

Directional motional control via engineered conical intersections in trapped Rydberg ions

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We demonstrate coherent control of motional dynamics in trapped Rydberg ions engineered to exhibit a conical intersection between adiabatic potential-energy surfaces. Using quantum optimal control, an optimally shaped electric field drives the motional wave packet between prescribed spatial configurations on microsecond timescales. Localized nonadiabatic coupling breaks the symmetry of the dynamics and produces a directed trajectory: after only a few early passages through the conical intersection region, the packet proceeds toward the target with high fidelity. In contrast, in the Born-Oppenheimer limit, where such coupling is absent, the optimized control yields symmetric, multicycle oscillations rather than a comparably directed displacement. While both approaches reach the target at the chosen final time, the underlying trajectories are qualitatively different. This work demonstrates that engineered conical intersections can serve as a potential control resource for directional motional dynamics, complementing pulse-shaping methods in trapped-ion systems. This directional motion of the ions, enabled by the conical intersection, may provide a route toward improved control of motional states in trapped-ion quantum information processing.

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I. INTRODUCTION

Trapped ions represent one of the most promising platforms for quantum information processing [1–12]. Achieving precise control over their motional degrees of freedom is essential for scalable quantum computation, as even small motional displacements can degrade entangling-gate performance [13]. Accordingly, several protocols have been developed to suppress residual excitations including motional squeezing [14] or tailored pulse shaping [15].

The Born-Oppenheimer (BO) approximation is a standard approach to treating coupled electronic and nuclear dynamics. It was introduced by Born and Oppenheimer in 1927 and exploits the separation of electronic and nuclear timescales arising from their large mass difference [16,17]. Within this framework, the electronic degrees of freedom define effective potential-energy surfaces (PESs) on which the nuclear motion evolves. The limitations of the BO approximation arise when strong nonadiabatic couplings between electronic and nuclear degrees of freedom are present, leading to a breakdown of the separation of their dynamics [16,18,19]. In particular, the BO approximation fails to describe the geometric and topological effects that arise in the vicinity of a conical intersection (CI), which corresponds to a degeneracy point between adiabatic PESs in the nuclear coordinate space. CIs are ubiquitous in molecular photochemistry and govern the dynamics of many

ultrafast photoinduced processes [20–23]. Recent theoretical proposals showed that CIs can also be engineered in synthetic quantum systems [24–26], including Rydberg atoms [27,28] and trapped Rydberg ions [29]. The latter provide an experimentally tunable platform to study nonadiabatic dynamics near CIs [29]. Their large electric polarizabilities and strong dipolar exchange interactions allow the shape of the PESs and the position of the CI to be engineered with external fields. Unlike molecular systems, where CIs occur on femtosecond timescales and nanometer length scales, Rydberg ions enable the same physics to be explored on microsecond and micrometer scales, where both the nuclear-like and electronic-like dynamics can be directly controlled and observed in real time within a state-of-the-art ion-trap setup [29].

In this paper, we aim to investigate the optimal control of Rydberg-ion motion near an engineered CI. Using a time-dependent electric field and shaping its temporal profile using quantum optimal control theory [30–36], we demonstrate coherent steering of a vibrational wave packet from an initial Gaussian state to a predefined spatial target. Our spinor model incorporates nonadiabatic couplings arising from the CI, allowing direct comparison with the BO limit where such couplings are absent. Near a CI, optimized fields induce a directed displacement of the wave packet with only a few early passages through the CI before reaching the target, whereas in the BO limit the control produces symmetric, multicycle oscillations. These results suggest that engineered CIs could provide a useful resource for realizing directed and robust motional control in trapped-ion platforms for quantum information science.

Our paper complements the recent work of Whitlow *et al.* [37] who simulated a CI using ground-state trapped ions

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by encoding the electronic and nuclear degrees of freedom in the spin and motional modes of the ions and observing the resulting geometric phase. In contrast, the present study employs Rydberg ions as a physical system in which a genuine CI arises from dipolar exchange and state-dependent polarizabilities [29]. This platform enables the exploration of nonadiabatic motion and optimal-control strategies on real PESs, extending beyond the quantum-simulation approach of Ref. [37].

This paper is organized as follows. In Sec. II, we present a model that enables the construction of a CI and the control of the motional states of two Rydberg ions confined in a Paul trap near the engineered intersection. In Sec. III, we apply this model to control the motional states of $^{88}\text{Sr}^+$ Rydberg ions and compare the results with those obtained in the absence of the CI under the BO approximation (Sec. IV). Finally, Sec. V summarizes our findings and outlines the main conclusions of this work.

II. EQUATIONS OF MOTION

We consider two Rydberg ions of mass m confined in a Paul trap, which generates an effective harmonic potential with frequencies ω_x , ω_y , and ω_z [38–40]. By assuming that $\omega_y \gg \omega_x > \omega_z$, the motion of the two ions can be analyzed in the X - Z plane. Hence the potential energy of the two trapped ions is given by

$$V_{\text{trap}} = \frac{m}{2} [\omega_x^2 (X_1^2 + X_2^2) + \omega_z^2 (Z_1^2 + Z_2^2)] + V_c, \quad (1)$$

where $\mathbf{R}_i = (X_i, Z_i)$ denotes the nuclear coordinates in the laboratory frame of the i th ion, with $i = 1, 2$. V_c is the repulsive Coulomb potential expressed as $V_c = k e^2 / |\mathbf{r}|$, where k is the Coulomb constant, e is the elementary charge, and $\mathbf{r} = \mathbf{R}_2 - \mathbf{R}_1$. By applying a static electric field u_0 along the X axis, a potential $V_m = u_0 \phi(X)$ is generated, where $\phi(X) = e(X_1 + X_2)$ [29]. The static electric field controls the transverse equilibrium positions of the ions and thus enables the construction of the CI.

Each trapped ion is modeled as a two-level Rydberg system $|\downarrow\rangle \equiv |nS\rangle$ and $|\uparrow\rangle \equiv |nP\rangle$, where n is the principal quantum number. These levels can be coupled by a microwave field with Rabi frequency Ω and detuning Δ [29]. Two such Rydberg ions interact through a resonant dipole-dipole exchange process, described by

$$H_{\text{ex}} = U_{\text{ex}}(r) \otimes (\sigma_1^+ \otimes \sigma_2^- + \sigma_1^- \otimes \sigma_2^+), \quad (2)$$

where $\sigma_i^+ |\downarrow\rangle_i = |\uparrow\rangle_i$ and $\sigma_i^- |\uparrow\rangle_i = |\downarrow\rangle_i$. This exchange potential couples the single-excitation states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, and its strength $U_{\text{ex}}(r)$ depends on the ion separation $r = |\mathbf{r}|$. In addition, the two Rydberg levels possess different polarizabilities, $\rho_\uparrow$ and $\rho_\downarrow$, which lead to state-dependent modifications of the trapping potential. This contribution can be written as

$$H_\rho = -\alpha^2 (X_1^2 \otimes \Pi_\rho \otimes \mathbb{1}_2 + X_2^2 \otimes \mathbb{1}_2 \otimes \Pi_\rho), \quad (3)$$

where $\Pi_\rho = \rho_\downarrow |\downarrow\rangle \langle \downarrow| + \rho_\uparrow |\uparrow\rangle \langle \uparrow|$ and α denotes the gradient of the radio-frequency field in the Paul trap. Together, the dipolar exchange and the state-dependent trapping potentials form the basis for engineering coupled PESs that intersect

when tuned by an external static field, thereby realizing a CI in a controllable trapped-ion environment [29].

