Electron cloud design for Rydberg multi-qubit gates

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This article proposes quantum processing in an optical lattice, using Rydberg electron’s Fermi scattering from ground-state atoms in spin-dependent lattices as a source of interaction. Instead of relying on Rydberg pair potentials, the interaction is controlled by engineering the electron cloud of a sole Rydberg atom. Here we specifically propose the implementation of two prominent multi-qubit gates i.e. the stabilizer-phase operator and the Toffoli gate. The new scheme addresses the main bottleneck in Rydberg quantum simulation by suppressing the population of short-lived Rydberg states over multi-qubit operations. This scheme mitigates different competing infidelity criteria, eliminates unwanted cross-talks, and allows operations in dense atomic lattices. The restoring forces in the molecule type Ryd-Fermi potential preserve the trapping over a long interaction period. The features in the new scheme are of special interest for the implementation of quantum optimization and error correction algorithms.

The recent experimental progress in the development of highly controllable quantum systems using Rydberg atoms enabled a parameter regime where fully functional quantum information processing algorithms are in reach. While individual control of atoms and their interactions has been achieved, the next step is the development of complex interactions between multiple quantum bits (qubits) which are of great interest for applications ranging from quantum optimization to error-correcting codes.

A particular application of near-term quantum devices is solving optimization problems using a gate model approach. The parity architecture [11 2], translates a problem with all to all connectivity to a simple nearest-neighbor problem-independent interaction. Hence, the quantum approximate optimization algorithm (QAOA) [3 4] implementation would be simplified to programming single-qubit operations, as well as applying problem independent four-body stabilizer-phase gate. The other prominent multi-qubit gate is Toffoli, playing a pivotal role in quantum error correction [5 6], fault tolerant quantum computation (QC) [7 8] and Shore’s algorithm [9].

The realization of multi-qubit gates with the concatenation of one- and two-qubit gates [10 11] results in a significant overhead [12 13]. The long-range many-body Rydberg interaction is vastly used in different quantum operations [14 25] including direct operation of multi-qubit gates [26 31]. The fidelities of these direct Rydberg multi-qubit gates are limited by the competing requirement of the presence (absence) of inter- (intra-) component interaction in addition to the short lifetime of the Rydberg level.

This article introduces a versatile toolbox to engineer multi-qubit operations by designing the Rydberg electronic cloud with respect to the lattice geometry. A spin-dependent lattice [32 31] is used to harvest the Fermi-scattering of the Rydberg electron [12 43] from neighboring lattice sites as a source of coherent interaction for the desired gates. The spin-dependent geometrical shift of atoms accommodates them inside or outside of the Rydberg electron’s wave-function, providing a spin-dependent nearest-neighbor interaction appropriate for gate operations. This double-encoding of qubits in internal and external degrees of freedom distinguishes the gate from previous proposals without spatial encoding of the qubit. In a previous work, spin-flip via Rydberg-Fermi interaction at very short inter-atomic distances below 50nm has been studied [44]. However such short lattice constants are not realizable in the experiment. The dual spin/spatial encoding proposed in this article provides strong qubit-dependent interaction within the present optical lattices.

In terms of scalability, making dense atomic lattices would be a promising approach in passing from the current era of intermediate-scale quantum devices. The new advances in sub-wavelength imaging and laser addressing of atoms [45 31] allow operation precisions in the nanometer scale. These advances call for new techniques for multi-qubit interactions at ultra-short distances. In the Rydberg-Fermi scheme, the interaction to loss ratio improves by going to smaller lattice constants, with examples studied here at 400nm and 500nm lattice constants. The restoring forces in the molecule type Rydberg-Fermi potential preserve the trapping over a long interaction period. The other bottleneck in the scalability of the Rydberg quantum processors comes from the lifetime of the Rydberg states. At small inter-atomic distances, the dipolar scheme is limited to short-lived Rydberg states with low principal number to avoid strong level-mixing and line-broadening [34 50]. In
the Rydberg-Fermi scheme, the absence of strong level-mixing close to the outer shell of the Rydberg wave-function, allows for choosing highly excited Rydberg states with longer lifetime. Furthermore, the Rydberg-Fermi gate schemes, significantly reduce the Rydberg population over the gate operation time. For example in C\textsubscript{k}-NOT, the Rydberg population averaged over 2\textsuperscript{k+1} qubit configurations scales by k in dipolar schemes [28] [29]. In contrast in the Rydberg-Fermi protocol the Rydberg population scale 2\textsuperscript{−(k+1)} is in favour of multi-qubit operations, see App. C. This would also be of special interest for quantum search algorithm [57] [58].

The Rydberg-Fermi scheme is especially appealing for fast multi-qubit operations. In an architecture of one vs many qubits, the presence/absence of inter/intra component interaction paves the way for the implementation of C\textsubscript{k}-NOT [26, 28, 29] and C-NOT\textsuperscript{c} [28] gates in minimal pulse steps as well as direct operation in logical basis [59]. In Rydberg-dipolar schemes, the fast operation is carried out by exciting all k control atoms in |0\rangle state to the Rydberg level followed by target Rydberg rotation [27] [29]. This results in competing requirements i.e. to preserve the lattice trapping against strong dipolar interaction, to overcome/preserve the blockade between inter/intra components, and to not excite the neighboring Rydberg levels [26, 28, 29, 60–62]. In the Rydberg-Fermi approach, multi-qubit operations are carried out by exciting a single atom to the Rydberg state. The system thus operates the many-body interaction at a different regime of energy hierarchy without the mentioned rivalry in Rydberg-dipolar systems. Furthermore, the absence of intra-component interaction eliminates the unwanted phase errors in multi-qubit gates, see the App. C.

RESULTS

Rydberg-Fermi interaction in a qubit-dependent lattice

In a two-dimensional lattice shown in Fig. 1a, atoms in spin-states |0\rangle, |1\rangle are trapped in shifted lattices distinguished by red and blue. The gate operations are carried out by exciting the central atom in a plaquette to the Rydberg level. Depending on whether the central atom is excited from |0\rangle or |1\rangle state, the plaquette atoms in |0\rangle or |1\rangle spin-lattice would be localized on the nodes and antinodes of the Rydberg electron’s last lobe, see Fig. 1a-d. This provides contrast on the Fermi scattering of the electron from distinguished qubit states of plaquette atoms. The qubit-dependent interaction could also be realized by the spin-dependent shift perpendicular to the lattice plane as depicted in Fig. 1b.

The spin-dependent lattice is formed by counter-propagating linearly polarized lights, see Fig. 1b,c. Introducing a relative shift between the fields’ polarizations of 2\theta, the total electric field can be written in terms of the sum of right and left circularly polarized lights \( E = E_0 \exp(-\text{i}vt)(\sin(k_0 \theta + \theta) + \sin(k_0 \theta - \theta)) \). To make a spin-dependent lattice-shift, the spin polarizabilities should be linked to different circular polarization components of lights [32]. To cancel the polarizabilities with unwanted light elements shown by dashed lines in Fig. 1b, the trapping laser must be tuned between \( P_{3/2} \) and \( P_{1/2} \) states so that the ac-Stark shifts of these two levels cancel each other. As a result the \( m_F = \pm 1/2 \) levels of the ground state would be trapped by \( V_{\pm} = \alpha |E_0|^2 \sin(kz \pm \theta) \). The hyperfine qubit states |0\rangle = |F = 1, m_F = 1\rangle and |1\rangle = |F = 2, m_F = 2\rangle experience \( V_0 = (V_+ + 3V_-)/4 \) and \( V_{11} = V_+ \). A spin-dependent

![Fig. 1. Rydberg-Fermi interaction in Spin-dependent lattice.](image-url)
lattice provides dual spin/spatial encoding of the qubit. A Raman transition coherently transfers atoms from one internal state to the other, thereby causing hopping between the two Wannier-functions \[63,65\]. The spin rotation Rabi frequency in qubit-dependent lattice would be modified by the Frank-Condon factor, see App. B.

**Ryd-Fermi Interaction** – The interaction between the Rydberg electron and the ground state atom is a Fermi type pseudo potential \[66,68\]. The electron wave-vector \(k(R)\) is defined by the kinetic energy of the Rydberg electron at energy \(E = -1/2n^2\) when it collides with a ground-state atom, i.e. \(k^2(R)/2 = E + 1/R\). The level-shift caused by the Rydberg electron scattering from the \(lth\) plaquette atom in the qubit state \(i = 0, 1\) would be characterized by two parameters

\[
\tilde{V}_{RF(i)} = \int |w(R - l_i)|^2 V_{RF}(R) dR
\]

and

\[
MD_{V_{RF(i)}} = \int |w(R - l_i)|^2 |V_{RF}(R) - \tilde{V}_{RF(i)}|^2 dR
\]

that are the average and the mean deviation of the scattering energy over the \(lth\) plaquette atom’s Wannier-state \(w\) centred at \(l_i\). Considering the symmetry of the Rydberg wave-function all plaquette atoms would experience the same qubit-dependent interactions. The Rydberg electron’s wave-packet dynamics are in the ps range \[70,71\]. Therefore, over the MHz scale of operation, the interaction of the Rydberg electron with all the plaquette atoms in \(|1\rangle\) qubit state would be alike and add up, see \[43\].

