

Numerical simulation of quantum nonequilibrium phase transitions without finite-size effectsEdward Gillman ^{1,2}, Federico Carollo,³ and Igor Lesanovsky ^{1,2,3}¹*School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom*²*Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, United Kingdom*³*Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany*

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Classical (1+1)-dimensional (D) cellular automata, as for instance Domany-Kinzel cellular automata, are paradigmatic systems for the study of nonequilibrium phenomena. Such systems evolve in discrete time steps, and are thus free of time-discretization errors. Moreover, they display nonequilibrium phase transitions which can be studied by simulating the evolution of an initial seed. At any finite time, this has support only on a finite light cone. Thus, essentially numerically exact simulations free of finite-size errors or boundary effects are possible, leading to high-accuracy estimates of critical exponents. Here, we show how similar advantages can be gained in the quantum regime: The many-body critical dynamics occurring in (1+1)D quantum cellular automata with an absorbing state can be studied directly on an infinite lattice when starting from seed initial conditions. This can be achieved efficiently by simulating the dynamics of an associated one-dimensional, nonunitary quantum cellular automaton using tensor networks. We apply our method to a model introduced recently and find accurate values for universal exponents, suggesting that this approach can be a powerful tool for precisely studying nonequilibrium universal physics in quantum systems.

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Introduction. One of the most intriguing aspects of nonequilibrium phase transitions (NEPTs) is the emergence of universal behavior: systems with very different microscopic details can display the same scaling laws at a macroscopic scale, both for key stationary and dynamical quantities. As in equilibrium, an understanding of such critical features comes from their classification into universality classes [1–3]. Each class groups systems with the same emergent behavior, as identified by the values of parameters known as critical exponents. However, in contrast to equilibrium settings, even the simplest critical nonequilibrium systems, e.g., those featuring absorbing state phase transitions in the directed percolation (DP) universality class, are not analytically solvable and their exponents cannot be determined exactly.

To overcome this problem, efficient numerical schemes for simulating nonequilibrium many-body dynamics are required. This concerns both continuous-time models, such as the contact process [4], and discrete-time evolutions such as in the paradigmatic Domany-Kinzel cellular automata (DKCA) [5]. To estimate the values of critical exponents with high precision, a particularly powerful approach is offered by studying critical behavior in discrete-time systems following a local perturbation of the absorbing state [4]. For instance, in the DKCA, this is a state with a single occupied site, as shown in Fig. 1(a).

The importance of such scenarios is twofold. First, numerically exact simulations can be performed directly in the limit of an infinite system, i.e., free of finite-size effects. This stems from the fact that the information about the presence of a local perturbation propagates with a strict light cone. Second, as

a consequence, critical exponents can be extracted directly from such evolutions by considering only a finite portion of the system; see Fig. 1(b). Put together, simulations of models such as the DKCA have allowed for unprecedented accuracy in the estimation of the critical exponents defining NEPTs in classical systems, and thus underpin the general understanding of out-of-equilibrium physics that results.

For quantum many-body systems (QMBSs), tracking the evolution of an initial seed also provides access to key universal quantities associated to NEPTs. However, the corresponding simulations in continuous [6,7] and discrete time [8,9] pose significant challenges. Indeed, owing to the substantial technical barriers present in studying out-of-equilibrium QMBSs, understanding the critical behavior and universality classes of even seemingly simple QMBSs displaying NEPTs remains an outstanding problem [10–13].

In this paper, we introduce a method to study NEPTs in QMBSs that builds on the advantages of classical seed simulations. We show that the discrete-time dynamics of (1+1)D quantum cellular automata (QCA) starting from a single seed can be simulated efficiently without finite-size effects. While the (unitary) (1+1)D QCA is represented by a 2D state, we consider the associated (nonunitary) reduced evolution of a 1D row. To this end, we use a tensor network (TN) [14–24] that grows dynamically, thus extending the range of application for infinite-size TN methods [25–27] to the case of NEPTs in QMBSs.

