{\text{tot}}/r$ and $\hat{U}(\phi) = \exp(-i\phi \hat{A})$. The expected angle applied by the total sequence $\hat{U}(\phi_{\text{tot}})$ is

$$\mathbb{E}[\phi_{\text{tot}}] = r \mathbb{E}_\phi[\phi]$$

(23)

where $\mathbb{E}_\phi[\phi]$ is the average angle applied by $\hat{U}(\phi)$. If the unitary gate errors in the system were modeled as Markovian, and therefore uncorrelated, the variance in the total angle would be

$$\text{Var} (\phi_{\text{tot}}) = r \text{Var} (\phi)$$

(24)

where $\text{Var} (\phi)$ is the variance in the angle applied by $\hat{U}(\phi)$. Regardless of the source of unitary error, this variance of each discretized gate will typically be proportional to $\mathbb{E}_\phi[\phi]^2$. Letting the constant of proportionality be $\beta$, defined through $\text{Var} (\phi) = \beta \mathbb{E}_\phi[\phi]^2$, the noise-to-signal ratio of the total gate sequence becomes:

$$\eta = \sqrt{\frac{\text{Var} (\phi_{\text{tot}})}{\mathbb{E}[\phi_{\text{tot}}]}} = \sqrt{\frac{\beta}{r}}.$$  

(25)

As an example, if we take the noise model developed in Sec. III and ignore temporal correlations, we have $\beta = (c_2 \tau)^2/(1 + 2c_2 \tau)$. This constant $\beta$ is computed by assuming that each gate angle is independent and identically distributed according to Eq. (14). We see that $\eta \to 0$ as $r \to \infty$, implying that discretizing the total intended gate, $\hat{U}(\phi_{\text{tot}})$, into a large number of steps eliminates the unitary error in the system, thus illustrating that unitary gate errors in experiments cannot be fully described using a Markovian noise model. Correlations between the unitary gate errors are responsible for decoherence observed in experiments, with an optimal gate depth being set by the timescale upon which this decoherence becomes too large.

To demonstrate how this optimal gate depth manifests in practice, we turn to the Hamiltonian simulation task described in Sec. III. The computed spectrum will have errors both due to discretization via the Trotter decomposition, Eq. (7), and unitary gate noise due to heating of the ions’ motion as described in Sec. III. Trotter error decreases as the number of gates in the circuit is increased, while unitary errors accumulate as the number of gates
is increased. Therefore, there is an optimal gate count balancing Trotter error and accumulated unitary error.

We can quantify the error in the computation use two different metrics. The first is to compute the average fidelity

\[ F(t) = \frac{1}{2^n} \text{Tr} \{ \hat{U}_1(t) \hat{U}(t) \}^2, \tag{26} \]

where \( \hat{U}(t) = e^{-i\hat{H}t} \), with \( \hat{H} \) given by Eq. (1), is the desired time evolution operator and \( \hat{U}_1(t) \) is the noisy Trotterized evolution we implement in the quantum circuit, given by Eq. (7), with noisy gate angles. Given that computation of a spectrum requires implementing time-evolution for a series of different times in order to generate samples of \( S(t) \), given by Eq. (5), we can define the time-integrated fidelity

\[ F_{\text{int}} = \frac{1}{T} \int_0^T \! F(t) \, dt \tag{27} \]

where \( T \) is the last sampled time. The optimal gate depth is then determined by the largest value of \( F_{\text{int}} \). This metric is not biased towards any particular choice of observable.

Alternatively, we can quantify the error in the spectrum by computing the Hellinger distance

\[ D_H^2(A_i, A_j) = \frac{1}{2} \int \frac{d\omega}{2\pi} \left( \sqrt{A_i(\omega)} - \sqrt{A_j(\omega)} \right)^2 \tag{28} \]

between a noiseless spectrum, \( A_i(\omega) \), generated by a noisy Trotterized evolution, \( \hat{U}_1(t) \). At the optimal gate depth, the Trotterized spectrum will have the most overlap with the true noiseless spectrum according to the Hellinger distance. This metric is biased towards the computation of the spectrum.

