

Pulse optimization in adiabatic quantum computation and control

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We present a robust pulse optimization method for adiabatic population transfer and adiabatic quantum computation. The approach relies on identifying control pulses that keep the evolving quantum system close to its instantaneous ground state. By combining advanced gradient-free optimization tools with specialized cost functions for adiabatic control, it achieves both efficiency and robustness. To demonstrate its generality, we apply the method to three examples involving both atomic and superconducting qubits. We test different optimization cost functions and discretization bases, showing that the approach outperforms ensemble optimization. Finally, to verify its performance on real quantum hardware, we implement digitized adiabatic qubit control using the optimized pulses on the IBM quantum cloud.

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I. INTRODUCTION

We present a robust pulse optimization method for adiabatic control protocols, including adiabatic population transfer (APT) [1] and adiabatic quantum computation (AQC) [2], where a driven quantum system follows the instantaneous eigenstate of the Hamiltonian and reaches a desired target state (in APT) or the solution to a computational problem (in AQC). While adiabatic protocols are inherently robust to fluctuations in the controlling pulses, their speed is limited by the requirement that the system must change slowly compared to its spectral gap [3]. Therefore, acceleration of adiabatic protocols is a topic of active research [4–9]. Motivated by the success of quantum optimal control (QOC) algorithms in enhancing the performance of gate-based quantum algorithms [10,11], we introduce a QOC pulse optimization method for adiabatic protocols. Our method achieves optimal performance by minimizing leakage from the instantaneous ground state during the propagation, i.e., the “diabatic error.” The resulting pulses possess both high fidelity—by using QOC—and robustness—due to adherence to the instantaneous ground state.

To analyze the performance of our method, we optimize two APT protocols—rapid adiabatic passage (RAP) in two-level systems and multilevel stimulated Raman adiabatic passage (STIRAP)—which are used as building blocks in AQC [12]. Our final example is an AQC algorithm for the maximum independent set (MIS) problem. While the robustness of our pulses to intensity fluctuations is similar to that of brute-force ensemble optimization [13], our approach is substantially more efficient.

According to the adiabatic theorem, suppressing diabatic errors requires control pulses to vary slowly compared to the spectral gap [14]. In adiabatic qubit control, increasing the pulse area—the product of the Rabi frequency and pulse duration—increases the spectral gap and, therefore, reduces the error. Specifically, in this work, we seek pulses with an integrated power of 4π [15]. However, practical limitations necessitate advanced pulse engineering methods to achieve optimal performance under realistically attainable pulse areas. Squared trigonometric, hyperbolic, and smooth polynomial pulses are known to effectively minimize diabatic errors [1,16]. Other methods for reducing diabatic errors include parallel-transported eigenvalues [17], superadiabatic states [18], and inertial pulses [5,8]. A widely used acceleration technique called shortcut to adiabaticity (STA) [19] involves engineering counterdiabatic driving forces that suppress diabatic transitions during the evolution [20]. While exact STA can eliminate diabatic errors altogether, its construction requires knowledge of all eigenstates and their derivatives [21]. When the latter are known, STA is extremely powerful [22–25]. However, in large systems, which are required for AQC, the eigenstates are generally unknown. In such cases, one can either use approximate STA solutions [26–28] or resort to alternative methods.

In this work, we present an acceleration method for adiabatic protocols with QOC. Previous applications of QOC to adiabatic control include searching within the subspace of STA solutions for pulses with minimal power and maximal robustness [29], and the application of the chopped random-basis (CRAB) method for optimizing adiabatic entangling gates [30]. Finally, Ref. [31] proposes improving approximate STA with additional control fields. Here, we generalize early work by Brif *et al.* [32], which focused on optimizing qubit control with the gradient ascent pulse engineering (GRAPE) method [33]. By combining gradient-free, multiobjective optimization methods with efficient simulation tools (Fig. 2), our approach can optimize the controls of few-body open quantum systems. We validate our method via classical simulations of the optimized pulses [34], as well as quantum execution of the digitized pulses [35] on the IBM quantum platform [36].