Just like their classical counterparts—which include the DKCA—(1+1)D QCA are free of time-discretization errors. As such, our approach offers an extremely clean, flexible, and

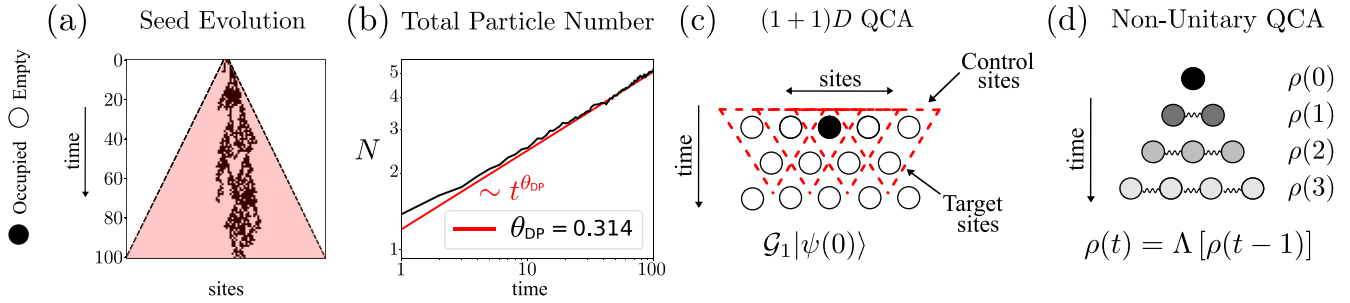


FIG. 1. Seed evolutions in a (1+1)D (quantum) cellular automaton. (a) Seed evolution of the classical Domany-Kinzel cellular automaton at the critical site-DP point [3] performed directly on an infinite lattice. Occupied sites only fall inside the indicated light cone (dashed lines and shaded region). (b) The total number of occupied sites, $N(t)$, is shown averaged over 1000 runs (solid black line). Even for relatively short times, the universal power law can be seen (straight solid red line), and the observed exponent is in agreement with the expected value for 1D DP: $\theta_{\text{DP}} = 0.314$. (c) In a (1+1)D QCA, a 2D lattice is initiated in a product state with all empty sites apart from the first row, which encodes the initial condition. The state $|\psi(1)\rangle$, obtained by updating the target sites in the subsequent row via the application of three-body unitary gates, is shown. The operator \mathcal{G}_1 is the product of the applied gates, and thus $|\psi(1)\rangle = \mathcal{G}_1 |\psi(0)\rangle$. (d) When (1+1)D QCA on an infinite lattice display a strict light cone, the reduced dynamics of a row with seed initial conditions are fully captured by those of a finite-size reduced state, $\rho(t)$. The size of this state grows proportionally with time. This allows for the dynamics of the underlying unitary (1+1)D QCA to be studied via the corresponding nonunitary dynamics of $\rho(t) = \Lambda[\rho(t-1)]$, free of finite-size effects.

efficient framework for studying NEPTs in quantum systems. To demonstrate its potential, we apply it to previously studied QCA [8]. The method introduced here allows for the accurate estimation of critical exponents at significantly reduced computational costs.

Single-seed dynamics in QCA. Similarly to the case of classical cellular automata [28] [cf. Fig. 1(a)], the full information about (1+1)D QCA is encoded in a two-dimensional (tilted) lattice, as shown in Fig. 1(c). The horizontal dimension represents space, while the vertical one provides a notion of time [8,9,29,30]. Each lattice site is described by a two-level system, with basis states $|\bullet\rangle$, $|\circ\rangle$ denoting an occupied or an empty site, respectively. The lattice is initialized with all sites in the empty state, except for those in the zeroth row, which encode the initial condition.

The evolution of this 2D lattice occurs via the action of unitary operators (gates) on lattice sites. These gates act on pairs of consecutive rows, such that at time step t , the “target” row t is updated according to the state of “control” row, $t-1$. For concreteness, we consider a local update rule with three-body gates, $G_{t,k}$, but the extension to gates with larger support (implementing longer-range interactions) is immediate.

