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Critical values for a non-attractive lattice gas model

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Abstract. We investigate the critical behaviour of a one-dimensional non-attractive lattice gas model that is the continuous-time, 'Hamiltonian limit' version of the Domany–Kinzel (Domany E and Kinzel W 1984 *Phys. Rev. Lett.* **53** 311) cellular automaton in one of its parameter subspaces. Our exact numerical diagonalizations and finite-size scaling data seem to indicate that the phase transition in the model is in the directed percolation (DP) universality class of critical behaviour, as would be expected on the basis of the DP conjecture.

The Domany–Kinzel (DK) probabilistic cellular automaton (PCA) [1] is one of the most studied PCAs in the physics literature, because it is the most general left–right symmetric one-dimensional PCA, and has the interesting property of having the mixed site–bond directed percolation (DP) process on the square lattice as one of its instances. Its defining rules are given in table 1. The mixed site–bond DP process is given by assigning a probability $s \in [0, 1]$ for a site to be present in the lattice, and a probability $b \in [0, 1]$ for a bond to exist between any two sites on the lattice. The mixed DP problem consists in finding the values of s and b for which an infinite cluster of sites connected by the bonds occurs such that one can walk unidirectionally in it, say to the south and to the east indefinitely. In the DK PCA this problem is obtained by choosing the transition probabilities $x = 0$, $y = sb$ and $z = sb(2 - b)$. For $s = 1$ one obtains the pure bond DP problem, whilst for $b = 1$ one obtains the pure site DP problem.

In this paper we investigate numerically the critical behaviour of a continuous-time one-dimensional non-attractive lattice gas for which some lower bounds on the critical points of the PCA version were given recently [2]. The model is related to the DK PCA in one of its parameter subspaces, and, although the model is not on the mixed site–bond DP parameter subspace of the DK PCA, our numerical data indicate that it presents a DP-compatible dynamical critical exponent, as would be expected on the basis of the DP conjecture [3].

Let $n_\ell(t) \in \{0, 1\}$ denote the occupation number of the site $\ell \in \Lambda$ at the integer instant t, with $\Lambda \subset \mathbb{Z}$ a finite lattice with $|\Lambda| = L$ sites and periodic boundary conditions $\ell + L \equiv \ell$. The model we are interested in is the continuous-time version of the PCA defined by the rules

$$n_\ell(t+1) = \begin{cases} (n_{\ell-1}(t) + n_{\ell+1}(t)) \bmod 2 & \text{with probability } p \\ 0 & \text{with probability } 1 - p. \end{cases} \tag{1}$$

The rule table for this PCA is given in table 2. From tables 1 and 2 we see that our PCA is equivalent to the DK PCA with rates $x = 0$, $y = p$ and $z = 0$. We thus see that unless we take the unphysical value $b = 2$ in the site–bond DP subspace of the DK PCA, this model does not belong to that subspace.

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Table 1. Rule table for the DK PCA. The first line gives the initial neighbourhood; the other two lines give the probability with which the state listed on the left is reached by the central bit.

	000	001	010	011	100	101	110	111
0	$1-x$	$1-y$	$1-x$	$1-y$	$1-y$	$1-z$	$1-y$	$1-z$
1	x	y	x	y	y	z	y	z

Table 2. The same as table 1 for the PCA defined by equation (1).

	000	001	010	011	100	101	110	111
0	1	$1-p$	1	$1-p$	$1-p$	1	$1-p$	1
1	0	p	0	p	p	0	p	0

Our approach in constructing the continuous-time version for the above PCA is to take its non-diagonal transitions, i.e. those transitions for which the final state differs from the initial state, and associate with them a stochastic lattice gas with transition rates given by the original PCA rules. This approach has been used before in the PCA literature [4], and is equivalent to the so-called 'Hamiltonian' or 'strong anisotropic' limit for the transfer matrixes of equilibrium lattice models [5].

