

Expanding the Neutral Atom Gate Set: Native iSWAP and Exchange Gates from Dipolar Rydberg Interactions

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We present a native realization of iSWAP and parameterized *exchange* gates for neutral atom quantum processing units. Our approach leverages strong dipole-dipole interactions between two dipole-coupled Rydberg states, and employs optimal control techniques to design time-efficient, high-fidelity gate protocols. To minimize experimental complexity, we utilize global driving terms acting identically on all atoms. We implement a noise-aware pulse selection strategy to identify candidate protocols with reduced susceptibility to certain noise sources, then analyze their performance under realistic noise sources – including atomic motion, Rydberg decay, and experimentally motivated laser phase and intensity noise. For a ⁸⁸Sr-based architecture, we demonstrate fast iSWAP gate protocols which exceed fidelities of 99.9% under realistic experimental conditions. These results pave the way for expanding the neutral atom gate set beyond typical Rydberg blockade-based entangling gates.

I. INTRODUCTION

Neutral atom quantum processing units (QPUs) have become a leading platform for quantum computing due to their unique capabilities, including high qubit numbers, flexible connectivity, and long coherence times. Their scalability has been demonstrated by capturing and coherent manipulation of up to thousands of individual atoms [1–4]. High-fidelity quantum gates have been demonstrated for several atomic species and qubit encodings [5–9], utilizing the Rydberg blockade effect for entangling two-, and even multi-body interactions [10–15]. Furthermore, the versatility to create arbitrary qubit arrangements [16–18] and to coherently shuttle atoms during experiments [5, 19] allows for an efficient implementation of long-range qubit interactions. These features have positioned neutral atom QPUs as a prime platform for quantum error correction (QEC) experiments, with demonstrations of planar and non-planar QEC codes [19–21], transversal logical gates [22], and non-Clifford logical gates through teleportation of magic resource states [21, 23].

In neutral atom QPUs, single atoms are trapped in a flexible arrangement of optical tweezers or, alternatively, in an optical lattice. Qubit states are encoded in two atomic low-energy levels, and laser light is used to coherently manipulate and read out the qubits [18, 24]. Entanglement between two or multiple atoms is usually generated through the Rydberg blockade effect, which relies on the strong van-der-Waals (vdW) interaction between two atoms when they are simultaneously excited to high-energy Rydberg levels [18, 24]. This interaction mechanism can natively realize CZ gates [5, 7–9, 13, 14], multi-control C^kZ gates [12, 25], and other diagonal multi-qubit gates [15, 26].

However, the vdW interaction is not the only possible interaction between Rydberg states, and not even

the most fundamental one. The large orbital size of electrons in Rydberg states leads to substantial atomic dipole moments and, consequently, strong dipole-dipole interactions (DDI) between atoms in Rydberg states [24]. This interaction has been utilized in quantum simulation experiments to explore, for example, coherent spin exchange [27], continuous symmetry breaking [28, 29], and symmetry-protected topological states [30, 31]. Also, ultrafast quantum operations [32] and fast two-qubit CZ gates [33] have been proposed using the exchange interaction.

In this paper, we utilize the dipole-dipole exchange interaction to realize a native iSWAP gate (and more generally parameterized exchange gates) between two qubits encoded in low-energy states of neutral atoms. The basic idea is to coherently map populations from the qubit manifold to dipole-dipole interacting Rydberg states during which the required interaction time is cumulated, using a single, optimally controlled pulse protocol.

Implementing native iSWAP gates (or arbitrary-angle exchange gates) on neutral atom QPUs promises significant advantages. In particular, the slower decay of the relevant exchange interaction with atomic distance, compared to the vdW interaction, offers the potential for faster operation speeds for atoms at larger distances and increased qubit connectivity. The combination of non-diagonal iSWAP and exchange gates together with the diagonal CZ gate in a single platform can speed-up algorithms and reduce gate count and depth [34–36]. In quantum optimization, arbitrary-angle exchange gates allow for particle-number conserving driver terms in VQA circuits [37], and to directly encode optimization sum-constraints within the Parity architecture for quantum optimization, leading to performance benefits [38]. The recently introduced Parity Twine method [39, 40] – providing, for example, the currently most efficient implementation of the quantum Fourier transformation – also benefits from iSWAP gates with further reduced

gate count and circuit depths. Beyond these, iSWAP gates are imperative for implementing promising novel quantum error correction ideas, for example the recently proposed dynamical surface codes [41] and directional qLDPC codes [42].

This paper is organized as follows: Section II details the considered neutral atom QPU setup and introduces the optimal control framework; Section III presents our optimal control results for the iSWAP gate for different driving schemes; Section IV is devoted to a careful analysis of the noise budget for the obtained iSWAP optimal control protocols for state-of-the-art hardware parameters of a ^{88}Sr QPU, considering atomic noise from atom position fluctuations and Rydberg decay, and laser noise modelled with power spectral densities (PSDs) for intensity and phase fluctuations. In Sec. V we present the sensitivity of gate fidelities for varying hardware noise, find optimal hardware parameters to push gate fidelities beyond 0.999, and showcase how pulses can be selected to minimize laser noise based on fidelity response theory [43]. Finally, we give our conclusions and outlook in Sec. VI. In the appendix, we provide supplemental information about optimal control results for the parameterized exchange gate, details about our noise modelling, and the calculation of Rydberg decay rates for ^{88}Sr .

II. SETUP AND OPTIMAL CONTROL ANSATZ

In this paper, we consider a neutral-atom quantum computing architecture where individual Rydberg atoms are trapped in optical tweezers, or in an optical lattice, each encoding a single qubit in two long-lived low-energy states $|0\rangle, |1\rangle$. Additionally, on each atom we consider two distinct, highly-excited, and strongly interacting Rydberg states $|r\rangle, |r'\rangle$, see Fig. 1(a).

Using two Rydberg states instead of one enables access to interactions beyond the usual vdW regime, in particular allowing the realization of a dipolar exchange interaction [18, 24, 27]. To illustrate this mechanism consider, as a toy model, two atoms in Rydberg states $|r_1\rangle$ and $|r_2\rangle$, denoted as “pair”-state $|r_1 r_2\rangle$, and a second pair-state $|r'_1 r'_2\rangle$. If these pair-states are dipole-dipole coupled the interaction takes the form

$$\hat{H}_{\text{Ryd}} = \Delta_F |r'_1 r'_2\rangle \langle r'_1 r'_2| + \frac{C_3}{R^3} (|r_1 r_2\rangle \langle r'_1 r'_2| + \text{h.c.}),$$

where $\Delta_F = E_{r'_1} + E_{r'_2} - E_{r_1} - E_{r_2}$ is the Förster defect (the difference of atomic energies), C_3 is the coupling coefficient and R is the distance between the atoms. Diagonalizing $\hat{H}_{\text{Ryd}}$ reveals two distinct interaction regimes. For $\Delta_F \gg C_3/R^3$ the interaction becomes diagonal, approximated by $\hat{H}_{\text{Ryd}} \rightarrow C_6/R^6 |r_1 r_2\rangle \langle r_1 r_2|$, with the vdW coefficient $C_6 \approx C_3^2/\Delta_F$. This is the typical regime for which current QPU setups implement CZ gates where just a single Rydberg state is used. In contrast, for $\Delta_F \ll C_3/R^3$, the interaction becomes off-diagonal and exchanges the two pair-states coherently,

$\hat{H}_{\text{Ryd}} \rightarrow C_3/R^3 (|r_1 r_2\rangle \langle r'_1 r'_2| + \text{h.c.})$. This regime can be reached with very small atomic distances, or by tuning the system to a Förster resonance with $\Delta_F \approx 0$, for example using precise electric fields [44, 45].

Yet another way to enter the dipolar exchange regime, without fine-tuning fields and independent of the lattice distance, is to make use of two, directly dipole coupled, Rydberg states $|r\rangle$ and $|r'\rangle$, as we do in this paper. Then the most resonant transition channel is $|rr'\rangle \leftrightarrow |r'r\rangle$, with $\Delta_F = 0$ by construction, leading to the exchange interaction with Hamiltonian [27]

$$\hat{H}_{\text{Ryd}} \rightarrow \hat{H}_{\text{exchange}} = \frac{C_3}{R^3} (|rr'\rangle \langle r'r| + \text{h.c.}). \quad (1)$$

exchanging coherently the two Rydberg states $|r\rangle$ and $|r'\rangle$ between two atoms, as illustrated in Fig. 1(a). Note that the Rydberg interaction coefficient C_3 depends on the chosen Rydberg states $|r\rangle$ and $|r'\rangle$ and increases strongly with their principal quantum number as $C_3 \propto n^4$.

To drive transitions between atomic states, we consider a set of distinct lasers and microwaves that globally illuminate the atoms to reduce experimental requirements. In particular, we examine the two distinct coupling schemes shown in Fig. 1(a) that, by necessity, allow to transfer the population from the qubit subspace to the two distinct Rydberg states:

- *Scheme A*: directly couples both qubit states to the Rydberg states: $|0\rangle$ with $|r'\rangle$, and $|1\rangle$ with $|r\rangle$

$$\frac{H_{\text{drive}}(t)}{\hbar} = \sum_i \frac{1}{2} \left(\Omega^{1r}(t) e^{i\phi^{1r}(t)} |r\rangle_i \langle 1| + \Omega^{0r'}(t) e^{i\phi^{0r'}(t)} |r'\rangle_i \langle 0| + \text{h.c.} \right). \quad (2a)$$

- *Scheme B*: couples only one qubit state to a Rydberg state, $|1\rangle$ with $|r\rangle$, and additionally the qubit states with each other, and the Rydberg states with each other

$$\frac{H_{\text{drive}}(t)}{\hbar} = \sum_i \frac{1}{2} \left(\Omega^{01}(t) e^{i\phi^{01}(t)} |1\rangle_i \langle 0| + \Omega^{1r}(t) e^{i\phi^{1r}(t)} |r\rangle_i \langle 1| + \Omega^{rr'}(t) e^{i\phi^{rr'}(t)} |r'\rangle_i \langle r| + \text{h.c.} \right). \quad (2b)$$

The driving Hamiltonians, Eq. (2a) and Eq. (2b), are written in the corresponding rotating frames. $\Omega^{ab}(t)$ denotes the time-dependent Rabi frequency of a laser/microwave that couples the atomic states $|a\rangle$ and $|b\rangle$, and $\phi^{ab}(t)$ denotes its time dependent phase, and we only consider resonant driving (i.e. zero detuning). The full system Hamiltonian is then the combination of H_{drive} (for the chosen scheme) and the exchange interaction H_{exchange} :

$$H(t) = H_{\text{exchange}} + H_{\text{drive}}(t). \quad (3)$$

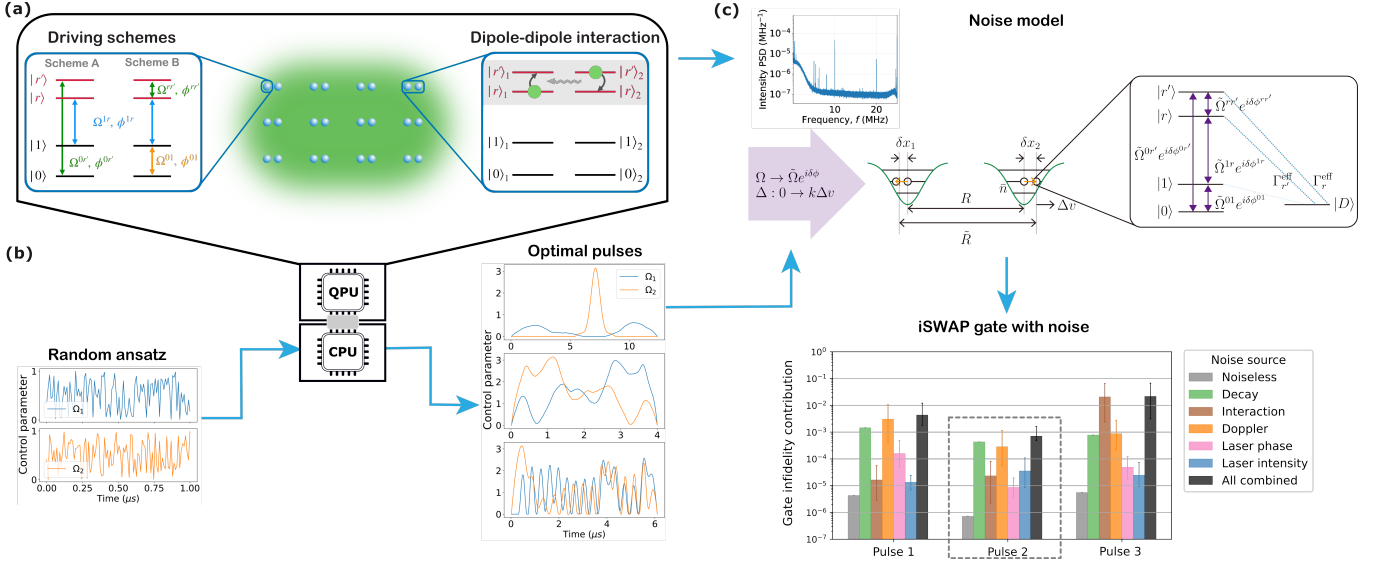


FIG. 1. Optimal control framework for iSWAP gates with Rydberg Atoms. (a) We consider a pair of neutral atoms with two low-energy (meta-)stable qubit states $|0\rangle, |1\rangle$ and two high-energy Rydberg states $|r\rangle, |r'\rangle$, which are dipole coupled and undergo the exchange interaction, Eq. 1. We consider global laser / microwave drives between qubit and Rydberg states using two different schemes A/B. (b) We use optimal control techniques to obtain high-fidelity pulse protocols for the iSWAP gate, starting from random ansatz pulse profiles. We use a regularization term in the cost function to obtain smooth pulses, which are easier to implement in an experiment. (c) A set of high-fidelity pulse candidates is then evaluated against a neutral-atom specific noise model to find the best performing pulse under experimentally realistic conditions. Our noise model contains noise from atomic motion in the traps, Rydberg decay, and laser phase and intensity noise modelled from PSDs.

Moreover, we define two types of pulses: Rabi modulated pulses, where only the Rabi frequencies $\Omega^{ab}(t)$ vary in time, and $\phi^{ab}(t) = 0$; and phase modulated pulses, where only the phases $\phi^{ab}(t)$ vary in time and the Rabi frequencies are set to one constant value $\Omega^{ab}(t) = \Omega_0$.

