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Dependence on initial conditions of an adsorption-desorption process

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A one-dimensional irreversible adsorption-desorption process is simulated. The critical parameters as well as the critical exponents are measured. At the critical point, the crossover between the accumulative state and the depleted state is described by a universal characteristic function.

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I. INTRODUCTION

The irreversible adsorption-desorption process (ADP) equivalent to a contact process [1] is a simple and representative model of nonequilibrium. Many important models belong to the same universal class as the ADP. They are, for instance, the stochastic cellular automata [2], directed percolation [3], Schlögl's first model [4,5], and the Reggeon field theory [6,7,5]. It is known that this class of models undergoes a dynamic phase transition. The critical parameters as well as the critical exponents have been calculated by various methods, such as the renormalization group ϵ expansion, the field theory, the series analysis, the high temperature expansion, the operator method, and the Monte Carlo simulation, etc. For the adsorption rate r larger than a critical value r_c (i.e., the subcritical phase), there is only one steady state in which all sites are occupied; while for $r<r_c$ (i.e., the supercritical phase) active steady states with finite fraction of vacancy emerge. Power laws of time evolution have been found for two initial states in the extreme conditions, i.e., (1) the state with only one (or few) vacant site (to be referred as accumulative initial state, or AIS in abbreviation), and (2) the state of no molecule (referred as depleted initial state, DIS in abbreviation). Since the model is nonequilibrium, the initial conditions could have important effects in all time of the evolution. Initial states with molecule number ranged from one to the maximum will be explored in the present paper.

In recent years, the dynamic Monte Carlo method based on the short-time dynamic scaling has been widely used in numerical evaluation of the critical parameters and exponents. The details of the algorithm can be found in Refs. [8–10]. The idea can be traced back to Grassberger and de la Torre twenty years ago [5] in their study on the Schlögl's first model that is believed to belong to the same universal class of the ADP to be studied in the present paper. We first apply the dynamic Monte Carlo method to the ADP. From the short-time evolution of the vacancy fraction with the AIS, the critical point is estimated. The critical exponents are attained at the critical points with either the AIS or DIS.

Though power laws are lost when molecule number is finite, it is found that the critical short-time behavior can be described by a universal characteristic function. Zheng first observed this phenomenon in the Ising model and Potts model [11]. In Ref. [12], authors attained an analytical expression of the universal function for the kinetic spherical model. In the present paper, we show that the universal characteristic function also exists in a dynamic process that is irreversible, nonergodic, and does not fulfil any detailed balance condition. To confirm the universality of the characteristic function, we simulate the model with both sequential and synchronous dynamic rules.

II. THE MODEL AND SCALING LAWS

The process is realized on discrete spacetime. Only periodic boundary condition will be considered. Each site could be occupied (denoted by $\sigma_i=1$) or nonoccupied (denoted by $\sigma_i=0$). For the sequential rule, the states of sites are updated one by one from left to right. A vacant site has a probability r to adsorb a molecule. The desorption probability of an occupied site depends on the states of its neighbors, $w_i(\sigma_i=1\rightarrow 0)=(2-\sigma'_{i-1}-\sigma_{i+1})/2$ with σ'_{i-1} the latest updated state of the $(i-1)$th site. If both neighbors are occupied, no desorption is possible. The synchronous rule is only different from the sequential one in that σ'_{i-1} is replaced by σ_{i-1}, i.e., the original state of the $(i-1)$th site, in the desorption probability w_i. The latter model is also called stochastic cellular automata.