We analyze the dynamics in the center-of-mass and relative coordinate frames, defined as $\mathbf{R} = \frac{\mathbf{R}_1 + \mathbf{R}_2}{2}$ and $\mathbf{r} = \mathbf{R}_2 - \mathbf{R}_1$, respectively. We restrict our analysis to the single-excitation subspace spanned by $|\pi_1\rangle = |\uparrow\downarrow\rangle$ and $|\pi_2\rangle = |\downarrow\uparrow\rangle$, realized by setting $\Omega = 0$ and holding Δ constant [29,41]. In this subspace, we define the effective Pauli operators as $S_0 = |\pi_1\rangle \langle \pi_1| + |\pi_2\rangle \langle \pi_2|$, $S_x = |\pi_1\rangle \langle \pi_2| + |\pi_2\rangle \langle \pi_1|$, and $S_z = |\pi_1\rangle \langle \pi_1| - |\pi_2\rangle \langle \pi_2|$. For typical experimental conditions, the harmonic trapping potential dominates the energy landscape, allowing the remaining interactions to be treated as perturbations. We perform an harmonic expansion around the equilibrium positions $\mathbf{R}_0 = (X_0, Z_0)$ for the center-of-mass coordinate and $\mathbf{r}_0 = (x_0, z_0)$ for the relative coordinate, introducing displacements $\mathbf{Q} = \mathbf{R} - \mathbf{R}_0$ and $\mathbf{q} = \mathbf{r} - \mathbf{r}_0$. The derivation of the equilibrium positions $X_0, Z_0 = 0$ and $x_0 = 0, z_0$ is provided in Appendix A.

Following Ref. [29], we neglect the center-of-mass motion ($\mathbf{Q} = 0$) and focus on the relative coordinate, which captures the key nonadiabatic effects (see Appendix A for details). The resulting effective Hamiltonian incorporating all relevant interaction terms is given as

$$H_0 = -\frac{\hbar^2}{2\mu} (\nabla_{q_x}^2 + \nabla_{q_z}^2) \otimes S_0 + H_{\text{spin}}, \quad (4a)$$

where

$$H_{\text{spin}} = S(\mathbf{q}) \otimes S_0 + W(\mathbf{q}) \otimes S_x + G(\mathbf{q}) \otimes S_z, \quad (4b)$$

with

$$S(\mathbf{q}) = \left[\frac{\mu}{2} \bar{\omega}_x^2 q_x^2 + \frac{\mu}{2} \bar{\omega}_z^2 q_z^2 \right], \quad (4c)$$

$$W(\mathbf{q}) = [U_{\text{ex}}(r_0) + F_z(r_0) q_z], \quad (4d)$$

$$G(\mathbf{q}) = \alpha^2 \rho_- X_0 q_x. \quad (4e)$$

Here, the reduced mass is $\mu = m/2$, $\hbar$ is the reduced Planck's constant, and the effective frequencies are $\bar{\omega}_x^2 = \omega_x^2 - \frac{\alpha^2}{2\mu} \rho_+ - \frac{k e^2}{\mu |z_0|^3}$, $\bar{\omega}_z^2 = \omega_z^2 + \frac{2k e^2}{\mu |z_0|^3}$, with $F_z(r_0) = \partial_z U_{\text{ex}}(r)|_{r=r_0}$ and $\rho_\pm = \rho_\uparrow \pm \rho_\downarrow$. Equation (4) is formulated within the pseudopotential approximation, where the fast radio-frequency (rf) micromotion of the ions in the Paul trap is averaged out. This treatment is standard and well validated for Rydberg-ion experiments operating under typical trapping conditions [29,38,39]. In this regime, the micromotion contributes only small periodic corrections to the harmonic potential and can be safely neglected on the microsecond timescales relevant to the control dynamics. A detailed derivation of the effective Hamiltonian, starting from the full spinor model and including the harmonic expansion around equilibrium, is provided in Appendix A. The PESs refer to the eigenvalues of the electronic Hamiltonian H_{spin} [16,42]. These eigenvalues are defined as

$$E_\pm = S(\mathbf{q}) \pm \sqrt{G(\mathbf{q})^2 + W(\mathbf{q})^2}. \quad (5)$$

In general, CIs occur at positions $\mathbf{q}^*$ where the adiabatic potentials become degenerate, i.e., $E_+(\mathbf{q}^*) = E_-(\mathbf{q}^*)$. According to Eq. (5), this condition is equivalent to $G(\mathbf{q}^*) = 0$ and $W(\mathbf{q}^*) = 0$. This implies that the system described by

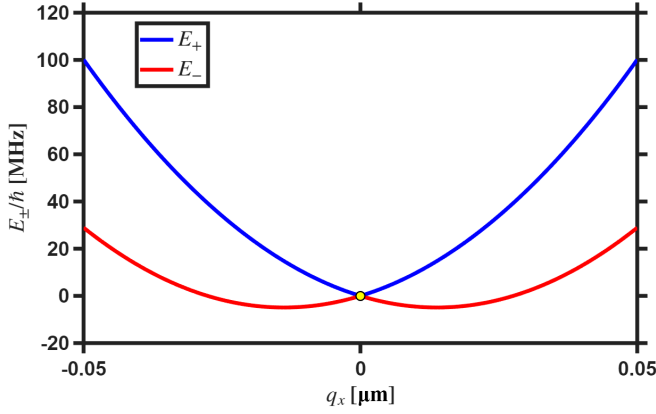


FIG. 1. One-dimensional slice of the PESs at $q_z = 0$, showing the lower (E_- , red) and upper (E_+ , blue) as functions of q_x (in μm). The yellow dot marks the position of the CI at ($q_x^* = 0$, $q_z^* = 0$). Parameters correspond to $^{88}\text{Sr}^+$ Rydberg ions: $m = 87.9 \times 1.66 \times 10^{-27}$ kg, $\rho_\downarrow = 8.9 \times 10^{-30}$ C² m²/J, and $\rho_\uparrow = -3.8 \times 10^{-31}$ C² m²/J (Corresponding to Rydberg $|nS\rangle$ and $|nP\rangle$ states with $n = 50$). Additional parameters used are $\omega_x = 2\pi \times 1.6$ MHz, $\omega_z = 2\pi$ MHz, $u_0 = 2.529$ V/m corresponding to $X_0 = -0.024 \mu\text{m}$, $\alpha = 8.17 \times 10^8$ V/m², $U_{\text{ex}}(r_0) = 0$, $z_0 = 4.31 \mu\text{m}$ and $F_0/\hbar = 2\pi \times 20$ MHz/ μm .