Our goal is to find optimal pulses that realize an exchange gate of angle θ between two qubits, given by the unitary (in the qubit subspace) [34]

$$U_{XY}(\theta) = e^{i\frac{\theta}{2}(X_1 X_2 + Y_1 Y_2)/2} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\frac{\theta}{2}) & i\sin(\frac{\theta}{2}) & 0 \\ 0 & i\sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (4)$$

where X_i, Y_i denote the Pauli-X, Pauli-Y matrix on qubit $i = 1, 2$. Importantly, the family of gates $U_{XY}(\theta)$ contains the iSWAP gate for $\theta = \pi$, which we will focus on in the remainder of the main text. Results for other target angles $\theta \neq \pi$ are shown in Appendix A.

Our approach goes beyond currently typical neutral atoms setups, where just a single Rydberg state $|r\rangle$ is used and the vdW interaction is utilized to create diagonal gates, such as CZ. With the setup considered here, the two atoms naturally perform an exchange interaction in the Rydberg states manifold $|r\rangle, |r'\rangle$, via Eq. (1). The main remaining challenge to implement an exchange gate $U_{XY}(\theta)$ is then to develop laser/microwave driving schemes that allow to “transfer” this interaction into the qubit subspace of the atoms. A simple, intuitive concept to realize $U_{XY}(\theta)$ would be a Ramsey-like pulse proto-

col with three steps: First, the atomic populations in the qubit manifold $\{|0\rangle, |1\rangle\}$ are transferred coherently to the Rydberg manifold $\{|r\rangle, |r'\rangle\}$, simultaneously for both atoms. Second, all driving lasers are switched off for a given duration (proportional to θ) during which the native DDI between the qubits, Eq. (1), generates the target exchange dynamics between the two atoms in the Rydberg manifold. Finally, the first step is inverted to coherently transfer the population back from the Rydberg manifolds to the qubit manifolds on both atoms. However, this simple protocol only works under the assumption that no DDI takes place during the two state transfer steps, which is difficult to realize in practice. It would either require infinitely fast state transfer (implying $\Omega \gg V_{\text{dipole}}$), or the ability to turn off the DDI during the state transfer steps. The latter could be in principle achieved using moving atoms [5, 19–21, 46] by performing the state transfer at large distance between the atoms and bringing them closer during the interaction step. This is, however, experimentally very demanding, as both qubit and Rydberg states must be simultaneously trapped in movable tweezers, the spatial requirements are substantial, and the required motion can lead to slow protocol durations.

In this paper, we therefore attempt to implement the state transfer and interaction steps concurrently within a single time-dependent control pulse and apply *quantum optimal control* methods [13, 14, 47] to find high-fidelity protocols for the target gate $U_{XY}(\theta)$, where the time evolution is governed by the Hamiltonian $H(t)$, Eq. (3) [see

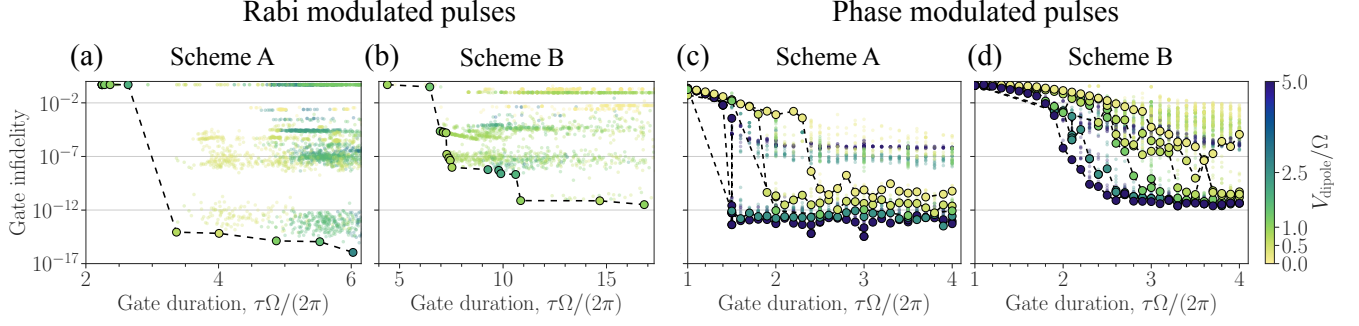


FIG. 2. Optimal control results for iSWAP gate. (a-b) Gate infidelity of different optimal control runs versus unitless gate duration $\tau\Omega$ for Rabi modulated pulse for (a) driving scheme A, (b) driving scheme B [c.f. Fig. 1]. (c-d) Same plots for phase modulated pulses for (c) driving scheme A, (d) driving scheme B. In all plots, each point corresponds to a single optimal control run with random initialization for a fixed gate duration τ . Highlighted points and dashed lines are visual guides to the eye tracking the lowest infidelity pulses vs duration. Different colors indicate different interaction strengths V_{dipole}/Ω . For each scheme and modulation type we can clearly identify a strong drop of infidelity at a certain duration τ^* , which indicates the corresponding iSWAP quantum speed limit for the given setting. For durations $\tau > \tau^*$ we obtain high-fidelity results with $1 - \mathcal{F} < 10^{-10}$.

Fig. 1(b) for an illustration]. In particular, we focus on global controls and smooth pulse shapes to lower required experimental capabilities. In more detail, for a given duration τ we try to find time dependent driving functions $\Omega^{ab}(t)$, $\phi^{ab}(t)$ (for the driving schemes A/B, and either Rabi modulated or phase modulated pulse ansätze) such that the Hamiltonian evolution at time $t = \tau$ generates the target unitary $U_{XY}(\theta)$. Specifically, we request that

$$U(\tau) = P\tilde{U}(\tau)P = P\mathcal{T}\exp\left(-i\int_0^\tau H(t')dt'\right)P, \quad (5)$$

where $\tilde{U}(t)$ denotes the Hamiltonian time evolution operator, and P the projector into the qubit subspace $\{|0\rangle, |1\rangle\}^{\otimes 2}$ is as close as possible to $U_{XY}(\theta)$. This closeness is quantified by a suitable figure of merit, for which we use the gate fidelity

$$\mathcal{F} = \frac{1}{d} |\text{tr}(U_{XY}(\theta)^\dagger U(\tau))|, \quad (6)$$

between $U(\tau)$ and the target unitary $U_{XY}(\theta)$, with $d = 2^2$ the dimension of the unitaries, and $0 \leq \mathcal{F} \leq 1$. Optimal pulse protocols maximize $\mathcal{F}$, and $\mathcal{F} = 1$ corresponds to a perfect implementation of the target unitary.

To find optimal pulses, we consider piecewise constant ansatz functions for the driving terms, similar to the GRAPE optimal control method [47]. In detail, a function $f(t)$, $0 \leq t \leq \tau$ is divided into N pieces f_i , such that $f(t) = f_i$, if $t \in [i\Delta t, (i+1)\Delta t]$ with $\Delta t = \tau/N$. The values f_i are the optimization parameters, and typically a large number of pieces N is used to receive a good approximation to a smooth function $f(t)$. We use gradient-based optimization algorithms (BFGS, L-BFGS-B) based on an automatic differentiation (AD) implementation using the software package JAX [48] to minimize the gate infidelity $1 - \mathcal{F}$. The advantage of AD is that gradients can be computed automatically even for complicated cost

functions and ansätze, which allows to use highly efficient gradient-based optimization algorithms also for problems where gradients are not known analytically. We leverage this potential to smooth the pulse wave functions by adding a regularization term to the cost function that penalizes large gradients in the control pulses [49]. In particular, for each control pulse $f(t)$ given as a piecewise function with N pieces f_i we compute its “smoothness” cost

$$C_{\text{smooth}}[f] = \sum_{i=0}^{N-1} \left(\frac{f_{i+1} - f_i}{2} \right)^2, \quad (7)$$

and the total cost function becomes

$$C_\lambda = (1 - \mathcal{F}) + \lambda \sum_{f \in \text{controls}} C_{\text{smooth}}[f]. \quad (8)$$

Here, f runs over all controls, $\Omega^{ab}(t)$ or $\phi^{ab}(t)$, and λ regulates how strongly the control pulses are smoothened. With this approach, we can find high-fidelity gates with smooth control profiles [15, 49], which is highly relevant for experimental implementations of the gates. Furthermore, the parameter λ balances smoothness and fidelity to produce optimal pulses compatible with limited control bandwidth, a necessary requirement for experimental implementation. In contrast to feeding already smooth ansatz pulses into the optimizer to achieve smooth high-fidelity gates, the method used here allows for initializing random pulses to avoid getting stuck in low-fidelity local minima. An illustration of our optimal control approach is shown in Fig. 1(b).

III. iSWAP GATE RESULTS

We run multiple optimal control optimisations, using random initial control pulses, for both driving schemes A

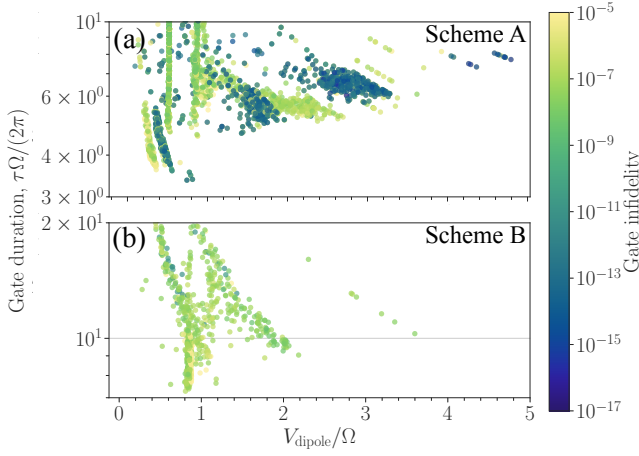


FIG. 3. Optimal control results for Rabi modulated drives for (a) Scheme A, (b) Scheme B with infidelity $1 - \mathcal{F} < 10^{-5}$. We plot the unitless gate duration τ/Ω as a function of the interaction strength V_{dipole}/Ω . High-fidelity, time optimal pulses are obtained for finite interaction strength $V_{\text{dipole}} \sim \Omega$. For $V_{\text{dipole}} \lesssim \Omega$ the gate duration is limited by finite interaction strength, for $V_{\text{dipole}} \gtrsim \Omega$ it is limited by finite Rabi frequency.

and B, and both modulation methods, Rabi and phase modulation, for different gate durations τ and interaction strengths $V_{\text{dipole}} = C_3/R^3$. For phase modulated pulse protocols we consider fixed, identical and constant Rabi frequencies $\Omega^{ab}(t) \equiv \Omega = 1$. For Rabi modulation we enforce a lower limit $\Omega^{ab}(t) \geq 0$ in the optimizer but don't constrain the upper limit, and define Ω as the maximal Rabi frequency among any of the drives throughout the entire pulse; for example for a scheme A $\Omega = \max \left\{ \max_{t \in [0, \tau]} \Omega^{1r}(t), \max_{t \in [0, \tau]} \Omega^{0r'}(t) \right\}$.

Our results are presented in Fig. 2. We find high-fidelity pulses with infidelities $1 - \mathcal{F} < 10^{-10}$ for all combinations of driving schemes and modulation methods with the best achieving infidelities approaching the limit of double-precision accuracy. This demonstrates the potential to realize high-fidelity iSWAP gates in diverse neutral-atom QPU setups with different experimental constraints. Furthermore, we can clearly identify a strong drop in infidelities after specific pulse durations τ^* , which indicate the quantum speed limit to realize an iSWAP gate for the given setup. In particular only for durations $\tau \geq \tau^*$ it is possible to realize an iSWAP gate. The value of τ^* varies between the driving schemes and modulation types, ranging from $\tau^*\Omega \sim 2\pi \times 1.5$ for “Scheme A” with phase modulated pulses to $\tau^*\Omega \sim 2\pi \times 7$ for “Scheme B” with Rabi modulated pulses. In general, we observe larger speed limits for “Scheme B” due to the fact that the state $|r\rangle$ cannot be populated directly from the qubit subspace, but only via the other Rydberg state $|r\rangle$, unlike in “Scheme A”.

The existence of this speed limit arises directly from the basic nature of our protocol which requires a finite amount of accumulated exchange interaction. Since the

interaction strength V_{dipole} is finite this yields a lower bound on the minimal pulse duration. Also finite Rabi frequencies restrict the rate of required transfer of populations from non-interacting qubit states to interacting Rydberg states, and back. However, since our protocols simultaneously perform the required amount of state transfer and interaction accumulation, the observed speed limit τ^* cannot be simply computed from the interaction strength and used Rabi frequencies.

This interplay between interaction and Rabi frequency strengths is prominently visible in the results for phase modulated pulses in Figs. 2(c, d). One can directly observe that increasing V_{dipole}/Ω lowers the gate speed limit due to the increased interaction accumulation for larger V_{dipole} . However, there is an upper limit for V_{dipole}/Ω beyond which no further reduction of the speed limit can be observed anymore and the system is limited by the finite Rabi frequencies, but not the interaction strength.

For the Rabi modulated pulses in Figs. 2(a, b) this effect is not so clearly visible. The reason is that the maximal Rabi frequency Ω is automatically optimized for the given interaction strength V_{dipole} during the optimization procedure. To gain more insight, we plot the optimal control results for the Rabi modulated pulses in Fig. 3 where we show the unitless pulse gate durations $\tau\Omega$ as a function of the relative interaction strength V_{dipole}/Ω for pulses with $1 - \mathcal{F} < 10^{-5}$. In particular, we find that the optimizer only finds results with $V_{\text{dipole}}/\Omega \lesssim 5$ throughout both schemes. Even more, high-fidelity, short duration pulses typically obey $V_{\text{dipole}} \sim \Omega$. For $V_{\text{dipole}} \lesssim \Omega$ the gate speed is limited by the strength of V_{dipole} which is necessary to generate the required exchange between the Rydberg states. On the other side, for $V_{\text{dipole}} \gtrsim \Omega$ the gate speed is limited by the Rabi frequency Ω which limits the speed of population transfer between non-interacting qubit states and interacting Rydberg states.

IV. iSWAP NOISE BUDGET

In the previous section, we optimized iSWAP pulses under the no-noise assumption. However, in real hardware, there are dynamics-deteriorating noise processes [50] that will reduce gate fidelities. We consider three kinds: noise induced by atomic motion caused by finite trapping temperatures of the atoms, noise from atomic decay, and noise induced from the driving lasers.

