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Introduction The Rydberg blockade mechanism intro-creating bipartite entanglement with fidelity of ~ 0.7 – 0.8[2, 3]. There is good reason to believe that the fidelity achieved to date is not a fundamental limit, but is due to experimental perturbations and the high sensitivity of Rydberg states to external fields [4]. With the expectation that experimental techniques will continue to improve it is important to address the question of the intrinsic fidelity limit of the Rydberg blockade gate. Detailed analysis with constant amplitude Rydberg excitation pulses revealed a Bell state fidelity limit of $F_B~\sim~0.999$ in Rb or Cs atoms in a 300 K environment[5]. Other work has sought to improve on this with optimal control pulse shapes [6, 7], adiabatic excitation[8, 9], or simplified protocols that use a single Rydberg pulse[10, 11]. However, none of the analyses to date that consistently account for Rydberg decay and ل provided a fidelity better than 0.999. This leaves open the question of whether or not the Rydberg gate will be capable of reaching the 0.9999 level or better that appears necessary for scalable quantum computation with a realisitc overhead in terms of qubit numbers for logical encoding[12].



$$\hat{\mathbf{H}}_{d} = \omega_{g} |g\rangle\langle g| + \omega_{q} |1\rangle\langle 1| + \sum_{r'} \omega_{r'} |r'\rangle\langle r'|$$
(1a)

$$\hat{\mathbf{H}}_{g} = \Omega(t) \sum_{r'} \left(\frac{n}{n'}\right)^{3/2} \left(|r'\rangle\langle 0| + |r'\rangle\langle 1|\right) + \text{h.c.}$$
(1b)

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$$\Omega(t) = \varepsilon_x(t) \cos\left(\omega_d t\right). \tag{2}$$

Usually, atoms are driven on resonance with the $|1\rangle \leftrightarrow |r\rangle$ transition, so that $\omega_d = \omega_r - \omega_1$ with ω_r being the frequency of the target Rydberg state $|r\rangle$. In order to remove any oscillation on the order of ω_d from the dynamics, we choose to work in a frame rotating with ω_d in the remainder of this work. The pulse sequence which we will use to implement a two-qubit entangling gate is il-觅 state $|r\rangle$ of the target atom will be Rydberg-blockaded by B₀ during the 2π -pulse due to the control atom's $|r\rangle$ state being populated. Hence, the 2π -pulse will ideally produce a phase shift of π on the state $|1\rangle$ of the target atom. This scheme implements an entangling C_Z gate[1], $\hat{U}_{C_z} = \text{diag}(1, -1, 1, 1)$ in the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. This differs from the phase gate matrix of [1] due to our use of $-\pi$ instead of π for the last pulse which results in slightly better gate fidelity.

The Hamiltonian of the compound system, control and target atom, can be written as

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_{\text{control}} \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes \hat{\mathbf{H}}_{\text{target}} + \sum_{i,j} \mathsf{B}_{r_i,r_j} |r_i, r_j\rangle \langle r_i, r_j|.$$
(3)

Here, the B_{r_i,r_j} quantify the Rydberg interaction strength between all relevant Rydberg states $|r_i\rangle$ of the control atom and $|r_j\rangle$ of the target atom, including all possible leakage levels depicted in Fig.1c). The desired excitation is resonant between $|1\rangle$ and $|r\rangle$, with leakage channels to both $(n \pm 1)p_{3/2}$ states (detunings Δ_{\pm}).

To remove leakage to $np_{1/2}$ states we assume a specific implementation in Cs atoms where qubit state $|1\rangle$ is mapped to $|1'\rangle = |f = 4, m = 4\rangle$ before and after the Rydberg gate. With σ_+ polarized excitation light $|1'\rangle$ only couples to states $|np_{3/2}, f = 5, m_f = 5\rangle$ so there is no leakage to $np_{1/2}$ states, and errors due to coupling to multiple hyperfine states within the $np_{3/2}$ levels are also suppressed. For compactness of notation we refer to $|1'\rangle$ as $|1\rangle$ in the following.

