Unitary and non-unitary quantum cellular automata with Rydberg arrays

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We propose a physical realization of quantum cellular automata (QCA) using arrays of ultracold atoms excited to Rydberg states. The key ingredient is the use of programmable multifrequency couplings which generalize the Rydberg blockade and facilitation effects to a broader set of non-additive, unitary and non-unitary (dissipative) conditional interactions. Focusing on a 1D array we define a set of elementary QCA rules that generate complex and varied quantum dynamical behavior. Finally we demonstrate theoretically that Rydberg QCA is ideally suited for variational quantum optimization protocols and quantum state engineering by finding parameters that generate highly entangled states as the steady state of the quantum dynamics.

Today there exists a wide variety of viable physical platforms for quantum information processing (QIP), including ultracold atoms, ions, impurities, photons and superconducting circuits. Each platform has its own unique advantages (and challenges) concerning important qualities such as isolation from the environment, qubit coherence time, gate speeds, scalability, addressability and interaction control. Therefore, to bring important and classically intractable problems within reach, protocols for quantum information processing must be robust and highly optimized to exploit the particular advantages of continually improving quantum hardware [1].

One promising platform for QIP is based on trapped ultracold Rydberg atoms [2–5]. Their distinguishing features include: (i) the availability of fast and switchable multiqubit interactions [2, 4, 6–10] and (ii) the possibility for non-trivial dissipative interactions, which rather than destroying entanglement can actually enhance and protect it [4, 11–17].

In this letter, we propose a physical implementation of the quantum cellular automata (QCA) paradigm [18–20] based on Rydberg atoms. This opens up an approach to QIP which is inherently parallelizable, does not require individual addressing of each qubit [21–26] and takes full advantage of both unitary and non-unitary multiqubit interactions, thus providing a viable alternative to gate-based [3, 4, 27, 28] and quantum adiabatic protocols [29–31]. The key idea is to use programmable multifrequency excitation and depumping of Rydberg states that implements a set of conditional interactions in analogy with classical cellular automata. We show that this leads to a rich diversity of controllable quantum dynamics in both discrete and continuous time evolution. Finally, we numerically demonstrate a powerful approach for generating highly entangled quantum states by embedding Rydberg QCA within a variational quantum optimization loop [32, 33].

Physical system:- As a physical platform we consider an array of three-level systems consisting of a ground state |g⟩ ≡ |0⟩, a strongly-interacting (Rydberg) state |r⟩ ≡ |1⟩ and a short-lived intermediate state |e⟩ used to mediate non-unitary interactions (Fig. 1a,b). This could be realized for example using single atoms [34–38], trapped ions [10, 39, 40] or Rydberg blockaded atomic ensembles [8, 41, 42]. For simplicity we consider an equidistant 1D chain of trapped atoms restricted to nearest neighbor interactions V. Two fields consisting of several discrete frequency components couple the |g⟩ ↔ |r⟩ transition and the |r⟩ ↔ |e⟩ transition (Fig. 1b). Within the rotating wave approximation the system is described by a time-
dependent quantum master equation in Lindblad form \((\hbar = 1)\): 
\[
\dot{\rho} = -i[H, \rho] + \mathcal{D}[\rho],
\]
where 
\[
\hat{H} = \sum_{j,k} \left( \frac{\theta_k^j}{2} e^{ikVt} \sigma_j^{\alpha} + \frac{\phi_k^j}{2} e^{ikVt} \sigma_j^{\beta} + h.c. \right) + V \sigma_j^{\alpha} \sigma_{j+1}^{\alpha},
\]
(1)
defining \(\sigma_j^{\alpha} = |\alpha\rangle \langle \alpha|\) acting on site \(j\) and the nearest neighbor interaction strength \(V\). The time dependent phase factors describe discrete components of the multifrequency fields with detunings \(kV\) \((k = \{0, 1, 2\})\) and coupling strengths \(\theta_k^j, \phi_k^j\). In the following we allow these couplings to be site dependent (e.g. applied independently to even and odd sites), but they can also be uniform for the whole system. Dissipation is included via the term 
\[
\mathcal{D}[\rho] = \sum_j \mathcal{L}_j \rho \mathcal{L}_j^\dagger - \left( \mathcal{L}_j^\dagger \mathcal{L}_j \rho + \rho \mathcal{L}_j^\dagger \mathcal{L}_j \right)/2
\]
where we define the jump operators \(\mathcal{L}_j = \sqrt{\mathcal{N}} \hat{\sigma}_j^{\alpha}\) describing spontaneous decay out of the \(|\alpha\rangle\) state. Rydberg state decay \(\sqrt{\mathcal{N}} \hat{\sigma}_j^{\alpha}\) is assumed to be much slower than the rest of the dynamics and will be neglected for the moment.