We model the noise induced by atomic motion with the semi-classical “frozen gas” approximation, assuming that the atomic motion is frozen during the gate operation, and its effect can be sampled on a shot-to-shot basis. Then atomic motion has two effects. First, it changes the position of both atoms and therefore their distance by a small amount ΔR , which directly affects the DDI strength $V_{\text{dipole}} \rightarrow \tilde{V}_{\text{dipole}} = C_3/(R + \Delta R)^3$. Second, atoms obtain finite velocities, in contrast to the noise-free case, which induce unwanted Doppler shifts of the lasers. We model this effect with additional detuning

terms

$$\frac{\tilde{H}_{\text{Doppler}}}{\hbar} = - \sum_i \left(\Delta^1 |1\rangle_i \langle 1|_i + \Delta^r |r\rangle_i \langle r|_i + \Delta^{r'} |r'\rangle_i \langle r'|_i \right), \quad (9)$$

in the Hamiltonian, where Δ^a denotes the Doppler induced detuning for atomic state $|a\rangle$.

The finite lifetimes of the Rydberg states $|r\rangle$ and $|r'\rangle$ are implemented with a non-hermitian Hamiltonian [51],

$$\frac{\tilde{H}_{\text{decay}}}{\hbar} = -\frac{i}{2} \sum_i \left(\Gamma_r^{\text{eff}} |r\rangle_i \langle r|_i + \Gamma_{r'}^{\text{eff}} |r'\rangle_i \langle r'|_i \right), \quad (10)$$

where $\Gamma_{r,r'}^{\text{eff}}$ represent the effective decay rates of the Rydberg states [see Appendix C].

For laser driving noise we consider both phase and intensity modulations described by power spectral densities (PSDs). Laser intensity phase noise alters the Rabi frequencies $\Omega^{ab}(t) \rightarrow \tilde{\Omega}^{ab}(t)$ and we consider the same intensity PSD for all Rabi drives. Similarly, laser phase noise changes $\phi^{ab}(t) \rightarrow \tilde{\phi}^{ab}(t)$ and again we assume an identical phase PSD for all phase drives. The modified $\tilde{\Omega}^{ab}(t)$ and $\tilde{\phi}^{ab}(t)$ can be obtained from the corresponding PSD in a Monte-Carlo sampling approach [see Appendix B 4 for details].

Combining all these terms, the full noisy Hamiltonian becomes

$$H_{\text{noisy}}(t) = \tilde{H}(t) + \tilde{H}_{\text{Doppler}} + \tilde{H}_{\text{decay}}, \quad (11)$$

where $\tilde{H}(t)$ corresponds to the noise-free Hamiltonian, Eq. (3), with the replacements $V \rightarrow \tilde{V}$, $\Omega^{ab}(t) \rightarrow \tilde{\Omega}^{ab}(t)$, $\phi^{ab}(t) \rightarrow \tilde{\phi}^{ab}(t)$.

Further details about the noise modelling are provided in Appendix B.

As a specific example, for the remainder of this paper we consider neutral atom QPUs based on ^{88}Sr atoms [9, 43, 52] to estimate interaction and noise model parameters, and to illustrate possible implementations of the proposed driving schemes. ^{88}Sr , as one of the alkaline-earth-like atoms, obeys a particularly promising atomic level scheme for quantum computing, and two different qubit encodings are commonly employed [see Fig. 4]: clock qubit scheme, where the qubit manifold $\{|0\rangle, |1\rangle\}$ is encoded in the levels $^1\text{S}_0, ^3\text{P}_0$, coupled by an ultranarrow optical clock transition [53–59]; fine-structure qubits, where the qubit manifold is encoded in the meta-stable fine-structure states $^3\text{P}_0$ and $^3\text{P}_2$ [60–62].

To match these qubit encodings with our driving schemes we propose the following:

- Scheme A, requiring a coupling between $|0\rangle$ and $|r'\rangle$, can be implemented in the fine-structure qubit, with an additional two-photon transition $^3\text{P}_0 \leftrightarrow n^3\text{P}_0$ compared to already available setups [see Fig 4(a)].

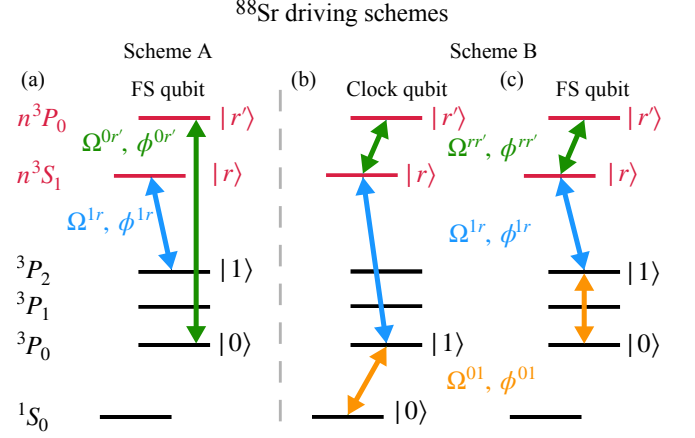


FIG. 4. Possible atomic driving scheme proposals for typical ^{88}Sr setups. (a) Driving scheme A, requiring a drive between $|0\rangle$ and $|r'\rangle$ can be implemented in the fine-structure qubit encoding with a two-photon drive between levels $^3\text{P}_0$ and $n^3\text{P}_0$. (b-c) Driving scheme B can be implemented with a MW drive between the Rydberg states $n^3\text{S}_1$ and $n^3\text{P}_0$, here shown for (b) the clock qubit encoding, and (c) the fine-structure qubit.

- Scheme B can be implemented straightforwardly for both encodings, only requiring an additional MW drive between the two Rydberg states $n^3\text{S}_1 \leftrightarrow n^3\text{P}_0$ compared to typical setups [see Figs. 4(b, c)].

Here, we want to mention that, depending on the available control drives, further combinations of the driving schemes proposed in this paper, and qubit encodings are possible.

In more detail, in this section we will focus on driving scheme A with Rabi modulation in the fine-structure qubit encoding. We consider an experimentally realistic maximal Rabi frequency, among all drives, of $\Omega = 2\pi \times 10$ MHz. We use Rydberg levels with principal quantum number $n = 61$, in particular $|r\rangle \equiv |5s61s^3\text{S}_1\rangle$ and $|r'\rangle \equiv |5s61p^3\text{P}_0\rangle$. Furthermore, we assume that the atoms are trapped by individual tweezers with trap frequencies $\omega_{xy} = 2\pi \times 100$ kHz and $\omega_z = 2\pi \times 20$ kHz, and assume a temperature of $T = 1$ μK for the atoms in the traps. To compute the Doppler induced detunings Δ^a , we consider the same effective wave vectors $k_{\text{eff}}^x = 3 \times 10^6 \text{ m}^{-1}$, $k_{\text{eff}}^y = k_{\text{eff}}^z = 0$ for all laser drives. A summary of the parameters is given in Tab. I, further details and derived effective noise parameters are given in App. B.

In the following we will analyze the effect of the individual noise sources on the optimal pulse protocols obtained in the noise-free setting [see Sec. III]. We divide the analysis into two categories of noise: First, we discuss atomic noise, arising from atomic motion and the finite lifetime of the Rydberg states. Second, we consider laser noise, caused by temporal fluctuations in both intensity and phase of the driving fields, which are modelled by PSDs.

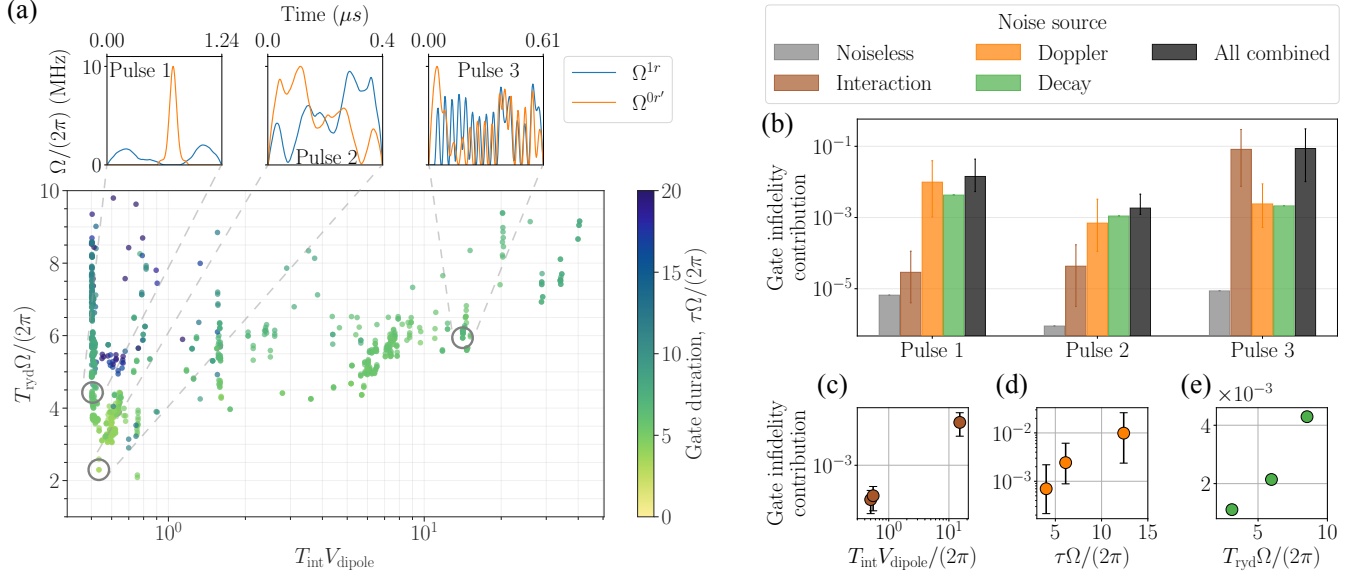


FIG. 5. Noise-aware pulse selection. (a) Pulse landscape for pulses with infidelities below 10^{-5} , where the time spent in Rydberg manifold, T_{ryd} is plotted against the cumulative interaction $T_{\text{int}} V_{\text{dipole}}$, and the gate duration τ is color coded. We select three different pulse protocols with different properties. Their pulse profiles are shown as insets on top of the main figure. (b) Gate infidelity contributions of the atomic noise sources for the selected pulses. “Pulse 2” shows the overall lowest gate infidelity (black bars). (c-f) Dependency of the infidelity contributions as a function of the relevant duration parameter; (c) Interaction noise, (d) Doppler noise, (e) Decay noise.

A. Atomic noise

As described above, we consider three distinct effects of atomic noise: interaction strength fluctuations due to atomic motion (interaction noise), Doppler effect induced fluctuations of the laser detunings (Doppler noise), and decoherence induced by the finite lifetime of the Rydberg states (decay noise).

Interaction noise is only influencing the atoms dynamics when the atoms are in the interacting Rydberg states, and its effect is expected to grow with the interaction strength V_{dipole} . Therefore, we expect that gate fidelity reductions induced by the interaction noise to depend on $T_{\text{int}} V_{\text{dipole}}$, where the interaction time T_{int} is defined as

$$T_{\text{int}} = \int_0^\tau dt [P_{|rr'\rangle}(t) + P_{|r'r\rangle}(t)], \quad (12)$$

where $P_{|ab\rangle}(t)$ denotes the population of pair state $|ab\rangle$ during the time evolution. Note, that we only include the pair states $|rr'\rangle$ and $|r'r\rangle$ in the definition of T_{int} , because these are the only interacting pair states under the exchange Hamiltonian H_{exchange} . With this definition, the accumulated exchange phase through the direct dipole-dipole interaction can be defined as $\theta_{\text{dipole}} \equiv T_{\text{int}} V_{\text{dipole}}$.

Decay noise from the Rydberg states fundamentally limits the achievable gate fidelities for neutral atom entangling gates [63]. It has been previously shown that it reduces the gate fidelity linearly with the time spent in Rydberg states, T_{ryd} , during the pulse [15, 51, 63]. For

our setup with two different Rydberg states, we define

$$T_{\text{ryd}} = \int_0^\tau dt \sum_{i=1,2} [P_{|r\rangle_i}(t) + P_{|r'\rangle_i}(t)], \quad (13)$$

where $P_{|r\rangle_i}$ and $P_{|r'\rangle_i}$ denote the populations in the states $|r\rangle_i$ and $|r'\rangle_i$ of atom i , respectively. We should emphasize that, for this definition, we expect deviations from the previously reported linear scaling when the decay rates for states $|r\rangle$ and $|r'\rangle$ are different. Nevertheless, T_{ryd} remains a good quantity to estimate the effect of decay noise in our setup. For the Doppler noise we find empirically, that it correlates with the gate duration τ [see below].

Therefore, to minimize the effects of atomic noise on the iSWAP gate fidelity we should try to select pulse protocols that minimize not only the noise-free gate infidelity $1 - \mathcal{F}$ but also the durations τ , T_{ryd} , and $T_{\text{int}} \cdot V_{\text{dipole}}$. This can be achieved either in noise-aware optimal control approaches where these additional quantities are added to the cost function [15], or by appropriately selecting from noise-free optimized pulse protocols. Given the vast amount of qualitatively different pulse protocols that we have already obtained from noise-free optimization, we here consider the second strategy. Figure 5(a), shows a subset of the pulse landscape with infidelities below 10^{-5} , where the unitless $T_{\text{ryd}} \cdot \Omega$ is plotted against $T_{\text{int}} \cdot V_{\text{dipole}}$, and the unitless total gate duration τ is color coded. This helps us to pick pulses which minimize the effect of the different atomic noise sources. However, the individual effects of the different noise sources can usually not all

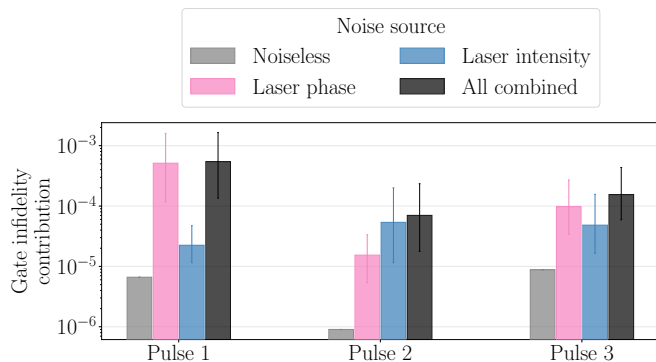


FIG. 6. Laser noise induced gate infidelities for the three pulses selected above [c.f. Fig. 5(a)]. Grey bars show the pulse infidelity without noise, magenta (blue) bars depict the infidelity contribution from laser phase (intensity) noise, black bars show their combined contribution.

be minimized simultaneously and their strength strongly depends on the given noise parameters. Therefore, one needs to find good trade-off between the noise-free gate infidelity and the individual noise contributions.