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$$S(f,\delta) = \int_{0}^{T} \mathrm{d}t \ f(t)e^{i\delta t}$$
(4)

$$S(f,\delta) = \left(\frac{i}{\delta}\right)^N \int_0^T \mathrm{d}t \; \frac{\mathrm{d}^N f(t)}{\mathrm{d}t^N} e^{i\delta t}.$$
 (5)

To obtain a control shape $\varepsilon_x(t)$ which satisfies $S(\varepsilon_x, \delta_j) = 0$ for all $j = 1, \ldots, m$ we make the expansion

$$\varepsilon_x(t) = \varepsilon_x^{(0)}(t) + \sum_{k=1}^{N/2} \alpha_{2k} \frac{\mathrm{d}^{2k} \varepsilon_x^{(0)}(t)}{\mathrm{d}t^{2k}},\tag{6}$$

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$$1 + \sum_{k=1}^{N/2} \alpha_{2k} \left(-i\delta_j \right)^{2k} = 0, \quad j = 1, \dots, m.$$
 (7)

Parameter	Value		Parameter	Value	
	51	52		51	52
n	107	141	$\tau_n (\mu s)$	538	969
n'	106	138	$\Delta_+/2\pi$ (GHz)	-5.534	-2.507
n''	105	137	$\Delta_{-}/2\pi$ (GHz)	5.694	2.562
$\Delta_{1/2}^{\prime}/2\pi$ (GHz)	-2.961	-1.245	$\Delta'_{3/2}/2\pi$ (GHz)	-3.161	-1.333
$\Delta_{1/2}^{\prime\prime}/2\pi ({\rm GHz})$	3.256	1.495	$\Delta_{3/2}''/2\pi$ (GHz)	3.051	1.405
$B_0/2\pi~(\mathrm{GHz})$	1.54	0.68	$b_{n,n}$	1	
$b_{n,n'}$	0.85		$b_{n,n^{\prime\prime}}$	0.80	
$b_{n,n+1}$	1.02		$b_{n,n-1}$	0.97	

Population error We proceed to demonstrate how Gaussian pulses with DRAG components help to improve over previous methods by several orders of magnitude. Since the main advantage of Gaussian and DRAG shapes is an exponential suppression of leakage, we first focus on population error arising from leakage channels to other Rydberg states as shown in Fig. 1c). For our simulations we use the system parameters that are listed in Tab. I. The two different settings, S1 and S2, respectively, belong to two possible one-photon-excitation schemes starting from the Cs $6s_{1/2}$ state. Leakage errors are expected to be worse in S2 due to smaller energy splittings at higher Rydberg states, whilst lifetimes in S2 are better by roughly a factor of two. As initial pulses for DRAG and Gaussian control, we utilize generalized Gaussians of duration T

$$\varepsilon_G(t) = A_\theta \left[\exp\left(-\frac{(t-T/2)^2}{2\sigma^2}\right) - \exp\left(-\frac{(T/2)^2}{2\sigma^2}\right) \right]_{(8)}^{N+1}$$

with a standard deviation $\sigma = 2T/3$ and a pulse area θ determined by the value of $A_{\theta}[23]$. The exponent N + 1 ensures that the first N = 2m derivatives of the Gaussian vanish at times t = 0 and t = T. Note that N here is the same as e.g. in (6), so that we meet the conditions for Eq.(5) to hold. Unless stated otherwise, we fix the pulse length τ_c for the $\pm \pi$ -pulses on the control atom to $\tau_c = \tau_t/2$.

In Fig. 2 we show the overall population error for a Rydberg blockade entangling gate according to the pulse sezicizieii dedin dedi

Leakage can further be reduced by minimizing the ئ الحاط الحال atom while also avoiding blockade leakage into the tar-get pulses can be shaped independently of each other. Hence, for the area π pulses we use N = 4 in Eq.(6) ل which in turn increases the amplitude of the control pulse ր ົin the term of term o to the frequencies Δ' and Δ'' being very similar, the spec-ሻ in the spectrum shown in Fig. 1d). Using these frequencyselective shapes additionally yields 1.5 orders of magnitude improvement over Gaussians, hence improving over square pulses by up to four orders of magnitude. Best population errors are achieved for excitations in S1, owing to larger separations of atomic levels. Under these conditions, DRAG pulses allow speeding up gates by a factor of three compared to Gaussians, while achieving the same error. Compared to square pulses, the speed up lies in the range of several orders of magnitude.