Two-color excitation of the superposition state \((|65F_{3/2}, 1/2\rangle + |65F_{1/2}, 1/2\rangle)/\sqrt{2}\) with in-plane quantization axis provides sites’ specific couplings along a line, see Fig. \[4\]. The two-color light could be obtained in a setup of beamsplitters and acusto-optical modulators. The generated superposition mainly contains the \(Y_{1,0}\) spherical harmonic term, which significantly concentrates the electron wave-function along the quantization axis and hence enhances the interaction strength. The atoms prepared in ground motional state \[72,73\] are considered delocalized over the Gaussian wave-function. Hence they would experience an effective Rydberg-Fermi interaction that is averaged over their spatial profile. The scattering energy of Rydberg electron over the qubit-dependent Wannier state of the \(lth\) plaquette atom with FWHM=20nm would be quantified by Eq. \[2\] as

\[
\tilde{V}_{RF(l)} = 2MHz, \quad MD_{V_{RF(l)}} = 0.1MHz
\]

\[
\tilde{V}_{RF(0)} = 0.3MHz, \quad MD_{V_{RF(0)}} = 0.2MHz
\]

**FIG. 2.** Superposition of Rydberg states. (a) The desired Rydberg superposition could be controlled by the polarization angles \(\theta_{R,B}\) of the two linearly polarized fields \(\Omega_{R,B}\) propagating along the \(z\) direction. (b) The transitions shown by dashed-lines would form destructive interference when \(\theta_{R} - \theta_{B} = \pi/2\), leading to the superposition of \(\langle e^{i(\theta_{R} + \theta_{B})}|m_j = 5/2\rangle + e^{-i(\theta_{R} + \theta_{B})}|m_j = -3/2\rangle/\sqrt{2}\) states of 6D Rydberg level. (c) Applying the qubit-dependent shift perpendicular to the lattice plane allows tunning the in-plane inter-atomic distance. The (d) \(xy\) and (e) \(xz\) cross-sections of Rydberg-Fermi interaction. The excited Rydberg superposition state would be further confined around the position of plaquette atoms and hence enhances the interaction. Red and White ovals present the qubit-dependent position of \(|0\rangle\) and \(|1\rangle\) states.

where the qubit-dependent lattice-shift of \(D = 36.8nm\) is considered.

To apply a uniform interaction on all the plaquette atoms, the polarization axis must be perpendicular to the lattice plane, see Fig. \[1\] and \[2\]. The interaction enhancement can be obtained by exciting superposition of Rydberg levels. The spatial constructive (destructive) interference of Rydberg wave-functions over the position of plaquette qubits (elsewhere) could further confine the electron and hence enhances the interaction. The desired Rydberg superposition could be controlled by the polarization angles \(\theta_{R,B}\) of the two linearly polarized lights \(\Omega_{R,B}\) used for Rydberg excitations, see Fig. \[2\]. These fields are propagating perpendicular to the lattice plane along the \(z\) direction. The linear polarized light could be expressed in terms of circular polarizations \(\Omega_{\pm} = (\exp(i\theta_{R})\Omega_{R}^{+} + \exp(-i\theta_{B})\Omega_{B}^{-})/\sqrt{2}\). Adjusting \(\theta_{R} - \theta_{B} = \pi/2\) the transition to \(|nD_{\pm}^{3/2}\rangle, m_j = 1/2\) would be canceled by destructive interference. Hence the excited state would be

\[
e^{i(\theta_{R} + \theta_{B})}\frac{|nD_{\pm}^{3/2}, \frac{5}{2}\rangle + e^{-i(\theta_{R} + \theta_{B})}|nD_{\pm}^{3/2}, \frac{-3}{2}\rangle}{\sqrt{2}}.
\]

The simultaneous excitation of both \(|nD_{3/2}\rangle\) and \(|nD_{5/2}\rangle\)

could be obtained by beam splitting and frequency adjustment of the blue laser. This could be realized in a setup of beamsplitters and acusto-optical modulators. The polarization angles in Eq. 4 would act as a controlling parameter to rotate the interaction maxima e.g. $\vartheta_R + \vartheta_B = \pi, 0$ are corresponding to Fig. 2, and the same pattern rotated by $\pi/4$ around the z axis. For the sake of presentation, Fig. 1 and 2 only plot the s-wave scattering part of $V_{RF}$, which is the dominant term at the desired last lobe in $^{87}$Rb atoms. The exciting laser’s polarization and propagation direction could act as a controlling knob to program different interaction connectivities among neighboring lattice sites.

In the setup of Fig. 1, with lattice constant of 400nm, exciting the central atom to the superposition state of Eq. 4 with $n=64$, the scattering energy of the Rydberg electron over the qubit-dependent Wannier state of the $1^{th}$ plaquette atom with $FWHM_{x,y}=20$nm and $FWHM_z=35$nm would be quantified by Eq. 2 as

$$V_{RF|1_i|} = 2.5\text{MHz}, \quad MD_{V_{RF|1_i|}} = 0.25\text{MHz} \quad (5)$$

$$V_{RF|0_i|} = 0.35\text{MHz}, \quad MD_{V_{RF|0_i|}} = 0.20\text{MHz},$$

where the magic lattice-shift of $D = 35.6$nm in the qubit-dependent structure results in uniform $V_{RF|0_i|}$ inside and outside the last lob. To further narrow the interaction induced line broadening $MD_{V_{RF|1_i|}}$, ultra-tight confinement of atoms could be obtained by the dark-state optical-lattices [51] and deep confinement to sub-nanometer scale is expected in Rydberg-empowered optical-lattices [52].

The scale of interaction to loss ratio improves by going to smaller Rydberg principal numbers. The volume of the Rydberg electron scales by $n^6$ [68]. Hence the electron density and the interaction scales by $V_{RF} \propto n^{-6}$. Since the lifetime of the Rydberg state scales by $n^3$ [70], the interaction to loss ratio would scale by $n^{-3}$, see Fig. 3. While the lattice configuration of Fig. 2 allows tuning the desired inter-atomic distance, going to a low principal numbers would raise concerns about single site addressing, see App. E. The new advances in sub-wavelength trapping, spin rotating and imaging [45–51] provide a wide range of opportunities for the Rydberg-Fermi QC. Also, dual-species lattices [77–79] could be used to suppress the laser-cross talk issues in compact lattices.

Applying the lattice shift perpendicular to the lattice plane provides a freedom in choosing the inter-atomic distance, see Fig. 2c–e. In the $\lambda = 1064$nm optical lattice [53], exciting the central atom to the superposition state of Eq. 4 with $n=74$, the scattering energy of the Rydberg electron over the qubit-dependent Wannier state of the $1^{th}$ plaquette atom with $FWHM_{x,y}=25$nm and $FWHM_z=35$nm would be quantified by Eq. 2 as

$$V_{RF|1_i|} = 1.1\text{MHz}, \quad MD_{V_{RF|1_i|}} = 0.07\text{MHz} \quad (6)$$

$$V_{RF|0_i|} = 0.1\text{MHz}, \quad MD_{V_{RF|0_i|}} = 0.05\text{MHz},$$

where the qubit-dependent lattice-shift of $D_z = 180$nm is considered.

![FIG. 3. The scaling of interaction to loss ratio. (a) The scattering interaction of Rydberg electron from the four plaquette atoms over the decay rate of the central Rydberg atom is plotted as a function of the principal number for Rydberg states $|nS_{1/2},1/2\rangle$, $|nP_{3/2},3/2\rangle$, and for the state presented in Eq. 4. While smaller $n$ enhances the coherence, (b) the smaller inter-atomic distance raises concerns about single site addressing.](image)

**IMPLEMENTATION OF MULTI-QUBIT GATES**

**Parallelized gate**

The Ryd-Fermi interaction in qubit-dependent atomic lattice could be used for the implementation of the parallelized gate

$$U_g = |0\rangle_c |0\rangle_i \otimes I + |1\rangle_c |1\rangle_i \otimes \prod_{i=1}^{4} \sigma_x^{il}\quad (7)$$

which is an essential element in realizing the stabilizer-phase gates [80], see Methods for detailed discussion.

In this proposal, the target atoms are localized on the square plaquette around the central control atom. Exciting the $|1_c\rangle$ state of the control atom to the Rydberg level, its electron creates potential energy shits via Fermi scattering. In the spin-dependent lattice, the contrast of scattering energy depends on the presence or absence of the Rydberg electron at the position of different qubit states. Over the operation time $\tau$, the effective Hamiltonian

$$H = a_{c1}^\dagger a_{c1} \sum_{i \in p} (V_{RF|1_i|} a_{i1}^\dagger a_{i1} + V_{RF|0_i|} a_{i0}^\dagger a_{i0}) \quad (8)$$

accumulates a contrast of $\pi$ phase on each target atom in $|1\rangle$ qubit state conditioned on the control atom being in state $|1_c\rangle$. Here $a_{i1}^\dagger$ annihilates (creates) the Wannier-state of the $l^{th}$ target qubit in the plaquette, centred at $l_i$ with $i \in \{0,1\}$ defining the qubit-dependent trap. Compensating the background phase [81] and applying Hadamard to the individual target atoms before and after the Rydberg excitation results in the desired operation of Eq. 4.