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II. QOC OF ADIABATIC CONTROL PULSES

Real quantum systems are open since they exchange energy and particles with their environment. Assuming a Markovian environment with relaxation rate faster than that of the system, the dynamics of the density matrix, ρ , is governed by the Lindblad master equation [37]:

$$\frac{d\rho}{dt} = -i[H(\mathbf{v}(t)), \rho] + \sum_k \left(\hat{L}_k \rho \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{L}_k^\dagger \hat{L}_k, \rho \} \right). \quad (1)$$

The terms in the sum correspond to dissipative dynamics, with operators $\hat{L}_k$ representing population relaxation and dephasing. The Hamiltonian H includes drift and control terms. The vector $\mathbf{v}(t)$ represents the control amplitudes and frequencies that we wish to engineer.

To accelerate adiabatic control protocols, we seek controls $\mathbf{v}(t)$ that drive the system along the instantaneous ground state of H . To do so, we minimize the functional

$$\mathcal{C}(\rho(t), \mathbf{v}(t), t_f) = \mathcal{C}_i + \eta \mathcal{C}_0, \quad (2)$$

where η balances infidelity ($\mathcal{C}_i$) and power ($\mathcal{C}_0$) constraints and t_f is the protocol duration. The term $\mathcal{C}_0 = \sum_v \int_0^{t_f} v_v^2(t) dt - \mathcal{C}_{\text{ref}}$ reduces total control power relative to the reference $\mathcal{C}_{\text{ref}}$ (summed over all controls) [38]. We consider three figures of merit for the infidelity:

$$\mathcal{C}_1 = 1 - \text{Tr} \sqrt{\sqrt{\rho_g(t_f, \mathbf{v})} \rho(t_f, \mathbf{v}) \sqrt{\rho_g(t_f, \mathbf{v})}}, \quad (3a)$$

$$\mathcal{C}_2 = \frac{1}{t_f} \int_0^{t_f} dt (1 - \text{Tr} \sqrt{\sqrt{\rho_g(t)} \rho(t, \mathbf{v}) \sqrt{\rho_g(t)}}), \quad (3b)$$

$$\mathcal{C}_3 = \frac{1}{M} \sum_{i=1}^M u_i \mathcal{C}_1 \{ \rho_i(t), \mathbf{v}(t), \alpha_i \}. \quad (3c)$$

The term $\mathcal{C}_1$ quantifies the deviation of the system's state at the end of the protocol, $\rho(t_f)$, from the desired eigenstate, $\rho_g(t_f)$, using the fidelity amplitude metric [39,40]. We refer to $\mathcal{C}_1$ as the diabatic error, and to pulses obtained by minimizing it as traditional QOC. The cost $\mathcal{C}_2$ is the accumulated diabatic error along the propagation, and we refer to pulses obtained by minimizing it as adiabatic QOC. In the numerical examples that follow, we use a weighted sum of the infidelity costs, $\mathcal{C}_1 + \lambda \mathcal{C}_2$, showing that by minimizing $\mathcal{C}_2$, one gains robustness. The choice of the weight factor λ is discussed in Sec. 1.1 of the Supplemental Material [41] and in the following examples (Sec. III). The cost $\mathcal{C}_3$ is used for ensemble optimization [13]. It is defined as the average diabatic error, $\mathcal{C}_1$, for an ensemble of systems whose states $\rho_i(t)$ evolve under controls shifted or scaled by α_i , with u_i denoting the averaging weights.

Figure 1 shows how pulse optimization affects qubit dynamics. We consider the RAP protocol for qubit population transfer (Sec. III A). In this case, the control fields $\mathbf{v}(t)$ are the Rabi frequency Ω and detuning Δ [Eq. (5)]. We compare three choices of control fields: (a) unoptimized (Gaussian Ω and linear Δ), (b) pulses optimized with traditional QOC, and (c) pulses optimized with adiabatic QOC. The bottom plots show the corresponding dynamics on the Bloch sphere, where the purple curve denotes the trajectory of the instantaneous ground state. Evidently, the system follows the ground state when driven with pulses obtained from adiabatic QOC.