In the limit \(V \gg \Gamma > \theta_k^j, \phi_k^j\) one can reduce the full quantum master equation to an effective two-level system (i.e. \(|0\rangle, |1\rangle\)) with time-independent 3-body conditional interactions (see Supplemental Material for the full derivation). Briefly, we transform the Hamiltonian (1) to an interaction picture with respect to the nearest neighbor Rydberg-Rydberg interactions [43] and then adiabatically eliminate the time-dependent phase factors using a large frequency expansion [44]. In a second approximation we adiabatically eliminate the rapidly decaying \(|\alpha\rangle\) states using the effective operator formalism [45], yielding an effective time-independent master equation defined by 
\[
\hat{H}^{\text{eff}} = \frac{1}{2} \sum_j \sum_{\alpha, \beta} \theta_j^\alpha P_j^\alpha \hat{X}_j P_j^\beta, \quad (2)
\]
\[
\hat{L}^{\text{eff}} = \frac{1}{2} \sum_j \sum_{\alpha, \beta} \sqrt{\phi_j^\alpha} P_j^\alpha \left( \hat{X}_j - i \hat{Y}_j \right) P_j^\beta, \quad (3)
\]
where \(\sqrt{\phi_j^\alpha} \approx \phi_j^\alpha/\sqrt{\mathcal{N}}\) and assuming \(\theta_j^k \in \mathbb{R}\). The double sum over \(\alpha, \beta\) goes from 0 to 1 with \(k = \alpha + \beta\), \(P^\alpha = |\alpha\rangle \langle \alpha|\) and \(\hat{X}_j, \hat{Y}_j\) are Pauli matrices. Higher order corrections to this model enter as effective level shifts and couplings \(\propto |\theta_j^k|^2/V, |\phi_j^k|^2/V\) which can be mostly neglected for experimentally relevant parameters. See Supplemental Material for benchmarking of the effective model Eqs. (2) and (3) against the full time-dependent three-level model Eq. (1). Although we concentrate on a 1D geometry with nearest neighbor interactions, the same model can be readily generalized to higher dimensions and more neighbors by including more frequency components to the driving fields.

Equations (2) and (3) describe an effective PXP model, previously applied to theoretically describe the Rydberg blockade and facilitation constraints in atomic chains [16, 43, 46–48], but generalized here to a wider set of unitary and dissipative conditional operators stemming from the multifrequency driving fields. Fig. 1c) depicts the unitary and non-unitary conditional update rules for the central site \(j\) of a three-site neighborhood. Each field component \(\theta_j^k\) effectuates transitions when there is precisely \(k\) Rydberg excitations in the neighborhood, constrained by the projection operators \(P_j^\alpha, P_{j+1}^\beta\) (i.e. \(\alpha = \beta = 1\) means the state will only change if both left and right neighbors are in state \(|1\rangle\)). The special case \(\theta_j^0 \neq 0, \theta_j^k = 0\) corresponds to the Rydberg blockade scenario, while for \(\theta_j^k = 0\) corresponds to facilitated excitation in the presence of \(k\) already excited neighbors. The inclusion of strong dissipative couplings via the second multifrequency field \(\phi_j^k\) realizes an additional set of irreversible conditional interactions that bring atoms back to the \(|0\rangle\) state.