Optimal Rydberg blockade The performance of the Ry-the blockade shifts. Scanning over the value of B_0 for a fixed gate time ($\tau_t = 30$ ns) reveals that the optimal value for $B_0/2\pi$ is around 1.5(0.7) GHz, for settings S1(S2) as illustrated in Fig. 3. This is explained qualitatively by analyzing the energies of all involved Rydberg states. For this purpose, we assume for simplicity that all blockades $\mathsf{B}_{r_i,r_j} \sim \mathsf{B}_0$. Starting in the initial state $\rho_{in} = |10\rangle \langle 10|$ we see that due to the first π -pulse populating $|np_{3/2}\rangle$, the Rydberg levels of the target atom are blockade-shifted by B_0 . As a consequence, for instance the leakage transitions into the $|n''\rangle$ subset are almost resonantly driven by the 2π -pulse if $B_0 \sim (\Delta_{1/2}'' + \Delta_{3/2}'')/2$, leading to even more undesired excitation. On the other hand, too small a blockade will produce large population errors since the 2π -pulse will leave population inside the almost resonant blockade-shifted $|np_{3/2}\rangle$ state. This motivates a careful



FIG. 2. (color online) Population error for a two-qubit Rydberg blockade entangling gate as a function of gate time $t_g = \tau_t + 2\tau_c$. Gaussian pulses reduce leakage errors by up to 2.5 orders of magnitude compared to conventional square controls, while additional supplementation with DRAG further improves by another 1.5 orders of magnitude for reasonable gate times. The DRAG pulses are designed to minimize primarily leakage into the $|n'\rangle$ subset of the control atom as well as blockade leakage in the target atom. The Rydberg blockades B₀/2 π are 1.54 GHz and 0.68 GHz for S1 and S2, respectively.



FIG. 3. (color online) Population error for a fixed gate time $\tau_t = 30$ ns as a function of the blockade shift B_0 in settings S1 and S2. The error is minimized for a value of $B_0/2\pi \sim 0.7$ GHz in S2. In S1, the population error is optimal for blockade shifts in the range of 0.7 - 2.7 GHz.

analysis of the Rydberg energies since an unsophisticated choice of B_0 might introduce severe frequency crowding issues and tremendously lower gate fidelities.

leakage states as

$$P_{\text{leak}} \propto \frac{1}{(n+1)^3 (\Delta_1 + \mathsf{B}_0)^2} + \frac{1}{(n-1)^3 (\Delta_1 - \mathsf{B}_0)^2} \\ + \frac{1}{(n')^3 (\Delta_2 - \mathsf{B}_0)^2} + \frac{1}{(n'')^3 (\Delta_2 + \mathsf{B}_0)^2} + \frac{1}{n^3 \mathsf{B}_0^2}.$$
(9)

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Entanglement fidelity The ideal unitary after the sequence in Fig. 1 is

$$\hat{\mathbf{U}}_{\mathrm{Cz},\vec{\phi}} = \mathrm{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}), \qquad (10)$$

with $\phi_{ij} \equiv \phi_{ij,ij}$ being a shorthand notation for phases on the diagonal elements. To turn the C_Z -like gate in Eq.(10) into an entangling CNOT-like gate we slightly modify the procedure that turns a C_Z into a CNOT gate: Applying a Hadamard on the target qubit before and after the C_Z results in a CNOT gate. Similarly, we find that a general $\pi/2$ rotation

$$\hat{\mathbf{R}}(\vec{h}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{ih_{00}} & e^{ih_{01}} \\ e^{ih_{10}} & e^{ih_{11}} \end{pmatrix}$$
(11)