Eq. (5) exhibits a CI at $q_x^* = 0$ and $q_z^* = -U_{\text{ex}}(r_0)/F_z(r_0)$. Figure 1 shows a one-dimensional slice of the PESs at $q_z = 0$ and the position of the CI for two trapped $^{88}\text{Sr}^+$ Rydberg ions.

In this paper, we demonstrate that the motional state of two trapped Rydberg ions near a CI can be coherently controlled using a time-dependent electric field applied to a single ion. This control field, designed through quantum optimal control theory, steers the system from an initial spatial configuration to a desired target at a fixed final time. We consider a spatially localized electric field $u(t)$ applied to the first ion along the X axis, resulting in an interaction term $V_u(t) = e u(t) X_1$. Spatially selective control is experimentally feasible using tightly focused laser beams or near-field microwave radiation [43–47]. In our work, we model the control field as a generic time-dependent electric drive, which makes the results broadly applicable independent of the specific implementation. After performing the harmonic approximation, the control Hamiltonian can be given by

$$H_u(t) = e u(t) (X_0 - \frac{1}{2} q_x) \otimes S_0. \quad (6)$$

The dynamics of the system are governed by the following Schrödinger equation:

$$\frac{\partial}{\partial t} |\psi(q_x, q_z, t)\rangle = \frac{-i}{\hbar} (H_0 + H_u(t)) |\psi(q_x, q_z, t)\rangle, \quad (7)$$

where $|\psi(q_x, q_z, t)\rangle$ belongs to the Hilbert space $\mathcal{H} = \mathcal{H}_q \otimes \mathcal{H}_{\text{spin}}$, with $\mathcal{H}_q$ is the single-particle motional Hilbert space in two spatial dimensions, and $\mathcal{H}_{\text{spin}} \cong \mathbb{C}^2$ is the two-dimensional Hilbert space associated with a spin- $\frac{1}{2}$ degree of freedom. For a known external electric field, the time-dependent Schrödinger equation given in Eq. (7) can be solved numerically. However, in quantum control problems, the form of the electric field is unknown and needs to be designed to minimize or maximize a cost function [30,31]. As seen

in Eq. (6), the control field couples directly to q_x , enabling efficient manipulation of the ions' relative motion. If instead the control field is applied symmetrically to both ions, the resulting control Hamiltonian becomes $H_u^B(t) = 2 e u(t) X_0 \otimes S_0$. Therefore, applying this control Hamiltonian introduces only a constant energy shift and does not provide the nuanced control achievable with the control Hamiltonian given in Eq. (6). We therefore apply the time-dependent electric field to a single ion to achieve full motional control.

III. CONTROL OF MOTIONAL STATES OF TRAPPED RYDBERG IONS

Our objective is to determine the optimal electric field $u(t)$ that drives the system from an initial to a target state at a fixed final time t_f . The initial state is

$$|\psi(q_x, q_z, 0)\rangle = \phi^0(q_x, q_z) |\pi_2\rangle, \quad (8)$$

where $\phi^0(q_x, q_z) = \ell_{xz} \exp\{-\frac{\mu}{2\hbar} [\bar{\omega}_x(q_x - q_x^0)^2 + \bar{\omega}_z(q_z - q_z^0)^2]\}$, with $\ell_{xz} = (\frac{\mu^2 \bar{\omega}_x \bar{\omega}_z}{\pi^2 \hbar^2})^{1/4}$. The target motional state $\phi^d(q_x, q_z)$ is a Gaussian with the same widths as $\phi^0(q_x, q_z)$ but centered at (q_x^d, q_z^d) . We define the target operator as

$$\hat{O} = \Pi_{|\phi^d\rangle\langle\phi^d|} \otimes S_0, \quad (9)$$

where the action of the projector $\Pi_{|\phi^d\rangle\langle\phi^d|}$ on a wave function $\Psi(q_x, q_z) \in \mathcal{H}_q$ is given by

$$\begin{aligned} (\Pi_{|\phi^d\rangle\langle\phi^d|} \Psi)(q_x, q_z) &= \phi^d(q_x, q_z) \\ &\times \iint dq'_x dq'_z [\phi^d(q'_x, q'_z)]^* \Psi(q'_x, q'_z). \end{aligned} \quad (10)$$

Our goal is to maximize the expectation value of the projector $\hat{O}$ while minimizing the energy of the control field, subject to the Schrödinger dynamics given in Eq. (7). Following Refs. [30,31], this objective can be equivalently expressed as the maximization of the following functional:

$$J = J_1 - J_2, \quad (11)$$

where

$$\begin{aligned} J_1 &= \langle \psi(q_x, q_z, t_f) | \hat{O} | \psi(q_x, q_z, t_f) \rangle \\ &- 2 \Re \int_0^{t_f} dt \langle \lambda(q_x, q_z, t) | \left(\frac{\partial}{\partial t} - \hat{L} \right) | \psi(q_x, q_z, t) \rangle, \end{aligned} \quad (12a)$$

$$J_2 = \alpha_0 \int_0^{t_f} [u(t)]^2 dt. \quad (12b)$$

The functional J_1 given in Eq. (12a) includes the expectation value of the target operator $\hat{O}$ and a constraint term that enforces the Schrödinger dynamics, while J_2 provided in Eq. (12b) penalizes large field amplitudes to limit the total fluence. Here, $|\lambda(q_x, q_z, t)\rangle$ is a Lagrange multiplier used to enforce the system's evolution, and $\hat{L}$ is the operator given on the right-hand side of Eq. (7). The parameter α_0 is a positive weighting factor that controls the contribution of the field fluence. To derive the optimal control capable of transitioning the system from the initial state to the target state, we apply the monotonically convergent algorithm (MCA) summarized