The optimal gate depth with the corresponding average fidelity and Hellinger distance for an example noisy computation is shown in Fig. 6 and Fig. 7 respectively, and we discuss these results in the next section. The total amount of error in the noisy computation can be reduced by appropriately modifying the angles of the gates comprising the quantum simulation circuit, Eq. (7), a method known as feedforward control. We develop a systematic, platform-independent protocol to determine the modified gate angles in the next section. We then illustrate the benefits of the feedforward control in the context of the Hamiltonian simulation task by showing improvements in the fidelity and Hellinger distance for an example Hamiltonian of the form in Eq. (1).

V. FEEDFORWARD CONTROL

A quantum computation or simulation involves applying a unitary operation \( \hat{U} \) to a system of qubits. Often, this unitary transformation is a composite of several single- and two-qubit unitary gates \( \hat{U}(\phi) = \exp \left( -i\phi \hat{A} \right) \), with \( \hat{A} \) typically linear or bilinear in spin-1/2 operators, \( \hat{S}_j^z = \sigma_j^z / 2 \). A unitary error in the system manifests...
as application of $\hat{U} (\phi)$ when we intend to apply $\hat{U} (\phi_p)$. We usually do not have deterministic knowledge of the value of the incorrect angle, $\phi$, and therefore describe it with a probability distribution $p_\phi (\phi; \phi_{in}, \vec{\lambda})$, where $\vec{\lambda}$ is a vector of latent variables characterizing the physical noise underlying the system and $\phi_{in}$ is the angle we input when applying the gate. If the gate was noiseless, we would have $p_\phi (\phi; \phi_{in}, \vec{\lambda}) = \delta (\phi - \phi_{in})$ and would input $\phi_{in} = \phi_p$, where $\phi_p$ is the desired output gate angle. The idea of feedforward control is to appropriately adjust the input gate angles of the computation to reduce the error accumulated from incorrect gate angles.

Formally, let the total unitary describing the actual computation be $\hat{U} = \prod_{m=1}^M \hat{U}_m (\phi^{(m)})$, where $\hat{U}_m (\phi^{(m)}) = \exp \left( -i \phi^{(m)} \hat{A}_m \right)$. The desired computation is $\hat{U}_p = \prod_{m=1}^M \hat{U}_m (\phi_p^{(m)})$. As the output angles are probabilistic, a particular manifestation of the output computation $\hat{U}$ depends on the joint probability distribution $p_\phi (\phi; \phi_{in}, \vec{\lambda})$, where $\phi_{in}$ and $\phi$ are the $m$ different input and output angles respectively. The goal of feedforward control is to pick the optimal input angles, $\phi_{in}^*$, such that the computation $\hat{U}$ is close to $\hat{U}_p$ on average. In general, $\phi_{in}^*$ will depend on both the set of desired output angles, $\phi_p$, and the latent noise variables, $\vec{\lambda}$.

Optimizing over the entire computation, however, can be challenging as it requires knowledge of the full joint distribution, $p_\phi$, which is generally non-trivial to compute, even for the model presented in Sec. III. Additionally, even if possible, such an optimization may not generalize well to other computations represented by different gate sequences. We therefore focus on optimizing each individual unitary gate independently of the others, which amounts to neglecting correlations between unitary gate errors and assuming that they are independent and identically distributed according to the marginal distribution, $p_\phi$. Mathematically, this amounts to the factorization

![Figure 5](image-url)  

**FIG. 5.** Time dependent fidelity of noisy Trotterized time evolution for a system of four spins evolving under the Heisenberg Hamiltonian, Eq. (1). Solid curves include both heating noise and Trotter error, while the dotted curves include only Trotter error and are given as a noiseless reference. (a) $c_2 = 0.005$ ms$^{-1}$ and no feedforward correction. (b) $c_2 = 0.02$ ms$^{-1}$ and no feedforward correction. (c) $c_2 = 0.005$ ms$^{-1}$ with feedforward correction. (d) $c_2 = 0.02$ ms$^{-1}$ with feedforward correction. The noisy computations are averaged over 40 runs.
of the joint distribution: $p_{\vec{\phi}} = \prod_{i=1}^{M} p_{\phi_i}$. Temporal correlations in the physical noise underlying the system lead to correlations in the angles $\vec{\phi}$ that are not captured by such a factorization. Feedforward optimization of individual gates can therefore only partially mitigate the error in the overall computation. Ignoring the non-Markovian effects discussed in Sec. III implies that the feedforward control is best applied at sufficiently shallow gate depths; when circuit discretization becomes comparable to temporal correlations of noise, the feedforward correction will be inaccurate. The advantage of ignoring error correlations, however, is that the correction can be easily applied to any computation, $U$, as it done at the level of individual gates.