As is well known [6], we may write the master equation for interacting lattice gases as a Schrödinger-like equation in Euclidean time,

$$\frac{\mathrm{d}}{\mathrm{d}t}|P(t)\rangle = -H|P(t)\rangle \tag{2}$$

with $|P(t)\rangle$ the generating vector of the probabilities $P(\boldsymbol{n},t) = \langle \boldsymbol{n}|P(t)\rangle$ of observing the configuration $\boldsymbol{n} = (n_1, n_2, \ldots, n_L) \in \{0,1\}^{\Lambda}$ at instant t, and with the infinitesimal generator H of the Markov semigroup playing the role of the Hamiltonian. For the non-diagonal transitions of the PCA defined by equation (1), the operator H can be written as

$$H = -\sum_{\ell=1}^{L} H_{\ell-1,\ell,\ell+1} \tag{3}$$

with the three-body stochastic transition matrix $H_{\ell-1,\ell,\ell+1}$ given by

$$H_{\ell-1,\ell,\ell+1} = \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -p & \cdot & 1-p & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & p & \cdot & -1+p & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -p & \cdot & 1-p & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & p & \cdot & -1+p & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 \end{pmatrix} \tag{4}$$

where the three-site basis vectors are ordered as usual, $(0,0,0) \prec (0,0,1) \prec \cdots \prec (1,1,0) \prec (1,1,1)$, and the dots indicate null entries. Proper tensorization of the above three-body matrix with unit matrices in order to obtain the full matrix H is understood. Notice that the elements in the columns of $H_{\ell-1,\ell,\ell+1}$ (and consequently of H) add to zero due to the conservation of probabilities, and that its non-diagonal elements are positive, since $0 \leqslant p \leqslant 1$. Identifying a particle with the up-spin state and a hole with the down-spin state in the σ^z basis, the transition matrix $H_{\ell-1,\ell,\ell+1}$ above is seen to be equivalent to the non-Hermitian quantum spin operator

$$H_{\ell-1,\ell,\ell+1} = \tfrac{1}{2}(\sigma_\ell^x - 1)[1 + (1-p)\sigma_\ell^z + p\sigma_{\ell-1}^z\sigma_\ell^z\sigma_{\ell+1}^z] \tag{5}$$

where σ^x and σ^z are the usual Pauli spin-$\frac{1}{2}$ matrixes. The transition matrix (4) resembles the analogous matrix for the basic contact process, but with non-standard rates and with the elementary process $101 \to 111$ lacking. This lack is the root of the non-attractiveness of the process. (Loosely speaking, attractive interacting particle systems present a tendency for clustering, as occurs in ferromagnetic models or in the basic contact process. The precise mathematical statement of attractiveness can be found in [7].)

The lowest gap in the spectrum of H may be used to perform a finite-size scaling analysis in the same way as one does in equilibrium problems [8]. Around the critical point $p \gtrsim p^*$, the correlation lengths of the infinite system behave as

$$\xi_\parallel \propto \xi_\perp^z \propto (p - p^*)^{-\nu_\parallel} \propto (p - p^*)^{-\nu_\perp z} \tag{6}$$

where $\xi_\parallel$ and $\xi_\perp$ are the correlation lengths respectively in the time and space directions, $\nu_\parallel$ and $\nu_\perp$ are the corresponding critical exponents, and $z = \nu_\parallel/\nu_\perp$ is the dynamical critical exponent. For finite systems of size L we expect that

$$\xi_{\parallel,L}^{-1} = L^{-z_L}\Phi(|p - p_L^*|L^{1/\nu_{\perp,L}}) \tag{7}$$

where p_L^*, z_L and $\nu_{\perp,L}$ are the finite versions of p^*z and $\nu_\perp$, and $\Phi(u)$ is a scaling function with $\Phi(u \gg 1) \sim u^{\nu_\parallel}$. On general grounds one expects $\lim_{L\to\infty} p_L^*, z_L, \nu_{\perp,L} = p^*, z, \nu_\perp$. From equations (6) and (7) we obtain

$$\frac{\ln[\xi_{\parallel,L}(p_L^*)/\xi_{\parallel,L'}(p_L^*)]}{\ln(L/L')} = \frac{\ln[\xi_{\parallel,L''}(p_L^*)/\xi_{\parallel,L}(p_L^*)]}{\ln(L''/L)} = z_L \tag{8}$$

which through the comparison of three different system sizes $L' < L < L''$ furnishes simultaneously p_L^* and z_L. Of course, $\xi_{\parallel,L}$ and the gap $E_L^{(1)} - E_L^{(0)} = E_L^{(1)}$ of H are related by $\xi_{\parallel,L}^{-1} = \mathrm{Re}\,\{E_L^{(1)}\}$.

We calculated the gaps of H with the power method, which requires only matrix-by-vector multiplications that can be carried out efficiently and does not require a diagonalization in the usual, 'QR' sense, a step that may lessen the quality of the data. The version of the power method we use takes advantage of the presence of absorbing states, and is also suitable for the investigation of time-dependent properties of Markov chains [9].