The gate $G_{t,k}$ performs a controlled unitary operation on the target site at (t, k) , with controls at $(t-1, k_-)$ and $(t-1, k_+)$, where k_- (k_+) refers to the control site to the left (right) of target site k . In order for the QCA to feature an absorbing state, we impose a constraint on $G_{t,k}$: we assume that target sites are not modified whenever the corresponding control sites are both found in the empty state [8]. As such, if a control row has all sites empty, no update takes place on their targets.

The global update for the entire row, \mathcal{G}_t , is then an ordered product of the gates $G_{t,k}$, one per target site. In contrast to classical systems, one must pay special attention to the ordering of the unitary quantum gates, as these do not commute in general. As such, to preserve a physical notion of causality—a concept which is also key to the definition of QCA in the field of quantum information (QI) [31,32]—only those gate orderings giving rise to a strict light cone, reminiscent of quantum

systems that feature a Lieb-Robinson bound [33], will be considered. Choosing specific gate orderings will certainly affect details of the evolution dynamics, but are not expected to impact universal features, such as critical exponents.

Due to the unitarity of the gates, the state of the 2D lattice after t time steps is pure, $|\psi(t)\rangle$. It contains the full space-time information of the QCA and can be used to compute unequal time observables, such as time-correlation functions. However, here we focus on observables which can be computed from the reduced state of the QCA on row t at time t . These observables provide sufficient information to determine the universality class of the considered model [3,4,8].

Mathematically, the reduced state is given by $\varrho(t) = \text{Tr}'(|\psi(t)\rangle \langle \psi(t)|)$, where Tr' is the partial trace over all sites with the exception of those in row t . The evolution of $\varrho(t)$ describes the discrete-time dynamics of a 1D system. Corresponding to the classical case where irreversible 1D CA can be simulated by reversible (1+1)D CA [34], the dynamics of $\varrho(t)$ are, in general, nonunitary. Since gates act solely on consecutive rows, the evolution of $\varrho(t)$ can be defined iteratively as

$$\varrho(t) = \text{Tr}_{t-1}[\mathcal{G}_t \varrho(t-1) \otimes |\Omega_t\rangle \langle \Omega_t| \mathcal{G}_t^\dagger], \quad (1)$$

where $|\Omega_t\rangle$ is the t th row configuration with all empty sites and Tr_{t-1} indicates the trace over the sites where $\varrho(t-1)$ is defined.

Turning now to dynamics ensuing from a single-seed initial condition, we set $\varrho(0)$, i.e., the zeroth row of the 2D lattice, to be $\varrho(0) = \sigma_{\text{seed}}^+ |\Omega_0\rangle \langle \Omega_0| \sigma_{\text{seed}}^-$, where $\sigma^+ = |\bullet\rangle \langle \circ|$ and $\sigma^- = (\sigma^+)^\dagger$, in such a way that the seed site (at the center of the initial row) is occupied. Clearly, for this choice of the initial state, $\varrho(0)$ factorizes as $\varrho(0) = \rho_\circ \otimes \rho(\bullet) \otimes \rho_\circ$, where the matrix ρ_\circ indicates an infinite tensor product of empty states, while $\rho(\bullet) = |\bullet\rangle \langle \bullet|$ has support only on a single site.

The most striking consequence of the existence of a strict light cone is that for dynamics starting from a state with finite nontrivial support such as the single seed, at any time, $\varrho(t)$ can be factorized as $\varrho(t) = \rho_\circ \otimes \rho(t) \otimes \rho_\circ$. Here, $\rho(t)$ has support only on a finite set of sites, \mathcal{L}_t , with size $L_t = |\mathcal{L}_t|$.