The error due to applying a gate $\hat{U}(\phi)$ when we desire to apply $\hat{U}(\phi_p)$ can be quantified by the gate fidelity

$$F(\phi, \phi_p) = \left| \frac{1}{2\pi} \text{Tr} \{ \hat{U}(\phi)^\dagger \hat{U}(\phi_p) \} \right|^2,$$

which describes the expected fidelity of an $n$-qubit gate for a random state drawn uniformly from the $n$-qubit state space $|\phi\rangle$. For example, let us consider a unitary gate corresponding to $\hat{A} = S_i S_j$ describing an interaction between two qubits $i$ and $j$. The fidelity then takes the simple form $F(\phi, \phi_p) = \cos^2((\phi - \phi_p)/4)$. The figure of merit we want to optimize with feedforward control is the average fidelity over all possible wrong angles $\phi$,

$$F(\phi_{in}, \phi_p, \lambda) = \int d\phi F(\phi, \phi_p).$$

The optimal input angle is then

$$\phi_{in}^*(\phi_p, \lambda) = \arg \max_{\phi_{in}} F(\phi_{in}, \phi_p, \lambda).$$

The optimal input angle, $\phi_{in}^*(\phi_p, c, \tau)$, for the trapped ion noise is the angle which satisfies the condition

$$F(\phi_{in}^*, \phi_p, c, \tau) = F(\phi_{in}, \phi_p),$$

where we recall that $F(\phi, \phi_p) = \cos((\phi - \phi_p)/4)$ is the fidelity of a gate imparting angle $\phi$ when we desire to apply $\phi_p$. We implement feedforward control by taking each desired output gate angle, $\phi_j$, of the $U^{xx}$ gates in Eq. (1) as $\phi_p$ at the experimental time $\tau$ that the gate is applied. The optimality condition, Eq. (33), is then solved numerically for each such gate and the angle $\phi_{in}^*$ is input into the noisy gate rather than $\phi_p$.

We show the optimal input angle, Fig. 3(a), and average gate fidelity, Fig. 3(b), for a range of desired output angles $\phi_p$. First, we note that the optimal feedforward angle, $\phi_{in}^*$, always yields a better average fidelity than inputting $\phi_p$. We see that for small output angles, there is always a finite optimal input angle. For sufficiently large output angles, however, the optimal input angle is $\phi_{in}^* = 0$, meaning we do not apply the gate. These angles are such that doing nothing leads to a better fidelity than any non-zero gate we apply. Furthermore, for times $\tau > 1/c_2$, meaning that the ions’ collective motion has undergone a considerable amount of diffusion, there is an intermediate range of angles where the optimal thing to do is apply a maximally strong laser pulse to make $\phi_{in}^*$ as large as possible. In this case, the gate essentially applies a random phase to the state and yields an average fidelity of 1/2.

To benchmark the utility of the feedforward control, we implement with Hamiltonian simulation task of Sec II using optimal input angles computed from Eq. (33). In Fig. 5 we plot an example of the time-dependent fidelity, Eq. (26), for different heating rate and gate counts with and without feedforward control. We see that for low gate counts such as computations with 100 gates, the drop in fidelity comes almost fully from Trotter error without heating noise having much of an effect. For larger gate counts, heating noise becomes the dominant cause of the drop in fidelity. While the fidelity for the zero heating case gets continuously better with increased gate count, finite heating causes computations with sufficiently large gate counts to decrease the overall fidelity.