**Gate fidelity:** The main sources of errors in quantifying the C-NOT gate’s operation are spontaneous emission and population rotation errors. The errors are averaged
over the $2^5$ qubit configurations. The average spontaneous emission error from the Rydberg level is given by $E_{sp,r} = \frac{1}{2} \frac{\pi}{\Gamma_r} \Gamma_r$, where $U_{RF}$ is the qubit-dependent contrast of $V_{RF}$ and $\Gamma_r$ is the decay rate of the Rydberg state \[^{10}\]. In a two-photon excitation scheme of Fig. 2a, partial population of the intermediate $|6P_{3/2}\rangle$ level results in an extra source of loss. Considering the effective two-photon excitation $\Omega_r = \frac{\Omega_{sp,rr}}{2 \delta_p}$, using high power lasers \[^{14}\] facilitates large Rabi frequencies $\Omega_{1013}/2\pi = 250\text{MHz}$, $\Omega_{420}/2\pi = 250\text{MHz}$ and $\delta_p/2\pi = 5\text{GHz}$. The corresponding average error would be $E_{se, p} = \frac{\pi}{4\delta_p} (q+1/q) = 4 \times 10^{-4}$ \[^{14}\] with intermediate level lifetime of $\tau_p = 113\text{ns}$ and $q = \Omega_{420}/\Omega_{1013}$. The control atom’s rotation error is due to the unwanted excitation of neighboring accessible Rydberg levels with $\delta_p/2\pi = 17\text{GHz}$, $21\text{GHz}$ and $6\text{GHz}$ energy separation in Fig. 1f, 1d and 2 respectively, summing up to an average error of $1/2 \frac{\Omega_r^2}{\delta_p^2}$. Finally, non-deterministic excitation of Rydberg atom due to qubit-dependent level-shift caused by Rydberg-Fermi interaction should be overcome by the strong exciting laser $\Omega_r$, tuned to the middle of the spectrum leading to average error of $1/2^{5} \sum_{j=0}^{4} \left( \frac{4}{j} \right) \left( \frac{\gamma_{2j} V_{RF}^2}{4 \delta_p} \right)^j$. Overall, using the schemes described in Fig. 1f, 1d, 2d with interactions quantified in Eq. 3, 5, 6 and with the respective Rabi-frequencies $\Omega_r = 200, 100, 40 \text{ MHz}$ results in high fidelity fan-out gate with the average fidelity of F=99.8%, 99.7%, 99.6% at the cryogenic environment of 77K and F=99.5%, 99.3%, 99.2% without cryogenic environment at 300K. The bottleneck in operation fidelity comes from the small lifetime of the Rydberg level. Using Rydberg circular state enhances the interaction to loss ratio by four orders of magnitude, see App. A.

Toffoli gate

The Toffoli gate $C_k$-NOT with $k = 4, 6$ could be realized in square and triangular lattices, by placing the control atoms over the plaqueette and exciting the central target atom in $|1\rangle_c$ state to the Rydberg level. The Fermi scattering of the Rydberg electron from control atoms forms an interaction-based level-shift on the target atom that depends on the spatial qubit configuration of the entire system. Unlike the C-NOT$^k$ gate, Toffoli does not operate with strong laser for deterministic Rydberg excitation. Here a weak transition $\Omega_r = \frac{\Omega_{sp,rr}}{2 \delta_p} \ll V_{RF}$ would selectively excite the Rydberg atom conditioned on the control atoms to be in $|0\rangle^\otimes^k_c$ state. The presence of any $|1\rangle_c$ state localized that control atom inside the Rydberg wave-function of the target atom, shifting the laser out of resonance and blocking the transition. The operation Hamiltonian would be

$$H_{tot} = (\Omega_1 \sigma_{1p} + \Omega_2 \sigma_{rp} + h.c.) + \delta_p \sigma_{pp} + \Delta \sigma_{rr}$$

where $\sigma_{ij} = |i\rangle\langle j|$ is the transition/projection operator acting on the target atom, $\Omega$ and $\delta_p$, $\Delta$ are the Rabi frequency, and laser detuning from the intermediate and Rydberg levels in a two-photon excitation. The last term would sum over the control qubits around the central target atoms and apply qubit-dependent Rydberg-Fermi interaction. Adjusting the laser to $\Delta = -k V_{RF}|0\rangle$, the $2\pi$ rotation of the target atom would be conditioned on the presence of $|0^k 1\rangle_c$ state, generates a $\pi$ phase, and apply the desired $C_k$-Z operation. Sandwiching the target atom with Hadamard gates results in the desired Toffoli operation. The Rydberg-Fermi interaction operates the $C_k$-Z with a single $2\pi$ pulse addressing the Rydberg level, leaving no Rydberg population unprotected from the laser. This would eliminate the errors associated with the conventional gate schemes with $\pi$-gap-$\pi$ Rydberg exciting pulses as discussed in \[^{20},^{34}\].

The main sources of errors in quantifying the $C_k$-NOT gate’s operation are spontaneous emission of the atomic levels, and population rotation errors. The spontaneous emission from the Rydberg level only occurs in the qubit configuration $|0^k 1\rangle_c$ where the single target atom gets excited to the Rydberg level. Hence the averaged operation error of $E_{sp,r} = \frac{1}{2\pi} \frac{\pi}{\Gamma_r}$ is expected. Off-resonant Rydberg excitation results in blockade leakage adding up to the average error of $E_{1} = \frac{1}{2\pi} \sum_{j=1}^{k} \left( \frac{k}{j} \right) \frac{\Omega_r^2}{\delta_p^2 V_{RF}^2}$, where $j$ is the number of control atoms in $|1\rangle_c$ qubit-dependent lattice. In the two-photon excitation, blockade is sensitive to the locking bandwidth of the lasers, which could be made less than $1\text{kHz}$ \[^{35}\]. Also in case of fast operation, the large frequency bandwidth of exciting pulses might affect the blockade at the heart of the scheme. Circle signs in Fig. 4 quantify the operation of the gate by simulating the master equation encountering the spontaneous emission from intermediate and Rydberg levels as well as the de-phasing terms associated with lasers’ line-width. Also, the frequency profiles of the laser pulses are encountered in the lasers’ detuning and Rabi frequencies as discussed in App. D. The analytic and numeric simulations of Fig. 4 suggest high fidelity operations of 99.8% could be expected in the setup of Fig. 1d. Other avenues in enhancing the fidelity are discussed in App. A. Which are based on improving the interaction and lifetime using the resonance scattering in Cs atoms and higher orbital angular momentum quantum numbers.
DISCUSSION

This article proposes highly controllable multi-qubit operations, based on engineering the electronic cloud of a single Rydberg atom with respect to the atomic lattice. The new scheme significantly reduces the population of short-lived Rydberg states during the multi-qubit operation compared to other fast conventional dipolar schemes. Restricting the Rydberg population to a single site eliminates unwanted intra-component interactions, facilitating high-fidelity multi-qubit gates. In a quantitative comparison of the conventional dipolar scheme with the proposed Rydberg-Fermi approach, App. C shows that the new approach is a significant step in the implementation of single-step multi-qubit operations.

The proposed Toffoli gate is operating with a continuous \(2\pi\) pulse, leaving no Rydberg population unprotected from the laser. This would eliminate the errors associated with the conventional schemes with \(\pi\)-gap-\(\pi\) Rydberg exciting pulses as discussed in \([20], [84]\). Another advantage of having a single Rydberg atom is closing the Anomalous broadening decoherence \([88], [89]\). Direct implementation of multi-qubit gates in this proposal would reduce the operation steps and hence the accumulative errors. As an example, the \(C_6\)-NOT gate operation with concatenated Rydberg C-NOT gates \([12], [13]\) requires 112 pulses. Significant contrast obtains in the Rydberg-Fermi scheme operating by three pulses.

In the outlook, the proposed Rydberg-Fermi interaction paves the way for long-distance entanglement and direct operations on the logical basis \([59]\). This would facilitate the investigation of phenomena, and protocols that arise in quantum information over a wide dimension of physical qubit state space while operating on the logical basis that is growing polynomially.

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METHODS

Implementing stabilizer phase-gate using parallelized gate

The implementation of the stabilizer operator $B_p = \prod_{i \in p} \sigma_x^{(i)}$ over the plaquette spins applies in three steps i.e. $B_p = H^{-1}U_sH$ where $H = \sum_{i \in [p,c]} \exp(i\pi/2\sigma_x^{(i)})$ is Hadamard applying over all the plaquette and control atoms and $U_s$ is the parallelized Ryd-Fermi gate of Eq. 7. For the control qubit prepared in $|0\rangle_c$, the gate $B_p$ coherently transfers the control qubit into the state $|1\rangle_c$ ($|0\rangle_c$) for the odd (even) parity of plaquette spin. Then $A_p = \prod_{i \in p} \sigma_x^{(i)}$ stabilizer would be obtained by exclusive application of Hadamard on control atom. The desired stabilizer-phase gate, would be implemented by application of a phase shift on the control qubit, sandwiched by applying/reverting the stabilizer operator $B_p$.

\[
U_{\square}(\theta) = e^{i\theta B_p} = B_p^{-1} e^{i\theta \sigma^{(c)}_z} B_p, \quad (10)
\]

with $\theta$ being optimized between $[0, \pi]$ in QAOA. At the end, the control atom would be factored out by transferring to the ground state.

