Small, Highly Accurate Quantum Processor for Intermediate-Depth Quantum Simulations

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Analog quantum simulation is widely considered a step on the path to fault tolerant quantum computation. With current noisy hardware, the accuracy of an analog simulator will degrade after just a few time steps, especially when simulating complex systems likely to exhibit quantum chaos. Here we describe a quantum simulator based on the combined electron-nuclear spins of individual Cs atoms, and its use to run high fidelity simulations of three different model Hamiltonians for \( \gtrsim 100 \) time steps. While not scalable to exponentially large Hilbert spaces, it provides the accuracy and programmability required to explore the interplay between dynamics, imperfections, and accuracy in quantum simulation.

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Absent errors, machines that process information according to quantum mechanics can in principle solve problems beyond the computational power of any classical computer. In practice, a scalable, general purpose quantum computer must include error correction and fault tolerance as an integral part of its operation, leading to requirements on the underlying quantum hardware that could be out of reach for years to come [1]. Thus, in the current era of noisy, intermediate-scale quantum (NISQ) devices [2], much of the effort in the field has focused on seemingly less ambitious challenges. High on the list is the development of analog quantum simulators, defined here as devices that operate without error correction but still have the potential to surpass classical computers for tasks such as modeling complex quantum systems [3,4]. Recent examples include work using trapped ions [5–7], Rydberg atoms [8,9], and superconducting qubits [10,11] to simulate phase transitions and other phenomena in large (> 50) spin systems. This is roughly the scale at which numerical modeling on classical computers is currently infeasible.

Quantum simulation generally requires access to highly entangled states of interacting many body systems. It has long been known that such systems also tend to support quantum chaos, in the sense that their time evolution is hypersensitive to perturbation [12–14]. This suggests two separate notions of complexity relevant for quantum simulation, one related to the nature of the quantum state, and another related to the nature of the system dynamics. Entangled states are complex because the information required to predict interparticle correlations grows exponentially with system size, while chaotic dynamics are complex because the information required to predict the quantum trajectory grows exponentially with time [15]. Both will contribute to the overall complexity and fragility of analog quantum simulation and related NISQ-era objectives such as quantum annealing [16,17]. Indeed, one can expect an inverse relationship between the accessible Hilbert space and the length of time one can meaningfully simulate, with those properties playing a role analogous to the width and depth in quantifying the complexity of a quantum circuit. So far, experiments have focused mostly on the width of a simulation (after all, this is the crucial resource when looking for a quantum advantage), with limited attention paid to the fidelity of the output state as one seeks to increase its depth in terms of simulated time.

Yet, to fully understand the computational power of an analog quantum simulation, it is necessary to look carefully at the accessible simulation depth and how it depends on the nature of the dynamics, before one can trust its outcome [18].

In this Letter we present a new platform for analog quantum simulation (AQS) with tradeoffs that are complementary to NISQ devices: it is modest in terms of accessible Hilbert space, but highly accurate and therefore uniquely suited to the study of dynamical complexity in time. Our small, highly accurate quantum (SHAQ) simulator is based on the combined electron-nuclear spins of individual Cs atoms in the electronic ground state, driven by phase modulated radio frequency (rf) and microwave (\( \mu \)w) magnetic fields, and provides access to a fixed 16-dimensional Hilbert space formally equivalent to four qubits. In place of the quantum circuit model where control is predicated on access to a universal gate set, we rely on a universal control Hamiltonian and quantum optimal control [19,20] to ensure that our simulator is fully programmable, in the sense that we can implement arbitrary unitary maps with average fidelities > 0.98 [21]. We show that optimal control can be further adapted for AQS, allowing us to set
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For future exploration of the interplay between dynamics, example, Refs. [27–30]. These are key elements required for future exploration of the interplay between dynamics, hardware imperfections, and accuracy in AQS. AQS falls into two broad categories sometimes referred to as “emulation” and “simulation.” A quantum emulator is a special-purpose device governed by the same Hamiltonian and having the same Hilbert space structure as the system of interest. Emulators have been realized on a variety of physical platforms and used to study a range of phenomena with considerable success [5,31–33]. A quantum simulator, by contrast, is a universal device that is controllable, in the sense that one can “program” it to implement any SU(d) map of Hilbert space onto itself. Given an arbitrary system Hamiltonian and a mapping of the system Hilbert space \( \mathcal{H}_{\text{sys}} \) onto the simulator Hilbert space \( \mathcal{H}_{\text{sim}} \), one can then implement unitary time steps on the simulator and iterate to perform stroboscopic simulations of the system dynamics (Fig. 1).