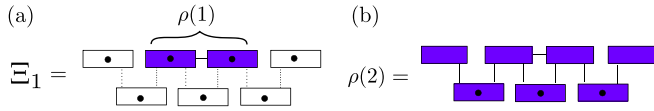


FIG. 2. Reduced dynamics of the (1+1)D QCA. (a) To evolve $\rho(t-1) \rightarrow \rho(t)$ through the map Λ , we begin via an MPO representation of $\rho(t-1)$, shown here for $t=2$. Empty sites are then added at locations where gates act nontrivially. This operation defines the state Ξ_{t-1} . We have depicted these states here using the standard diagrammatic notation for TNs [14,22]. In this notation, tensors are represented by shapes with a number of legs corresponding to their order. Each tensor corresponding to operators in a local Hilbert space must have two legs for the “physical” indices, here represented by a solid black circle. Other “virtual” legs which join the shapes (solid black lines) encode correlations between these, and we denote the trivial legs (indicating no correlations) as dashed lines. (b) The gates are then applied in MPO form to update the state. By tracing out the sites of row $t-1$, indicated diagrammatically by removing physical legs, the exact TN representation of $\rho(t)$ is obtained. Approximating this by an MPO allows the scheme to be iterated.

Consequently, the entire reduced dynamics of the (1+1)D QCA can be captured without finite-size effects through the evolution of $\rho(t) = \Lambda[\rho(t-1)]$, where Λ is the map that implements this update; see Fig. 1(d).

In general, starting from any $\rho(t-1)$ and for any gate ordering, the reduced dynamics can be implemented via Eq. (1) as follows. First, $\rho(t-1)$ is mapped into $\varrho(t-1)$ by attaching an infinite product of empty sites in row $t-1$ to the left and right of \mathcal{L}_t . Second, row t is included in a product state of all empty sites. Third, the gates are applied via \mathcal{G}_t before, finally, the sites of row $t-1$ are traced out.

For orderings with strict light cones, this procedure simplifies since sites outside the support \mathcal{L}_t are in the absorbing state and, thus, only a finite number of gates in \mathcal{G}_t act nontrivially. Therefore, the map Λ can be implemented by considering only a finite number of extra empty sites and gates (see, also, Fig. 2). In addition, for any given t , $L_t \leq L_{t-1} + v$ for some fixed integer v determined by the gate and the ordering. In what follows, we show how Λ can be expressed in terms of a finite TN that updates a matrix product operator (MPO) representation for $\rho(t-1)$ into an MPO representation of $\rho(t)$. This enables efficient numerical simulations of the dynamics of $\rho(t)$, allowing us to investigate universal aspects of the QCA, directly in the infinite lattice limit.

TNs for seed evolutions on infinite lattices. For the sake of clarity, we now specify a gate ordering. We choose an alternating leftmost-rightmost ordering, where first the leftmost target site is updated, then rightmost, then the second leftmost, and so on. Generalization to other gate orderings is possible (see the Supplemental Material [35] for a discussion of another example). The alternating leftmost-rightmost ordering leads to the lowest possible increase in L_t , i.e., $v=1$, and thus has minimal computational cost.

It is convenient to represent $\rho(t)$ as an MPO. The map Λ , which connects two MPOs with different supports, can then be understood in terms of a TN; see Fig. 2. At any given time, $\rho(t-1)$ is represented as an MPO [cf. Fig. 2(a)] with maximum bond dimension χ . To find the representation for $\rho(t)$,

with our choice of the ordering, we first expand $\rho(t-1)$ by introducing a single empty site at both boundaries and $t+1$ empty sites (the target sites) representing the subsequent row. This defines a new state Ξ_{t-1} , with the same nontrivial part. At this point, we can apply all the gates acting nontrivially on the QCA, as shown in Fig. 2(b). This is achieved by representing gates as three-site MPOs and applying these to the previous TN for Ξ_{t-1} . To obtain a TN for $\rho(t)$, we then trace out all sites related to row $t-1$. An exact representation of $\rho(t)$ as an MPO can be achieved by factorizing the tensors in row $t-1$ and contracting them into those of row t . However, such an operation will, in general, lead to an exponential growth of the bond dimension χ with time, making numerical simulations infeasible. To avoid this, the last step of the update consists in constructing an approximate MPO for $\rho(t)$. There are several strategies for approximating $\rho(t)$ using an MPO with fixed χ . For TNs, a natural approach is to first map the MPO into a matrix product state (MPS), apply standard approximation methods available for MPS [14,18], and, finally, map the MPS back into an MPO [35].