To investigate the time-dependent states, one must specify the initial state. The initial state with only one vacant site has been extensively studied. Denote the survival probability as $P(t)$, the vacancy fraction as $n(t)$, and the average square distance as $R^2(t)$. At the critical point, one expects the power laws

$$P(t)\sim t^{-\delta}, \tag{1}$$

$$n(t)\sim t^{\eta}, \tag{2}$$

$$R^2(t)\sim t^{z}. \tag{3}$$

Here z is the critical dynamic exponent. Since the average size of occupied domains is finite (not divergent as t grows), the domain number follows the same scaling law as $n(t)$. There is a hyperscaling relation between the three exponents, $Dz=3\eta+4\delta$ with $D=1$, the space dimension. Notice that here z is different from that defined in Ref. [5]. The latter is

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$z-\eta$ in our notation. The original vacant seed will produce a spreading active region in the following time. The active region contains vacant domains and occupied domains that do not reach the boundary sites of the lattice. Since the domains have finite average sizes, the width Γ of the active region is proportional to the domain number $m(t)$ and follows the same scaling law as $m(t)$. On the other hand, the domain number is proportional to the vacancy fraction averaged only over the active states, hence we have the scaling laws

$$m(t)\sim t^{c_m}=t^{\eta+\delta}, \tag{4}$$

$$\Gamma\sim t^{c_g}=t^{\eta+\delta}. \tag{5}$$

In the limit of zero rate, it is known that $c_g=1/2$ in one dimension [5]. A nontrivial correction at the critical point is expected.

For initial states of zero correlation length, we assume that the initial molecule number $n_0=n(0)$ is transformed to $\phi(n_0,b)$ in the scale transformation with ϕ a universal function of n_0 and the scale factor b. It has the general properties: $\phi(n_0\rightarrow+0,b)=b^{x_0}n_0$, $\phi(1,b)=1$, and $\phi(n_0,1)=n_0$. The vacancy fraction, for instance, has the finite-size scaling relation

$$n(t,n_0,\tau,L)=b^{-\beta/\nu}n(b^{-z}t,\phi(n_0,b),b^{1/\nu}\tau,b^{-1}L), \tag{6}$$

where $\tau=r-r_c$. Let $b=(-\tau)^{\nu}$ and choose $n_0=1$, $t\rightarrow\infty$, and $L\rightarrow\infty$, one recognizes that β is the exponent for the steady order in supercritical phase: $n(\tau)\sim(-\tau)^{\beta}$. For $n(0)=1$, Eq. (6) at the critical point implies a power law

$$n(t)\sim t^{-\beta/\nu z}. \tag{7}$$

For the Reggeon field theory, Grassberger and De La Torre [5] has proved that $\beta/\nu z=\delta$. Due to the universality, this relation should also be valid for the AD process. In the limit $n_0\rightarrow+0$, assuming that the vacancy fraction is an analytic function of n_0, one can recover the power laws for the AIS and has $x_0=z\eta+\beta/\nu$. The derivative of $\ln n(t)$ with respect to τ in the vicinity of the critical point provides a relation for determination of $1/\nu$,

$$\left.\frac{\partial \ln n(t)}{\partial\tau}\right|_{\tau=0}\sim t^{1/\nu}. \tag{8}$$

Define a time-dependent cumulant as

$$U(t)=\frac{n^{(2)}(t)}{n(t)^2}-1 \tag{9}$$

with $n^{(2)}$ the second moment of the order (i.e., the vacancy fraction). Its scaling relation is

$$U(t,n_0,\tau,L)=U(b^{-z}t,\phi(n_0,b),b^{1/\nu}\tau,b^{-1}L). \tag{10}$$

For $n(0)=1$, at the critical point one has a power law in the infinite L limit

$$U(t)\sim t^{D/z} \tag{11}$$

with $D=1$ the dimension.