**Numerical simulation of QCA dynamics** :- The effective two-level representation given by equations (2) and (3) can be interpreted as a set of unitary and non-unitary elementary QCA [26], parameterized by \([\theta_0^0, \theta_1^0, \theta_2^0, \phi_0^1, \phi_1^1, \phi_2^1]\), analogous to the binary string representation used in classical CA. In the following, we consider either discrete or continuous time evolution, described by the application of an (in general non-unitary) operator 
\[
\rho(t) = \exp(\mathcal{L}t) \rho(0), \quad (4)
\]
where \(\mathcal{M} = \exp(\mathcal{L}_B) \exp(\mathcal{L}_A)\) is separated according to two sub-
lattices $A$ (odd sites) and $B$ (even sites), which are updated in alternating fashion an integer number of times $t$. Block partitioned QCA could be experimentally implemented using two different sets of atomic states/species or spatially structuring the Rydberg excitation lasers to address even and odd sites independently. In both cases we solve the master equation using a linear multistep method and the QuTiP package [49].

Fig. 2 shows numerical simulations of the effective master equation for both discrete time (block partitioned, where we restrict unitary rotations to 0 or $\pi$ and dissipative jump probabilities to 0 or $1 - e^{-2\pi}$ in each step) and the corresponding continuous (non-partitioned) time evolution. We choose 12 representative rule sets (out of $2^6 = 64$ digital combinations of the parameters $\theta^k, \phi^k$), which are assumed to be equal for the $A$ and $B$ sublattices. The panels with solid green borders correspond to purely unitary rules ($\phi^k = 0$). The numerical simulations are performed for 9 atoms, starting from the initial state with the central atom in the $|1\rangle$ state and all others in $|0\rangle$. This state is evolved for 20 time units via Eq. (4) assuming open boundary conditions (which can be treated as two additional fictitious spins on the left and right fixed to $|0\rangle$). Bright (dark) colors reflect high (low) magnetization $\langle Z_j \rangle \approx 1$ ($\langle Z_j \rangle \approx -1$).

The simulated dynamics reveal a variety of different dynamical structures reminiscent of classical CA, including fixed point, periodic, and complex/fractal like structures (comparable to those studied in Ref. [50]). Furthermore, discrete and continuous time evolution show qualitatively similar features (especially for early times, i.e. time index roughly equal to lattice size), except for a generally lower contrast for the continuous time case. This does not necessarily indicate a loss of coherence however, as it is also seen for the purely unitary rules which can be explained by the build up of entanglement during QCA evolution.

Careful inspection of the continuous time evolution shows additional periodicities and non-trivial stationary states that are not present in the discrete time evolution. As a specific example we highlight the non-unitary rule $[0, 1, 0, 0, 0, 2] \times \pi$ (Fig. 2-second row, first column). Initially, both discrete and continuous time evolution show similar light-cone like propagation of the excitation. Upon reaching the boundary however, the two cases deviate strongly. Rather than simply reflecting from the boundary, the continuous time evolution evolves toward a steady state that exhibits an antiferromagnetically ordered pattern. Qualitatively this can be understood as the competition between the conditional $k = 1$ neighbor driving which favors spreading of the excitations while the $k = 2$ neighbor depumping suppresses nearest-neighbor excitations. Thus the final state $|101010101\rangle$ is a dark state for both terms. This highlights the possibility to use unitary and non-unitary QCA dynamics to generate correlated many-body states as the stationary state of the open system dynamics and it is an interesting question whether it can also be used to generate highly entangled quantum states.

Steering QCA evolution to highly entangled states:- Quantum state engineering via open system dynamics is typically cast in terms of finding a Liouvillian $\mathcal{L}$ that yields a desirable (e.g., entangled) state as the stationary state of the dynamics [4, 11–17]. However in general it is a hard problem to find $\mathcal{L}$ (and a corresponding set of physically available interactions) that result in this state. We show here that an appropriate combination of QCA rules may be found that steer quantum dynamics into desired quantum states on demand.