Critical exponents for (1+1)D QCA. To demonstrate the potential of the method introduced here, we consider the (1+1)D QCA defined by the local gate,

$$G_{t,k} = \exp[-i\Gamma(U_{t-1,(k-,k_+)}P_{t-1,(k-,k_+)}\sigma_{t,k}^+ + \text{H.c.})]. \quad (2)$$

This gate implements a generalized rotation of the target by an angle Γ , conditioned on the controls by a two-body projector,

$$P_{t,(k-,k_+)} = \mathbb{1}_{t,(k-,k_+)} - |\circ\circ\rangle\langle\circ\circ|_{t,(k-,k_+)}. \quad (3)$$

This dynamics thus has the absorbing state $|\dots\circ\dots\rangle$, which follows from $P_{t,(k-,k_+)}|\circ\circ\rangle_{t,(k-,k_+)} = 0$ [29]. In order to control the degree of quantum correlations [8], we introduce the two-body unitary

$$U_{t,(k-,k_+)} = \exp(-i\omega[\sigma_{t,k-}^z\sigma_{t,k_+}^y + \sigma_{t,k-}^y\sigma_{t,k_+}^z]), \quad (4)$$

where $\sigma^y = -i|\bullet\rangle\langle\circ| + i|\circ\rangle\langle\bullet|$, $\sigma^z = |\bullet\rangle\langle\bullet| - |\circ\rangle\langle\circ|$. When $\omega=0$, no entanglement is created in $\varrho(t)$ and it is always separable. As ω is increased, $\varrho(t)$ can become entangled, before again becoming separable when $\omega = \pi/2$.

This particular (1+1)D QCA was studied previously for $\omega=0$ [29] and with $\omega>0$ [8]. In the first case, the separability of $\varrho(t)$ allowed for the universality class to be established as 1D DP, via a mapping to the site-DP critical point of the DKCA. For $\omega>0$, TNs were used to find bounds on the critical exponent α , associated to the decay of the average particle density when starting from homogeneous—all sites occupied—initial conditions [3]. These exponents were also found to be consistent with 1D DP. However, the accuracy of the estimates was limited by the computational difficulty of the simulation. This was found to depend strongly on the value of ω , and cases where $U_{t,(k-,k_+)}$ generated significant entanglement were particularly challenging. As such, simulations with values such as $\omega=1$ led to rather loose bounds on the estimate of α .

Here, we study the dynamics of this (1+1)D QCA starting from an initial seed state and using an alternating leftmost-rightmost gate ordering. To test our method, we consider the challenging $\omega=1$ case, using $\omega=0$ for comparison.