Feedforward control can improve the situation in two different ways, which can be seen by comparing, for example, the 300 gate and 700 gate curves. The first effect is to improve the total fidelity over all time values, as quantified by the improvement in $F_{\text{int}}$, Eq. (27), depicted in Fig. 6. This improvement indicate that the computation of $U(t)$ is closer on average to the desired computation $\hat{U}(t)$ for all values of $t$, with the feedforward correction bringing the fidelity of a computation closer to the upper bound set by the Trotter error. The second effect is that for computations with large gate counts, the fidelity for samples at late times, corresponding to large values of $t$, is improved more significantly than for short time (32) samples. This improvement causes the fidelity to have a
FIG. 6. Optimal fidelity resulting from balancing Trotter and decoherence errors for a system of four spins evolving under the Heisenberg Hamiltonian, Eq. (1). The heating rate $c_2$ is given in units of $\text{ms}^{-1}$. (a) Optimal gate count. (b) Integrated fidelity. The noisy computations are averaged over 10 runs.

FIG. 7. Optimal spectra resulting from balancing Trotter and decoherence errors for a system of four spins evolving under the Heisenberg Hamiltonian, Eq. (1). The heating rate $c_2$ is given in units of $\text{ms}^{-1}$. (a) Optimal gate count. (b) Hellinger distance between optimal noisy spectra and noiseless spectrum. The noisy computations are averaged over 10 runs.

more shallow decay, and creates windows of time samples where it may be more advantageous to use circuits with different gate counts. For example, in Fig. 5(c), a computation with 300 gates is advantageous for samples with $c_2t \lesssim 3$, while a computation with 700 gates is advantageous for samples with $c_2t \gtrsim 3$. The significance of this result is that a particular observables of interest may have information that is more concentrated in a particular time window. For example, the resolution between peak of the spectrum, Eq. (2), comes from samples at late times. Therefore, the optimal gate count determined by the accuracy of the spectrum may be larger than the optimal gate count determined by the integrated fidelity. Indeed, this is what is seen when comparing Fig. 6 and Fig. 7.

In Fig. 7(a) and (b), we show the optimal gate count and associated Hellinger distance of spectra computed both with and without the feedforward correction. We see that the accuracy of the optimal noisy spectrum is significantly improved. An example spectrum for a system with heating rate $c_2 = 0.02 \text{ms}^{-1}$ is depicted in Fig. 2. The feedforward control both directly mitigates
decoherence error from the motion of the ions and indirectly reduces the Trotter error by increasing the optimal gate count. Therefore, by effectively increasing the optimal gate depth of the circuit, feedforward control can be used to partially mitigate both discretization error and accumulated unitary gate error in the system.

VI. DISCUSSION & CONCLUSION

This improvement in the quality of the Hamiltonian simulation can be helpful for practical applications, such as the NMR spectrum inference task discussed in Ref. [9]. In that work, a hybrid quantum-classical algorithm is used to infer the parameters of a Hamiltonian, Eq. (1), that models the system of nuclear spins which produce a given experimental NMR spectrum. The premise of the algorithm is to iteratively simulate the spectrum corresponding to different Hamiltonian parameters on quantum hardware and guess parameters that are closer to the target experimental spectrum using classical optimization techniques. After a sufficient number of iterations, the learned Hamiltonian parameters can be used to gain insight into the chemical structure of the sample that produced the given NMR spectrum. In Fig. 8, we demonstrate the benefit of feedforward correction in this inference algorithm. Figure 8(a) shows the Hellinger distance between the average noisy Trotterized spectrum and a given target spectrum at each iteration of the protocol. We see that the feedforward correction allows the algorithm to converge faster, as the increased resolution in the simulated spectra allows the classical optimization to more easily guess better Hamiltonian parameters. In Fig. 8(b), we take the Hamiltonian parameters for the initial and last iterations of the noisy protocol with feedforward correction and compute the corresponding spectra without noise to compare how well the learned parameters correspond to the true parameters underlying the given target spectrum. We see that even though the quantum simulation is noisy, we are still able to iteratively infer the Hamiltonian parameters underlying the target spectrum.