The basic idea is to embed the Rydberg QCA within a variational optimization loop which iteratively adjusts the QCA parameters to reach a desired target state (Fig. 3a). The role of the quantum system is to generate trial states with a fixed population size of 10 (gray lines) towards states with large covariance coefficient ($C$). The solid blue line highlights the best individual. The optimal parameters are shown in the inset. (c) Graphical representation of the density matrix of the optimized state. (d) Time evolution of the fidelity between the resulting QCA state using the optimal variational parameters and the GHZ$^N$ state. The system evolves to a highly entangled state within approximately 200 time units. The dashed orange line shows the same evolution including a Rydberg state decay rate of $\gamma/2\pi = 2$ kHz (see the text for other parameters).
fully demonstrated for finding ground states of unitary quantum systems [51–54], we show it can also apply to non-unitary quantum evolution and stationary states.

To steer the system to highly correlated states we choose to maximize elements of the covariance matrix \(C_{ij} = \text{Tr}[\rho(\hat{Z}_i - \langle \hat{Z}_i \rangle)(\hat{Z}_j - \langle \hat{Z}_j \rangle)]\). For the following we average over all neighbours, i.e. \(\langle C \rangle = 1/N \sum C_{ij+1} = 0\) for a separable state while \(\langle C \rangle = \pm 1\) for a pairwise inseparable state. Here we restrict to proof-of-principle numerical simulations for relatively small system sizes of \(N = 6\) sites, although this provides valuable guidance for finding optimal parameter regimes for larger systems. In the following we numerically solve for the steady state of the continuous time QCA evolution with periodic boundary conditions and global variational parameters \(\theta^k, \phi^k\). We use \(|0\rangle^\otimes N = |000000\rangle\) as the initial state, but we observe similar behavior for other initial states. We maximize \(\langle C \rangle\) using the particle swarm optimization (PSO) algorithm [55].

Figure 3b shows the convergence of the variational optimization algorithm as a function of the number of PSO iterations. We use a population of 10 individuals (gray lines), with the best individual highlighted in blue. We find that convergence is robust and relatively fast (within 100 iterations), saturating at a value close to the maximum value \(\langle C \rangle = 1\). Inspecting the resulting density matrix (Fig. 3c) we find that the final state is very close to the \(|\text{GHZ}^N\rangle = 1/\sqrt{2}(|0\rangle^\otimes N - |1\rangle^\otimes N\rangle\) state. This can be understood since both \(|0\rangle^\otimes N\) and \(|1\rangle^\otimes N\) are dark with respect to the projectors associated to \(\theta^1\) and \(\phi^0\). However, as these separable states both yield \(\langle C \rangle = 0\), it appears that a relatively weak contribution from \(\theta^0\) and \(\phi^2\) is important to stabilize the \(|\text{GHZ}^N\rangle\) state with a well defined relative phase.

The evolution towards this state using the optimized parameters is shown in Fig. 3d, quantified by the fidelity \(F_{\text{GHZ}}(t) = \text{Tr}\left[\sqrt{\rho(t)}|\text{GHZ}^N\rangle\langle\text{GHZ}^N|\sqrt{\rho(t)}\right]\), which reaches \(\geq 0.99\) within 200 time units. The \(|\text{GHZ}^N\rangle\) state is very promising as a resource for quantum metrology [56] and measurement-based quantum computing [57], as it is, e.g., a stabilizer state (+1 co-eigenstate) of stabilizer operators generated from the set of \(n\) independent operators \(\{Z_1Z_2Z_3\ldots, Z_{n-1}Z_n, X_1X_2\ldots X_n\}\). We have also performed minimization of \(\langle C \rangle\) and the resulting solution is the entangled antiferromagnetically ordered state \(|\text{AF}\rangle = 1/\sqrt{2}(|010101\rangle - |101010\rangle\) which shows that variational quantum optimization combined with Rydberg QCA provides a powerful and rather general approach to quantum state engineering.