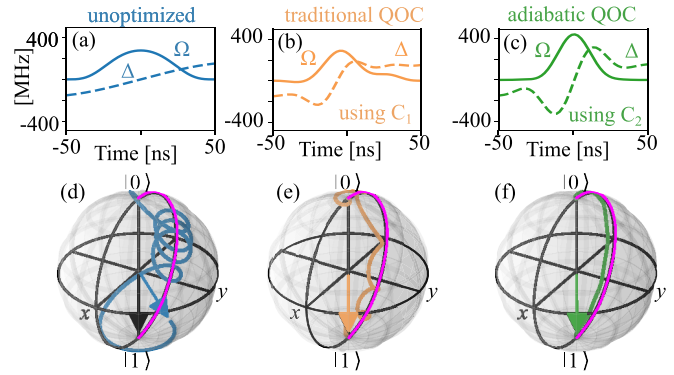


FIG. 1. Three RAP pulses for adiabatic excitation in a two-level system with Rabi frequency Ω and detuning Δ : (a) an unoptimized polynomial pulse, (b) a pulse obtained with traditional QOC, and (c) a pulse obtained with adiabatic QOC. (d)–(f) State trajectories on the Bloch sphere under pulses from panels (a)–(c). Purple curve is the ground-state trajectory.

An overview of our optimization procedure is given below. A flow chart is provided in Fig. 2. For efficient pulse representation, we write the control pulses as a sum of a reference pulse—which we *a priori* know provides good and adiabatic performance—and, on top of it, a correction written as a finite sum of basis elements whose weights we seek. This is similar to the chopped random basis [42]. For optimal performance, we choose between three different of bases depending on the case of study:

$$v^{(1)}(t) = v_0(t) + \sin^2 \left(\frac{\pi t}{t_f} \right) \sum_n w_n \exp \left(-\frac{(t - \mu_n)^2}{\sigma_n^2} \right), \quad (4a)$$

$$v^{(2)}(t) = v_0(t) + \sin^2 \left(\frac{\pi t}{t_f} \right) \sum_n w_n \sin \left(\frac{n\pi t}{t_f} \right), \quad (4b)$$

$$v^{(3)}(t) = v_0(t) + \sin^2 \left(\frac{\pi t}{t_f} \right) \sum_n w_n T_n \left(\frac{2t}{t_f} - 1 \right), \quad (4c)$$

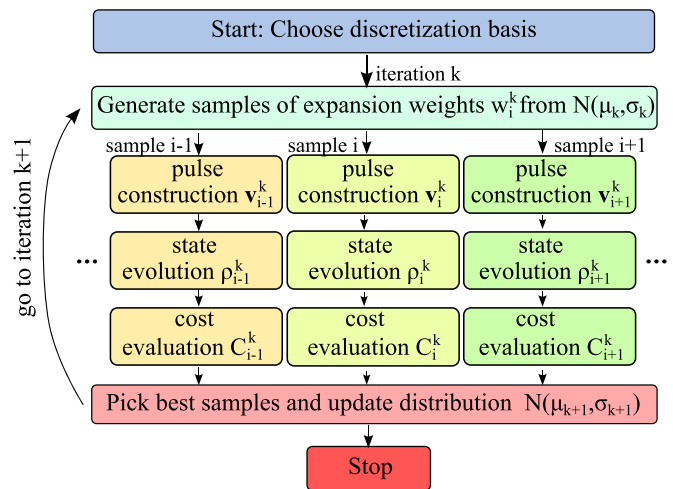


FIG. 2. Flow chart of iterative adiabatic QOC algorithm. In each iteration (k), generate random samples of expansion coefficients (w_i^k). For each sample (i), construct pulse, evolve system, and evaluate cost using Eq. (3) (including the adiabatic infidelity cost $\mathcal{C}_2$). Select best samples and update the distribution to lower the cost.

where $v_0(t)$ is a fixed reference pulse and the sums represent corrections spanned in bases of Gaussians, sine functions, and Chebyshev polynomials, $T_n(z)$, respectively. The squared sine envelope in Eq. (4c) guarantees smoothness of the basis functions at the start and end of the protocol [8]. In Sec. 1.2 of the Supplemental Material [41], we compare the performance across different bases to justify our basis selection. We find that Chebyshev polynomials consistently yield the lowest infidelity, while Gaussian functions provide the fastest convergence. The sinusoidal basis offers a trade-off between convergence rate and fidelity.