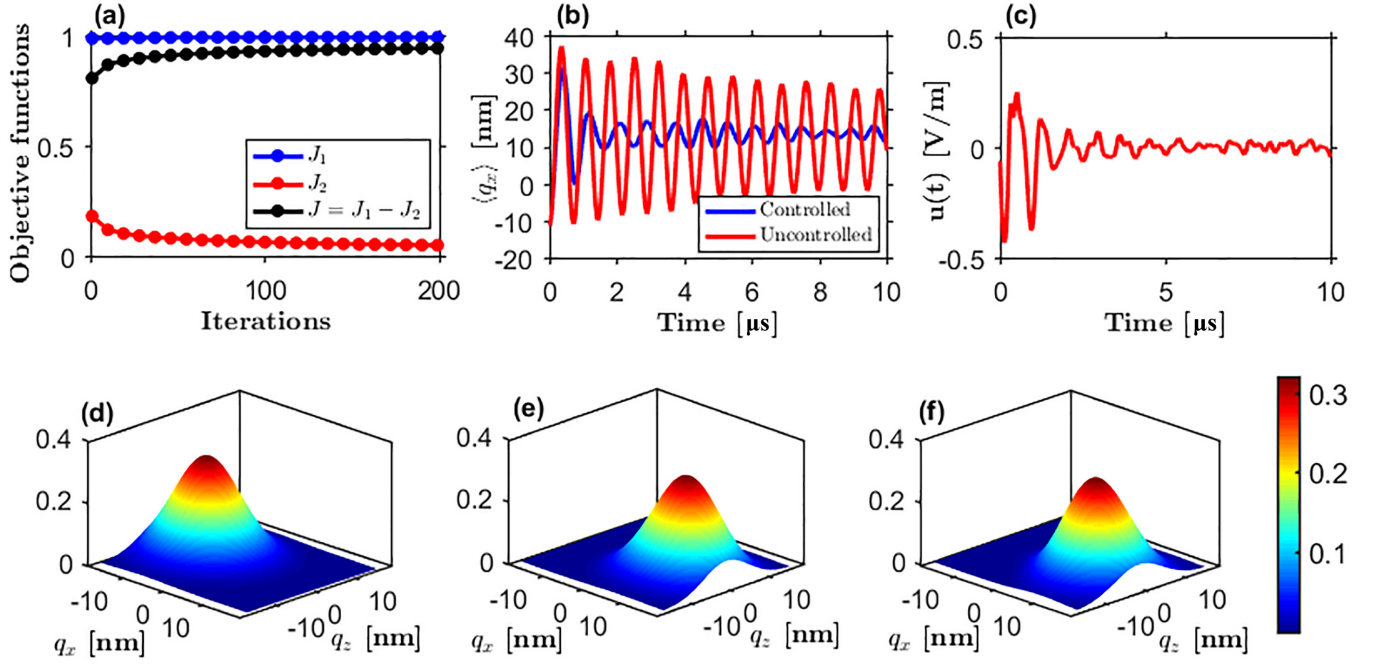


FIG. 2. Optimal control of spatial dynamics near a CI. (a) Convergence of the target functional J_1 , the penalty J_2 , and the total $J = J_1 - J_2$ over the MCA iterations. (b) Time evolution of $\langle q_x(t) \rangle$ with (blue) and without (red) the control field, demonstrating successful steering. (c) Temporal profile of the optimized electric field $u(t)$. (d)–(f) Probability density $|\psi(q_x, q_z, t)|^2$ at (d) $t = 0$ μs, (e) $t = 5$ μs, and (f) $t = 10$ μs, illustrating transport to the target region under control. Additional parameters are provided in the main text and in Fig. 1.

in Appendix B. The MCA iteratively updates the control field to maximize the objective functional while ensuring stable convergence. Before starting the optimization, an initial guess for the control field is specified. Then, the control field is refined over successive iterations of the algorithm until the objective functional reaches its maximum.

In our simulations, the initial wave-packet center is set to $(q_x^0, q_z^0) = (-11.4 \text{ nm}, 0)$, the target wave-packet center to $(q_x^d, q_z^d) = (11.4 \text{ nm}, 0)$, and the final time to $t_f = 10$ μs. For the trap parameters considered in this work, rf-driven micromotion remains well below the nanometer scale for the ~ 10 nm secular displacements relevant to our control protocol (see Appendix C). For the optimization parameters listed in Appendix B, we take $\eta = \zeta = 1$. The fluence penalty in Eq. (12b) is $\alpha_0 = 0.01$. The initial electric field used to seed the optimization is a rectangular pulse, $\mathcal{E}(t) = -14.39 \text{ V/m}^{-1}$ for $t \in [0, 20] \text{ ns}$ and 0 otherwise.

In Fig. 2(a), we show the target function J_1 , the penalty term J_2 , and the total functional $J = J_1 - J_2$ as a function of the algorithm iteration number. The functional J increases rapidly in the first 20 iterations, then stabilizes after approximately 100 iterations. At the final iteration, J_1 reaches 99.08%, indicating a high overlap with the target operator $\hat{O}$, while J_2 decreases. To confirm the control objective, Fig. 2(b) shows the time evolution of the position operator q_x with and without the optimized electric field $u(t)$. The relative position between the ions exhibits oscillatory behavior, and under the action of the optimal field, it reaches the desired value at the final time, indicating successful spatial control. By contrast, in the absence of the control field the final expectation value is $\langle q_x(t_f) \rangle = 8.96 \text{ nm}$, compared to the desired $q_x^d = 11.4 \text{ nm}$. From Fig. 2(b), one can conclude also that the optimized

field induces a directed displacement toward the target: the wave packet traverses the vicinity of the CI point twice at early times and does not return thereafter. In Fig. 2(c), we show the optimized electric field $u(t)$, which is responsible for achieving the control objective.

Figures 2(d)–2(f) show the density $|\psi(q_x, q_z, t)|^2$ at three representative times: initial, intermediate, and final. These snapshots illustrate the real-space dynamics of the wave function under the optimized field, and demonstrate that the control objective is achieved by driving the system from the initial to the target configuration.

The optimal control fields obtained here should not be viewed as prescriptions for direct experimental implementation. Rather, they serve to demonstrate the control concept and to elucidate the underlying dynamical mechanisms enabled by the engineered Rydberg-mediated coupling structure. In particular, while the finite Rydberg-state lifetime (70–100 μs) implies a nonnegligible decay probability over the ~ 10 μs control times considered here, leading to a reduction of the achievable fidelity by an amount of order 0.1, this effect primarily reduces the overall success probability and does not invalidate the coherent control mechanism identified by the optimization.

In practice, experimental realizations of quantum optimal control should rely on closed-loop optimization protocols in which control fields are iteratively refined directly in the laboratory [48,49]. Such approaches automatically incorporate all relevant physical effects, including spontaneous decay, micromotion, and technical noise, without requiring their explicit inclusion in the theoretical cost functional. From this perspective, the present results identify engineered Rydberg-induced structures as a control resource that can be exploited by