Experimental feasibility:- Rydberg QCA could be implemented in a number of physical systems that support a simple (three) level scheme and strong state-dependent nearest-neighbor interactions. But to estimate realistic experimental parameters we consider an array of ultracold \(^{39}\text{K}\) atoms. The \(|g\rangle \leftrightarrow |r\rangle\) coupling could be achieved using a two-photon resonance with large detuning from the \(|e\rangle\) state, while \(|r\rangle \leftrightarrow |e\rangle\) could be a single-photon transition, with multiple tones generated by electro-optical modulators. Parameters corresponding to those used for Fig. 2 (and Fig. 3) are \(V/2\pi = 50\) MHz (typical for the \(|r\rangle = |801_{1/2}\rangle\) state at a distance of \(a = 6\mu m\), \(\phi^k/2\pi \leq 1\) MHz, \(\phi^k/2\pi \leq 2\) MHz. This gives a characteristic time unit of \(t = \pi/\phi^k = 500\) ns. Therefore, within a typical Rydberg state lifetime (\(\gamma^{-1} \approx 200\) µs) one could realize up to \(\sim 400\) time steps and prepare highly entangled states with high fidelity. To quantify this, we find in Fig. 3d that the fidelity for preparing a 6 atom \(|\text{GHZ}^N\rangle\) state still reaches \(F \approx 0.9\) when additional jump operators describing Rydberg state decay are included (dashed line). This could be further improved using error correction schemes [58, 59] or using longer-lived Rydberg states in cryogenic environments [60].

To conclude, we have put forward a promising approach to quantum state engineering and QIP that is highly parallelizable and exploits both unitary and non-unitary multiqubit interactions. Already a very basic set of conditional QCA rules acting under continuous time evolution can generate a rich variety of complex quantum dynamics and highly entangled states. Allowing for different rules to be applied at different times would enable the generation of deeper quantum circuits opening up the possibility for universal quantum computing [21, 22].

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Supplemental Material

Unitary and non-unitary quantum cellular automata with Rydberg arrays

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DERIVATION OF THE EFFECTIVE TWO-LEVEL HAMILTONIAN

To derive the effective time-independent master equation [Eqs. (2) and (3) in the manuscript] from the full time-dependent Hamiltonian [Eq. (1)] we assume that the nearest-neighbor interaction \( V \) and the intermediate state decay rate \( \Gamma \) are the dominant scales. This makes it possible to neglect the non-resonant couplings of the driving field and to adiabatically eliminate the \( |e\rangle \) state. In the following we use units where \( \hbar = 1 \).

We consider a multifrequency coupling field of the form \( E_j = E_j^r + E_j^\phi + \text{c.c.} \), where

\[
E_j^r = \frac{1}{2} \sum_k \theta_j^k e^{i E_{j \text{r}} t + i k V t}
\]

(1)

\[
E_j^\phi = \frac{1}{2} \sum_k \phi_j^k e^{i (E_{j \text{e}} - E_{\text{c}}) t + i k V t},
\]

(2)

acting on the time-dependent Hamiltonian

\[
\hat{H}(t) = \sum_j \left( \hat{\sigma}_{j r}^g E_j^r(t) + \hat{\sigma}_{j r}^e E_j^\phi(t) + h.c. + \hat{V}_{\text{int}} + \hat{H}_{\text{atom}} \right)
\]

(3)

where \( \hat{\sigma}_{ab} = |a\rangle \langle b| \), \( \hat{H}_{\text{atom}} = E_{\text{r}} \hat{\sigma}_{rr}^r + E_{\text{e}} \hat{\sigma}_{rr}^e \) and we restrict to nearest neighbor interactions between sites \( j \) only

\[\hat{V}_{\text{int}} = V \hat{\sigma}_{j r}^r \hat{\sigma}_{j+1 r}^r.\]

The first step is to transform away the time dependence due to the carrier frequencies \( E_{\text{r}} \), \( (E_{\text{e}} - E_{\text{c}}) \). We transform to a rotating frame via the unitary \( \hat{U} = U \hat{U}_{\text{int}} U \) where \( \hat{U} = \exp(-i \hat{H}_{\text{atom}} t) \) and average out the rapidly varying phases that depend on \( E_{\text{r}} \), \( E_{\text{e}} \).