Once choosing an expansion basis, we employ the covariance matrix adaptation evolution strategy (CMA-ES) algorithm [43] to find optimal expansion coefficients. Evolutionary algorithms like CMA-ES are widely used in experimental QOC [12,44–46] because they handle multi-objective cost functions well [45], as also required in our adiabatic QOC setting. We use the open-source Python library Nevergrad [47] to implement CMA-ES. The algorithm works by drawing random samples of expansion coefficients from a normal distribution and iteratively updating the distribution. At each iteration, one generates samples of expansion coefficients. For each sample, one constructs the corresponding pulses, evolves the state under Eq. (1) (using QuTiP [34]), and evaluates the cost using Eq. (2). Finally, the algorithm picks samples with minimal costs to update the mean and covariance of the distribution and reiterate until a stop criterion is reached. The convergence of CMA-ES is analyzed in Sec. 1.3 of the Supplemental Material [41]. Next, we apply the optimization algorithm just described to three numerical examples.

III. NUMERICAL EXAMPLES

A. Optimization of adiabatic qubit control

First, we study rapid adiabatic passage, a protocol for population transfer between the ground and excited states of a two-level system using a chirped pulse. The Hamiltonian in the rotating-wave approximation is [48]

$$H_{\text{RAP}} = \Omega(t)\hat{\sigma}_x + \Delta(t)\hat{\sigma}_z, \quad (5)$$

where $\Omega(t)$ is the Rabi frequency and $\Delta(t)$ is the detuning. In RAP, Ω vanishes at the beginning and end of the protocol, so the Hamiltonian reduces to $\Delta\hat{\sigma}_z$. Because Δ changes sign during the sweep, the instantaneous ground state evolves from $|0\rangle$ to $|1\rangle$, enabling population transfer by adiabatically following the ground state.

To improve state-transfer fidelity under a fixed pulse area, we apply our QOC method. We compare qubit dynamics under an unoptimized polynomial pulse (blue) [49] with dynamics under two optimized pulses [using the sine basis; Eq. (4b)]: a “traditional pulse” obtained using C_1 [Eq. (3a)] (orange) and an “adiabatic pulse” obtained using $C_1 + C_2$ for the infidelity cost [Eq. (3b)] (green). The pulses are shown in Figs. 1(a)–1(c), and corresponding Bloch-sphere trajectories in Figs. 1(d)–1(f). As discussed conceptually above, only the adiabatic QOC pulse tracks the instantaneous ground state.

Since the adiabatic QOC trajectory adheres to the instantaneous eigenstate, we expect robustness to fluctuations in the control amplitude and frequency, which are prevalent in

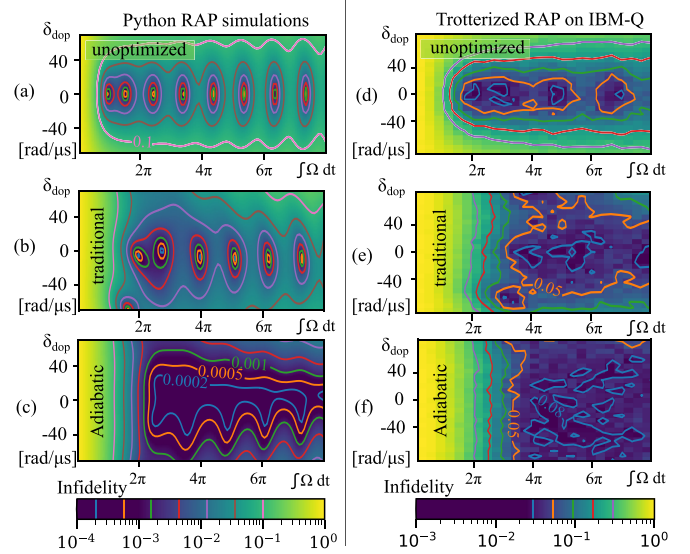


FIG. 3. Robustness of optimized RAP pulses. (a)–(c) Python simulations showing infidelity of state transfer [Eq. (3a)] (colorbar) for the three pulses from Fig. 1 under variations in pulse amplitude, $\int_0^t \epsilon \Omega(t) dt$, and frequency shifts, $\Delta(t) + \delta_{\text{dopp}}$. (d)–(f) Infidelity of a Trotterized RAP protocol under variations in the controls pulse area and detuning, obtained from quantum simulations on the IBM quantum cloud [36].

atomic qubits [50]. To assess the robustness under such noise, we evolve the system under control fields with a rescaled Rabi frequency, $\Omega(t) \rightarrow \epsilon \Omega(t)$, and shifted detuning, $\Delta \rightarrow \Delta + \delta_{\text{dopp}}$, and compute the state-transfer infidelity. Figures 3(a)–3(c) summarize the results for the three pulses from Fig. 1, showing the infidelity over a range of control parameters [51]. Both the unoptimized pulse and the pulse obtained from traditional QOC show high-fidelity islands (dark blue) arising from Rabi oscillations and a sharp fidelity drop for nonzero Doppler shifts. However, the pulse obtained from adiabatic QOC achieves high state-transfer fidelity over a wider range of parameters (dark blue).