Data availability

All data needed to evaluate the conclusions in the article are presented in the article and/or the Supplementary Figures. Additional data related to this paper may be requested from the corresponding author.

Competing interests

The authors declare no competing interests.

Author contribution

The project is defined, derived and written by M. Khazali. The project is benefited from the scientific advice of W. Lechner.

SUPPLEMENTAL MATERIAL

APPENDIX A: RYDBERG CLOUD ENGINEERING IN A TRIANGULAR LATTICE

Rydberg states with high orbital angular momentum in rubidium lattice

Going to high orbital angular momentum numbers, the centrifugal force pushes the electron away from the core towards the neighboring ground-state atoms. This could enhance the interaction strength. In the extreme limit, the maximum angular momentum $l = n - 1$ in the circular Rydberg state forms an ideal torus wave-function, see below.

Exciting $|nL_j, m_j = j\rangle$ Rydberg state would exclusively excite the $Y_{L_j}$ spherical harmonic. With the quantization axis being perpendicular to the lattice, the electron wave-function would be confined close to the 2D lattice plane providing a homogenous interaction for all plaquette atoms. The electronic cloud of two Rydberg states $|64D_{5/2, 5/2}\rangle$ and $|62G_{9/2, 9/2}\rangle$ are plotted in Fig. 5. Please note that $|nD\rangle$ and $|nG\rangle$ state could be excited via a single photon [90] and double photon quadrupole transitions respectively. Corresponding Rydberg-Fermi interaction and gate fidelities in a triangular lattice are quantified in table I.

| #   | State                  | $D_z$ (nm) | $(\sigma_{x,y}, \sigma_z)$ (nm,nm) | $V_{RF|1\rangle}$ (MHz) | $V_{RF|0\rangle}$ (MHz) | $MDV_{RF|1\rangle}$ (MHz) | $MDV_{RF|0\rangle}$ (MHz) | 1-Fid Cg-NOT |
|-----|------------------------|------------|-----------------------------------|-------------------------|-------------------------|-------------------------|-------------------------|---------------|
| 1   | $|64D_{5/2, 5/2}\rangle$ | 150        | (25,30)                            | 12                      | 13                      | 17                      | 17                      | 0.002         |
| 2   | $|62G_{9/2, 9/2}\rangle$ | 150        | (25,30)                            | 1.7                     | 1.6                     | 1.6                     | 1.6                     | -             |
| 3   | $|64D_{5/2, 1/2}\rangle$ | 100        | (25,30)                            | 0.45                    | 0.047                   | 0.04                    | 0.015                   | 0.003         |
| 4   | $|62G_{9/2, 1/2}\rangle$ | 45         | (20,20)                            | 0.45                    | 0.08                    | 0.08                    | 0.017                   | -             |

Table I: The wavelength of the in-plain optical-Lattice in #1,3 is $\lambda = 795$nm and in #2,4 is $\lambda = 780$nm [91]. In calculating the fidelity, spontaneous emission of $nD$ state at 300K environment temperature is considered [76].

Further confinement of electron cloud perpendicular to the lattice, allows smaller qubit-dependent lattice-shift $D_z$. This would enhance the Franc-Condone factor and facilitates the qubit rotation on the spin-dependent lattice. Exciting $|nL_j, 1/2\rangle$ forms a cloud with $L$ angular nodes. The two examples of $|64D_{5/2, 1/2}\rangle$ and $|62G_{9/2, 1/2}\rangle$ are
FIG. 5. Designing the Rydberg cloud with respect to the lattice sites depicted by red/white ovals corresponding to the $|0\rangle/|1\rangle$ qubit states. (a) Shining the laser perpendicular to the lattice plane (that defines the quantization axis along $z$), the symmetry of the wave function in the lattice plane results in a uniform interaction with all plaquette qubits. (b,c) Exciting $|nL_j, m_j = j\rangle$ would confine the cloud close to the lattice plane providing larger interaction. (d,e) Exciting $|nL_j, m_j = 1/2\rangle$ increases the number of the angular nodes, allowing significant reduction of the qubit-dependent lattice-shift with the price of reducing the interaction strength.

These states allow operation in small $D_z$ qubit-dependent lattices with significant overlap of two-qubit Wannier states. The drawback in choosing these types of states is the weak strength of the interaction, see table I.

### Realization with Circular states

The recent advances in fast transition to the Rydberg circular states $^{92,93}$, would make them an ideal choice for Rydberg-Fermi gates’ application. The ponderomotive potential of focused Laguerre-Gauss (LG) beams, enables site addressing in exciting circular states $^{93}$. Exciting the circular state $|58C\rangle$ of a $^{87}$Rb atom, the electron would be confined at the position of neighbouring qubits at 176nm, see Fig. 6. Considering a plaquette atom with Gaussian ground motional state of FWHM=18nm and qubit dependent lattice shift of $D = 50$nm, the interaction would be quantified according to $\bar{V}$ as

$$
\bar{V}_{RF|1\rangle} = 39\text{MHz}, \quad \text{MD}_{V_{RF|1\rangle}} = 4\text{MHz}
\bar{V}_{RF|0\rangle} = 0.5\text{MHz}, \quad \text{MD}_{V_{RF|0\rangle}} = 0.27\text{MHz}
$$

The other advantage of the circular state comes from the minimized overlap of the wave-function with the ionic-core which results in an enhanced lifetime in the order of minutes $^{94}$. In an alternative approach one can encode the central atom’s $|0_c\rangle$ and $|1_c\rangle$ qubit states in the ground $|g\rangle$ and the circular state $|nC\rangle$. The laser transition between close circular states $|1_c\rangle = |nC\rangle$ and $|(n+11)C\rangle$ $^{95}$ could be used to turn on the Ryd-Fermi interaction. The radial interaction profile of $|58C\rangle$ and $|47C\rangle$ are plotted in Fig. 6, showing maximum and minimum overlap with a plaquette atom confined at 176nm. The interaction of $|1_c\rangle$ central qubits would be compensated with global dynamical decoupling (DD) sequences such as WAHUHA $^{96}$.

### Strong resonance scattering in Cs atoms

Another approach to enhancing the interaction to loss ratio is harnessing the p-wave near resonance scattering from $^{133}$Cs atoms, available at smaller electron kinetic energies at larger interatomic distances compared to the
resonance position in $^{87}\text{Rb}$ [97]. Fig. 7 plots the potential energy curves (PEC) of $|46D_{5/2}, 5/2\rangle + |6S\rangle$ coupled with the neighbouring Rydberg states $|43H + 42H + 47P + 48S\rangle + |6S\rangle$ under Ryd-Fermi interaction

$$V_{\text{RF}} = (2\pi \tan(\delta^*)/k(R) - 6\pi \tan(\delta^*)/k^3(R) \nabla_r \cdot \nabla_r) \delta(r - R).$$

Here $|nH\rangle = \sum_{l,m} |n, l, m\rangle$ represents the Hydrogen state encountering semi degenerate orbital angular momentum numbers $2 < l < n$. The matrix elements in the manifold of coupled states are given by

$$H_{nlm,n'l'm'}(R) = \langle \psi_{nlm}(R)|V_{\text{RF}}|\psi_{n'l'm'}(R)\rangle,$$

$$H_{nlm,nlm} = -\frac{R_y}{n^{*2}},$$

where $R_y$ is the Rydberg constant of Cs atoms and $n^*$ is the effective Rydberg principal number. Diagonalizing 8000 coupled states, the energy potential is plotted in Fig. 7. In a UV optical-lattice with $\lambda = 350$nm, the Fermi scattering of Rydberg electron from the neighbouring lattice site would result to about 400MHz level-shift of the Rydberg level ideal for fast quantum operations.

For the p-wave scattering of Rydberg electron from the neighboring ground state atom, the gradient of the Rydberg wave-function $\psi = R_{nl}(r)Y_i^m(\theta, \phi)$ at the position of the neighboring lattice site is required which is

$$\nabla \psi(r, \theta, \phi) = \left[ \frac{\partial R_{nl}(r)}{\partial r} Y_i^m(\theta, \phi) \right] \left[ \frac{\partial Y_i^m(\theta, \phi)}{\partial \theta} \right] = \left[ \frac{1}{r} \frac{\partial R_{nl}(r)}{\partial r} Y_i^m(\theta, \phi) \right] \left[ \frac{1}{r \sin \theta} \frac{\partial Y_i^m(\theta, \phi)}{\partial \theta} \right],$$

in the spherical coordinate. The radial wave-function and its derivative are calculated numerically using the Numerov technique [98].