The resulting (still time-dependent) Hamiltonian in the rotating wave approximation is

\[
\hat{H}(t) = \sum_j \sum_k \left( \frac{\theta_j^k}{2} \hat{\sigma}_{j r}^r e^{i k V t} + \frac{\theta_j^k}{2} \hat{\sigma}_{j r}^e e^{-i k V t} \right)
\]

(4)

\[
+ \left( \frac{\phi_j^k}{2} \hat{\sigma}_{j r}^e e^{i k V t} + \frac{\phi_j^k}{2} \hat{\sigma}_{j r}^e e^{-i k V t} \right) + V \hat{\sigma}_{j r}^r \hat{\sigma}_{j+1 r}^r.
\]

Next we transform to an interaction picture with respect to the nearest neighbor interaction using the unitary transformation \( U = \exp \left(-i V t \sum_j \hat{\sigma}_{j r}^r \hat{\sigma}_{j+1 r}^r \right) \) where \( U^\dagger \hat{\sigma}_{j r}^a \hat{U} = [P_{j-1 r} + P_{j-1 r} e^{-i V t}] \hat{\sigma}_{j r}^a [P_{j+1 r} + P_{j+1 r} e^{-i V t}] \) [1], with \( \alpha = g, e \), the projection operators \( P_{j r} = 1 - \hat{\sigma}_{j r}^r \) and \( P_{j r} = \hat{\sigma}_{j r}^r \). After transformation the Hamiltonian reads

\[
\frac{\hat{H}}{\hat{H}_{\text{int}}} = \sum_j \sum_k \left( \frac{\theta_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^g P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r} \right) e^{i k V t}
\]

(5)

\[
+ \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r} + \frac{\phi_j^k}{2} \hat{\sigma}_{j r}^e P_{j+1 r} \right) e^{i(k-1) V t}
\]

\[
+ \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r} \right) e^{i(k-2) V t}
\]

\[
+ h.c.
\]

This can be written as

\[
\hat{H}(t) = \sum_{j} \sum_{k,k'} \hat{H}_{k,k'}(j)e^{i(k-k')Vt} + h.c.
\]

(6)

where \( k,k' = \{0 \ldots 2\} \) and the non-hermitian time-independent operators \( \hat{H}_{k,k'} \) are given by

\[
\hat{H}_{k,0}(j) = \frac{\theta_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^g P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r}
\]

(7)

\[
\hat{H}_{k,1}(j) = \frac{\theta_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^g P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r}
\]

\[
+ \frac{\theta_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^g P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r} \right) e^{i(k-2) V t}
\]

\[
\hat{H}_{k,2}(j) = \frac{\theta_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^g P_{j+1 r} + \frac{\phi_j^k}{2} P_{j-1 r} \hat{\sigma}_{j r}^e P_{j+1 r}
\]

Next we approximate Eq. (6) using the formalism described in [Ref. 2 Eq.(35)]. This approach is equivalent to second order adiabatic elimination in the Floquet picture. The effective Hamiltonian [3] reads

\[
\hat{H}' = \sum_{k} \left( \hat{H}_{k,k} + \hat{H}_{k,k}^\dagger \right) + \frac{1}{V} \sum_{k \neq k'} \frac{1}{k' - k} \left[ \hat{H}_{k,k'}^\dagger, \hat{H}_{k,k'} \right]
\]

(8)

where the first term describes the resonant couplings and the last term includes leading order corrections due to off-resonant cross-talk couplings. These terms enter as
effective light shifts and couplings between states within constant \( k \) manifolds (scaling with \((\theta k)^2/V\) and \((\phi k)^2/V\)).

For the manuscript we restrict to the resonant terms only. Thus one can write the time-independent Hamiltonian as

\[
\hat{H}' = \frac{1}{2} \sum_j \sum_{\alpha, \beta} \mathcal{P}_{j-1}^{\alpha} \left[ \theta_j^k \hat{\sigma}_j^{\alpha \beta} + \phi_j^k \hat{\sigma}_j^{\alpha \beta} + h.c. \right] \mathcal{P}_{j+1}^{\beta}
\]  

(9)

where we introduce the projection indices \( \alpha, \beta = \{0, 1\} \), with \( k = \alpha + \beta \).