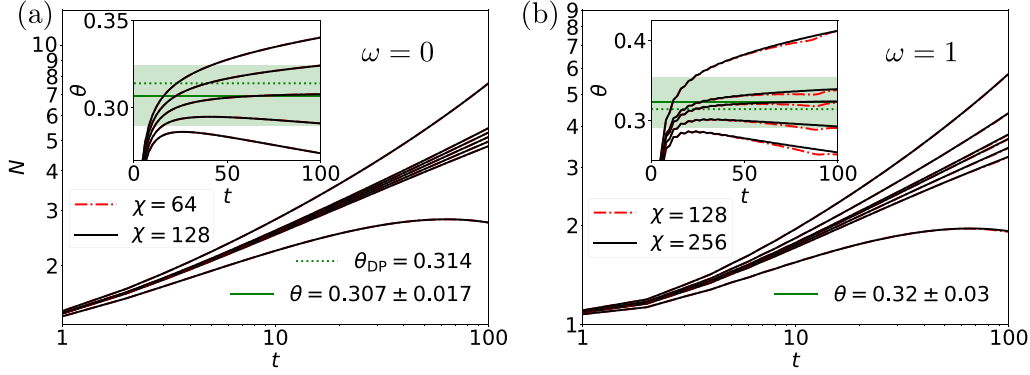


FIG. 3. Critical behavior. (a) The evolution of the total number of occupied sites, $N(t)$, is shown for $t \in [1, 100]$ for various values of Γ . This includes five intermediate values close to the critical point—as indicated by the almost linear behavior in the log-log plot—and two values (the bottom-most and top-most lines) further from the critical point, illustrating the NEPT from a state of zero particles to one with a diverging number. In ascending order from the lowest line, the values of Γ are 0.98, 0.995, 0.996, 0.997, 0.998, 0.999, 1.01. The inset shows $\theta(t)$ for the central five values. From these, the flattest curve provides the estimate for the critical point, $\Gamma_c = 0.997 \pm 0.01$, and exponent, $\theta = 0.307 \pm 0.017$. The shaded region represents the error [35]. The estimated value of θ is consistent with that of 1D DP, indicated by the dotted green line. χ is the maximum MPO bond dimension used. (b) Corresponding plots for $\omega = 1$ with $\Gamma = 1.015, 1.03, 1.032, 1.034, 1.035, 1.04, 1.05$. These produce the estimates $\Gamma_c = 1.034 \pm 0.02$ and $\theta = 0.32 \pm 0.03$, also consistent with 1D DP.

We focus on the total number of occupied sites at time t ,

$$N(t) = \sum_{k \in \mathcal{L}_t} \text{Tr}[\hat{n}_k \rho(t)], \quad (5)$$

where \hat{n}_k is the operator $\hat{n} = |\bullet\rangle\langle\bullet|$ at a given site. At the critical Γ , this average value is expected to display a universal power-law behavior with critical exponent θ , $N(t) \sim t^\theta$ [see Fig. 1(c)]. We can thus use $N(t)$ both to determine the critical point Γ_c for each ω and to estimate the value of θ , as shown in Fig. 3.

For fixed ω , we take several values of Γ and simulate $\rho(t)$ up to $t = 100$ for different χ , the two highest of which are shown in Fig. 3. We then calculate the effective exponent, $\theta(t) = \log_2 [N(t)/N(t/2)]$, which converges to a constant for power-law behavior and provides an approximation for the exponent θ at criticality. Using the highest value of χ available and taking the curve for which $\theta(t)$ is closest to a constant, we estimate the critical value Γ_c as well as the exponent θ . Errors due to finite χ are estimated via the difference of curves with alternative χ values. For errors associated to the estimation of the critical point, values of θ extracted from curves with $\Gamma \approx \Gamma_c$ are used. For both $\omega = 0$ and $\omega = 1$, the errors due to the estimate of Γ_c are far larger than those attributable to finite χ . As such, the errors stated in Fig. 3 correspond to those induced by the estimate of the critical point [35].

For $\omega = 0$ and $\omega = 1$, the estimated values of θ were $\theta = 0.307 \pm 0.017$ and $\theta = 0.32 \pm 0.03$, respectively. Both are consistent with 1D DP. Since the errors on these estimates are dominated by the resolution of the grid used to find Γ_c , they can be reduced easily by finer searches. This is in stark contrast to the homogeneous case. Not only are the overall errors there larger due to the presence of finite-size effects, but it is the error due to finite χ that limits the accuracy [8].

Conclusions and outlook. We have introduced a general scheme for the simulation of seed evolutions in (1+1)D QCA with an absorbing state. This allows for the study of quantum NEPTs free of finite-size effects. This method

can be used to provide an accurate estimate of the critical exponents related to the universal dynamics of these models. Owing to the universality of continuous NEPTs, the method introduced here can be more broadly applied well beyond the particular considerations of QCA to the study of out-of-equilibrium quantum many-body systems with absorbing states. Furthermore, by considering systems with trivial (infinite-temperature) steady states, it can easily be extended to the study of systems without absorbing states as well.

Nonetheless, QCA are also of interest in their own right. Not only can they be considered as computational models and analyzed from the perspective of QI [31,36–38], but, as they are quantum many-body systems, their emergent physical properties can be intriguing [39]. In this regard, our method, along with (1+1)D QCA more generally, may be rather useful as it allows for the explicit study of emergent behavior in QCA—including nonunitary QCA, far less studied than their unitary counterparts [9,32,40,41]. Applying these tools to characterize nonequilibrium universality classes will potentially provide general insights into the relationships between the computational properties of QCA and their collective many-body behavior.

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