In a triangular lattice of Fig. 7a, the in-plane $x-y$ Cs trap is formed by 350nm UV laser dressing the ground state to $|10P\rangle$ state. Considering the Gaussian ground motional state with a half-width at 1/e maximum of $\sigma_{x,y} = 8.7$nm, the atom would accommodate within a single lobe of $V_{\text{RF}}$, see Fig. 7c. Alternative trapping schemes are discussed in [99]. For spin-dependent trap perpendicular to the plane (along the $z$) the $\lambda = 870$nm laser could be used for dressing $|6S\rangle$ to $|6P\rangle$, with $U/2\pi = 2$MHz, $\sigma_z = 20$nm, $D_z = 100$nm. Exciting the target atom to $|46D_{5/2}, 5/2\rangle$, the Rydberg-Fermi interaction averaged over the $i^{th}$ plaquette atom’s wave-function in the ground motional state would be

$$\tilde{V}_{RF|i_1\rangle} = 365$MHz, \hspace{1cm} MD$_{V_{RF|i_1\rangle}} = 0.07$MHz

$$\tilde{V}_{RF|o_1\rangle} = 2$MHz, \hspace{1cm} MD$_{V_{RF|o_1\rangle}} = 0.06$MHz

see Eq. 2 for the definitions. This contrast of spin-dependent level-shift with narrow lines allows fast selective laser excitation of central atom conditioned on the plaquette qubits’ configurations. This would result in high fidelity operation of Cs-NOT gate as depicted in Fig. 7. The fidelity is quantified along the same lines described in Fig. 4.

Single site addressing requires ultra strong focusing with large NA microscope [100][101], see App. E. Alternatively, the sub-wavelength localized population rotation via semi interferometer techniques [45][46] or dual-species atomic lattice [4][59][77][79] with central $^{87}\text{Rb}$ and plaquette $^{133}\text{Cs}$ atoms could be used to improve single site addressing.
APPENDIX B: QUBIT-ROTATION IN THE SPIN-DEPENDENT LATTICE

Qubit-rotation in the spin-dependent lattice – A spin-dependent lattice provides dual spin/spatial encoding of the qubit. A Raman transition coherently transfers an atom from one internal state to the other, thereby causing hopping between the two Wannier-functions \( |A\rangle \) and \( |B\rangle \). The polarizability of the qubit states \( |0\rangle \) and \( |1\rangle \) and the intermediate electronic-level \( |5P_{1/2}, 1/2\rangle \) in the optical lattice are given by different light polarization elements, see Fig. 8a,b, and do not need to be orthogonal. Also using the Condon approximation, the dipole transition of electronic states is equivalent to the Franck-Condon principle in molecular physics. Under the Born-Oppenheimer approximation, the electronic and centre of mass positions are belonging to different traps and do not need to be orthogonal. Also using the Condon approximation, the dipole transition of electronic states is assumed independent of nuclear coordinates. In conclusion, the dipole transition would be modified by the overlap of the wave functions i.e. Franck-Condon factor \( f = \langle w(R - l_A) \rangle \langle w(R - l_B) \rangle \).

Effective qubit-rotation rate: The Hamiltonian \( H = H_0 + H_d \) consists of the energy level of electronic states \( H_0 \), and the dipole transitions \( H_d \). The Hamiltonian of the system in the rotating wave approximation and in the basis

\[
\psi_{i_1}(R, r) = w(R - l_1) \psi_{e,i}(R, r)
\]  

where \( r \) and \( R \) are addressing the electronic and centre of mass positions. The Wannier function of the \( i \)th site in the \( i \in \{0, 1, p\} \) spin dependent lattices is given by \( w(R - l_i) \). The electric dipole transition from a state \( A \) to an excited state \( B \) is given by

\[
\langle \psi_A | (R + r) | \psi_B \rangle = \langle w(R - l_A) | w(R - l_B) \rangle \langle \psi_e, A | r | \psi_e, B \rangle.
\]  

Here we have the orthogonality of the electronic eigenstates but the vibrational states are belonging to different traps and do not need to be orthogonal. Also using the Condon approximation, the dipole transition of electronic states is assumed independent of nuclear coordinates. In conclusion, the dipole transition would be modified by the overlap of the wave functions i.e. Franck-Condon factor \( f = \langle w(R - l_A) \rangle \langle w(R - l_B) \rangle \).
\[ \tilde{H} = \begin{bmatrix} 0 & 0 & f_{0p_0} \Omega_0 / 2 & f_{0p_1} \Omega_0 / 2 & \cdots & f_{0p_n} \Omega_0 / 2 \\ 0 & \delta & f_{1p_0} \Omega_1 / 2 & f_{1p_1} \Omega_1 / 2 & \cdots & f_{1p_n} \Omega_1 / 2 \\ f_{0p_0} \Omega_0 / 2 & f_{1p_0} \Omega_1 / 2 & \Delta - 1/2 \omega_{tr} & 0 & \cdots & 0 \\ f_{0p_1} \Omega_0 / 2 & f_{1p_1} \Omega_1 / 2 & 0 & \Delta - 3/2 \omega_{tr} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ f_{0p_n} \Omega_0 / 2 & f_{1p_n} \Omega_1 / 2 & 0 & 0 & \cdots & \Delta - (n + 1/2) \omega_{tr} \end{bmatrix} \]

where \( \Delta = \omega_{L0} - (\omega_p - \omega_0) \), \( \delta = (\omega_{L0} - \omega_{L1}) - (\omega_1 - \omega_0) \). The Frank-Condon factors \( f_{in} = \int w^*_n (x - l_i) w_{p_n} (x - l_p) dx \) quantify the overlapping of the qubit states \( i = 0, 1 \) and intermediate \( |p\rangle \) state’s Wannier function \( w_{p_n} \) for the nth motional state. The Schrödinger equation in the interaction picture could be written in terms of coupled equations:

\[
\frac{dC_0}{dt} = i \sum_{j=0}^{n} f_{0j} \Omega_0 C_j / 2
\]

\[
\frac{dC_1}{dt} = i \sum_{j=0}^{n} f_{1j} \Omega_1 C_j / 2
\]

\[
\frac{dC_{p_j}}{dt} = i \left( \frac{f_{0j} \Omega_0}{2} C_0 + \frac{f_{1j} \Omega_1}{2} C_1 + [\Delta - (j + 1/2) \omega_{tr}] C_{p_j} \right)
\]

Under the condition that \( \Delta \) is the dominant term the amplitudes \( C_{p_j} \) would oscillate much faster than \( C_0 \) and \( C_1 \). Hence we can apply adiabatic elimination by substituting

\[
C_{p_j} = -\frac{f_{0j} \Omega_0 C_0 + f_{1j} \Omega_1 C_1}{2(\Delta - (j + 1/2) \omega_{tr})}
\]

into equations 10, 11. Hence the system would be represented by an effective two-level system:

\[
\frac{dC_0}{dt} = -i \sum_{j=0}^{n} f_{0j} \Omega_0^2 C_0 + f_{0j} \Omega_0 f_{1j} \Omega_1 C_1 / 4(\Delta - (n + 1/2) \omega_{tr})
\]

\[
\frac{dC_1}{dt} = -i \sum_{j=0}^{n} f_{0j} \Omega_0 f_{1j} \Omega_1 C_0 + f_{1j} \Omega_1^2 C_1 / 4(\Delta - (n + 1/2) \omega_{tr}) + i\delta C_1 + i\delta C_1
\]

Assuming that \( \Delta \gg U_{tr} \) the effective Rabi frequency in the two-level system would be

\[
\tilde{\Omega} = \frac{\Omega_0 \Omega_1}{4\Delta} \sum_{j=0}^{n} f_{0j} f_{1j}
\]

and the effective detuning of the two-level system would be

\[
\delta_{eff} = \delta - \sum_{j=0}^{n} \frac{f_{0j} \Omega_0^2 - f_{1j} \Omega_1^2}{4\Delta}
\]
The qubit-rotation is performed in the regime of $\hat{\Omega} \ll \omega_{\text{tr}}$ to avoid exciting the motional Bloch bands.

**APPENDIX C: COMPARING RYDBERG-DIPOLAR AND RYDBERG-FERMI GATES**

Rydberg decay

The main bottleneck in the Rydberg quantum computation/simulation is the short lifetime of Rydberg levels. The Rydberg dipolar multi-qubit Toffoli $C_k$-NOT gate could be realized by two approaches as explained in [29]. In the fast scheme, all control atoms in $|0\rangle$ qubit state would get excited to the Rydberg level with simultaneous pulses. In that case, the control atoms would be out of the intra-component blockade and the average population of Rydberg levels in control atoms over the $2k + 1$ qubit configurations would scale by $k$ leading to an average Rydberg decay error of $k\Gamma(\pi/2\Omega + 3\pi/2\Omega)$ see Eq. 5 in [29]. In the other scheme operating with sequential excitation steps, the Rydberg population is limited to one due to the global blockade effect but the $2k+3$ sequence of excitation would result in a long operation time leading to the same scaling of average Rydberg decay error of control atoms $k\Gamma(\pi/2\Omega)$ [29]. This is in contrast to the Rydberg-Fermi scheme where the only qubit configuration with a single Rydberg population is $|0^{k+1}\rangle$ qubit state. In the other $2^{k+1} - 1$ qubit configurations, the target laser would be out of resonance and no population would be excited. Hence the Rydberg decay error averaged over all qubit configurations would be $\frac{1}{2^k}\pi/2\Omega$. Please note that the scheme could operate for $k = 6$ in a triangular lattice and $k > 6$ by increasing the principal number. This results in a significant difference compared to the dipolar scheme.