Finally we include the spontaneous decay of the \(| e \rangle\) state and derive an effective master equation for the dynamics of the form \( \partial_t \rho = -i[\hat{H}_\text{eff}, \rho] + \mathcal{D}_\text{Lett}[\rho] \). Spontaneous emission from the \(| e \rangle\) state to the \(| g \rangle\) state with rate \( \Gamma \) is described by the jump operators \( \hat{L}_j = \sqrt{\Gamma} \hat{\sigma}_j^e \). To adiabatically eliminate the manifold containing short lived \(| e \rangle\) states and to derive effective jump operators \( \hat{L}_j^{\text{eff}} \) acting on the \( g, r \) subspace we use the effective operator formalism of [4].

We start by defining operators for the slow and fast evolving subspaces according to \( \mathcal{P}|e\rangle = 0 \) and \( \mathcal{Q} = 1 - \mathcal{P} \), such that \( \mathcal{Q}\sigma_j^{\alpha \alpha} = \sigma_j^{\alpha \alpha} \) and \( \mathcal{P}\sigma_j^{\alpha \alpha} = 0 (\alpha = g, r) \). Following Ref. [4] we also define the non-hermitian Hamiltonian

\[
\hat{H}_{nh} = \mathcal{Q}\hat{H}'\mathcal{Q} - i \sum_j \hat{\mathcal{L}}_j^i \hat{L}_j.
\]  

(10)

As a first approximation we neglect states with more than one \(| e \rangle\) excitation which is justified for \( \Gamma \gg |\phi_k| \). In this case \( \mathcal{Q}\hat{H}'\mathcal{Q} = 0 \), which leaves

\[
\hat{H}_{nh} = -\frac{i\Gamma}{2} \sum_j \hat{\sigma}_j^e.
\]  

(11)

The effective Hamiltonian can be written as

\[
\hat{H}_\text{eff} = \mathcal{P}\hat{H}'\mathcal{P} - \frac{1}{2} \mathcal{V}^- [\hat{H}_{nh}^{-1} + (\hat{H}_{nh}^{-1})^\dagger] \mathcal{V}^+ \]  

(12)

where \( \mathcal{V}^- = \mathcal{P}\hat{H}'\mathcal{Q} \) and \( \mathcal{V}^+ = \mathcal{Q}\hat{H}'\mathcal{P} \). Since the inverse of \( \hat{H}_{nh} \) is a purely imaginary diagonal matrix the term in the brackets cancels, leaving

\[
\hat{H}_\text{eff} = \mathcal{P}\hat{H}'\mathcal{P} \]  

(13)

which coincides with Eq. (2) in the manuscript. The effective jump operators can be written

\[
\hat{L}_j^{\text{eff}} = \hat{L}_j \hat{H}_{nh}^{-1} \mathcal{V}^+ \]  

\[
= \frac{i}{\sqrt{\Gamma}} \hat{\sigma}_j^{ee} (\sum \hat{\sigma}_i^{ee})^{-1} \]  

\[
\times \mathcal{Q} \sum_{j'} \sum_{\alpha, \beta} \mathcal{P}_{j'-1}^{\alpha} \left[ \theta_{j'}^k \hat{\sigma}_{j'}^{\alpha \beta} + \phi_{j'}^k \hat{\sigma}_{j'}^{\alpha \beta} + h.c. \right] \mathcal{P}_{j'+1}^{\beta} \mathcal{P} \]  

(14)