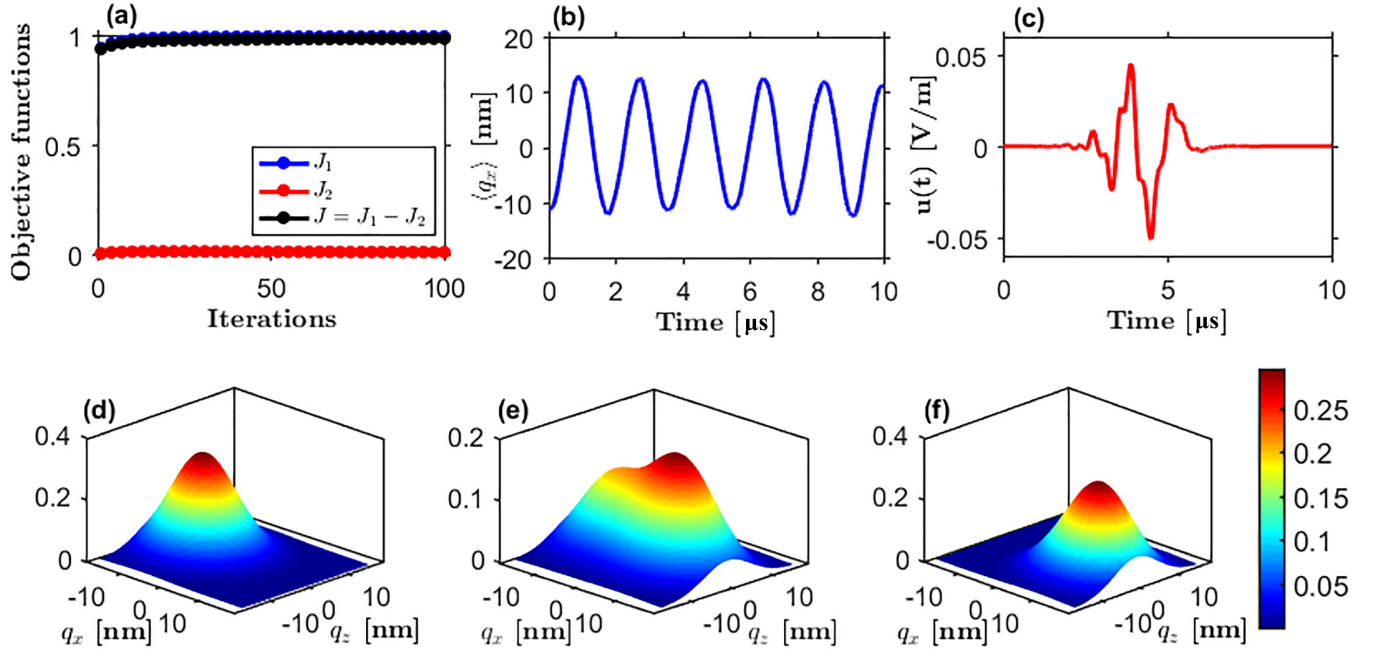


FIG. 3. Optimal control of wave-packet dynamics under the BO approximation. (a) Evolution of the target functional J_1 , penalty J_2 , and total $J = J_1 - J_2$ over the MCA iterations. (b) Time evolution of $\langle q_x(t) \rangle$ under optimal control. (c) Time profile of the optimized electric field $u(t)$. (d)–(f) Density $|\psi(q_x, q_z, t)|^2$ at representative times: (d) $t = 0 \mu\text{s}$, (e) $t = 5 \mu\text{s}$, and (f) $t = 10 \mu\text{s}$. Additional parameters are provided in the main text and in Fig. 1.

experimental optimization schemes, rather than as a requirement to reproduce a specific theoretically optimized pulse shape.

IV. CONTROL DYNAMICS IN THE ABSENCE OF THE CI (BO LIMIT)

To isolate the effects of the CI on the control of the motion dynamics, we solve the same optimal control problem within the BO approximation. This approximation confines the system's dynamics to a single adiabatic PES, neglecting nonadiabatic couplings between electronic states. Under this approach, the full spinor structure of the Hamiltonian is removed, and the dynamics is governed by the time-dependent Schrödinger equation with the Hamiltonian

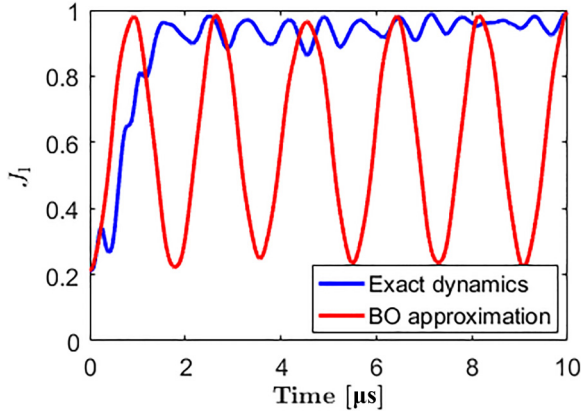
$$H^{\text{BO}} = -\frac{\hbar^2}{2\mu} \nabla_{q_x}^2 - \frac{\hbar^2}{2\mu} \nabla_{q_z}^2 + E_- + e u(t) \left(X_0 - \frac{1}{2} q_x \right), \quad (13)$$

where E_- is given in Eq. (5). We apply the same optimization procedure to the reduced model, targeting the same objective operator $\hat{O}$. The optimization parameters, shown in Appendix B, are $\eta = \zeta = 1$ and the fluence penalty $\alpha_0 = 0.1$. The initial electric field used before optimization is a simple Gaussian-shaped pulse along the X direction, defined as $\mathcal{E}(t) = \mathcal{E}_0 \times \exp[-\frac{(t-t_0)^2}{2\tau^2}]$ where the pulse center $t_0 = 4 \mu\text{s}$, $\mathcal{E}_0 = -0.719 \text{ mV/m}$, and $\tau = 0.85 \mu\text{s}$. This field served as the initial guess for the optimization algorithm.

In Fig. 3(a), we show the evolution of the target function J_1 , the penalty term J_2 , and the total functional $J = J_1 - J_2$ as a function of the algorithm iteration number for the BO limit. By comparing the evolution of the objective functional J in the BO case with that in the full spinor dynamics case (including

the CI) shown in Fig. 2(a), we observe that in the BO case, the total functional J converges to its optimal value in significantly fewer iterations, approximately 30 compared to 100 for the exact dynamics. This indicates that the CI complicates the control process due to the presence of nonadiabatic couplings. In Fig. 3(a), the curves for J_1 and $J = J_1 - J_2$ nearly overlap because the fluence penalty J_2 is much smaller than J_1 during the optimization.

In Fig. 3(b), we show the time evolution of the expectation value $\langle q_x(t) \rangle$ under optimal control for the BO approximation. The control field produces regular oscillations, such that the wave packet repeatedly traverses the spatial region corresponding to the CI point in the full spinor model. The absence of nonadiabatic coupling preserves symmetry in the motion, resulting in periodic dynamics with $\langle q_x(t) \rangle$ spanning a broad range (approximately from -12 nm to $+12 \text{ nm}$). In contrast, as seen in Fig. 2(b), the dynamics exhibits two early passages through the vicinity of the CI point, after which the wave packet proceeds toward the target without further return. At later times ($t \rightarrow t_f$), the motion becomes localized near the desired position ($\approx 11.4 \text{ nm}$), with $\langle q_x(t) \rangle$ oscillating within a narrow interval around this value. This contrast suggests that the localized nonadiabatic coupling near the engineered CI, together with optimal field shaping, is responsible for the emergence of directional motional control. It is known that even a small amount of displacement of trapped ions erodes the performance of entangling gates [13], while protocols based on motional squeezing have been shown to enable clean, residual-free transport and separation of ions [14]. Moreover, tailored pulse shaping has been successfully employed to design robust motional trajectories for high-fidelity gate operations in trapped-ion experiments [15]. In this context, the directional movement of the relative

FIG. 4. Time evolution of J_1 .

ions induced by the presence of the CI may provide a useful resource for quantum information science. Figure 4 compares the time evolution of the target functional J_1 for the exact dynamics including the CI and for the BO approximation. With the CI, J_1 rapidly approaches unity and remains stable (typically ≈ 0.9 – 1 after $t \approx 2$ μ s), whereas in the BO limit it exhibits large oscillations over the same time interval, ranging from near unity down to ≈ 0.2 , signaling repeated departures from the target and increased sensitivity to timing. Directed motion in trapped-ion systems has also been demonstrated in the transport of topological solitons in Coulomb crystals [50]. In analogy, the engineered CI provides a complementary route to convert oscillatory dynamics into robust directed transport, a feature that is promising for enhancing coherence and stability in future trapped-ion applications.