We have shown how to tailor gate-based quantum simulation algorithms for particular hardware platforms. Specifically, we demonstrate how knowledge of hardware noise leading to unitary gate errors can be exploited to implement feedforward control to improve the simulation outcome. The ion noise model we derive applies to an array of computations and simulations performed in trapped ions. Feedforward control, albeit being unable to correct for temporal correlations in the noise, can be used to partially mitigate errors in these applications. A similar approach may ameliorate errors other than the leading order rotation error captured by our noise model, but would require the development of noise models accurately describing such errors.

In addition to feedforward control, it may be possible to incorporate feedback control to mitigate the motional noise. For example, the motional state of an ancilla ion can be periodically measured. Such a strong mea-
measurement, or relatedly mid-circuit cooling, would restart the ions’ diffusion process, effectively reducing the time $\tau$ over which the system undergoes diffusion. Knowledge of the motional state can then be used to generate feedforward corrections until they are recalibrated by the next measurement.

Other common quantum platforms such as superconducting qubits and Rydberg atoms also suffer from unitary gate errors. The physical mechanisms underlying these errors, however, is quite different from that of trapped ions and understanding the structure of the optimal feedforward correction in these systems may provide insight into which quantum algorithms and simulations are best suited to different platforms.

ACKNOWLEDGMENTS

We thank Marko Cetina and Christopher Monroe for stimulating discussions. K.S. and E.D. acknowledge funding from ARO grant number W911NF-20-1-0163, Harvard-MIT CUA, NSF EAGER-QAC-QCH award No. 2037687, and the NSF grant No. OAC-1934714. The Flatiron Institute is a division of the Simons Foundation. D.S. acknowledges funding from the Harvard Quantum Initiative Seed Funding program and AFOSR; Grant FA9550-21-1-0236. The Flatiron Institute is a division of the Simons Foundation.