Our Cs-atom-based “device” is a quantum simulator in the second sense, and requires unitary control over the entire accessible Hilbert space. As shown in [19], the spin degrees of freedom of a Cs atom in its electronic ground state are controllable with a combination of phase modulated rf and \( \mu \text{W} \) magnetic fields whose piecewise constant phases \( \{ \phi_1^x, \phi_2^y, \phi_3^z \} \), \( 1 \leq i \leq N_{\phi} \), serve as control variables (“controls” for short). We can then apply the generic toolbox of quantum optimal control to find (non-unique) controls that accomplish the control task at hand. In this Letter, we focus on the adaptation of optimal control to AQS, and refer the reader to past work [19–22] and [34] for details of the laboratory implementation.

To set up an AQS we first choose orthonormal bases in \( \mathcal{H}_{\text{sys}} \) and \( \mathcal{H}_{\text{sim}} \). Having done so, a straightforward way of mapping from system to simulator is to represent states and operators by identical vectors and matrices in the two bases. Next, given a unitary time propagator \( W \) acting on the system, we seek controls \( \{ \phi_i \} \) for which the transformation \( U(\{ \phi_i \}) \) acting on the simulator is a good approximation to \( W \). Note that \( W \) can be chosen as the exact propagator for a time step of any length; there will be no Trotter errors [3,4] unless deliberately introduced as part of the simulation. Given \( W \), we then use one of two versions of optimal control to find high-performing controls.

Conventional control: This version uses an objective function \( F(\{ \phi_i \}) = \frac{1}{N_{\phi}} \text{Tr}[W^r U(\{ \phi_i \})^r]^2 / d^2 \) (the fidelity). Numerical optimization of \( F(\{ \phi_i \}) \) as a function of \( \{ \phi_i \} \) will find controls for which the matrices \( W \) and \( U(\{ \phi_i \}) \) are near identical in the chosen bases. That is, within a global phase, they have the same eigenvalues and eigenstates. In prior work we have found that \( N_{\phi} = 150 \) phase steps (450 phase values) is sufficient to consistently achieve a theoretical \( F(\{ \phi_i \}) \geq 0.99999 \) for any \( W \). In the laboratory where control errors and decoherence are present, the corresponding controls achieve \( F \geq 0.98 \) on average, as measured by randomized benchmarking [21].

Eigenvalue only (EVO) control: In AQS there are in principle no restrictions on the map from system to simulator. To take advantage of this, we note that it suffices for \( W \) and \( U(\{ \phi_i \}) \) to have near identical eigenvalues, in which case \( V = \text{Tr} \Phi VU(\{ \phi_i \})V^\dagger \) will be nearly identical for some \( V \). Accordingly, the EVO approach uses an objective function

\[
F_{\text{EVO}}(\{ \phi_i \}, \{ v_j \}) = \frac{1}{d^2} \text{Tr}[W^r V U(\{ \phi_i \}) V^\dagger]^2,
\]