We note that identical optimization parameters were not used in the CI and BO cases, as applying the same settings in the BO limit leads to poor convergence and limited motional displacement. The parameters were therefore adapted in each case to ensure effective optimization. We find that moderate variations of the initial guess and control parameters do not qualitatively affect the observed behaviors and results, and the emergence of directional motion in the presence of the CI remains preserved.

In Fig. 3(c), we present the optimized electric field $u(t)$ under the BO approximation. Compared to the full dynamics with the CI, the control energy is significantly lower. This reduction reflects the simplified optimization landscape in the absence of nonadiabatic couplings. As a result, the optimization algorithm requires a less intricate field to reach the target, reducing the field amplitude and total fluence needed for optimal control.

Figures 3(d) to 3(f) display the wave-function density $|\psi(q_x, q_z, t)|^2$ at representative times under the BO approximation, showing the evolution from the initial to the target configuration.

V. CONCLUSION

We demonstrated coherent control of motional dynamics in trapped Rydberg ions near a CI using an optimally shaped time-dependent electric field. To isolate the role of nonadiabatic effects, we compared the full spinor dynamics with

the BO approximation. With the CI present, the optimized field drives the wave packet toward the target on microsecond timescales, producing a directed motional displacement. In the BO limit (no CI), the control produces symmetric, multi-cycle oscillations of large magnitude rather than a comparably directed displacement within the same time interval. This contrast suggests that the localized nonadiabatic coupling near the engineered CI, together with optimal field shaping, as the mechanism enabling directional motional control. While both cases reach high fidelity at the chosen final time, the CI case achieves it through a qualitatively different trajectory. This prospect suggests a potential pathway toward overcoming a key challenge in trapped-ion quantum computing: residual motional excursions that degrade gate fidelity. By adding CIs to the trapped-ion control toolbox, this work lays the groundwork for implementing future strategies that could contribute to improving the fidelity and scalability of ion-based quantum information platforms.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: DERIVATION OF THE EFFECTIVE HAMILTONIAN

We provide here the derivation of the effective Hamiltonian used in the main text. The total Hamiltonian includes the trap potential, Coulomb repulsion, exchange interaction, polarizability-induced potential, the microwave coupling, and the external control field. The full Hamiltonian is given by

$$H = H_0 + H_u(t), \quad (\text{A1})$$

where

$$H_0 = [T_n + V_{\text{trap}} + V_m] \otimes \mathbb{1}_2 \otimes \mathbb{1}_2 + H_{\text{ex}} + \mathbb{1}_n \otimes H_{\text{MW}} + H_\rho, \quad (\text{A2})$$

and

$$H_u(t) = V_u(t) \otimes \mathbb{1}_2 \otimes \mathbb{1}_2, \quad (\text{A3})$$

where V_{trap} , V_m , H_{ex} , H_ρ , and $V_u(t)$ are defined in the main text, $\mathbb{1}_n$ is the nuclear identity operator, and T_n is the kinetic energy operator expressed as

$$T_n = -\frac{\hbar^2}{2m} \nabla_{\mathbf{R}_1}^2 - \frac{\hbar^2}{2m} \nabla_{\mathbf{R}_2}^2. \quad (\text{A4})$$

The two Rydberg levels are coupled by a microwave field with Rabi frequency Ω and detuning Δ [29]. This coupling Hamiltonian appearing in Eq. (A2) can be described by

$$H_{\text{MW}} = \hbar \Omega (\sigma_x^1 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \sigma_x^2) + \hbar \Delta (\sigma_z^1 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \sigma_z^2). \quad (\text{A5})$$

We now recast the Hamiltonian H_0 in center-of-mass and relative coordinates $\mathbf{R} = \frac{\mathbf{R}_1 + \mathbf{R}_2}{2}$, $\mathbf{r} = \mathbf{R}_2 - \mathbf{R}_1$. This leads to

$$H_0 = H_{\text{CoM}} + H_{\text{rel}} + H_{\text{CoM-rel}}, \quad (\text{A6})$$

where H_{CoM} depends solely on the center-of-mass coordinates, H_{rel} depends on relative coordinates, while $H_{\text{CoM-rel}}$ depends on both sets of coordinates [29]. The expressions of these Hamiltonians are as follows:

$$H_{\text{CoM}} = \left[-\frac{\hbar^2}{2M} (\nabla_X^2 + \nabla_Z^2) + \frac{M}{2} (\omega_x^2 X^2 + \omega_z^2 Z^2) + 2u_0 e X \right] \otimes \mathbb{1}_2 \otimes \mathbb{1}_2 - \alpha^2 X^2 \otimes [\Pi_\rho \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \Pi_\rho], \quad (\text{A7})$$

$$H_{\text{rel}} = \left[-\frac{\hbar^2}{2\mu} (\nabla_x^2 + \nabla_z^2) + \frac{\mu}{2} (\omega_x^2 x^2 + \omega_z^2 z^2) + V_c \right] \otimes \mathbb{1}_2 \otimes \mathbb{1}_2 - \alpha^2 \frac{x^2}{4} \otimes [\Pi_\rho \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \Pi_\rho] + H_{\text{ex}} + \mathbb{1}_n \otimes H_{\text{MW}}, \quad (\text{A8})$$

and

$$H_{\text{CoM-rel}} = \alpha^2 X x \otimes [\Pi_\rho \otimes \mathbb{1}_2 - \mathbb{1}_2 \otimes \Pi_\rho], \quad (\text{A9})$$

where Π_ρ is defined in the main text and $M = 2m$. In the following, we restrict our analysis to the case where only one ion is excited to the Rydberg state $|\uparrow\rangle$, while the second ion is prepared in the Rydberg level $|\downarrow\rangle$. This condition requires that $\Omega = 0$ and Δ remains constant [29,41]. Hence, the dynamics can be fully described within the Hilbert space spanned by the vectors $|\pi_1\rangle = |\uparrow\downarrow\rangle$ and $|\pi_2\rangle = |\downarrow\uparrow\rangle$. It follows that