Our results for p^* and z are summarized in figure 1. Curiously enough, despite the translational invariance of the lattice gas rules the finite-size estimates behaved better for triplets of lengths of the form $L', L, L'' = 2\ell - 1, 2\ell, 2\ell + 1$, $\ell \in \mathbb{N}$; i.e., whilst for these triplets of lengths it was possible to find a p_L^* satisfying the first equality in equation (8), for the other type of triplets (the even–odd–even ones) that was not always possible, although in general the difference between the first and the second terms in equation (8) could be made small, and with a reasonable value of z_L, of the same order as the other values found. Both sets of data behaved irregularly with the system sizes, preventing us from applying the usual extrapolation algorithms [10, 11] to them. We are presumably in the presence of strong finite-size effects and corrections to scaling. Unfortunately, we were not able to go beyond $L = 22$ in our diagonalizations. The $L = \infty$ values for p_L^* were obtained through a least-squares fit to the curve $x_L = x_\infty + aL^{-1}$, since the data scale well with L^{-1} (although they do so with L^{-2} also, but with a smaller correlation coefficient), whilst for z_L we only estimated the mean value of our data. As expected on the basis of the DP conjecture, namely, that the phase transition about a single absorbing state in single-component systems with a scalar order parameter and in the absence of internal symmetries should be in the DP universality class of critical behaviour [3], our lattice gas shows a DP-compatible exponent $z = 1.58 \pm 0.04$. The most precise value of z for the DP universality class to date is given by $z = 1.580\,745 \pm 0.000\,010$ [12]. The critical point of the model is estimated as $p^* = 0.926 \pm 0.004$ (LS correlation coefficient $\gamma = -0.944$). This value is slightly higher than the critical value $p_{\mathrm{DK}}^* = 0.82 \pm 0.01$ of the

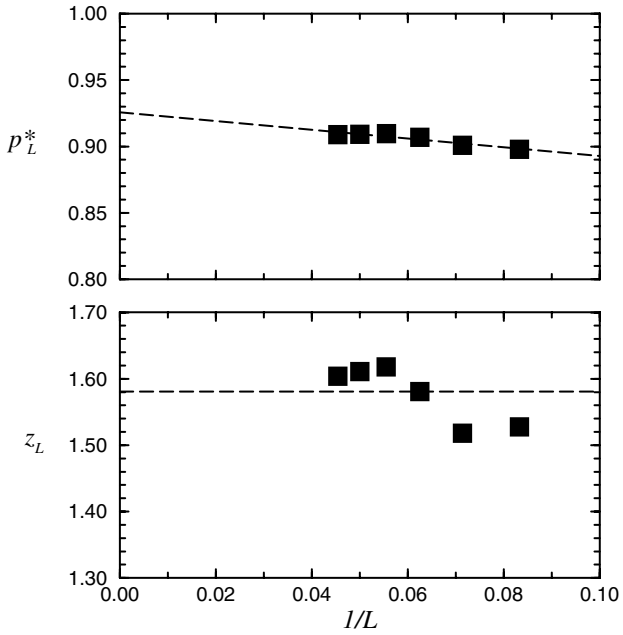

Figure 1. Finite-size data for the critical point p^* and the dynamical critical exponent z of the model defined in equation (4). The dashed line in the graph for p_L^* is the least-squares linear fit to the data, whilst the dashed line in the graph for z_L represents the best known value of the dynamical critical exponent of the DP universality class.

corresponding point ($x = 0$, $y = p$, $z = 0$) in the DK PCA [1]. This shift in the critical point for the lattice gas version of the PCA was observed before in a study similar to the present one, where the properties of the lattice gas on the line $x = 0$, $y = z$ (corresponding to the pure site DP problem) was investigated [4], and is probably a general feature, since asynchronous dynamics tend to be more noisy than synchronous dynamics.

In summary, we conducted numerical diagonalizations of the infinitesimal generator of the continuous-time version of a non-attractive PCA that is an instance of the DK PCA. Although our PCA is not in the site–bond DP subspace of the DK PCA, our data seem to indicate that its continuous-time version shows DP critical behaviour. Our finite-size data showed an irregular approach to the infinite-system limit, and this prevented us from obtaining good estimates of the critical values. It would be interesting to study this lattice gas by time-dependent Monte Carlo methods in order to obtain more accurate critical values.

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