To illustrate this, we pick three different pulses spread across this landscape, along its lower boundary: “Pulse 1”, minimizing $T_{\text{int}} \cdot V_{\text{dipole}}$; “Pulse 2” with the lowest value of T_{ryd} and τ ; and “Pulse 3” with the highest $T_{\text{int}} \cdot V_{\text{dipole}}$. For the selected pulses we compute the individual contributions of the different atomic noise sources to the gate infidelity in the noisy setting. The results are shown in Fig. 5(b). We indeed observe that interaction noise contribution to the gate infidelity is several orders of magnitude smaller for “Pulse 1” and “Pulse 2” compared to “Pulse 3” which has a much larger $T_{\text{int}} V_{\text{dipole}}$ [see also Fig. 5(c)]. Doppler noise appears as the dominant noise source for “Pulse 1” with the longest gate duration τ . Reducing τ can strongly reduce the corresponding infidelity contribution, for the chosen pulses by almost one order of magnitude [see Fig. 5(d)]. Finally, the infidelity contribution from decay noise is on the order of 10^{-3} for all selected pulses, but shows the expected scaling with T_{ryd} [see Fig. 5(e)].

Overall, “Pulse 2” performs best when combining all considered atomic noise sources, reaching an overall infidelity of $\sim 10^{-3}$, dominated by the effects of decay and Doppler noise.

B. Laser noise

After analyzing atomic noise in the previous section, we now investigate the effect of laser noise from temporal fluctuations of its intensity and phase, described by PSDs, on the previously selected pulses. Laser PSDs quantify how phase and intensity fluctuations are distributed over frequency, thereby characterizing the temporal correlations of the laser noise. As a realistic example, we assume previously measured PSDs for the

laser phase and intensity noise from Ref. [43] [see also Figs. 7(b, e)]. For the phase PSD, we suppose that the laser is additionally cavity-filtered [43]. The noise effect from a PSD on the gate fidelities can be evaluated in a Monte-Carlo sampling based approach [50, 64] which modifies the time-dependent Rabi frequencies $\Omega^{ab}(t) \rightarrow \tilde{\Omega}^{ab}(t)$, and phases $\phi^{ab}(t) \rightarrow \tilde{\phi}^{ab}(t)$ for each shot [see App. B 4 for details]. For simplicity, we here consider identical intensity (phase) PSDs for each Rabi (phase) drive term $\Omega^{ab}(t)$ ($\phi^{ab}(t)$).

The contributions of the laser intensity and phase noise on the gate fidelity for the previously selected three pulses [c.f. Fig. 5] are shown in Fig. 6. We clearly observe that the different pulses behave very differently under the laser noise for the given PSDs. In particular, for “Pulse 1” the infidelity contribution from laser phase noise is much larger than the laser intensity noise contribution, while for “Pulse 2” it is the opposite, and for “Pulse 3” the infidelities from these two sources are comparable. Overall, “Pulse 2” shows the lowest fidelity degradation from laser noise with in total less than 10^{-4} infidelity contribution [c.f. Fig. 6, black bars], for the given PSDs. This is an order of magnitude lower than the total noise contribution from atomic noise [c.f. Fig. 5(b)], so that “Pulse 2” has a total infidelity of only about $1 - \mathcal{F} \sim 1.85 \times 10^{-3}$ for the given noise parameters.

This analysis allowed us to select the best pulse among candidates based on given laser noise properties. However, to shed more light on the intricate structure of infidelity contributions for different pulses we employ the recently developed *fidelity response theory* (FRT) [43]. FRT constructs a pulse response function (RF) which characterizes the sensitivity of a given pulse shape to noise of a certain type, at a given frequency. Combined with the corresponding PSD, the RF allows to determine how much phase or intensity noise at each frequency contributes to the fidelity loss of a given pulse. In more detail, in FRT the infidelity for a given pulse, for laser noise channel α (here intensity or phase), is approximated as

$$(1 - \mathcal{F})_{\alpha} = \int_0^{\infty} df S_{\alpha}(f) I_{\alpha}(f), \quad (14)$$

where $S_{\alpha}(f)$ is the related PSD with noise frequency f , and $I_{\alpha}(f)$ is the corresponding RF, evaluated as [43]

$$I_{\alpha}(f) = \int_0^T \int_0^T dt d\tau \cos(2\pi f(t - \tau)) \times \langle \hat{O}_H(t), \hat{O}_H(\tau) \rangle_c, \quad (15)$$

where $\hat{O}_H(t)$ denotes the noise operator $\hat{O}(t)$ in the Heisenberg picture and $\langle \hat{A}, \hat{B} \rangle_c$ is the connected correlation function between operators $\hat{A}$ and $\hat{B}$. Details about the FRT approach and derivations of the RFs are provided in Appendix D.

Figure 7 depicts the FRT analysis for the three selected pulse protocols. The phase noise response functions for the three pulses are shown with different colors

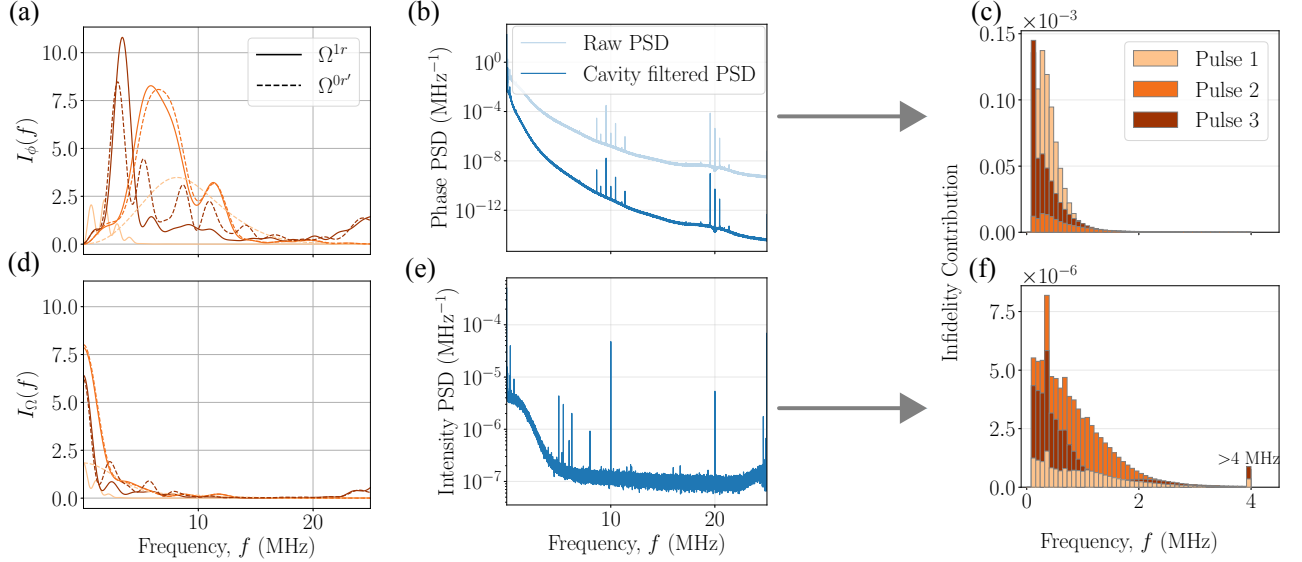


FIG. 7. FRT based analysis of selected pulses [c.f. Fig. 5(a)]. (a-c) FRT analysis of laser phase noise showing (a) the pulses' RF $I_\phi(f)$ for the two driving terms $\Omega^{0r'}$ and Ω^{1r} , (b) the corresponding PSD, and (c) the resulting infidelity contributions as a function of the noise frequency f , obtained from multiplying the RF with the PSD. The total contribution of the laser phase noise on the infidelity (within the FRT approximation) is given by integration over f . In (b) we show the raw laser PSD (light blue) and the same one filtered through a cavity (dark blue). To compute the infidelity contribution in (c), we consider the cavity filtered PSD. (d-f) Same data for laser intensity noise. Different colors in (a, c, d, f) correspond to different pulse protocols.

in Fig. 7(a), where solid (dashed) lines correspond to the driving between $|0\rangle \leftrightarrow |r'\rangle$ ($|1\rangle \leftrightarrow |r\rangle$). They show qualitatively distinct behaviour: “Pulse 1”, having the longest duration, shows peaks at low frequencies $f \lesssim 5$ MHz for the drive $|0\rangle \rightarrow |r'\rangle$, and a broader peak around 8 MHz for the drive $|1\rangle \rightarrow |r\rangle$; “Pulse 2” and “Pulse 3”, on the other hand, show much higher peaks, but shifted to larger frequencies, and the two different drives have a more similar profile. This qualitative difference between the pulses might look surprising at first glance, given that we consider only Rabi modulated pulses here, and $\phi^{ab}(t) = 0$. This can be explained by the fact that the formula for the phase noise RF contains the Rabi terms $\Omega^{ab}(t)$ [see derivation in App. D].

Figure 7(b) depicts the corresponding phase PSD, which shows a strong decay with frequency f . Also, we show the PSD after cavity-filtering [43] which effectively reduces the phase noise, and which we assume for the results in this paper. The frequency resolved infidelity contributions (within the FRT framework) are obtained by multiplying the RFs with the PSD, the corresponding graph is shown in Fig. 7(c). We observe large contributions to the infidelity for “Pulse 1” which stem from the RF peaks at very small frequencies $f \lesssim 1$ MHz. The larger peaks of the RFs for the other pulses at larger f have overall less effect on the infidelity because of the strong decay of the phase PSD with f . Integrating up the frequency resolved infidelity contributions gives an approximate value for the full infidelity contribution from laser phase noise for the chosen pulses, and we observe

a qualitatively good match with the Monte-Carlo sampled results [c.f. Fig. 6]. Furthermore, we want to emphasize that the phase RFs for all selected pulses vanish for $f = 0$, indicating stability against shot-to-shot phase fluctuations.

We perform the same FRT analysis for the laser intensity noise in Figs. 7(d-f). Here, the RFs are dominated by a peak at $f = 0$ [see Fig. 7(d)] with varying height and width, which dominates the final infidelity contributions [Fig. 7(f)]. The width of these peaks can be related to the overall strength of the Rabi frequencies. This is clearly visible for “Pulse 1” which has very distinct maximal Rabi frequencies for the two drives and correspondingly different widths of the $f = 0$ peaks in the RF [see also App. D]. The dominance of low-frequency features in the intensity RFs indicates that our pulses are sensitive to low-frequency and shot-to-shot intensity noise. However, we also observe that the size of these peaks can be reduced by appropriate pulse selection. In particular, $I_\Omega(f = 0)$ is strongly reduced for “Pulse 1” compared to the other pulses, and it obeys the smallest overall infidelity contribution from intensity noise. Since phase noise is dominating over intensity noise for the given parameters and PSDs, “Pulse 2” still reduces overall laser noise.

We have demonstrated that the FRT framework provides valuable insight into the laser noise susceptibility of different optimal pulse protocols and can be utilized to select pulses that perform particularly well for a given set of PSDs. On the other side, using this tool one

Parameter		Standard	Optimal ("Pulse 2")
Rabi frequency	$\Omega/(2\pi)$	10 MHz	20 MHz
Trap frequency	$\omega_{xy}/(2\pi)$	100 kHz	50 kHz
Trap frequency	$\omega_z/(2\pi)$	20 kHz	20 kHz
Rydberg level	n	61	65
Temperature	T	1 μ K	≤ 1 μ K
Laser wavevector	k_{eff}^x	$3 \times 10^6 \text{ m}^{-1}$	–
Laser wavevector	$k_{\text{eff}}^{y,z}$	0	–
"Pulse 2":			
Interaction	$V_{\text{dipole}}/(2\pi)$	5 MHz	10 MHz
Distance	R	6.8 μ m	6.0 μ m
Gate fidelity	$\mathcal{F}$	99.81%	99.92%

TABLE I. Experimental parameters used in the noise analysis for a ^{88}Sr setup. "Standard" denotes the values we assume for a standard setup and are commonly used throughout Sec. IV and Sec. V. "Optimal" refers to the optimized parameters we suggest for "Pulse 2" based on the noise sensitivity analysis in Sec. V. Note, that we do not optimize the laser wavevectors $k_{\text{eff}}^{x,y,z}$, but use fixed values throughout the manuscript. The final rows show pulse dependent values of the interaction strength and corresponding distance only for the "Pulse 2" pulse protocol. Note, that the distance R can be computed from the interaction strength and the C_3 coefficient for the chosen Rydberg levels.

could also try to adjust laser PSDs to a given pulse RF to further reduce noise. Finally, FRT could also be included already in the cost-function for the optimal control runs to directly find laser phase or intensity noise robust pulses [43], which we leave for future work.

V. NOISE SENSITIVITY ANALYSIS

In Sec. IV, we have analyzed the fidelity of the iSWAP gate protocols for a ^{88}Sr setup with fixed experimental parameters. Here, we investigate the sensitivity of the gate fidelity to variations in several experimental parameters: maximum Rabi frequency Ω , principal quantum number of the Rydberg states n , temperature T of the atoms in the traps, and trapping laser frequencies ω_{xy} and ω_z . For this analysis, we will focus on the best performing pulse under noise conditions, "Pulse 2", identified above. Then, we vary the experimental parameters one by one by keeping the other parameters fixed at their "standard" values used before [see Tab. I].

For this analysis, we assume all parameters that are not being varied to be $n = 61$ (which means $C_3 = 2\pi \times 1570.34 \text{ MHz } \mu\text{m}^3$, and $R = 6.8 \text{ } \mu\text{m}$ for optimal "Pulse 2" with $V_{\text{dipole}} = 2\pi \times 5 \text{ MHz}$), $\Omega = 2\pi \times 10 \text{ MHz}$, $T = 1 \text{ } \mu\text{K}$, $\omega_{xy} = 2\pi \times 100 \text{ kHz}$ and $\omega_z = 2\pi \times 20 \text{ kHz}$, which we denominate as "Standard parameters". Figures 8(a-d) show the gate infidelity contributions from atomic and laser noise sources for varying experimental parameters. For each plot only the relevant, non-constant

noise sources are shown; the black lines ("all combined") still include all considered atomic and laser noise sources.