**Phase errors due to intra-component interaction**

One of the advantages of implementing multi-qubit operations with the single step Rydberg-Fermi scheme compared to the fast Ryd-dipolar counterpart is in the absence of intra-component interaction. To quantify the effects of this unwanted phase on gate performance, the phase sensitive form of fidelity is used

$$F_{\text{id}} = \text{Tr}((M + M^\dagger))/2n, \quad \text{(28)}$$

where $M = U_{\text{id}}^U U_{\text{gate}}$, with $U_{\text{id}}$ and $U_{\text{gate}}$ representing the ideal and realistic gate operations. Dimension of the qubit configurations in $C_k$-NOT or C-NOT$^k$ is given by $n = 2^{k+1}$.

Evaluating the fidelity of Rydberg-dipolar $\text{Toffoli gate}$ $C_k$-NOT proposed in [29], with the phase dependent definition of fidelity in Eq. 28 reveal the effects of unwanted phase. In [29], control and target atoms are getting excited to $|60S\rangle$ and $|60P\rangle$, with optimum laser couplings of $\Omega_c/2\pi = 180\text{MHz}$, $\Omega_t/2\pi = 0.8\text{MHz}$ and lattice separation of $4\mu\text{m}$. Simulating the gate operation under the Schrödinger equation, encountering spontaneous emission and population rotation errors in addition to the infidelity encountered by unwanted phases leads to the average infidelity of $5\%$ quantified by Eq. 28. Importantly, large phase-dependent infidelities would occur for specific qubit configurations with large Rydberg population e.g. $|1111\rangle_c |1(0)\rangle_t$ experience $52\%$ (12\%) infidelity. This is while the phase independent conventional definition leads to $2\%$ average infidelity. In the proposed Ryd-Fermi approach the absence of intra-component interaction, reduced rotation errors at the lower principal numbers, and reduced Rydberg population results in high-fidelity operations that surpass the conventional counterparts [28, 29] while the scheme allows orders of magnitude compression of the atomic quantum processor. Notably, the assigned fidelity is below the 1.4\% fidelity threshold for surface error correction codes.

The implementation of Rydberg-dipolar parallelized gate [102] is also sensitive to the intra-component interaction. Using the parameters of Ref. [102], in the absence of the Rydberg control atom, each of the target atoms would follow the dark state $|D\rangle = (\Omega_t |A\rangle - \Omega_p |R\rangle)/N$ with the Rydberg population of $P_k = (\frac{\Delta}{\Omega})^2$ on each target atom. For the abbreviation, the readers are referred to [102] for the scheme explanation and parameter definitions. With phase independent definition of fidelity, Ref. [102] predicts the gate operation to be insensitive to strong intra-component interaction $V_{jk}$, see Fig. 9. However, using the parallelized gate for the implementation of the stabilizer operator [80] makes the operation

![Figure 9](image-url)
phase-sensitive. Applying phase-dependent definition of fidelity Eq. 23, the dipolar Rydberg gate is significantly sensitive to $V_{jk}$ as shown in Fig. 9. This comparison shows the value of Rydberg-fermi gates in the implementation of quantum simulation and optimization algorithms.

**APPENDIX D: ADIABATICITY AND PULSE DURATION**

In the parallelized gate, the Rydberg-Fermi potential modifies the optical trapping experienced by the plaquette atoms in $|1_i⟩$ Wannier states. It is important to apply the changes adiabatically to avoid an unwanted entanglement between the computational and the motional states. Over the Rydberg excitation of the control atom, target atoms in $|1_i⟩$ Wannier state would experience trap evolution $U_{trap} = U_{op} + P_c(t)V_{RF}$ where $U_{op}$ is the optical trap, $P_c$ is the Rydberg population of the central atom. As long as the dynamic is adiabatic, i.e. $\omega_{trap} ≪ \omega^2_{trap}$ [103], the Wannier states of the $|1_i⟩$ can adapt continuously and stays close to the instantaneous ground motional state. Operating the C-NOT gate with shorter pulses $τ_f$ frequencies compared to Toffoli and in principle could operate Rydberg level would be 17GHz, 21GHz and 6 GHz respectively. In Fig. 1 and 2, the level spacing to the next dipole accessible Rydberg wave-function blocks the Rydberg excitation. Hence no bound state would be formed and the above adiabaticity discussion does not limit the Toffoli scheme. Stronger confinement of atoms in dark-state optical-lattices [51] or twist-optical-lattices [52] with sub-nanometer trap width, allows faster adiabatic operations.

The other concern about pulse duration is related to the pulse bandwidth. While fast operation makes short pulses desirable, short pulses would be wide in bandwidth and might excite the neighboring Rydberg levels [104] in fan-out or disturb the blockade in Toffoli gate. For the chosen Rydberg levels $|65P_{3/2}⟩$, $|64D⟩$ and $|75D⟩$ in Fig. 1 and 2, the level spacing to the next dipole accessible Rydberg level would be 17GHz, 21GHz and 6 GHz respectively. The fan-out gate operates with stronger Rabi frequencies compared to Toffoli and in principle could operate with shorter pulses $τ_f ≳ 140ns$. Corresponding pulse bandwidths would be at least three orders of magnitude smaller than the level spacing in the above-mentioned cases.

In the fast operation of the Toffoli gate, the laser pulse bandwidth might be comparable with the interaction-induced level-shift suppressing the blockade at the heart of the scheme. Circle signs in Fig. 4 quantify the gate’s operation by simulating the master equation encountering the pulse bandwidth, the spontaneous emissions in two-photon excitation, and the dephasing terms associated with laser line-widths as described below. The effective Rabi frequency in two-photon excitation $Ω_r = \frac{Ω_{RF}B_{l}}{2\hbar}$ is obtained by $Ω_{RF} = \frac{Ω_{lock}}{2\hbar}$ lasers that are detuned from intermediate $|p⟩$ level by $δ_p/2\pi = 5GHz$. The Gaussian pulses $Ω_r e^{-\frac{(t-T)^2}{\sigma^2}} e^{-\frac{(T/\pi)^2}{\sigma^2}}$ are considered in the numerics with $σ = T/5$ and a pulse duration $T$ given $\int_0^T Ω(t)dt = 2π$. Over the two-photon excitation, the Fourier transform of the two laser pulses would be $Ω_1(ω1) = Ω_{RF} e^{-\frac{ω^2}{ω^2_{l}}}$ and $Ω_2(ω2) = Ω_{lock} e^{-\frac{ω^2}{ω^2_{l}}}$ with $ω_i$ indicating the central frequency of the pulse and the pulse bandwidth is presented by $w = 1/σ$.

The driving Hamiltonian of Eq. 9 is a function of the pulse frequency elements $ω_{12}$ and $ω_{11}$ both in Rabi frequencies and detunings. The Fourier transform of the two laser pulses would be $Ω_1(ω1) = Ω_{RF} e^{-\frac{ω^2}{ω^2_{l}}}$ and $Ω_2(ω2) = Ω_{lock} e^{-\frac{ω^2}{ω^2_{l}}}$ with $ω_i$ indicating the central frequency of the pulse and the pulse bandwidth is presented by $w = 1/σ$. The laser detunings from the intermediate and Rydberg levels $δ_p = ω_{12} - ω_{1p}$ and $Δ = ω_{21} + ω_{2r} - ω_{1r}$ are also a function of the pulse frequency elements. In Fig. 4a,b the master equation (Eq. 29) is simulated for distinct pulse frequencies $ω_{12}$, $ω_{21}$ and the final results are averaged over the Gaussian frequency profile of the two laser pulses.

In the operation, the target atom is subject to dephasing and decay terms that are encountered by the master equation

$$\dot{\hat{ρ}} = -i[\hat{H}, \hat{ρ}] + \mathcal{L}(\hat{ρ}) \tag{29}$$

where the Liouvillian term $\mathcal{L}(\rho) = \sum_β \mathcal{D}(c_β) \rho$ with

$$\mathcal{D}(c)\rho = cρc^† - 1/2(c^† cρ + ρ c^† c)$$

in the Lindblad form governs the dissipative time evolution. Lindblad terms encounter spontaneous emission from the intermediate level to the qubit states $c_{1p} = \sqrt{γ_l/2}|1⟩⟨1|$, $c_{op} = \sqrt{γ_{p}/2}|0⟩⟨p|$ as well as the loss of population from Rydberg state to other electronic states $c_{op} = \sqrt{γ_τ}|0⟩⟨τ|$. Furthermore, the dephasing terms associated by the lasers’ linewidth are included as $c_{11} = \sqrt{γ_l}|1⟩⟨1|$, $c_{pp} = \sqrt{γ_{pp}}|p⟩⟨p|$, $c_{rr} = \sqrt{γ_{rr}}|r⟩⟨r|$, where $γ_l = (γ_{lock} + γ_{11} - γ_{12})/2$, $γ_{pp} = (-γ_{Lock} + γ_{11} + γ_{22})/2$, $γ_{rr} = (γ_{Lock} - γ_{11} + γ_{22})/2$ [105] with $γ_{11}$ and $γ_{22}$ being the line-widths of $Ω_1$ and $Ω_2$ lasers (corresponding to 420m and 1013nm lasers respectively). The coherence in two-photon excitation would be sensitive to the linewidth of the Lock $γ_{Lock}$ when the lasers are locked out of phase [105], which could be suppressed to less than 1kHz [30].