where \( V = e^{iA} \), \( A = \sum_{j=1}^d \lambda_j N_j \), \( \{ \lambda_j \} \) is a set of generalized Gell-Mann matrices forming a basis of traceless Hermitian \( d \times d \) matrices, and \( \{ v_j \} \) is a set of \( d^2 - 1 \) real-valued variables, sufficient to generate all \( V \in \text{SU}(16) \). Simultaneous optimization of \( F_{\text{EVO}}(\{ \phi_i \}, \{ v_j \}) \) with respect to \( \{ \phi_i \} \) and \( \{ v_j \} \) will then find co-optimal controls and system-simulator maps.
Our experience suggests the search complexity and computational effort is comparable for conventional and EVO control. Furthermore, we find that optimizing for computational effort is comparable for conventional and EVO control, which works in every scenario we have explored. Therefore, when necessary, we revert to conventional control fields from atom to atom, but ensures excellent microscopic record of the expectation value $\langle \hat{\chi}(0) \rangle$, take k time steps, measure the observable $M$ of interest, and repeat for $1 \leq k \leq K$ to build up a stroscopic record of the expectation value $\langle M(k) \rangle$. In AQS of systems such as the TI and LMG models, $M$ might be a spin observable. As a measure of the accuracy of the simulation we can also look at the fidelity of the quantum state itself, $\mathcal{F}_{\text{AQS}}(k) = \text{Tr}[\rho_s(k)|\chi(k)\rangle\langle\chi(k)|]$, where $|\chi(k)\rangle$ and $\rho_s(k)$ are the predicted and actual states after $k$ steps. To access this quantity we measure the projector $M(k) = |\chi(k)\rangle\langle\chi(k)|$, i.e., the probability of finding the simulator in the predicted state after $k$ steps. In practice, using laser cooling to prepare a large sample of noninteracting Cs atoms allows us to run as many as $10^7$ identical quantum simulators in parallel. This leads to small variations in the control fields from atom to atom, but ensures excellent averaging over noise in the controls and the measurement. In our setup the time per phase step is $4 \mu s$ and the maximum overall duration of a quantum simulation is
The meaningful time step is one period of the Floquet operator, and the only meaningful time step is one period of $H_{\text{QKT}}$. This assures that the propagator $W$ is far from the identity for all but a small subset of parameters, and thus ideally suited for EVO control. Figures 2(a) and 2(d) show simulations of $\langle \sigma_z^2 \rangle$ for the TI model, and collective spin components $\langle J_x \rangle$ and $\langle J_y \rangle$ for the LMG model; these examples were chosen because of their varied and nontrivial behavior. Each AQS extends over $1 \leq k \leq 40$ steps, enough to densely sample for long enough that the nature of the dynamics becomes apparent. Overall, quantum simulation of the TI model appears somewhat more challenging than the LMG model, but both track the spin dynamics with good accuracy. Notably, 40 time steps is enough for a considerable loss of fidelity, $\mathcal{F}_{\text{AQS}}(k) \sim 0.5$, showing that useful simulation of physical observables can be achieved even when accuracy at the level of the quantum state is fairly poor.

As a third test we apply our simulator to the quantum kicked top. An AQS of the QKT consists of repeated applications of the Floquet operator, and the maximum number of QKT steps are $N_{\phi} = 150$, $K = 20$ (circles), EVO control with $N_{\phi} = 60$, $K = 50$ (squares), and $N_{\phi} = 20$, $K = 150$ (diamonds), and finally randomized EVO control with $N_{\phi} = 20$, $K = 150$ where coherent errors are scrambled (triangles). Thin lines connect the data points to guide the eye. Error bars are the standard error of the mean for the chosen sample of initial states.

12 ms, limited by the time a free-falling atom spends in the region of uniform control fields.