A very relevant experimental parameter is the maximal achievable Rabi frequency of the laser drives Ω , which can be modified for example by changing the laser powers. Our results for varying Ω are shown in Fig. 8(a). The gate duration τ is inversely proportional to the maximal Rabi frequency, $\tau \propto \Omega^{-1}$. This directly influences time-dependent error sources, and we clearly observe a reduction of gate infidelity contributions from Doppler, decay and laser phase noise with increasing Ω . For Doppler noise, we have already identified this behavior with τ in Fig. 5(d). Decay noise is known to depend directly on T_{ryd} , which is directly proportional to τ , explaining the observed results.

For laser phase noise changing the Rabi frequency by a factor c , $\Omega \rightarrow c\Omega$ only scales the frequency axis in the corresponding response function, $I_\phi(f) \rightarrow I_\phi(c \cdot f)$ [see Fig. 11 in Appendix D], and since there are no $I_\phi(f = 0) = 0$ for our selected pulse [c.f. Fig. 7(a)], increasing Ω moves the peaks in $I_\phi(f)$ to larger f . Given that the PSD $S_\phi(f)$ strongly decreases with f , this leads to the observed decay of the laser phase induced noise when Ω is increased. Laser intensity noise, by contrast, leads to larger contributions to gate infidelity with increasing Ω , as expected. This can also be nicely illustrated from the FRT perspective: the intensity RFs $I_\Omega(f)$ have peaks at $f = 0$ [c.f. Fig. 7(d)], and that they obtain the same scaling with Ω as $I_\phi(f)$ [see Fig. 11 in the appendix]. Therefore, increasing Ω results in a larger noise frequency window to be relevant for the pulse and, thus, increases the infidelity.

Finally, we find that interaction noise also increases with increasing Ω , which is mainly related to the required increase of the interaction strength to keep V_{dipole}/Ω constant and maintain a valid optimal pulse. For fixed Rydberg states, this is achieved by reducing the distance R between the two atoms, which directly increases the interaction fluctuations induced by atom movement in the traps.

In Fig. 8(b) we show the dependence of iSWAP gate infidelities for modified trapping frequencies. The main plot shows the dependency with in-plane trap frequency ω_{xy} . Increasing ω_{xy} reduces position fluctuations of the atoms and, thereby, reduces the infidelity from interaction noise. However, at the same time it increases the average velocity of the trapped atoms, leading to larger Doppler noise. In total, we find a sweet spot $\omega_{xy} \sim 2\pi \times 50 \text{ kHz}$ where the combined effect is minimized. The inset of Fig. 8(b) shows the results for varying the out-of-plane trapping frequency ω_z . Within the considered range we find a rather stable behaviour of the noise contributions for $\omega_z \gtrsim 2\pi \times 20 \text{ kHz}$.

Figure 8(c) analyzes the dependence on the principal quantum number n of the two Rydberg states $|r\rangle = |5s n s^3 S_1\rangle$ and $|r'\rangle = |5s n p^3 P_0\rangle$. This has diverse implications on all sources of noise. First, it changes the interaction coefficient $C_3 \propto n^4$ and subsequently the re-

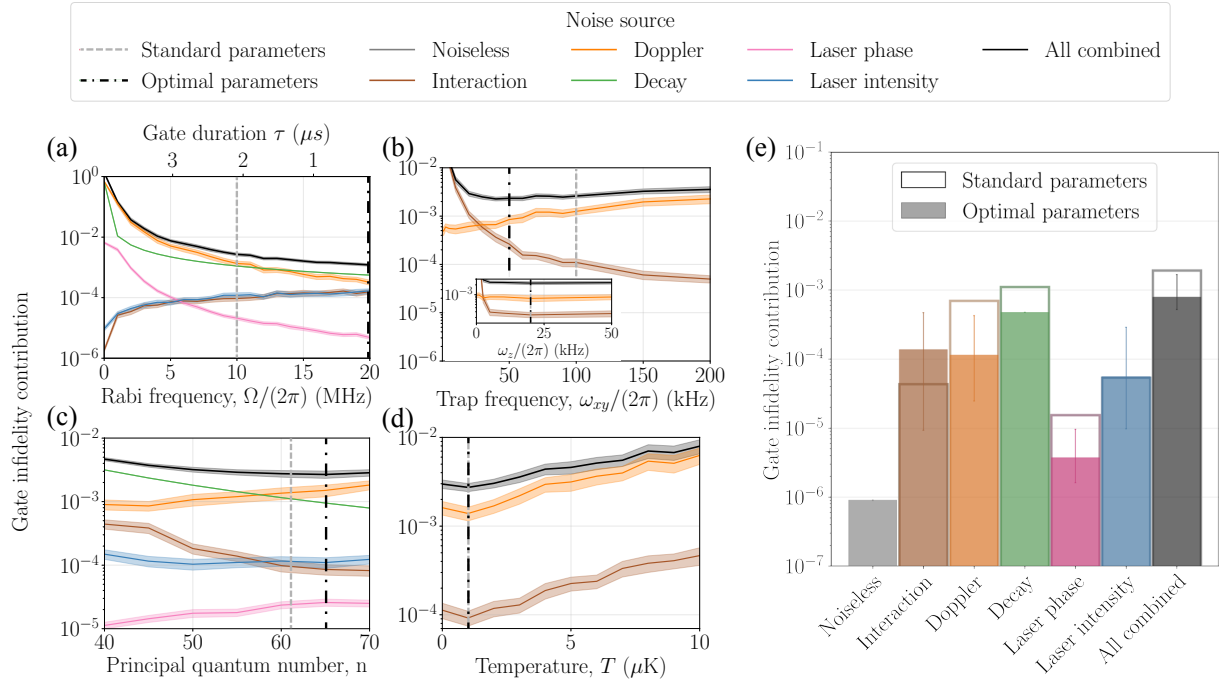


FIG. 8. Noise sensitivity of “Pulse 2”. (a-d) Gate infidelity contributions of different noise sources under variations of, (a) maximal Rabi frequency Ω , (b) in-plane trap frequency ω_{xy} (inset out-of-plane trap frequency ω_z), (c) Rydberg states’ principal quantum number n , and (d) temperature of atoms in the trap T . In these plots, only the non-constant noise sources under the varied parameters are depicted, but black lines show the full infidelity of all considered noise sources. Dashed vertical lines indicate the “standard” parameters assumed in this manuscript, dash-dotted vertical lines depict the “optimal” parameters obtained from this noise sensitivity analysis minimizing the overall gate infidelity. (e) Noise budget for the “optimal” parameters (filled bars) compared to the “standard” parameters (outlined bars). See Tab. I for the parameter values.

quired atomic spacing R to maintain the targeted interaction strength V_{dipole} . The Rydberg decay rates are modified as $\Gamma \propto n^{-3}$. Then, under the assumption of fixed laser powers, changing n modifies the Rabi frequencies $\Omega^{ab} \propto n^{-3/2}$ [24]. Lastly, the driving laser wavelength λ between qubit and Rydberg states scales as $\lambda \propto n^{-2}$ [see Fig. 14 in Appendix E] and, consequently, affects effective wave vector associated with the driving lasers, $k_{\text{eff}} \propto n^2$. Considering all these effects we find that the decay noise decreases with n , as expected. The Doppler noise, however, increases with n and counteracts the advantages from the reduced decay noise. The other noise sources are less relevant for the considered range of n . Overall, for our pulse we find an optimum at $n \sim 65$ for “Pulse 2”. More details about the dependence on n are given in App. E.

Eventually, Fig. 8(d) shows the behaviour of interaction and Doppler noise for varying temperature T of the atoms in the trap. As expected, for the regime above the quantum limit $k_B T \gg \hbar \omega_\alpha$ increasing the temperature increases the effect of interaction and Doppler noise. Below this quantum limit the infidelities from Doppler and interaction noise remain constant, so that we do not find any further improvements for $T \lesssim 1 \mu\text{K}$ for the given parameters.

Based on this noise sensitivity analysis, we finally de-

rive a set of “optimal” parameters for which the overall noise contribution is minimized for “Pulse 2”. They are listed in Tab. I, and the corresponding noise budget is shown in Fig. 8(e). Compared to the “standard” parameters the “optimized” parameters allow to substantially reduce the Doppler and decay noise, which were the dominant noise sources before, at the cost of increasing the interaction noise. Overall, the optimized parameters allow to reach an overall gate fidelity above 99.9% ($1 - \mathcal{F} < 10^{-3}$) for the iSWAP gate.

Finally, we want to note, that we have repeated the noise-aware pulse selection and noise modelling presented here also for “Scheme A” with *phase modulated* pulses and obtain similar fidelity of $\sim 99.9\%$ for the iSWAP gate with similar experimental parameters [see App. F for details].

VI. CONCLUSIONS

In summary, this work demonstrates a pathway towards implementing high-fidelity native iSWAP entangling gates for Rydberg atoms using tailored control protocol. By concurrently implementing state transfer and interaction within a single time-dependent control pulse and leveraging quantum optimal control methods, we

achieve high-fidelity protocols for the iSWAP gate for different driving schemes and both Rabi-modulated and phase-modulated pulses. Our approach considers global controls and smooth pulse shapes to minimize experimental demands.

We perform extensive noise modelling to analyze the gate fidelities one could reach in an experiment. In particular, we consider a neutral atom setup with ^{88}Sr atoms and include noise from the motion of atoms in the traps, noise due to decay of the Rydberg states, and time-dependent laser phase and intensity noise modelled with PSDs. Using a noise-aware pulse selection process we identify pulses that minimize gate degradation from different noise sources and obtain a pulse protocol that reaches $\sim 99.8\%$ fidelity for the iSWAP gate under state-of-the-art experimental parameters.

Finally, we conducted a detailed analysis of the influence of experimental parameters on the infidelity contributions of individual noise sources for our optimized pulse protocol. This analysis allowed us to identify “optimal” parameters, achieving iSWAP gate fidelities exceeding 99.9% with realistic near-term experimental constraints.

Our findings highlight the potential to extend the neutral atom gate set beyond the usually considered diagonal entangling gates by using and controlling a second Rydberg state. Extending our approach to include atomic and laser noise directly in the gate optimization could further improve gate infidelities and robustness against noise for specific experimental neutral atom QPU setups. For that, noise-aware optimization cost functions [15] and the FRT approach to laser noise [43] could be very useful to reduce noise sampling costs throughout the optimization

process. Another interesting direction would be to design specifically tailored noise robust iSWAP gate implementation using previously established techniques [13, 14]. Considering the entire exchange gate family, $U_{XY}(\theta)$, finding analytically parameterized pulses for the angle θ would simplify the implementation of a continuous set of gates by reducing experimental calibration efforts [6].

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Note added — During the final stages of preparing this manuscript we became aware of related work [65].

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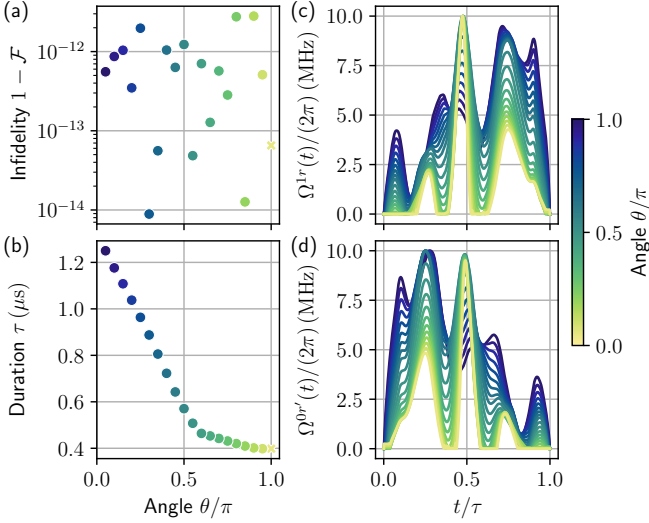


FIG. 9. Parameterized exchange gate optimization. Optimal pulses for different angles θ are obtained by sequential optimization starting from the iSWAP gate result at $\theta = \pi$ and fixing the maximal Rabi frequency $\Omega = 2\pi \times 10$ MHz. (a) Infiltrity of $U_{XY}(\theta)$, and (b) gate duration τ plotted vs the gate angle θ . (c, d) Optimized pulse drives, (c) $\Omega^{1r}(t)$, (d) $\Omega^{0r'}(t)$, plotted versus relative time t/τ to illustrate the continuous pulse deformation with the angle θ .

Appendix A: Parameterized exchange gate

The exchange interaction between the two Rydberg states $|r\rangle$ and $|r'\rangle$ allows to implement parameterized exchange gates $U_{XY}(\theta)$ in the qubit manifold, where θ denotes the gate angle. In the main text, we focused our discussion on the iSWAP gate which is realized by $U_{XY}(\theta = \pi)$. The same techniques used there can be applied for arbitrary angles θ .

Here, we adopt a slightly different strategy: we use an optimal pulse for the iSWAP gate with $\theta = \pi$, and then use this result to initialize our optimal control engine for a slightly smaller angle. We continue this strategy to obtain a sequence of pulse protocols for $\theta \in (0, \pi]$. Within this section, we focus on “Scheme A” with Rabi modulated pulses and choose “Pulse 2” (see main text) as our initial optimal protocol for the iSWAP gate. Figure 9(a) shows the so obtained infiltrities, which are all below 10^{-11} . Fixing the maximal Rabi frequency Ω , leads to increased pulse durations for angles $\theta < \pi$ for the given Rabi modulated pulse, as shown in Fig. 9(b). The advantage of such an approach can be observed by looking at the pulse protocols for the different angles θ , depicted in Figs. 9(c, d), which show a continuous deformation when the angle is changed. This could allow to obtain high-fidelity pulses for the continuous range $\theta \in (0, \pi]$ using interpolation methods. Furthermore, experimental calibration for the different angles could be simplified, and noise characteristics are expected to be qualitatively similar.

The results shown here demonstrate that even this simple protocol allows to generate an entire family of high-fidelity exchange gates $U_{XY}(\theta)$. The increase of the gate duration τ with decreasing θ is most likely an artifact of the approach taken here, since the iSWAP gate with $\theta = \pi$ is the most entangling gate in the exchange gate family $U_{XY}(\theta)$. Therefore, we expect to be able to find faster pulses for $\theta < \pi$ when optimization with random ansatzes is directly performed. However, this would most likely lead to qualitatively different pulse shapes. More elaborate approaches that identify families of similar pulses and allow for their interpolation [66] could be investigated in future work to overcome some of these limitations.

Appendix B: Noise model

1. Interaction noise

Atomic motion due to finite temperature leads to position fluctuations in optically trapped atoms, which in turn induce fluctuations in the dipole-dipole interaction (DDI) between two atoms. Since the DDI strength determines the exchange frequency, any deviation from the target value V_{dipole} results in non-optimal Rydberg population and consequently reduces the overall gate fidelity.