$$H_{\text{CoM}} = \left[-\frac{\hbar^2}{2M} (\nabla_X^2 + \nabla_Z^2) + \frac{M}{2} (\omega_x^2 X^2 + \omega_z^2 Z^2) - \alpha^2 X^2 \rho_+ + 2u_0 e X \right] \otimes S_0, \quad (\text{A10})$$

$$H_{\text{rel}} = \left[-\frac{\hbar^2}{2\mu} (\nabla_x^2 + \nabla_z^2) + \frac{\mu}{2} (\omega_x^2 x^2 + \omega_z^2 z^2) + \frac{k e^2}{(x^2 + z^2)^{1/2}} - \alpha^2 \rho_+ \frac{x^2}{4} \right] \otimes S_0 + U_{\text{ex}}(x, z) \otimes S_x, \quad (\text{A11})$$

and

$$H_{\text{CoM-rel}} = \alpha^2 \rho_- X x \otimes S_z, \quad (\text{A12})$$

where $\rho_\pm = \rho_\uparrow \pm \rho_\downarrow$ and S_0 , S_x , and S_z are defined in the main text. Thus, the Hamiltonian H_0 of Eq. (A6) can be expressed in the following form:

$$H_0 = \left[-\frac{\hbar^2}{2M} (\nabla_X^2 + \nabla_Z^2) - \frac{\hbar^2}{2\mu} (\nabla_x^2 + \nabla_z^2) \right] \otimes S_0 + H_{\text{spin}}, \quad (\text{A13})$$

where the Hamiltonian H_{spin} is given by

$$H_{\text{spin}} = (V_{\text{CoM}} + V_{\text{rel}}) \otimes S_0 + U_{\text{ex}}(x, z) \otimes S_x + H_{\text{CoM-rel}}, \quad (\text{A14})$$

with

$$V_{\text{CoM}} = \frac{M}{2} (\omega_x^2 X^2 + \omega_z^2 Z^2) - \alpha^2 X^2 \rho_+ + 2u_0 e X, \quad (\text{A15})$$

and

$$V_{\text{rel}} = \frac{\mu}{2} (\omega_x^2 x^2 + \omega_z^2 z^2) + \frac{k e^2}{\sqrt{x^2 + z^2}} - \alpha^2 \rho_+ \frac{x^2}{4}. \quad (\text{A16})$$

The control Hamiltonian becomes

$$H_u(t) = V_u(t) \otimes S_0. \quad (\text{A17})$$

For particular values of the system parameters, the terms $U_{\text{ex}}(x, z) \otimes S_x$, $H_{\text{CoM-rel}}$, and $H_u(t)$ can be treated as small perturbations to $(V_{\text{CoM}} + V_{\text{rel}}) \otimes S_0$ [29]. Hence, the equilibrium positions R_0 and r_0 of the ions can be determined by solving $\frac{\partial V_{\text{CoM}}}{\partial X}|_{X_0, Z_0} = 0$, $\frac{\partial V_{\text{CoM}}}{\partial Z}|_{X_0, Z_0} = 0$, and $\frac{\partial V_{\text{rel}}}{\partial x}|_{x_0, z_0} = 0$, $\frac{\partial V_{\text{rel}}}{\partial z}|_{x_0, z_0} = 0$. As suggested in Ref. [29], we choose $x_0 = 0$ and z_0 can be numerically determined from $\frac{\partial V_{\text{rel}}}{\partial z}|_{x_0, z_0} = 0$. By performing a harmonic approximation of V_{CoM} and V_{rel} around

the corresponding ions' equilibrium positions, we find

$$V_{\text{CoM}} \approx \left[\frac{M}{2} \omega_x^2 - \alpha^2 \rho_+ \right] Q_X^2 + \frac{M}{2} \omega_z^2 Q_Z^2, \quad (\text{A18})$$

and

$$V_{\text{rel}} \approx \left[\frac{\mu}{2} \omega_x^2 - \frac{\alpha^2}{4} \rho_+ - \frac{k e^2}{2|z_0|^3} \right] q_x^2 + \left[\frac{\mu}{2} \omega_z^2 + \frac{k e^2}{|z_0|^3} \right] q_z^2, \quad (\text{A19})$$

where

$$Q = R - R_0 = (X - X_0, Z - Z_0), \\ q = r - r_0 = (x - x_0, z - z_0).$$

Therefore, Eq. (A14) can be written in terms of operators Q and q as

$$H_{\text{spin}} \approx S(Q, q) \otimes S_0 + W(Q, q) \otimes S_x + G(Q, q) \otimes S_z, \quad (\text{A20})$$

where

$$S(Q, q) = \left[\left(\frac{M}{2} \omega_x^2 - \alpha^2 \rho_+ \right) Q_X^2 + \frac{M}{2} \omega_z^2 Q_Z^2 \right. \\ \left. + \left(\frac{\mu}{2} \omega_x^2 - \frac{\alpha^2}{4} \rho_+ - \frac{k e^2}{2|z_0|^3} \right) q_x^2 \right. \\ \left. + \left(\frac{\mu}{2} \omega_z^2 + \frac{k e^2}{|z_0|^3} \right) q_z^2 \right], \quad (\text{A21})$$

$$W(Q, q) = U_{\text{ex}}(r_0) + F_z(r_0) q_z, \quad (\text{A22})$$

$$G(Q, q) = \alpha^2 \rho_- (Q_X + X_0) q_x, \quad (\text{A23})$$

and we expand $U_{\text{ex}}(r)$ around r_0 with

$$F_z(r_0) = \nabla_r U_{\text{ex}}(r)|_{r=r_0}.$$

The PESs refer to the eigenvalues of the electronic Hamiltonian H_{spin} [16,42]. These eigenvalues are defined as

$$E_{\pm} = S(Q, q) \pm \sqrt{G(Q, q)^2 + W(Q, q)^2}. \quad (\text{A24})$$

The corresponding eigenvectors are expressed as

$$|\varphi_+(Q, q)\rangle = \cos[\Lambda(Q, q)]|\pi_1\rangle + \sin[\Lambda(Q, q)]|\pi_2\rangle, \quad (\text{A25})$$

and

$$|\varphi_-(Q, q)\rangle = -\sin[\Lambda(Q, q)]|\pi_1\rangle + \cos[\Lambda(Q, q)]|\pi_2\rangle, \quad (\text{A26})$$

where $\Lambda(Q, q)$ is defined by the relation $\tan[2\Lambda(Q, q)] = W(Q, q)/G(Q, q)$.

The control Hamiltonian provided in Eq. (A17) can be written in terms of Q and q as

$$H_u(t) = e u(t)(Q_X + X_0 - \frac{1}{2}q_x) \otimes S_0. \quad (\text{A27})$$

By using Eq. (A20), the CI is located at $(q_x^*, q_z^*) = [0, -U_{\text{ex}}(r_0)/F_z(r_0)]$. In this configuration, the CI lies entirely in the subspace of the relative nuclear coordinate, and its position is therefore not affected by the center of mass degrees of freedom, as discussed in the Supplemental Material of Ref. [29].