To verify our results on real quantum hardware, we ran a trotterized version of the pulses from Fig. 1 on IBM’s brisbane quantum computer [35,36]. We generated 625 Hamiltonian parameter sets, corresponding to 25 Doppler shifts and pulse areas, and then simulated the system evolution and recorded the fidelity for each set. Infidelity averaged over 1024 runs is shown in Figs. 3(d)–3(f). The measured results resemble the Python results, but the fidelity of the former is lower due to the limited repetition number at each parameter set. In Sec. 2.1 of the Supplemental Material [41], we compare our method with ensemble optimization. While both methods find pulses that are robust to Doppler shifts and intensity variations, adiabatic optimization is substantially more efficient.

B. Adiabatic QOC of a multilevel system

Next, we accelerate a protocol for adiabatic state transfer between superconducting qubits mediated via a multimode waveguide [52]. The energy level diagram of the system (reproduced from Ref. [15]) is shown in Fig. 4(a), where qubits A and B couple to the n th guided mode with amplitudes

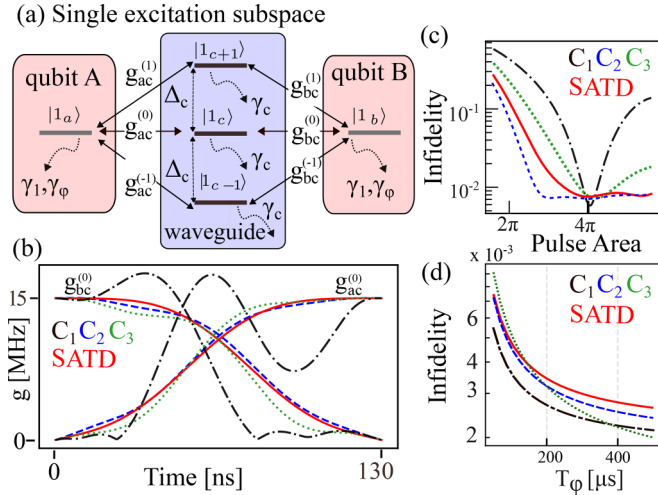


FIG. 4. (a) Single-excitation subspace of two qubits coupled to a multimode waveguide with couplings $g_{ac}^{(n)}$ and $g_{ab}^{(n)}$, and FSR Δ_c . Decay rates γ_1 , γ_ϕ , γ_c representing qubit relaxation, dephasing, and waveguide decay. (b) Coupling amplitudes $g_{ac}(t)$ and $g_{ab}(t)$ of SATD pulses and pulses obtained with C_1 , $C_1 + \frac{1}{2}C_2$ (labeled as C_2), and C_3 [Eq. (3)]. (c), (d) State-transfer infidelity for varying $T_\phi = 1/\gamma_\phi$ (where C_1 is optimal) and pulse areas of the qubit-waveguide couplings (where C_2 is optimal) for pulses from panel (b), and assuming $Q_c = 10^5$ where $Q_c = \omega_c/\gamma_c$, $\omega_c = 5$ GHz, and $\Delta_c = 500$ MHz.

$g_{ac}^{(n)}(t)$ and $g_{bc}^{(n)}(t)$, respectively. The protocol is a generalized STIRAP scheme [1], in which one first applies $g_{bc}^{(n)}(t)$ and then $g_{ac}^{(n)}(t)$ [Fig. 4(b)]. By doing so, the instantaneous ground state changes and excitation is transferred from A to B. We optimize the pulse shapes, $g_{bc}^{(n)}(t)$ and $g_{ac}^{(n)}(t)$, using our adiabatic QOC algorithm. To benchmark our method, we compare it with superadiabatic transitionless driving (SATD), which relies on eliminating diabatic errors in the dressed-state basis [53]. The details of the SATD pulses are given in Sec. 4 of the Supplemental Material [41]. We include population relaxation (T_1) and dephasing (T_ϕ) noise using the Lindblad master equation [Eq. (1)]. Its use can be justified as follows. While non-Markovian dynamics are generally required for qubits coupled to multimode waveguides [54–58], when using meter-long microwave waveguides, qubit couplings to high-order interconnect modes are nearly frequency independent justifying the Markov approximation underlying Eq. (1) [15,52].