The positions of two atoms, (x_1, y_1, z_1) and (x_2, y_2, z_2) , fluctuate as $\tilde{x}_i = x_i + \delta x_i$, $\tilde{y}_i = y_i + \delta y_i$, and $\tilde{z}_i = z_i + \delta z_i$, where $i = 1, 2$. If we approximate the optical tweezer potential as an harmonic oscillator, each displacement δ_α for $\alpha = \{x, y, z\}$ follows a Gaussian distribution with the standard deviation

$$\sigma_{\text{pos}}^\alpha = \sqrt{\frac{\hbar}{2m\omega_\alpha}}(1 + 2\bar{n}_\alpha), \quad (\text{B1})$$

where

$$\bar{n}_\alpha = \frac{1}{e^{\hbar\omega_\alpha/k_B T} - 1}. \quad (\text{B2})$$

Here, k_B is the Boltzmann factor, T is the temperature, m is the atomic mass, and ω_α is the trap frequency. In typical tweezer geometries, we assume $\omega_x = \omega_y \equiv \omega_{xy}$.

The noisy interatomic separation is then

$$\tilde{R} = \sqrt{(\tilde{x}_2 - \tilde{x}_1)^2 + (\tilde{y}_2 - \tilde{y}_1)^2 + (\tilde{z}_2 - \tilde{z}_1)^2}, \quad (\text{B3})$$

which induces a fluctuating DDI,

$$\tilde{V}_{\text{dipole}} = \frac{C_3}{\tilde{R}^3}. \quad (\text{B4})$$

Finally, the interaction term in the Hamiltonian takes the form

$$\frac{\tilde{H}_{\text{exchange}}}{\hbar} = \tilde{V}_{\text{dipole}} \left(|r\rangle_i |r'\rangle_j \langle r'|_i \langle r|_j + \text{h.c.} \right). \quad (\text{B5})$$

For example, we choose the radial and axial trap frequencies respectively as $\omega_{xy} = 2\pi \times 100$ kHz and

$\omega_z = 2\pi \times 20$ kHz, which are realistic in the current experimental system. With a temperature $T = 1$ μ K, one obtains a position standard deviation of $\sigma_{\text{pos}}^\alpha = (0.02, 0.02, 0.08)$ μ m for each spatial dimension.

2. Doppler noise

Atomic motion not only perturbs the DDI, but also generates unwanted detuning stemming from the Doppler shift, which is known as Doppler noise. Finite velocity

$$\Delta v_\alpha = \sqrt{\frac{\hbar \omega_\alpha}{2m}} (1 + 2\bar{n}_\alpha), \quad (\text{B6})$$

shift the resonance for each atomic level $a = \{1, r, r'\}$. This shift is characterized by a Gaussian standard deviation in detuning as follows:

$$\begin{aligned} \sigma_{\text{det}}^a &= k_{\text{eff}}^{\alpha,a} \Delta v_\alpha \\ &= k_{\text{eff}}^{x,a} \Delta v_x + k_{\text{eff}}^{y,a} \Delta v_y + k_{\text{eff}}^{z,a} \Delta v_z, \end{aligned} \quad (\text{B7})$$

where k_{eff}^a represents the effective wave vector for each laser coupled with the atomic level a . Finally, we can extract the Doppler shift Δ^a from sampling from the Gaussian distribution, which adds the following detuning term to the Hamiltonian:

$$\begin{aligned} \frac{\tilde{H}_{\text{Doppler}}}{\hbar} &= - \sum_i \left(\Delta^1(t) |1\rangle_i \langle 1| + \Delta^r(t) |r\rangle_i \langle r| \right. \\ &\quad \left. + \Delta^{r'}(t) |r'\rangle_i \langle r'| \right) \end{aligned} \quad (\text{B8})$$

For example, take the scheme A $|1\rangle \leftrightarrow |r\rangle$ transition, where $|1\rangle = |5s5p^3P_2\rangle$ and $|r\rangle = |5s61s^3S_1\rangle$ case, with transition wavelength $\lambda = 323$ nm and effective wave vector $k_{\text{eff}}^x = (2\pi)3.10 \times 10^6$ m⁻¹ and $k_{\text{eff}}^y = k_{\text{eff}}^z = 0$. Using the values from the previous subsection, $\omega_x = \omega_y = 2\pi \times 100$ kHz, $\omega_z = 2\pi \times 20$ kHz, and $T = 1$ μ K, one obtains a detuning standard deviation of $\sigma_{\text{det}}^r = k_{\text{eff}}^r \Delta v = 2\pi \times 47$ kHz.

3. Decay noise

We consider an approximate method to implement the finite lifetimes of the Rydberg states $|r\rangle$ and $|r'\rangle$ into our modelling. We considered the non-hermitian Hamiltonian [51]

$$\frac{\tilde{H}_{\text{decay}}}{\hbar} = -\frac{i}{2} \sum_i \left(\Gamma_r^{\text{eff}} |r\rangle_i \langle r|_i + \Gamma_{r'}^{\text{eff}} |r'\rangle_i \langle r'|_i \right) \quad (\text{B9})$$

where $\Gamma_{r,r'}^{\text{eff}}$ represent the effective decay rates of the Rydberg states [see Appendix C for a detailed derivation]. While approximate, this method offers high enough accuracy for the tasks performed in this paper and can be very efficiently implemented.

4. Laser Phase and Intensity noise

The laser drive couples the two states with a strength coefficient $\Omega e^{i\phi}$, where ϕ is the phase and Ω is the Rabi frequency. Due to the finite stability of the laser, both the phase and the intensity fluctuate as $\phi \rightarrow \tilde{\phi}$ and $\Omega \rightarrow \tilde{\Omega}$ [50]. We model these fluctuations as [64]:

$$\tilde{\phi}(t) = \phi(t) + \delta\phi(t) \quad (\text{B10})$$

$$\tilde{\Omega}(t) = \Omega(t) \left(1 + \frac{\alpha_I(t)}{2} \right) \quad (\text{B11})$$

where $\delta\phi$ and α_I denote the phase noise and the relative intensity noise (RIN). These noise contributions are quantified by their respective power spectral densities (PSDs), S_ϕ and S_{α_I} . Accordingly, we express them as

$$\delta\phi(t) = \sum_f 2\sqrt{S_\phi(f)\Delta f} \cos(2\pi ft + \varphi_f) \quad (\text{B12})$$

$$\alpha_I(t) = \sum_f 2\sqrt{S_{\alpha_I}(f)\Delta f} \cos(2\pi ft + \varphi_f) \quad (\text{B13})$$

where $\Delta f = f_{j+1} - f_j$ is the spacing between sampled frequency components, and each φ_f is a random phase drawn from a uniform distribution $[0, 2\pi]$ for each frequency component $f = f_j$ [64].

These are then implemented in the dynamics of the system via the driving terms of the Hamiltonian,

$$\begin{aligned} \frac{\tilde{H}_{\text{drive}}(t)}{\hbar} &= \sum_i \left[\left(\frac{1}{2} \tilde{\Omega}^{01}(t) e^{i\tilde{\phi}^{01}(t)} |1\rangle_i \langle 0| \right. \right. \\ &\quad + \frac{1}{2} \tilde{\Omega}^{1r}(t) e^{i\tilde{\phi}^{1r}(t)} |r\rangle_i \langle 1| \\ &\quad + \frac{1}{2} \tilde{\Omega}^{0r'}(t) e^{i\tilde{\phi}^{0r'}(t)} |r'\rangle_i \langle 0| \\ &\quad \left. \left. + \frac{1}{2} \tilde{\Omega}^{rr'}(t) e^{i\tilde{\phi}^{rr'}(t)} |r'\rangle_i \langle r| + \text{h.c.} \right) \right] \end{aligned} \quad (\text{B14})$$

Appendix C: Atomic parameters for ⁸⁸Sr

The inverse radiative lifetime of an atomic state Γ_i , in the absence of black-body radiation, is given by

$$\Gamma_i = \sum_j \frac{4}{3} \frac{|\langle i|\hat{D}|j\rangle|^2}{\hbar c^3} \omega_{ij}^3, \quad (\text{C1})$$

where the sum runs over all possible atomic states j with lower energies $E(j) < E(i)$. Here $\omega_{ij} = |E_i - E_j|/\hbar$, and the set of allowed lower states is determined by the electric-dipole selection rules, through the dipole matrix elements $\langle i|\hat{D}|j\rangle$, whose evaluation we describe in details below.

Our object of interest is the alkaline-earth atom ^{88}Sr . This isotope has no nuclear spin, and therefore exhibits no hyperfine structure. On the other hand, the presence of two valence electrons requires the coupling of spin and orbital angular momenta of individual electrons. This is handled using the non-relativistic LS -coupling scheme,

$$\vec{J} = \vec{L} + \vec{S}, \quad (\text{C2a})$$

$$\vec{L} = \vec{l}_1 + \vec{l}_2, \quad (\text{C2b})$$

$$\vec{S} = \vec{s}_1 + \vec{s}_2, \quad (\text{C2c})$$

where $\{J, L, S\}$ are the total atomic quantum numbers. Atomic terms are labeled as $^{2S+1}L_J$, while $l_{1,2}$ and $s_{1,2}$ denote the quantum numbers of individual valence electrons.

Let $\hat{\vec{D}} = \hat{\vec{d}}_1 + \hat{\vec{d}}_2$ be an operator of electric dipole moment of both electrons. Assuming only one electron is excited by the incident field and neglecting two-electron excitations, we take $\hat{\vec{D}} = \hat{\vec{d}}_2$. We now evaluate the dipole moment matrix element $\langle i | \hat{\vec{D}} | j \rangle$ between a pair of states $|i\rangle = |J'M_{J'}\rangle$ and $|j\rangle = |JM_J\rangle$, where only one electron is excited (here the primed and unprimed denotations do not refer to $|r'\rangle$ and $|r\rangle$ from the main text). Following the coupling scheme (C2), we obtain

$$\begin{aligned} \langle J'M_{J'} | \hat{\vec{D}} | JM_J \rangle &= \delta_{SS'} (-1)^{l_2+l_1+S+J'} \sqrt{[L][l'_2][J'][L']} \\ &\quad C_{JM_J, 1q}^{J'M_{J'}} \begin{Bmatrix} L & S & J \\ J' & 1 & L' \end{Bmatrix} \begin{Bmatrix} l_2 & l_1 & L \\ L' & 1 & l'_2 \end{Bmatrix} \\ &\quad \langle n'_2 l'_2 | \hat{\vec{d}}_2 | n_2 l_2 \rangle, \end{aligned} \quad (\text{C3})$$

where $[k] = 2k + 1$, and the remaining reduced single-electron dipole matrix element is given by

$$\begin{aligned} \langle n'l' || \hat{\vec{d}} || nl \rangle &= (-1)^{l'} \sqrt{2l+1} \begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad \int_0^\infty R_{n'l'}(r) R_{nl}(r) r^3 dr, \end{aligned} \quad (\text{C4})$$

the remaining integral includes radial parts of wave-functions on the active electron.

Hence, the evaluation of radiative lifetimes (C1) reduces to computing transition frequencies ω_{ij} and radial integrals from (C4). A rigorous *ab initio* computation of the radial integrals is an extra theoretical problem, which requires many-body methods such as multi-configuration Hartree-Fock [67] or the random phase approximation with exchange [68]. Instead, we use the method proposed in [69], based on quantum defect (QD) theory. Within this approach, the radial wave-functions are taken as a hydrogen-like ones:

$$\begin{aligned} R_{nl}(r) &= \frac{1}{n^{*2}} \sqrt{(2Z)^3 \frac{\Gamma(n-l-I(l))}{2\Gamma(n^*+l^*+1)}} \left(\frac{2Zr}{n^*} \right)^{l^*} \\ &\quad e^{-\frac{Zr}{n^*}} L_{n-l-1-I(l)}^{2l^*+1}(2Zr/n^*), \end{aligned} \quad (\text{C5})$$

where $n^* = n - \delta_l(n)$ and $l^* = l - \delta_l(n) + I(l)$. An integer parameter $I(l)$ has an arbitrariness of choice with the following constraint: $l^* + \frac{1}{2} > 0$ and $I(l) \leq n_{\min} - l - 1$, where $n_{\min} = 5$ is the principal quantum number of the lowest unoccupied state with the given l . It should be chosen for a given angular momentum value l in a way for the best reproduction of a target result.

To apply this method, we need the QD values. For highly excited rydberg states ($n \gg 1$), the QD is approximately constant for each angular momentum l . For lower states, its variation can be described by the extended Rydberg-Ritz formula:

$$\delta_l(n) = \delta_l^{(0)} + \frac{\delta_l^{(2)}}{(n - \delta_l^{(0)})^2} + \frac{\delta_l^{(4)}}{(n - \delta_l^{(0)})^4} + \dots, \quad (\text{C6})$$

where the parameters $\{\delta_l^{(m)}\}$ are determined by fitting to known data. For low-lying excited states, QD values are extracted directly from the Rydberg-Ritz formula

$$E_{nl} = I[^{88}\text{Sr}] - \frac{\tilde{R}y[^{88}\text{Sr}]}{[n - \delta_l(n)]^2}, \quad (\text{C7})$$

where the ionization energy $I[^{88}\text{Sr}] = 1\,377\,012.72$ GHz [70], the reduced Rydberg constant accounts for the finite nuclei mass $\tilde{R}y[^{88}\text{Sr}] = 3\,289\,821.43$ GHz.

The radiative lifetime in Eq. (C1) does not include black-body-radiation (BBR) effects; in other words, the terms proportional to the mean thermal photon number $n(\omega_{ij}, T) = [\exp(\tau_R \omega_{ij}) - 1]^{-1}$ are omitted. Here $\tau_R = \frac{\hbar}{k_B T}$ is so-called photon reservoir correlation time, the temperature entering here refers to the photon reservoir. At room temperature ($T = 300\text{K}$) we have $\tau_R^{-1} \sim 10^{14} \text{ sec}^{-1}$. This value is larger than typical energy spacing between neighboring rydberg levels, which makes the BBR-induced transitions to the neighbor Rydberg states significant. In the regime $\tau_R \omega_{ij} > 1$, however, even a small uncertainty in the transition frequency ω_{ij} leads to a sizable error in $n(\omega_{ij}, T)$, while the available data on highly excited $5snp(^3P_J)$ states [71] do not resolve the fine-structure splittings. Consequently, incorporating BBR-induced transitions into the lifetime calculation becomes unreliable. For this reason, we proceed under the assumption that BBR can be neglected. This is realistic in a real experimental environment supported by cryogenic apparatus [72, 73].