**APPENDIX E: SINGLE SITE ADDRESSING**

Applying local light-shift

The Laser cross-talk and misalignment could affect the accuracy of gate operation in compact lattices. The population that does not return to the qubit basis over the
Rydberg excitation would be considered as loss. Inspired by \cite{50}, single-site addressing could be performed by applying site-selective differential light-shift to the $|1\rangle r$ transition. Focusing the 788nm auxiliary laser to the targeted site, only the desired atom would get in-resonance with the Rydberg exciting laser.

To quantify the single site addressing efficiency, we consider a microscope with NA=0.68 that focuses the 788nm light to $1/e^2$ intensity waists of $w$ =370nm and 500nm \cite{53}. The alignment accuracy of 25nm has been achieved for single-site addressing \cite{50}, which is subject to improvement by e.g. sub-wavelength localization of atoms \cite{17,18}. The generated light-shift by the focused laser has the form of $U_{LS}(x,y) = U_{LS} e^{-2((x-x_0)^2+(y-y_0)^2)/w^2}$ with $r_0 = \sqrt{x_0^2 + y_0^2}$ being the laser misalignment. At the central site, this misalignment would cause a detuning $\Delta (r_0) = U_{LS}(1 - e^{-2r_0^2/w^2})$ in $|1\rangle r$ transition that changes the effective Rabi frequency $\tilde{\Omega} = \sqrt{\Omega^2 + \Delta^2}$. Hence for the central atom, starting at $|1\rangle$ qubit state, after the gate operation time $\tau = \frac{\pi}{2\tilde{\Omega}}$, the qubit state would not be fully retrieved, which results in an error of $E_c = \frac{\Omega^2}{2\tilde{\Omega}} \sin^2 (\Omega \tau/2)$. Considering the uncertainty in addressing a specific site within distance $r_0$, the error of the centred atom must be averaged $\tilde{E}_c = \frac{1}{\pi r_0^2} \int E_c(r) 2\pi r \, dr$. Taking into account the error distribution profile, the optimum operation time would be modified from $\tau = \frac{\pi}{2\tilde{\Omega}}$ to $\tau_{opt} = \frac{2\pi}{\sqrt{\Omega^2 + \Delta^2(r_0)}}$.

The averaged error of the centered atom $\tilde{E}_c$ is plotted by dashed lines in Fig. 10 as a function of $U_{LS}/\Omega$. The infidelities caused by laser misalignment could be suppressed by spatial beam shaping \cite{108}.

Concerning the laser cross talk, the detuning experienced by the neighbouring plaquette atoms must be large enough to avoid population leakage out of the qubit basis. The leakage probability of a plaquette atom in $|1\rangle$ qubit state over the operation time $\tau_{opt}$ is given by $E_p = \frac{\Omega^2}{\Omega^2 + \Delta^2(|r|)^2} \sin^2 \left( \frac{\Omega^2}{12} \Delta (|r|)^2 \pi \right)$ where $|r| = |a - r_1 - r_p|$ is the distance from the centre of the laser beam to the neighbouring plaquette atom. Here $a$ is the distance vector between centered and a plaquette site, and one needs to average over the laser misalignment $r_1$ and also over the position of the plaquette atom $r_p$, considering its Wannier wave-function to find the average loss population $E_p$ of a plaquette atom in $|1\rangle$ state. The variation of the averaged plaquette error is plotted by solid lines in Fig. 10 as a function of $U_{LS}/\Omega$. The Oscillation is due to the change of effective Rabi frequency $\tilde{\Omega}$, which leads to different values of Rydberg leakage at the plaquette sites after the gate operation. At large $U_{LS}/\Omega$ and also for weak laser focusing (large $w$) the variation of detuning over the plaquette atoms’ wave-functions would be large and hence averaging the error over $r_1$ and $r_p$ washes the oscillation pattern. The laser cross talk could be suppressed by using two species lattices \cite{59,77,79}. Considering both plaquette error $\tilde{E}_p$ and the central atom error $\tilde{E}_c$, Fig. 10 shows that single-site operations with high fidelity is achievable in the designed setups discussed in the main text.

The scattering of the auxiliary laser could also affect the fidelity. To give an example a 420nm auxiliary laser focused to 370nm, dresses the $|1\rangle$ qubit state by $|6P_{1/2}\rangle$ with $\Omega_{LS}/2\pi = 200\text{MHz}$ and the laser detuning of $\Delta_{LS}/\Omega_{LS} = -150$. This laser imposes a differential light-shift of $U_{LS} = \Omega_{LS}^2/4\Delta_{LS} = -2.1\text{MHz}$ on the $|1\rangle - |r\rangle$ transition. In a Toffoli gate with $\Omega_c/2\pi = 30\text{kHz}$ (Fig. 4), the single-site addressing infidelity of 0.003 is expected, see Fig. 10b. Over the 30$\mu$s operation time, the photon scattering from the $|6P_{1/2}\rangle$ state would cause 0.0015 gate infidelity. An alternative approach is to initially change the hyperfine state of the desired site \cite{50} and then excite the new auxiliary hyperfine state to the Rydberg level. In this case, it would be important that both hyperfine states get trapped at the same position in the qubit-dependent lattice of Fig. 11a-c. A possible choice is changing $|0\rangle = |F = 1, m_f = 1\rangle$ to $|F = 2, m_f = -1\rangle$ which has the same distribution of $m_f$ components and hence experiences the same trapping potential.

![FIG. 10. Effects of Laser cross-talk and misalignment on gate fidelity. The population that does not return to the qubit basis after gate operation would be considered as loss. The errors are averaged over the laser’s misalignment area which is a circle with radius $r_0$ and also over the Wannier state of atoms. The reported error is averaged over all qubit configurations in a C1b-NOT gate. Red and blue lines are corresponding to systems described in Fig. 1 and 2 with lattice constants $a = 400$ and 532 nm. The solid and dashed lines are corresponding to errors of plaquette $E_p$ and central atoms $E_c$. To apply the single-site addressing the 788nm laser is focused to $1/e^2$ intensity waist of (a) $w$ =500nm and (b) $w$ =370nm with alignment accuracy of $r_0 = 25$nm, generating a differential light-shift $U_{LS}$ on $|1\rangle r$ transition. The Oscillation is due to the change of effective Rabi frequency $\tilde{\Omega}$, which leads to different values of Rydberg leakage at the plaquette sites after the gate operation.](image)
Interferometric approach

Single site addressing could be realized with precisions below the diffraction limit using an interferometer technique applied before in sub-wavelength localization [45,49]. Over this process the qubit state $|0\rangle = |5S,F=1,m_f=1\rangle$ of the desired site would be changed to an auxiliary hyperfine state $|g\rangle = |5S,F=2,m_f=-1\rangle$ via an intermediate level $|6P\rangle$. The three-level $\Lambda$ transition is operated by a standing-wave driving field ($\Omega_c$) and a focused laser ($\Omega_p$), see Fig. 11. The standing wave is formed in each dimension by counter-propagating fields $\Omega_{c1q}\exp(ikq)$ and $\Omega_{c2q}\exp(-ikq + \phi_q)$ where $q \in \{x,y\}$. The transition occurs under the dark state STIRAP mechanism. The dark-state in the described $\Lambda$ system is a superposition of the $|g\rangle$ and $|0\rangle$ states with spatially varying amplitudes:

$$|D(r)| = \frac{1}{\sqrt{\Omega_c(r)^2 + \Omega_p(r)^2}}(\Omega_c(r)|0\rangle - \Omega_p(r)|g\rangle). \quad (30)$$

To apply the transition, first the $\Omega_{c1x}$ field would be applied. The probe field would then be applied focused on the targeted site with a Gaussian profile $\Omega_p(r) = \Omega_p e^{-(r-r_0)^2/w^2}$ and $\Omega_p \ll \Omega_c$. In the next step $\Omega_{c2y}$ would be applied adiabatically [48] to form the standing-wave with a node being adjusted on the position of the targeted site via the $\phi_{2q}$ angle. At the nodes of $\Omega_c$ standing-wave $\Omega_p(r) \gg \Omega_c(r)$ the dark-state composition is predominantly $|g\rangle$ while away from the nodes $\Omega_p(r) \ll \Omega_c(r)$ the dark state would remain at $|0\rangle$ qubit state.

Considering the wave-function density $|\psi(r)|^2$ of atoms initialized in $|0\rangle$ states, the local population of $|g\rangle$ state after applying $\Omega_{p,c}$ fields would be $f(r)|\psi(r)|^2$ where $f(r)$ is obtained from Eq. 30 as

$$f(r) = \frac{\Omega_p^2 e^{-2(r-r_0)^2/w^2} + \Omega_c^2 \sin^2 k(x-x_0) \sin^2 k(y-y_0)}{\Omega_p^2 e^{-2(r-r_0)^2/w^2} + \Omega_c^2 \sin^2 k(x-x_0) \sin^2 k(y-y_0)}, \quad (31)$$

where $k = k \sin \theta/2$ with $\theta$ being the angle between the $\Omega_{c1}$ and $\Omega_{c2}$ lasers. Figure 11 plots the narrow peaks of $f(r)$ at the nodes of $\Omega_c$. Going away from the focusing point of $\Omega_p$ at $r_0$, the profile width of $f(r)$ gets narrower and disappears. The full width at half maximum of an $f$ peak located at $r'$ would be given by $\text{FWHM}_{f(r')} = 2\Omega_p \exp(-r'^2/r_0^2)/\dot{k}\Omega_c$ [47,48]. While the nearest peaks of $f$ shown in Fig. 11b do not overlap with the atomic lattice sites the next nearest neighbors are at the position where the amplitude of $\Omega_p$ would approach zero. In the next step, the $\Omega_p$ and $\Omega_c$ lasers would be turned off simultaneously keeping the ratio of $\Omega_c(t)/\Omega_p(t)$ constant to preserve the dark state components. At this stage, only the desired site would be in the $|g\rangle$ state and hence would get excited to the Rydberg level by the subsequent $\Omega_c$ laser. Considering the qubit-dependent lattice of Fig. 1b, the auxiliary state $|g\rangle$ would experience the same trapping potential as $|0\rangle$ state since the distribution of $m_f$ components in the two hyperfine states are the same.