Figure 4(b) shows optimized pulse shapes $g_{ac}^{(0)}(t)$ and $g_{ab}^{(0)}(t)$ obtained with SATD and QOC using the infidelity costs from Eq. (3). The dashed blue curve is obtained with adiabatic QOC by minimizing the weighted sum $C_1 + \frac{1}{2}C_2$. Here, we use a basis of Chebyshev polynomials since we prioritize high fidelity over fast convergence. Figures 4(c) and 4(d) show the robustness of the pulses from panel (b) to intensity and lifetime variations, respectively. In panel (c), we compute infidelity upon scaling the amplitude of the pulses from panel (b) by an overall scale factor, replacing $g_{ac}^{(n)} \rightarrow \epsilon g_{ac}^{(n)}$ and $g_{bc}^{(n)} \rightarrow \epsilon g_{bc}^{(n)}$. We assume $T_1 = T_\phi = 100 \mu$ s and a waveguide quality factor of $Q = 10^5$. In panel (d), we plot the state-transfer infidelity versus T_ϕ for the pulses from panel (b). The pulses are optimized assuming $T_1 = 50 \mu$ s.

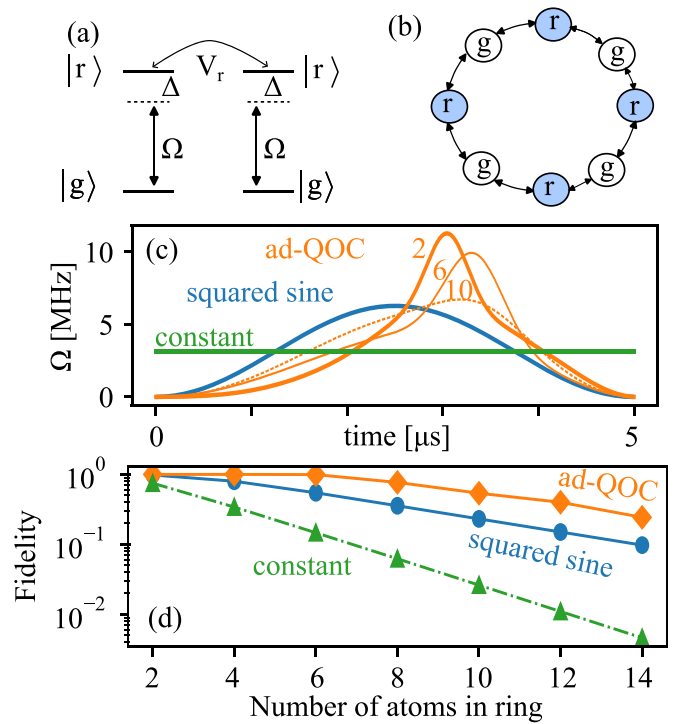


FIG. 5. (a) Rydberg qubits with levels $|g\rangle$ and $|r\rangle$. V_r is the Rydberg interaction, while Ω and Δ are the Rabi frequency and detuning of the control. (b) An eight-node ring graph and one of its MIS solutions. (c) Rabi frequency $\Omega(t)$ of a constant field (green), a squared sine pulse (blue), and pulses obtained with adiabatic QOC for rings containing $N = 2, 6, 10$ atoms (orange). (d) Fidelity defined as the overlap of the final state and MIS solution, $1 - C_1$, vs ring length for the pulses from panel (c).

Our analysis shows that pulses obtained with adiabatic QOC have improved robustness for intensity fluctuations, but not to variations in dephasing lifetime. The robustness to amplitude variations can be attributed to the fact that when forcing $g_{bc}^{(0)} = 0$ at t_f , an overall scale factor does not affect the final ground state. Finally, we note that ensemble optimization produces robust results but is significantly less efficient than adiabatic QOC; it takes approximately one hour compared to several minutes with adiabatic QOC.