TABLE II. Parameters of Rydberg-Ritz formula (C6) for the states of interest.

	$5sns(^3S_1)$ ($15 \leq n$) [70]	$5snp(^3P_0)$ ($15 \leq n$)	$5snd(^3D_1)$ ($28 \leq n$) [70]
$\delta_l^{(0)}$	3.370778	2.883326	2.67517
$\delta_l^{(2)}$	0.418	0.255	-13.15
$\delta_l^{(4)}$	-0.3	4.07	-4444

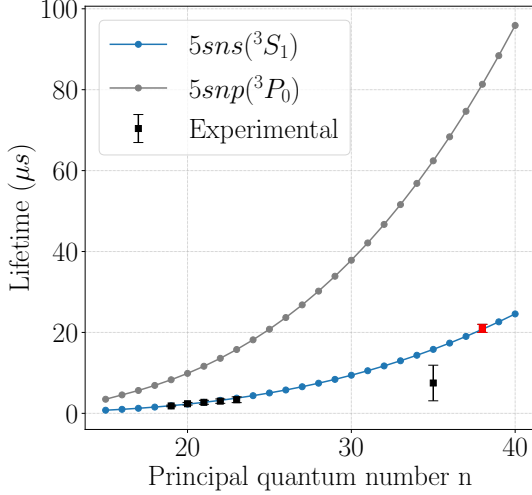


FIG. 10. Radiative lifetimes $\tau_{\text{decay}} = \Gamma^{-1}$ of triplet $5sns(^3S_1)$ and $5snp(^3P_0)$ states obtained via calculation of Equation (C1) with dipole moments evaluated with QD-based wave functions (C5). The calculated values are shown by blue and grey dots, respectively. Black squares are the experimental results from [74], the red square value is reported in Ref. [75]. Vertical bars denote measurement uncertainties.

a. Lifetimes of triplet states $5sns(^3S_1)$

The triplet states $5sns(^3S_1)$ are dipole-coupled to $5sn'p(^3P_{J=0,1,2})$ manifold. Therefore, to construct radial wave functions for these states and calculate the radiative lifetimes, we must know the QD of the corresponding Rydberg levels.

For the $5sns(^3S_1)$ series, the quantum defects for $15 \leq n$ are well described by the extended Rydberg-Ritz formula (C6), using the parameters listed in Table II. These parameters were derived from high-precision transition-frequency measurements reported in Ref. [70] (the accuracy is up to 1 MHz). For the lower-lying states ($6 \leq n \leq 14$), the QD values are obtained directly from the Rydberg formula (C7) using the available experimental dennergies.

Experimental data for the $5snp(^3P_J)$ states are less precise [71]. For $n > 15$, the energies of states $5snp(^3P_0)$ states are not available, and the fine structure is unresolved. Thus, we proceed under an assumption that all fine-structure share the same QD. For $n \geq 15$, the extracted QD values follow the extended Rydberg-Ritz formula (C6) with the parameters given in Table II. For lower-lying states $5 \leq n \leq 15$, QDs are again determined manually from available experimental energies via (C7).

We use the QD values to construct radial wavefunctions (C5), using $I(0) = 4$, $I(1) = 2$. The wave-functions were used to calculate the radial integrals for transition dipole moments (C4). The latter ones are used for calculations for the radiative decay rates (C1). The results

for the radiative lifetimes are shown in Fig. 10.

The results for the calculated radiative lifetimes are shown in Fig. 10 and listed in Table IV. Although experimental data of radiative lifetimes are limited, some values are available. The measurements reported in Ref. [74] for $19 \leq n \leq 23$ are consistent with our results within experimental uncertainties. There is a discrepancy at $n = 35$, but our result for $n = 38$ agrees with [75].

The calculated radiative decay rate for the target state $|5s61s(^3S_1, M_J = 0)\rangle$ is

$$\frac{1}{2\pi} \Gamma[5s61s(^3S_1, M_J = 0)] = 1.66 \text{ kHz},$$

and the corresponding radiative lifetime $\tau_{\text{decay}} = \Gamma^{-1}$ is

$$\tau_{\text{decay}}[5s61s(^3S_1, M_J = 0)] = 96 \mu\text{s}.$$

b. Lifetimes of triplet states $5snp(^3P_0)$

These states have two decay channels: $|5snp(^3P_0)\rangle \rightarrow |5sns(^3S_1)\rangle$ and $|5snp(^3P_0)\rangle \rightarrow |5snd(^3D_1)\rangle$. The QDs of the $|5snp(^3P_0)$ and $|5sns(^3S_1)\rangle$ states are discussed above.

The energies of the triplet states $5snd(^3D_1)$ were measured and reported in Ref. [70] for $12 \leq n \leq 50$ with high precision (up to 1 MHz). For $n \geq 28$, these energies are well reproduced with the use of QDs that obey the extended Rydberg-Ritz formula (C6), with the parameters listed in Table II.

TABLE III. Quantum defects for selected low-excited states $|5snd(^3D_1)\rangle$. Values marked by '*' are obtained by numeric interpolation of available data.

n	QD	n	QD
4	2.01224	12	1.91164
5	1.83073	13	1.97945
6	1.80857	14	2.08210
7	1.80610	15	2.21470
8	1.80708*	16	2.37302
9	1.81482*	17	2.44031
10	1.83263*	18	2.50352
11	1.86380*	19	2.54444

For the lower-lying states, the QD are extracted manually from the Rydberg formula (C7) using available experimental data: Ref. [70] for $n \geq 12$ and Ref. [76] for $4 \leq n \leq 7$. No experimental energy data could be found for $8 \leq n \leq 11$, the QDs for these states were therefore obtained here via numerical interpolation of known data, the results are listed in Table III. These QDs were used to construct the radial wave functions (C5). The integer parameter entering the effective orbital quantum number is taken as $I(2) = 2$, except for the first two states with $n = 4$ and $n = 5$, for which we take $I(2) = 0$.

The calculated radiative decay rate for the target state $|5s60p(^3P_0, M_J = 0)\rangle$ is:

$$\frac{1}{2\pi}\Gamma[5s61p(^3P_0, M_J = 0)] = 0.44 \text{ kHz},$$

and the corresponding radiative lifetime defined as $\tau_{\text{decay}} = \Gamma^{-1}$ is

$$\tau_{\text{decay}}[5s61p(^3P_0, M_J = 0)] = 365 \mu\text{s}.$$

The radiative lifetimes have been calculated for $15 \leq n \leq 70$ for both $5sns(^3S_1)$ and $5snp(^3P_0)$ manifolds. The are partially shown and listed in Fig. 10 and Table IV, respectively. These values are used also in the analysis in Section V and in Figure 8.

TABLE IV. Calculated radiative lifetimes $\tau_{\text{decay}} = \Gamma^{-1}$ of some rydberg states, the values are given in μs units.

n	$5sns(^3S_1)$	$5snp(^3P_0)$
15	0.77	3.49
20	2.28	9.89
25	5.04	20.80
30	9.42	37.85
35	15.81	62.42
40	24.58	95.88
45	36.10	139.62
50	50.76	195.03
55	68.92	263.48
60	90.99	346.37
65	117.23	445.07
70	148.15	560.98

c. Lifetimes of metastable states $5s5p(^3P_0)$ and $5s5p(^3P_2)$

The state $5s5p(^3P_0)$ can potentially decay only into the physical ground state $5s^2(^1S_0)$. The value of the corresponding radiative decay rate has been reported in Ref. [77], where the measurements were performed for fermionic isotope ^{87}Sr

$$\frac{1}{2\pi}\Gamma[5s5p(^3P_0)] = 1.35 \text{ mHz}.$$

The state $5s5p(^3P_2)$ has the highest energy among all states of the spin-orbit manifold $5s5p(^3P_J)$. Thus, it can undergo through the radiative decay into the lower spin-orbit states with $J = 1, 0$ as well as into the physical ground state $5s^2(^1S_0)$. The corresponding radiative lifetime resulting from all these processes has been reported in theoretical work [78]

$$\Gamma[5s5p(^3P_2)] = 9.55 \times 10^{-4} \text{ sec}^{-1}.$$

Finally, the effective decay rates we used in equation (B9) are

$$\Gamma_{r'}^{\text{eff}} = 2\pi \times 0.44 \text{ kHz}, \quad (\text{C8})$$

$$\Gamma_r^{\text{eff}} = 2\pi \times 1.66 \text{ kHz}, \quad (\text{C9})$$

$$\Gamma_1^{\text{eff}} = 2\pi \times 0.15 \text{ mHz}, \quad (\text{C10})$$

$$\Gamma_0^{\text{eff}} = 2\pi \times 1.35 \text{ mHz}. \quad (\text{C11})$$

Note that because the decay rates of the metastable and the Rydberg state are differs by 6-7 orders of magnitude, we can ignore $\Gamma_{0,1}^{\text{eff}}$ for decay noise modeling.

Appendix D: Fidelity Response Theory on Laser noise

Fidelity response theory (FRT) [43] is a powerful tool for understanding and predicting the behavior of fidelity depending on the noise. We apply FRT to phase and intensity noise. We consider these two noises as a perturbation,

$$\hat{H}(t) = \hat{H}_0(t) + \sum_j h_j(t) \hat{O}_j(t), \quad (\text{D1})$$

where $\hat{H}_0(t)$ is the noiseless Hamiltonian, $\hat{O}_j(t)$ is a noise operator that encodes information about the noise type, and $h_j(t)$ is a function that encodes the amplitude of the noise. $h_j(t)$ is depending on the PSD $S_j(f)$, where $h(t) = \sum_f 2\sqrt{S(f)\Delta f} \cos(2\pi ft + \varphi_f)$. FRT expect the fidelity by using the first-order perturbation,

$$1 - \mathcal{F} = \int_0^\infty df S(f) I(f, \Omega), \quad (\text{D2})$$

where $I(f, \Omega)$ is denoted the response function (RF),

$$I(f, \Omega) = \int_0^T \int_0^T dt d\tau \cos(2\pi f(t - \tau)) \langle \hat{O}_H(t, \Omega) \hat{O}_H(\tau, \Omega) \rangle_c. \quad (\text{D3})$$

$\langle \hat{A}\hat{B} \rangle_c = \langle \hat{A}\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$ represents the connected correlator function, where $\langle \hat{A} \rangle$ is short for $\langle \Psi_0 | \hat{A} | \Psi_0 \rangle$. $\hat{O}_H(t)$ represents the noise operator $\hat{O}(t)$ in the Heisenberg picture $\hat{O}_H(t) = \hat{U}^\dagger(t) \hat{O}(t) \hat{U}(t)$ for the unitary evolution operator $\hat{U}(t)$ under $\hat{H}_0(t)$.

1. Phase noise

For fluctuations in the phase of the lasers we replace the phase in driving term of the Hamiltonian by $\tilde{\phi}(t)$ (from equation (B10)), obtaining the driving term,

$$\tilde{H}_{\text{drive}}(t) = \sum_{ab} \sum_i \frac{\Omega^{ab}(t)}{2} \left(e^{i\tilde{\phi}^{ab}(t)} |b\rangle_i \langle a| + h.c. \right)$$

where we sum over the different atomic transitions $ab = \{01, 1r, 0r', rr'\}$. Expanding the exponential terms to first order,

$$e^{\pm i\tilde{\phi}^{ab}(t)} \sim e^{\pm i\phi^{ab}(t)} (1 \pm i\delta\phi^{ab}(t)) \quad (\text{D4})$$

one can separate the noiseless from the noisy Hamiltonian terms,

$$\sum_{ab} \sum_i \left[\frac{\Omega^{ab}(t)}{2} \left(e^{i\phi^{ab}(t)} |b\rangle_i \langle a| + e^{-i\phi^{ab}(t)} |a\rangle_i \langle b| \right) + \delta\phi^{ab} \frac{i\Omega^{ab}(t)}{2} \left(e^{i\phi^{ab}(t)} |b\rangle_i \langle a| - e^{-i\phi^{ab}(t)} |a\rangle_i \langle b| \right) \right] \quad (\text{D5})$$

Here the noisy operators, for each of the atomic transitions, are,

$$\hat{O}_{\phi^{ab}}(t) = \frac{\Omega^{ab}(t)}{2} \sum_i i \left(e^{i\phi^{ab}(t)} |b\rangle_i \langle a| - h.c. \right) \quad (\text{D6})$$

Lastly, the infidelity becomes

$$1 - \mathcal{F}_\phi = \sum_{ab} \int df S_\phi(f) I_{\phi^{ab}}(f, \Omega), \quad (\text{D7})$$

with the phase response function

$$I_{\phi^{ab}}(f) = \int_0^T \int_0^T dt d\tau \cos(2\pi f(t - \tau)) \times \left\langle \hat{O}_{\phi^{ab}}(t) \hat{O}_{\phi^{ab}}(\tau) \right\rangle_c. \quad (\text{D8})$$

2. Intensity noise

For intensity noise, the derivation is slightly simpler since the driving term with intensity/Rabi frequency noise can be separated into noisy and noiseless terms (see (B11)) without any approximate expansions,

$$\begin{aligned} \tilde{H}_{\text{drive}}(t) &= \sum_{ab} \sum_i \frac{\tilde{\Omega}^{ab}(t)}{2} \left(e^{i\phi^{ab}(t)} |b\rangle_i \langle a| + h.c. \right) \\ &= \hat{H}_{\text{drive}}(t) + \sum_{ab} \alpha_I^{ab}(t) \hat{O}_{\Omega^{ab}}(t), \end{aligned} \quad (\text{D9})$$

where the relative intensity noise $\alpha_I^{ab}(t)$ is given by (B13), leading to the following noise operators:

$$\hat{O}_{\Omega^{ab}}(t) = \frac{\Omega^{ab}(t)}{4} \sum_i \left(e^{i\phi^{ab}(t)} |b\rangle_i \langle a| + h.c. \right) \quad (\text{D10})$$

Therefore, the infidelity becomes

$$1 - \mathcal{F}_\Omega = \sum_{ab} \int df S_{\alpha_I}(f) I_{\Omega^{ab}}(f, \Omega), \quad (\text{D11})$$

with the intensity noise response function

$$I_{\Omega^{ab}}(f) = \int_0^T \int_0^T dt d\tau \cos(2\pi f(t - \tau)) \times \left\langle \tilde{O}_{\Omega^{ab}}(t) \tilde{O}_{\Omega^{ab}}(\tau) \right\rangle_c. \quad (\text{D12})$$

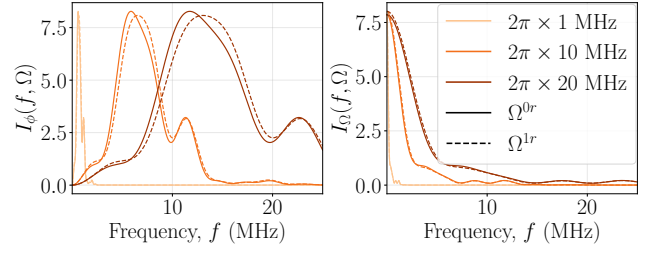


FIG. 11. Phase and intensity response functions of scheme A, Rabi modulated, Pulse 2 for different maximum Rabi frequencies [see Fig. 5].