[1] John Preskill, “Quantum Computing in the NISQ era and beyond,” Quantum 2, 79 (2018).
[2] I. M. Georgescu, S. Ashhab, and Franco Nori, “Quantum simulation,” Rev. Mod. Phys. 86, 153–185 (2014).
[3] Andrew M. Childs, Dmitri Maslov, Yunseong Nam, Neil J. Ross, and Yuan Su, “Toward the first quantum simulation with quantum speedup,” Proceedings of the National Academy of Sciences 115, 9456–9461 (2018).
[4] Bela Bauer, Sergey Bravi, Mario Motta, and Garnet Kin-Lic Chan, “Enabling quantum leap: Quantum algorithms for quantum chemistry and materials,” (2019).
[5] B. P. Lanyon, C. Hempel, D. Nigg, M. Müller, R. Gerritsma, F. Zähringer, P. Schindler, J. T. Barreiro, M. Rambach, G. Kirchmair, M. Henrich, P. Zoller, R. Blatt, and C. F. Roos, “Universal digital quantum simulation with trapped ions,” Science 334, 57–61 (2011).
[6] Y. Salathé, M. Mondal, M. Oppliger, J. Heinsoo, P. Kurpiers, A. Potoczniak, A. Mezzacapo, U. Las Heras, L. Lamata, E. Solano, S. Filipp, and A. Wallraff, “Digital quantum simulation of spin models with circuit quantum electrodynamics,” Phys. Rev. X 5, 021027 (2015).
[7] Ivan Kassal, Stephen P. Jordan, Peter J. Love, Masoud Mohseni, and Alán Aspuru-Guzik, “Polynomial-time quantum algorithm for the simulation of chemical dynamics,” Proceedings of the National Academy of Sciences 105, 18681–18686 (2008).
[8] F. J. J. O’Malley, R. Babbush, T. D. Kivlichan, J. Romero, J. R. McClean, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, E. Jeffrey, E.Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. C. White, P. V. Covonev, P. J. Love, H. Neven, A. Aspuru-Guzik, and J. M. Martinis, “Scalable quantum simulation of molecular energies,” Phys. Rev. X 6, 031007 (2016).
[9] Dries Sels, Hesam Dashti, Samia Mora, Olga Demler, and Eugene Demler, “Quantum approximate bayesian computation for nmr model inference,” Nature Machine Intelligence 2, 396–402 (2020).
[10] P. Hauke, D. Marcos, M. Dalmonte, and P. Zoller, “Quantum simulation of a lattice schwinger model in a chain of trapped ions,” Phys. Rev. X 3, 041018 (2013).
[11] Esteban A. Martinez, Christine A. Muschik, Philipp Schindler, Daniel Nigg, Alexander Erhard, Markus Heyl, Philipp Hauke, Marcello Dalmonte, Thomas Monz, Peter Zoller, and Rainer Blatt, “Real-time dynamics of lattice gauge theories with a few-qubit quantum computer,” Nature 534, 516–519 (2016).
[12] T. D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe, and J. L. O’Brien, “Quantum computers,” Nature 464, 45–53 (2010).
[13] Michael A. Nielsen and Isaac L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000).
[14] Hui Khoon Ng and John Preskill, “Fault-tolerant quantum computation versus gaussian noise,” Phys. Rev. A 79, 032318 (2009).
[15] John Preskill, “Sufficient condition on noise correlations for scalable quantum computing,” (2012), arXiv:1207.6131 [quant-ph].
[16] Gerardo A Paz-Silva, Seung-Woo Lee, Todd J Green, and Lorenza Viola, “Dynamical decoupling sequences for multi-qubit dephasing suppression and long-time quantum memory,” New Journal of Physics 18, 073020 (2016).
[17] David Layden and Paola Cappellaro, “Spatial noise filtering through error correction for quantum sensing,” npj Quantum Information 4, 30 (2018).
[18] K. Stannigel, P. Hauke, D. Marcos, M. Hafezi, S. Diehl, M. Dalmonte, and P. Zoller, “Constrained dynamics via the zeno effect in quantum simulation: Implementing non-abelian lattice gauge theories with cold atoms,” Phys. Rev. Lett. 112, 120406 (2014).
[19] Rich Rines, Kevin Obenland, and Isaac Chuang, “Empirical determination of the simulation capacity of a near-term quantum computer,” (2019), arXiv:1905.10724 [quant-ph].
[20] Elbio Dagotto, “Correlated electrons in high-temperature superconductors,” Rev. Mod. Phys. 66, 763–840 (1994).
[21] Rahul Nandkishore and David A. Huse, “Many-body localization and thermalization in quantum statistical mechanics,” Annual Review of Condensed Matter Physics
[22] David J. Luitz, Nicolas Laflorencie, and Fabien Alet, “Many-body localization edge in the random-field heisenberg chain,” Physical Review B 91 (2015), 10.1103/physrevb.91.081103.

[23] Arijeet Pal and David A. Huse, “Many-body localization phase transition,” Physical Review B 82 (2010), 10.1103/physrevb.82.174411.

[24] Kristan Temme, Sergey Bravyi, and Jay M. Gambetta, “Error mitigation for short-depth quantum circuits,” Phys. Rev. Lett. 119, 180509 (2017).

[25] Kushal Seetharam, Debopriyo Biswas, Crystal Noel, Andrew Risinger, Daiwei Zhu, Or Katz, Sambuddha Chatopadhyay, Marko Cetina, Christopher Monroe, Eugene Demler, and Dries Sels, “Digital quantum simulation of nmr experiments,” Science Advances 9, eadh2594 (2023), https://www.science.org/doi/pdf/10.1126/sciadv.adh2594.

[26] M. Cetina, L.N. Egan, C. Noel, M.L. Goldman, D. Biswas, A.R. Risinger, D. Zhu, and C. Monroe, “Control of transverse motion for quantum gates on individually addressed atomic qubits,” PRX Quantum 3, 010334 (2022).

[27] M. Brownnutt, M. Kumph, P. Rabl, and R. Blatt, “Ion-trap measurements of electric-field noise near surfaces,” Rev. Mod. Phys. 87, 1419–1482 (2015).

[28] Michael A Nielsen, “A simple formula for the average gate fidelity of a quantum dynamical operation,” Physics Letters A 303, 249 – 252 (2002).