Now we use \((\sum \hat{\sigma}^{ee})^{-1} \mathcal{Q} = (\sum \hat{\sigma}^{ee})^{-1} \) and the action of \( \mathcal{P} \) from the right hand side changes \( \mathcal{P}_{j+1}^\beta \rightarrow |q\rangle \langle g| \) and restricts \( \hat{\sigma}_j^{tr} \) to states that initially have no \(| e \rangle\) excitations (i.e. exactly one \(| e \rangle\) at site \( i' \) after application of the operator). This allows us to remove the sums over \( i, i' \)

\[
\hat{L}_j^{\text{eff}} = \frac{i}{\sqrt{\Gamma}} \sum_{\alpha, \beta} \mathcal{P}_{j-1}^{\alpha} \theta_{j}^k \hat{\sigma}_j^{ee} (\sum \hat{\sigma}_i^{ee})^{-1} \hat{\sigma}_j^{tr} \mathcal{P}_{j+1}^{\beta} \]  

(15)

\[
= \frac{i}{\sqrt{\Gamma}} \sum_{\alpha, \beta} \theta_{j}^k \mathcal{P}_{j-1}^{\alpha} \hat{\sigma}_j^{ee} \hat{\sigma}_j^{tr} \mathcal{P}_{j+1}^{\beta}. \]

To arrive at Eq. (3) in the manuscript we drop the \( i \) prefactor, since it is of no physical consequence [canceling out in the Lindblad term \( \mathcal{D}[\rho] = \sum_j \hat{L}_j \rho \hat{L}_j^\dagger - (\hat{L}_j^\dagger \hat{L}_j \rho + \rho \hat{L}_j^\dagger \hat{L}_j)/2 \)].

**NUMERICAL COMPARISON BETWEEN THE THREE-LEVEL MULTI-FREQUENCY HAMILTONIAN AND THE EFFECTIVE TWO-LEVEL MODEL**

To verify the validity of the effective two-level model we compare numerical simulations of the effective model and the full three-level Rydberg excitation Hamiltonian (including time-dependent couplings). Fig. S1 shows the time evolution of the magnetization \( \langle \hat{Z}_j \rangle \) for the same 12 representative rules that were chosen in Fig. 2 in the manuscript for 5 sites with open boundary conditions. For each rule we display three panels: on the left is the result of the three-level master equation [Eq. (1) in the manuscript]; in the middle is the effective two-level master equation results [Eqs. (2) and (3) in the manuscript]; and the right panels show the difference between the three-level and two-level results, where more homogeneous colors indicate better agreement. The simulations are performed with with a nearest neighbor Rydberg-Rydberg interaction energy \( V = 50\pi \) (in units where \( t = 1 \)), an intermediate state decay rate of \( \Gamma = 6\pi \) and coupling parameters \( \theta^k, \phi^k \) indicated in the figure labels, with \( \phi^k = \sqrt{\Gamma}\phi^k \).

We additionally include jump operators for Rydberg state decay with the dimensionless rate \( \gamma = 8\pi \times 10^{-4} \). Each rule is evolved starting in the initial state \(|00100\rangle\) for a duration of 20 time units.

Inspecting the results in Fig. S1 we see good agreement between the effective model and the full three-level time-dependent master equation for the majority of rules. This agreement is especially good considering the chosen parameters are close to the limit of validity for the approximations used in deriving the effective model (i.e. \( V \gg \Gamma \gg \theta^k, \phi^k \gg \gamma \)). Certain rules do show some deviations though, e.g. rule \([0, 0, 1, 0, 2, 0] \times \pi\), where the excited state population of the central site in the three-level case is seen to decay with a time constant of around.
Figure S1. Numerical simulations of the evolution of the magnetization $\langle \hat{Z}_j \rangle$ for the full three-level model as well as its effective two-level description for 12 representative QCA rules indicated in the label of each subfigure with the notation $[\theta^0, \theta^1, \theta^2, \tilde{\phi}^0, \tilde{\phi}^1, \tilde{\phi}^2]$. For each QCA rule there are three panels: left: three-level master equation simulation including time-dependent couplings, center: two-level effective master equation simulation and right: residual between three-level and two-level result.

50 time units, which is not captured by the effective two-level model. This can be attributed to slow off-resonant depumping caused by the $\phi^{k=1}$ coupling acting on the $k=0$ subspace which is neglected in the effective model. Increasing $V/\Gamma$ further improves the agreement between the two models.

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