3. Response function and Rabi frequency

The example in Figure 7 showed the RF profile of pulses rescaled to have a maximum Rabi frequency of $2\pi \times 10$ MHz. Changing this value means expanding or contracting the RF horizontally (see Figure 11). Higher Ω , for example, would expand the RF horizontally to higher noise frequencies and lead to different effects on the sensitivity of the pulse to laser noise depending on whether the later arises from phase or intensity noise. For phase noise, since we are essentially shifting the maximum of the RF to the right the pulse becomes more(less) sensitive to high(low) noise frequencies; for intensity noise, however, since the RFs are maximum for lower frequencies, increasing Ω leads to expanding the maximum RF to a larger set of frequencies, that is, the pulse becomes more sensitive to a larger range of noise frequencies. In short, increasing Ω improves(worsens) the performance of the pulses in the presence of intensity(phase) noise, as is shown.

Appendix E: Principal quantum number analysis

Changing the principal quantum number n of the Rydberg states, as is shown in the plot (c), has diverse implications on all sources of noise, which we want to discuss in-depth within this appendix. Firstly, and the one that affects all sources of noise, is the requirement that the Rabi frequency for a specific atomic transition changes accordingly due to changing of the dipole matrix element,

$$\Omega^{a,b} = \frac{\langle a | \hat{D} | b \rangle \cdot \vec{E}}{\hbar}, \quad (\text{E1})$$

assuming the laser, with electric field amplitude E , is linearly polarized. Here, for the coupling scheme A, $|a\rangle$ would represent Rydberg state, $|r\rangle$ or $|r'\rangle$, with principal quantum number n , and $|b\rangle$ would represent the Qubit states, $|0\rangle$ or $|1\rangle$. One can fix the electric field amplitude E so that when $n = 61$ the Rabi frequency is $\Omega = 2\pi \times 10$ MHz, and scale the Rabi frequencies for the remaining n as: $\Omega_{\text{new}} = \Omega \Omega^{1,r}(n) / \Omega^{1,r}(61) \propto n^{-3/2}$ [79], where

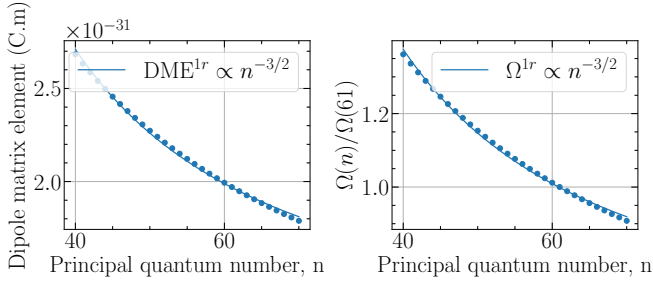


FIG. 12. Scaling of dipole matrix element and Rabi frequency with n [79]

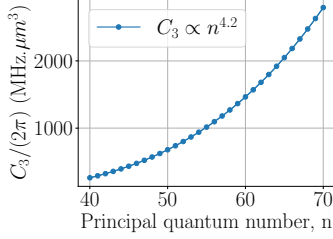


FIG. 13. Scaling of C_3 coefficient with n .

$|\tilde{r}\rangle \equiv |n^3 S_0\rangle$ and $|r\rangle \equiv |61^3 S_0\rangle$ [see Fig. 12]. Since we change the maximum Rabi frequency the whole pulse is rescaled as in the Rabi frequency analysis, therefore increasing the duration of the pulse linearly with n , which affects all sources of noise. Second and thirdly, and solely dependent on the choice of atomic species, is the scaling of the decay rate from the Rydberg states with n , which is approximately $\Gamma \propto n^{-3}$ [see Fig. 10], and the scaling of the C_3 coefficient mediating the DDI between the Rydberg states $|r\rangle$ and $|r'\rangle$, which is approximately $C_3 \propto n^4$ [see Fig. 13]. Lastly, the scaling of the driving laser wavelength with n , which for atomic transitions of the type $|0\rangle\langle r'|$ or $|1\rangle\langle r|$, scales as $\lambda \propto n^{-2}$ [see Fig. 14], will consequently have an effect on the effective wave vector associated with each driving laser, increasing the wave vector as $k_{\text{eff}} \propto n^2$ for increasing n .

As such, the scaling of the infidelity contributions from each source of noise scales differently with n . Interaction noise is both affected by the scaling of the Ω and by the scaling of the C_3 coefficient. Increasing n means first decreasing Ω , and due to Hamiltonian rescaling, decrease the V_{dipole} , which is equivalent to increasing the interatomic distance as $R \propto n^{1/3}$. This effect effectively reduces the interaction noise. Additionally, increasing the C_3 translates into scaling $R \propto n^{4/3}$, to keep the strength of the interaction V_{dipole} constant. Combining all scalings, the interaction strength scales as $V_{\text{dipole}} \propto n^{-1}$ and

the interatomic distance as $R \propto n^{5/3}$, with the standard deviation (B1) remaining constant. We indeed observe that interaction noise is reduced for larger n . Doppler noise, has a considerably simpler scaling. Although, the detuning scales as $\Delta \propto n^{-1}$ due to the scaling of Ω , since we assume our system to be resonance, this has

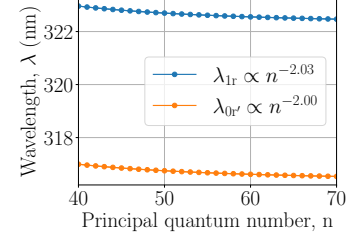


FIG. 14. Scaling of the transition wavelength with n .

no effect. Instead, the scaling of the noisy detunings arises from the scaling of the standard deviation (B8), that is, $\Delta \propto n^2$, meaning that increasing n increases the strength of Doppler noise. Decay noise has, in this case, two different scales: a scaling on the pulse duration – from the scaling of the Ω – given by $\tau \propto n$; and a scaling from the decay rate $\Gamma \propto n^{-3}$. Overall, since the the infidelity contribution from decay is approximately $1 - F_{\text{decay}} \sim \Gamma_r T_r + \Gamma_{r'} T_{r'}$, where T_r and $T_{r'}$ scale as τ , the final scaling is $1 - F_{\text{decay}} \propto n^{-2}$, that is, larger n reduce the strength of decay noise. Lastly, phase and intensity noise, scale solely with Ω as in the Rabi analysis, where in this case we expect that larger n increase(decrease) the effect of phase(intensity) noise.

Appendix F: Results for “Scheme A” with phase modulation

In this appendix, we repeat the approach of pulse selection and noise modelling presented in Secs. IV,V in the main text for “Scheme A” with *phase modulation*.

Again, we first select a set of candidate pulses from noise-free optimization by considering the noise-relevant duration quantities τ , T_{Ryd} , and $T_{\text{int}} V_{\text{dipole}}$ [see Fig. 15(a)]. For three candidate pulses, we evaluate the gate infidelity contributions from atomic noise [see Fig. 15(b-e)] and from laser noise [not shown]. Based on this analysis, “Pulse 2” (different pulse from the main text) is selected as best performing one. We then repeat the noise sensitivity analysis from Sec. V in the main text [see Fig. 16] for this pulse and find similar “optimal parameters” [see Tab. V]. Eventually, we obtain a gate fidelity $F \sim 99.95\%$ using this phase modulated pulse in “Scheme A”.

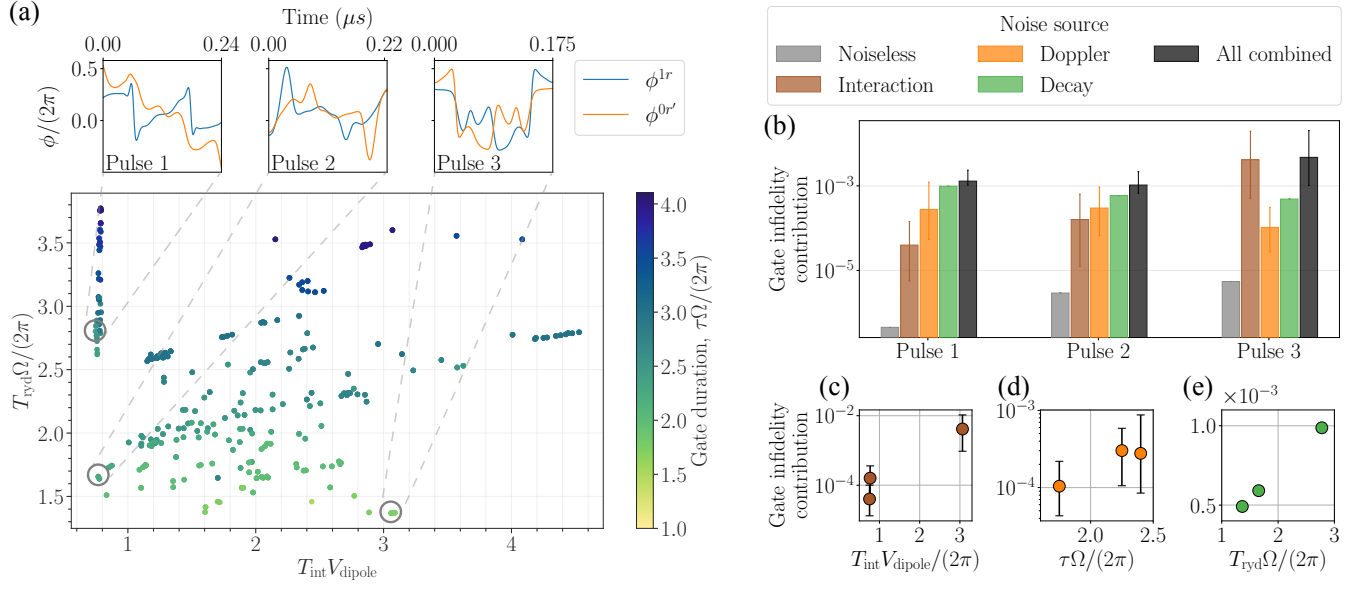


FIG. 15. Noise-aware pulse selection for “Scheme A” with phase modulation. See Fig. 5 in the main text for details.

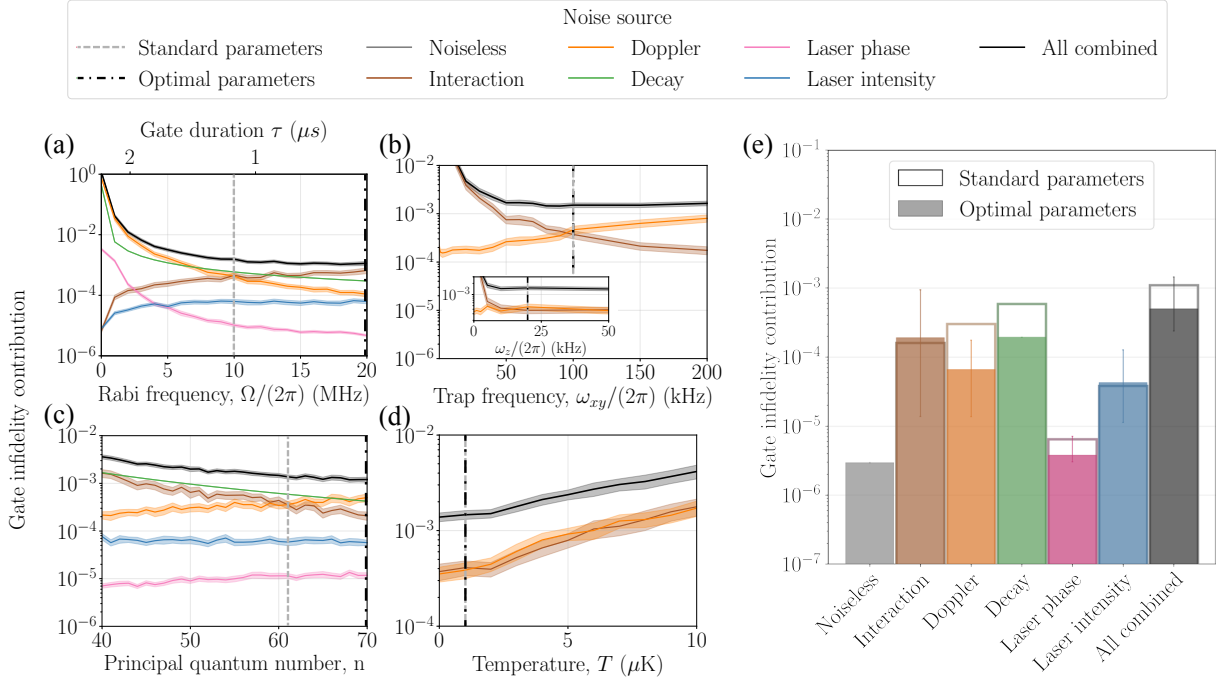


FIG. 16. Noise sensitivity for “Scheme A” with phase modulation. Here we consider “Pulse 2” selected in Fig. 15. See Fig. 8 in the main text for details.

Parameter		Standard	Optimal ("Pulse 2")
Rabi frequency	$\Omega/(2\pi)$	10 MHz	20 MHz
Trap frequency	$\omega_{xy}/(2\pi)$	100 kHz	100 kHz
Trap frequency	$\omega_z/(2\pi)$	20 kHz	20 kHz
Rydberg level	n	61	70
Temperature	T	1 μ K	≤ 1 μ K
Laser wavevector	k_{eff}^x	$3 \times 10^6 \text{ m}^{-1}$	–
Laser wavevector	$k_{\text{eff}}^{y,z}$	0	–
"Pulse 2":			
Interaction	$V_{\text{dipole}}/(2\pi)$	5 MHz	20 MHz
Distance	R	5.4 μ m	5.2 μ m
Gate fidelity	$\mathcal{F}$	99.89%	99.95%

TABLE V. Experimental parameters for the noise analysis for "Scheme A" with phase modulation in Appendix F. See Tab. I in the main text for details.