Moreover, by introducing the characteristic oscillation length associated with the center-of-mass motion

$$\ell_Q = \sqrt{\frac{\hbar}{M\bar{\omega}_x}},$$

where $\bar{\omega}_x^2 = \omega_x^2 - \alpha^2 \rho_+/m$, one finds that $\ell_Q < |X_0|$. As a result, the center of mass undergoes limited oscillations around its equilibrium position and does not significantly affect the structure of the potential energy surfaces or the CI-induced dynamics. The dominant nonadiabatic effects are governed by the relative coordinate, which justifies neglecting the center of mass motion and setting $Q = 0$ to a good approximation, yielding Eqs. (4) and (5).

APPENDIX B: MONOTONICALLY CONVERGENT OPTIMIZATION ALGORITHM

To solve the control problem defined by the objective functional in Eq. (11), we begin by choosing an initial electric field $u^0(t)$. The state vector is then propagated forward in time over the interval $[0, t_f]$ using

$$\frac{\partial}{\partial t} |\psi^0(t)\rangle = [A + iNu^0(t)]|\psi^0(t)\rangle, \quad |\psi^0(0)\rangle = |\psi_0\rangle, \quad (\text{B1})$$

where the operators A and N can be determined from Eq. (7), and $|\psi^0(t)\rangle \equiv |\psi^0(q_x, q_z, t)\rangle$. The index 0 indicates the initial iteration [32].

For subsequent iterations $k \geq 1$, the Lagrange multiplier $|\lambda^k(t)\rangle \equiv |\lambda^k(q_x, q_z, t)\rangle$ is propagated backward in time from $t = t_f$ to $t = 0$, starting from the final condition $|\lambda^k(t_f)\rangle = \hat{O}|\psi^{k-1}(t_f)\rangle$ with $|\psi^k(t)\rangle \equiv |\psi^k(q_x, q_z, t)\rangle$. The backward evolution is given by

$$\frac{\partial}{\partial t} |\lambda^k(t)\rangle = [-A^\dagger + iN^\dagger \bar{u}^k(t)]|\lambda^k(t)\rangle, \quad (\text{B2})$$

where

$$\bar{u}^k(t) = (1 - \eta)u^{k-1}(t) - \frac{\eta}{\alpha_0} \text{Im}[\langle \lambda^k(t) | N | \psi^{k-1}(t) \rangle]. \quad (\text{B3})$$

Next, the state vector is propagated forward again via

$$\frac{\partial}{\partial t} |\psi^k(t)\rangle = [A + iNu^k(t)]|\psi^k(t)\rangle, \quad |\psi^k(0)\rangle = |\psi_0\rangle, \quad (\text{B4})$$

where the updated control field is given by

$$u^k(t) = (1 - \zeta)\bar{u}^k(t) - \frac{\zeta}{\alpha_0} \Im[\langle \lambda^k(t) | N | \psi^k(t) \rangle]. \quad (\text{B5})$$

At each iteration k , the states $|\psi^k(t)\rangle$, $|\lambda^k(t)\rangle$, and the control field $u^k(t)$ are used to evaluate the objective functional J . The algorithm continues until convergence is reached.

APPENDIX C: MICROMOTION ESTIMATE

The confinement of an ion in a linear Paul trap is generated by static and rf electric fields. Near the trap center, the electric potential can be given by

$$\Phi(x, y, z, t) = \alpha(x^2 - y^2) \cos(\Omega_{\text{rf}} t) + \beta(2z^2 - x^2 - y^2) + \gamma(x^2 - y^2), \quad (\text{C1})$$

where α denotes the curvature of the rf quadrupole potential, while β and γ describe static confinement and Ω_{rf} is the rf frequency [51].

The motion of an ion along a radial direction in this potential is described by a Mathieu equation [51]. The solution of the Mathieu equation along the x direction can be written as a modulation of the secular motion

$$\hat{x}(t) = \hat{x}_{\text{sec}}(t) \left[1 + \frac{q_x^{(\text{rf})}}{2} \cos(\Omega_{\text{rf}} t) \right], \quad (\text{C2})$$

with the Mathieu parameter

$$q_x^{(\text{rf})} = \frac{4e\alpha}{m\Omega_{\text{rf}}^2}, \quad (\text{C3})$$

where m is the ion mass and e is the elementary charge [51]. Here $\hat{x}(t)$ denotes the position operator of the ion along the x direction in the laboratory frame and $\hat{x}_{\text{sec}}(t)$ denotes the secular component of the ion motion.

The secular trap frequencies [38–40] are given by

$$\omega_x = \frac{2e}{m\Omega_{\text{rf}}} \sqrt{\alpha^2 - \frac{m\Omega_{\text{rf}}^2}{e}(\beta - \gamma)}, \quad (\text{C4})$$

$$\omega_y = \frac{2e}{m\Omega_{\text{rf}}} \sqrt{\alpha^2 - \frac{m\Omega_{\text{rf}}^2}{e}(\beta + \gamma)}, \quad (\text{C5})$$

$$\omega_z = \sqrt{\frac{4e\beta}{m}}. \quad (\text{C6})$$

In this work, we use an ion of mass $m = 1.46 \times 10^{-25}$ kg and trap parameters $\alpha \simeq 8.2 \times 10^8$ V m $^{-2}$, $\beta \simeq 9.0 \times 10^6$ V m $^{-2}$, $\gamma \simeq -1.5 \times 10^6$ V m $^{-2}$, with $\Omega_{\text{rf}} = 2\pi \times 18.12$ MHz. This yields secular frequencies $\omega_x = 2\pi \times 1.60$ MHz, $\omega_y = 2\pi \times 1.65$ MHz, and $\omega_z = 2\pi \times 1.00$ MHz, and a Mathieu parameter $q_x^{(\text{rf})} \simeq 0.277$.

The ground-state wave-packet size is

$$\tilde{x}_0 = \sqrt{\frac{\hbar}{2m\omega_x}} \simeq 6\text{--}7\text{ nm}. \quad (\text{C7})$$

The corresponding rf micromotion amplitude is therefore

$$\delta x_{\text{mm}} = \frac{q_x^{(\text{rf})}}{2} \tilde{x}_0 \approx 0.80\text{ nm}. \quad (\text{C8})$$

Even for secular excursions (or quantum wave-packet extents) of order 10 nm, micromotion remains at the ~ 1 nm level [29]. Micromotion therefore constitutes only a small, fast oscillatory modulation of the ion position and is neglected in the effective Hamiltonian used in the main text. The ion motion remains confined to a region much smaller than the characteristic trap length scales. Since the micromotion amplitude is at least an order of magnitude smaller than the secular displacement and oscillates at the rf frequency, it averages out on the microsecond timescales relevant to the control dynamics.

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