Figures 2(a) and 2(d) show $\mathcal{F}_{\text{AQS}}(k)$ for two versions of a four-site TI model and a $J = 15/2$ LMG model, each for $0 \leq k \leq 100$ time steps. The simulations use EVO control with $N_{\phi} = 20$ phase steps, the fidelities are averaged over 10 randomly chosen initial states, and the cutoff at $K = 100$ is to ensure the fidelity of the time steps does not vary with $k$. The TI data corresponds to ferromagnetic and paramagnetic regimes respectively, while the LMG data correspond to regimes below and just above the critical point. In all cases the simulation fidelity declines smoothly with time but remains well above that of a mixed state, $\mathcal{F}_{\text{AQS}}(k) > 1/16 = 0.0625$, even after $k = 100$ time steps. As examples of AQS of dynamical observables, Figures 2(b) and 2(d) show simulations of $\langle J_z \rangle$ for the TI model, and collective spin components $\langle J_x \rangle$ and $\langle J_y \rangle$ for the LMG model; these examples were chosen because of their varied and nontrivial behavior. Each AQS extends over $1 \leq k \leq 40$ steps, enough to densely sample for long enough that the nature of the dynamics becomes apparent. Overall, quantum simulation of the TI model appears somewhat more challenging than the LMG model, but both track the spin dynamics with good accuracy. Notably, 40 time steps is enough for a considerable loss of fidelity, $\mathcal{F}_{\text{AQS}}(k) \sim 0.5$, showing that useful simulation of physical observables can be achieved even when accuracy at the level of the quantum state is fairly poor.

FIG. 3. AQS of the quantum kicked top, Eq. (2c). (a) Measured $\mathcal{F}_{\text{AQS}}(k)$, averaged over 10 initial coherent states, in the globally chaotic regime ($p = 1, \kappa = 7$). Insert: classical phase space map for the hemispheres $J_z > 0$ and $J_z < 0$ showing global chaos. (b) Measured $\mathcal{F}_{\text{AQS}}(k)$ in a mixed regime ($p = 0.99, \kappa = 2.3$), averaged over five initial coherent states in the large regular island in the $J_z > 0$ hemisphere (triangles), over five initial coherent states in the sea of chaos in the $J_z < 0$ hemisphere (diamonds), and over all 10 initial states (circles). Insert: classical phase space map. (c) Measured $\mathcal{F}_{\text{AQS}}(k)$ ($p = 1, \kappa = 7$), averaged over 10 initial coherent states, for different control strategies: conventional control with $N_{\phi} = 150$, $K = 20$ (circles), EVO control with $N_{\phi} = 60$, $K = 50$ (squares), and $N_{\phi} = 20$, $K = 150$ (diamonds), and finally randomized EVO control with $N_{\phi} = 20$, $K = 150$ where coherent errors are scrambled (triangles). Thin lines connect the data points to guide the eye. Error bars are the standard error of the mean for the chosen sample of initial states.
have the potential to compound much faster than random noise. We can explore the role of coherent errors versus noise by comparing to a scenario akin to randomized benchmarking [45]. To do so, we use EVO optimization with $N_\phi = 20$ to find a number of time propagators $U(\{\hat{\phi}_i\})$, all with identical eigenvalues but different and effectively random controls $\{\hat{\phi}_i\}$ and maps $V$. These are put together in random sequences of various lengths, at the end of which we measure the fidelity of the output state relative to the output predicted in the absence of errors. As seen in Fig. 3(c), the resulting decline in fidelity is significantly slower than for each of the three quantum simulations, with an end point fidelity of $F_{\text{AQS}}(k) \sim 0.6$ at $k = 150$, and an average fidelity per step of 0.997. We take this as evidence that quantum simulations such as those studied here are more strongly affected by coherent errors than random noise, and that efforts to improve the simulation fidelity should focus on the former.

In conclusion, we have demonstrated a small, universal and highly accurate analog quantum simulator based on the spin-dieges of freedom in the ground state of individual Cs atoms. We have further shown how optimal control can be adapted to program such a simulator, and we have established its baseline performance by applying it to both integrable and chaotic model systems. Notably, the idea of looking for co-optimal controls and system-simulator maps is not restricted to quantum simulation, and could lead to similar gains in other contexts where a generic control task is mapped onto a specific piece of hardware. Going forward, we plan to use our Cs atom quantum simulator to develop and test a general model of the interplay between the native errors of a generic quantum simulator and the types of observables one might use it to access. Ultimately, we hope testbeds such as ours can help better understand the computational power of analog quantum devices and their use in lieu of error corrected and fault tolerant quantum computers.

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