with phases $\vec{h} = (h_{00}, h_{01}, h_{10}, h_{11})$ can be used to turn, up to relative phases, Eq.(10) into a CNOT. If the entangling phase $\phi_{\text{ent}} = \phi_{00} - \phi_{01} - \phi_{10} + \phi_{11}$ of Eq.(10) is exactly π , the transformation

$$\left(\hat{1} \otimes \hat{R}(\pi, \tilde{\phi}, -\tilde{\phi}, 0)\right) \hat{U}_{C_{\mathbf{Z}}, \phi} \left(\hat{1} \otimes \hat{R}(0, 0, 0, \pi)\right)$$
(12)

$$F = \left(\operatorname{Tr}_{\mathbb{Q}} \left\{ \sqrt{\sqrt{\rho}\rho_{\mathrm{id}}\sqrt{\rho}} \right\} \right)^2.$$
 (13)

Here, we take the partial trace over the computational subspace $\mathbb{Q} = \operatorname{span}\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ to disregard irrelevant information about non-computational states.

For $\rho_{\rm id} = |\Phi_+\rangle\langle\Phi_+|$ we denote the fidelity as Bell state fidelity F_B . The results are shown in the upper plot of Fig. 4 whereby we assume that the $\pi/2$ gates on the qubit subspace are perfect gates. We observe that Gaussian controls seem to achieve better results than a naive DRAG control. However, the main reason for DRAG pulses to perform poorly at a first glance is wrong phases. Originally, it was proposed to change the drive frequency ω_d as a function of time to account for this effect [13]. However, it is also possible to employ a constant detuning Λ from resonance, i.e. $\omega_d = \omega_r - \omega_q + \Lambda$ [26], with the benefit of less experimental effort being required. We find, that detuning the target 2π pulse is sufficient to achieve low enough errors. As a consequence of offresonant drive, rotation errors will be induced which can be corrected by rescaling the amplitudes of the pulses (by up to 3% only for the fastest gates). The difference between the solid black line and the dotted red one in Fig. 4 illustrates that a constant detuning and a rescaled amplitude indeed account for this induced error, yielding at least two orders of magnitude improvement over Gaussian waveforms. As one would expect from previous results [13], the detuning scales proportionally to the Rabi frequency squared, yielding approximately a $1/\tau_t^2$ power law whereby the optimal detuning for a 2π pulse of 25 ns is 124.07 MHz. We find that we are able to produce Bell states with a fidelity of 0.9999 for $t_g \sim 50$ ns using detuned DRAG pulses with amplitude correction.

An alternate approach to account for phase issues is by waiting an appropriate time $t_{\rm gap}$ between the pulses [2] or to track phases in software and correct for them afterwards. The former approach will noticeably prolong the gate times compared to our approach. Overall, detuned DRAG pulses yield an improvement of more than two orders of magnitude compared to conventional shapes. Furthermore, the necessary gate times are less than 10^{-7} of the few second coherence times that have been demonstrated with neutral atom qubits[27], substantiating that Rydberg gates are a promising approach for scalable quantum computing.

Including spontaneous emission All results in the previous section are based on unitary evolution of the atoms. A more realistic model incorporates decay due to finite lifetimes of the energy levels. We employ a Lindbladian model to simulate the effects of decoherence, whereby we assume that population of Rydberg levels decays by a fraction of 7/8 into some auxiliary level $|g\rangle$ that has zero effect on the rest of the dynamics. The residual part decays with equal probabilities into the states $|0\rangle$ and $|1\rangle$ of the atoms. Hence, the full dynamics of our system are goverened by the Lindblad master equation for the density operator $\hat{\rho}$

$$\dot{\hat{\rho}} = -i\left[\hat{\mathbf{H}}, \hat{\rho}\right] - \frac{1}{2}\sum_{r} \left(\hat{\mathbf{C}}_{r}^{\dagger}\hat{\mathbf{C}}_{r}\rho + \rho\hat{\mathbf{C}}_{r}^{\dagger}\hat{\mathbf{C}}\right) + \sum_{r}\hat{\mathbf{C}}_{r}\hat{\rho}\hat{\mathbf{C}}_{r}^{\dagger}.$$
(14)