The initial calibration of the $\Omega_c$ standing wave with the optical lattice could be done by fluorescence imaging with the approach of [45]. The nodes of the $\Omega_c$ standing wave could be then moved by high resolution adjusting of the $\Omega_{c2g}$ phase [109]. For the chosen parameters of Fig. 1b applied in a lattice of $a = 532nm$ with the atom confinement of $\text{FWHM}=20nm$, and focusing $\Omega_p$ laser to the Gaussian width of $2\mu m$, the single site addressing infidelity averaged over the qubit configurations would be 0.01. This calculation encounters the population leakage of the neighboring lattices as well as the imperfect tran-
Considering the setups described before Eq. 5 and Eq. 6 the Hadamard combinations of the long-lived hyperfine states with longer coherence times. One example is -independent lattices [39, 50, 85], the dual encoding of the quantum information experiments in spin-dependent motional state $e^{ik\hat{z}}$ with $k = k_{1013} - k_{420}$. We can rewrite the vibrations of the position operator as $\hat{z} = \sigma/2(\hat{a}^\dagger + \hat{a})$, where $\sigma = \sqrt{\frac{\hbar}{m_\nu_{\sigma_r}}}$ is the spread of the ground motional state wave-function, $\nu_{\sigma_r}$ is the trap frequency and $(\hat{a}, \hat{a}^\dagger)$ are the phononic annihilation-creation operators of the targeted site. In the Lamb-Dicke regime $\eta = k\sigma/2 \ll 1$ one can expand the exponential to get
\begin{equation}
e^{ik\hat{z}} = (I + i\eta(\hat{a} + \hat{a}^\dagger)) + O(\eta^2). \tag{32}\end{equation}
The Hamiltonian describing the laser excitation can now be written in the new basis $|1e, 0m\rangle$, $|r_e, 0m\rangle$, $|r_e, 1m\rangle$ as:
\begin{equation}
\begin{pmatrix}
0 & \eta\Omega_r & \eta\Omega_r & \eta\Omega_r \\
\Omega_r & 0 & 0 & 0 \\
\eta\Omega_r & 0 & \omega_{tr} & 0 \\
\eta\Omega_r & 0 & 0 & \omega_{tr}
\end{pmatrix}
\begin{pmatrix}
|1e, 0m\rangle \\
|r_e, 0m\rangle \\
|r_e, 1m\rangle
\end{pmatrix} = \begin{pmatrix}
\langle 1e, 0m | \langle r_e, 0m | \\
\langle r_e, 0m | \langle r_e, 1m |
\end{pmatrix}
\tag{33}\end{equation}
Considering the setups described before Eq. 5 and Eq. 6 with FWHM$_z$=35nm, the probability of exciting a motional state $|r_e, 1m\rangle$ over the Toffoli and fan-out operations with $\Omega_r/2\pi = 30$ kHz and 30MHz would be 0.3% and 1.5% respectively.

APP. G: ALTERNATIVE ENCODING OF THE QUBIT STATES

While the chosen qubit states have been widely used in the quantum information experiments in spin-dependent and -independent lattices [29, 20, 52], the dual encoding of the qubit could also be realized in other hyperfine states with longer coherence times. One example is the Hadamard combinations of the long-lived hyperfine states $|F = 1, m_f = 0\rangle$ and $|F = 2, m_f = 0\rangle$:
\begin{equation} |0\rangle = (|F = 2, m_f = 0\rangle - |F = 1, m_f = 0\rangle)/\sqrt{2} \tag{34} \end{equation}
\begin{equation} = |I = 3/2, m_I = 1/2\rangle |J = 1/2, m_j = -1/2\rangle \end{equation}
\begin{equation} |1\rangle = (|F = 2, m_f = 0\rangle + |F = 1, m_f = 0\rangle)/\sqrt{2} \tag{35} \end{equation}
\begin{equation} = |I = 3/2, m_I = -1/2\rangle |J = 1/2, m_j = 1/2\rangle \end{equation}

In this arrangement the qubit states $|0\rangle$ and $|1\rangle$ would exclusively contain $m_j = -1/2$ and $m_j = 1/2$ respectively.

Hence they would get trapped by different polarizations of the qubit-dependent lattice as discussed in Fig. 11-c. In a Rydberg two-photon excitation with $\sigma^+$ circularly polarized lasers that are red detuned from the $|6P_{1/2}\rangle$ intermediate state, only the $|1\rangle$ state would get excited to the Rydberg level as discussed below. Dipole transitions between the hyperfine states are given by
\begin{equation}
\langle n'lj'F'M'|\sigma\rangle nljFM = (-1)^{1+l'+s+j'+J'+l-M'} \sqrt{\max(l'J')} \sqrt{(2J'+1)(2F'+1)} \sqrt{(2F+1)} \tag{36}
\end{equation}
\begin{equation}
\langle F'F\rangle |J\rangle l1 \langle F F'\rangle |J\rangle 11 \langle M q -M'\rangle |n'lj'||nlj\rangle
\end{equation}
where $q = 0, \pm 1$ for the linear $\sigma^0$ and $\sigma^\pm$ circular polarizations of the exciting light. Under the $\sigma^-$ circularly polarized laser $\langle 6P_{1/2}; 1, -1|7S_1/2; 1, 0\rangle = (6P_{1/2}; 1, -1|7S_1/2; 2, 0\rangle$, hence the dipole transition from the $|0\rangle (|1\rangle)$ qubit states of Eq. 34 into the $|0\rangle (|1\rangle)$ intermediate state would be forbidden (allowed) due to destructive (constructive) interference, see Fig. 12.

In the upper transition of Fig. 12a, a two-color transition excite a superposition of the Rydberg levels $|6D_{3/2}, -3/2\rangle + |6D_{5/2}, -3/2\rangle/\sqrt{2}$. The two-color laser could be obtained in a setup of beamsplitters and acusto-optical modulators. The spatial profile of the Rydberg-Fermi interaction relative to the position of plaquette atoms is plotted in Fig. 12b. The generated Rydberg superposition state mainly contains the $Y_{-2}$ spherical harmonic term, which concentrates the electron wave-function close to the lattice plane and enhances the interaction strength. The plaquette atoms experience an effective Rydberg-Fermi interaction that is averaged over their spatial profile. The scattering energy of Rydberg electron over the qubit-dependent Wannier state of the $l$th plaquette atom in the geometry of Fig. 1 with FWHM$_{x,y}=20$nm and FWHM$_z=35$nm would be quantified by Eq. 2 as
\begin{equation}
\bar{V}_{RF|1i} = 1.1\text{MHz}, \quad MD_{\bar{V}_{RF|1i}} = 0.14\text{MHz} \tag{36}
\end{equation}
\begin{equation}
\bar{V}_{RF|0i} = 0.27\text{MHz}, \quad MD_{\bar{V}_{RF|0i}} = 0.16\text{MHz}
\end{equation}
where the in-plane qubit-dependent lattice-shift of $D = 34.5$nm is considered. The same Rydberg state in the geometry of Fig. 2 reduces the unwanted level shift of the $|0\rangle$ qubit state to
\begin{equation}
\bar{V}_{RF|0i} = 0.16\text{MHz}, \quad MD_{\bar{V}_{RF|0i}} = 0.09\text{MHz} \tag{37}
\end{equation}
with the qubit-dependent lattice shift of $D_z = 150$nm being perpendicular to the lattice plane.

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FIG. 12. Qubit encoding in the Hadamard combination of long-lived hyperfine states $|F = 2, m_F = 0\rangle$ and $|F = 1, m_F = -1\rangle$ intermediate state, see Eq. $\frac{\sqrt{3}}{2}$. The two-qubit states have distinct $m_j$ components allowing qubit-dependent trapping, see Fig. 1b-c. (a) Applying a two-photon Rydberg excitation via $\sigma^\pm$ circular polarized lasers that are red detuned from the $|F = 1, m_F = -1\rangle$ intermediate state, only the $|1\rangle$ qubit state would get excited to the Rydberg level, see the main text. The space-dependent Rydberg-Fermi interaction of the excited Rydberg level $(\frac{64a_3/2, -3/2}{2} + \frac{64a_3/2, -3/2}{2})/\sqrt{2}$ is plotted in (b) where $z$ is perpendicular to the lattice plane.
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The same order of lattice constant could also realized by the conventional 6S – 6P transition via dark state approach or by using dual species that are node and antinode seekers. Also the subwavelength confinement could be arranged using the dark state approach inspired by [45, 107]. The recently proposed twist-optical lattice could confine atoms down to sub-nanometer scale [52].

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