C. Adiabatic QOC of a few-body quantum system

Finally, we accelerate an AQC algorithm for finding the maximum independent set of a graph. Following Refs. [12,59–61], we use Rydberg qubits—two-level atoms with a low-energy hyperfine state and a highly excited Rydberg state [Fig. 5(a)]. Rydberg states have a large dipole moment, preventing atoms separated by less than the critical “blockade radius” r_B from being simultaneously excited. A lattice of Rydberg qubits represents a unit-disk graph, $G(N, E)$, where each qubit corresponds to a node $i \in N$, and nodes represented by qubits with mutual distance $d < r_B$ are connected by an edge $(i, j) \in E$. The AQC for finding the MIS of $G(N, E)$ proceeds as follows [59]: All qubits are initialized in the ground state. Then, a global RAP pulse is applied, attempting to excite all atoms. Rydberg blockade

prohibits excitations of qubits with mutual distance $d < r_B$, so the system naturally finds the maximum number of allowed Rydberg excitations—corresponding to the MIS of $G(N, E)$.

The Hamiltonian of the driven Rydberg lattice is

$$H_{\text{MIS}} = \sum_{i \in N} [\Omega(t)\hat{\sigma}_x^i - \Delta(t)\hat{\sigma}_z^i] + V_r \sum_{(i,j) \in E} \hat{n}_i \hat{n}_j, \quad (6)$$

where the first sum represents the global RAP pulse, with $\Delta(t)$ a cubic polynomial swept from positive to negative and $\Omega(t)$ an optimized pulse, shown in Fig. 5(c). The second sum represents Rydberg interactions, with V_r the Rydberg interaction strength and $\hat{n}_i$ the projector of qubit i onto the Rydberg state; i.e., the product $\hat{n}_i \hat{n}_j$ is nonzero when both i and j are excited.

We apply our method to study ring graphs with an even number of nodes. The MIS is known—consisting of every other node [Fig. 5(b)]—and is used to evaluate the error of the AQC. We analyze the error in finding the MIS when using the pulses shown in Fig. 5(c): A constant Rabi intensity (green), a squared sine pulse (blue), and pulses obtained from adiabatic QOC for rings containing 2, ..., 14 atoms (orange) when using the squared sine pulse as an initial guess. (For clarity, only three optimized pulses are shown.) Here, we use a weighted sum of fidelity costs, $C_1 + 0.1C_2$. Upon increasing the Hilbert space dimension, we find that convergence improves when decreasing the weight of C_2 . We demonstrate the robustness of the optimized pulses to intensity fluctuations in Sec. 2.2 of the Supplemental Material [41]. We discretize the control pulses with Gaussian basis functions since fast convergence is crucial in multiqubit control. To facilitate convergence for large rings, we reduce the Hilbert space dimension by projecting the Hamiltonian onto the subspace of states without neighboring Rydberg excitations [59]. We analyze the error induced by this projection in Sec. 3 of the Supplemental Material [41]. To ensure a fair comparison with the unoptimized pulses in Fig. 5(c), we normalize all pulse areas to 4π after pulse optimization and before running the AQC. Figure 5(d) shows the fidelity (defined as the overlap between the final and true MIS states) versus chain length for the pulses from panel (c), demonstrating the superiority of adiabatic QOC over other methods. For short chains ($N = 2, \dots, 8$), we find slightly asymmetric pulses (orange), while for longer chains, the asymmetry becomes less pronounced. Details about the convergence of our algorithm are given in Sec. 1.3 of the Supplemental Material [41].

IV. CONCLUSION

This work presents a powerful optimization tool for adiabatic control of open few-body quantum systems. Generalizing Ref. [32], we seek pulses under which the evolving system adheres to the instantaneous eigenstate along its propagation. Combining efficient optimization and simulation tools, we can optimize technologically relevant systems, as demonstrated by the three numerical examples above. We conclude by mentioning directions for further research. Adherence to the instantaneous ground state along the propagation requires knowledge of the state, which is not available in large-scale AQC. Nevertheless, we hypothesize that AQC can be improved by seeking pulses that adhere to approximate ground states or by using knowledge of the ground state during early stages of the protocol. Furthermore, optimization of AQC requires classical computation resources in the optimization stage and quantum resources in the evolution stage. Optimizing the division between classical and quantum resources in adiabatic QOC is key to advancing the present approach.

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DATA AVAILABILITY

The data in the manuscript was generated by numerical simulations described in the manuscript. The code is available from the corresponding author upon request, and the results are fully reproducible from the parameters provided in the paper.

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