Here, the operators $\hat{\mathbf{C}}_r = \hat{\mathbf{c}}_r \otimes \hat{\mathbf{1}} + \hat{\mathbf{1}} \otimes \hat{\mathbf{c}}_r$ describe decay of all relevant Rydberg states $|r\rangle$ in both atoms into $|g\rangle$,



FIG. 4. (color online) Unitary Bell state infidelity as a measure for entanglement generated by the pulse sequence in Fig. 1 using square pulses, Gaussians, DRAG, detuned (d) DRAG controls and detuned DRAG controls with amplitude correction (d/r) for the setting S1 as well as optimized DRAG controls in S2. Detuning DRAG pulses on the target atom accounts for wrong phases and combines less leakage with high degrees of entanglement. The necessary detuning Λ decreases proportionally to $1/\tau_t^2$ with a value of $\Lambda/2\pi = 124.07$ MHz at $\tau_t = 25$ ns.

 $|0\rangle$ and $|1\rangle$, i.e.

$$\hat{\mathbf{c}}_r = \sqrt{\Gamma_r} \left(\frac{7}{8} \left| g \right\rangle \langle r \right| + \frac{1}{16} \left| 0 \right\rangle \langle r \right| + \frac{1}{16} \left| 1 \right\rangle \langle r \right| \right).$$
(15)

The decay rate Γ_r is the inverse of the lifetime τ_r of a Rydberg state $|r\rangle$. Values for the target Rydberg states in both settings are given in Tab. I. For an experiment at room temperature (~ 300 K) in setting S1, we find that Bell states are generated with a fidelity of better than 0.9999 at a gate time of \lesssim 60 ns. The results for optimized DRAG pulses are plotted in Fig. 5. As expected because of shorter lifetimes, non-unitary errors become visible earlier in S1 than in S2. However, unitary errors are dominant, so that gates in S1 apear to be more promising than those in S2, despite the shorter lifetimes. Since the π pulses on the control atom do not require blockade effects, we may run them faster without losing performance. The dotted red curve in Fig. 5 confirms this observation. For $\tau_c = \tau_t/3$ we achieve slightly better results, yielding errors less than 10^{-4} at only 50 ns gate time. In a 4 K environment lifetimes will be on the order of a few ms, allowing for performance very similar to that for the unitary analysis.

We have characterized the gate performance in terms of the Bell state fidelity. While the fidelity is the most widely used measure of gate performance, others have been proposed[28]. In particular the trace distance has been shown to be linearly sensitive to Rydberg gate phase errors that affect the fidelity only quadratically[5]. Using the rescaled and detuned DRAG gates that optimize the fidelity we find that the trace distance error is an order of magnitude larger. As it is an open question as to which performance measure is most relevant for specific quantum computational tasks we have not studied the trace distance in more detail, although we anticipate



FIG. 5. (color online) Bell state infidelity including decay from all Rydberg levels for optimized detuned DRAG controls in both settings S1 and S2. Bell states are generated with a fidelity of 0.9999 at a total gate time of only 50 ns.

that the trace distance error could also be reduced with appropriate pulse design,

Summary In conclusion we have presented DRAG pulses with x quadrature control for Rydberg blockade gates that lead to Bell state fidelity $F_B > 0.9999$ with gate times of 50 ns. The pulses are generated with an analytical method that could readily be extended to the

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level structure of other atoms. The results fully account for all the dominant leakage channels as well as Rydberg decay in a room temperature environment. The 50 ns gate time is orders of magnitude faster than high fidelity art superconducting qubit gates, while the ratio of coherence time to gate time is orders of magnitude better. Together with recent progress in high fidelity single qubit gates [27, 29] DRAG pulses establish neutral atom gubits with Rydberg gates as a promising candidate for scalable quantum computation. Our result specifically applies to the case of one-photon Rydberg excitation. We leave extension to the more common case of two-photon excitation for future work. We also emphasize that the predicted gate fidelity assumes no technical errors and ground state laser cooling. Demonstrating real performance close to the theoretical level established here re-

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mains an outstanding challenge.

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