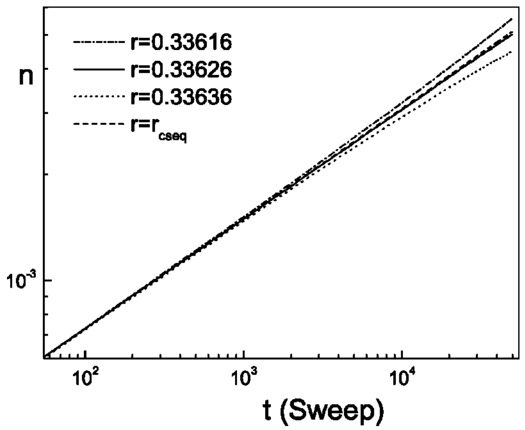

FIG. 1. The log-log plot of the order parameter $n(t)$ of the sequential rule with $n_0=1/L$, $L=10\,000$. Three curves from up to down are corresponding to $r=0.336\,16$, 0.336 26, and 0.336 36, respectively. The dash line is the fitted straight line corresponding to $r_{cseq}=0.336\,241$.

Let us take R^2 as the last example. The definition of R^2 in continuous space is

$$R^2(t)=\int_0^L dx x^2\rho(x,t). \tag{12}$$

For the depleted states, the molecule density $\rho(t)$ does not depend on x, hence $R^2(t)\sim L^3 n(t)$. The scaling relation is

$$R^2(t,n_0,\tau,L)=b^{3-\beta/\nu}R^2(b^{-z}t,\phi(n_0,b),b^{1/\nu}\tau,b^{-1}L). \tag{13}$$

This implies that for $n_0=1$ and a fixed L, a power law

$$L^{-3}R^2\sim t^{-c_r} \tag{14}$$

with $c_r=\beta/\nu z$.

It is remarkable that the same characteristic function ϕ enters all the scaling relations. Among all critical exponents introduced in this section, only three are independent.

III. CRITICAL POINT AND EXPONENTS

Initialize the lattice in the AIS then release it to evolve with the sequential rule, we produce Fig. 1 for $n(t)$ vs time in a log-log plot for $r=0.336\,16$, $0.336\,26$, and $0.336\,36$. A periodic lattice of $L=10\,000$ sites is used. For each line, 0.4×10^6 of samples are generated. In fact, difference between such lattice and that of a smaller order is not big for time up to 10 000 sweeps (one sweep is to update the whole lattice one time). One sees that the middle line is very straight from a hundred until 50 000 sweeps. The first 100 sweeps would contain nonuniversal microscopic detail or corrections to the scaling hence should be skipped. In the macroscopic short time, $n(t)$ follows the power law (2). Using the three curves of Fig. 1, from $t=1000$ to 50 000, to interpolate for a straight line, we attain the critical rate $r_{cseq}=0.336\,241(10)$ and exponent $\eta=0.3137(28)$. The errors quoted here and in the following are estimated from the statistical fluctuations among subgroups of samples. Each subgroup typically contains 20 000 samples. From this set of samples, one can measure other quantities such as $P(t)$, $R^2(t)$, $\Gamma(t)$, and the number of domains $m(t)$. For each quantity, one can estimate the critical point and attain the corresponding critical exponent. Critical points estimated from various quantities have discrepancy of 2 at the fifth effective digit. With $r_{cseq}=0.336\,241$ as input, we attain: $\delta=0.1594(14)$, $z=1.578(9)$, $c_g=0.4728(54)$, and $c_m=0.4802(52)$. One may check that our results fulfill the hyperscaling relation $z=3\eta+4\delta$ within the errors.

The relaxation from $n(0)=1$ at r_{cseq} with the sequential rule has the power law of Eq. (7). The exponent $\beta/\nu z$ estimated in a range $t=1000\sim 10\,000$ is 0.1597(5) in $L=3000$ and 0.1597(4) in 2000. One sees that the finite-size effect has been smaller than the statistical errors. Typically, $(80\text{–}120)\times 10^3$ samples are generated for each set of parameters. The same set of samples gives $c_r=0.1603(7)$ for the exponent of Eq. (14). By fitting the power law (11) for $U(t)$, we attain $1/z=0.631(2)$ in $L=3000$ and $0.634(2)$ in $L=2000$. The cumulant U contains the second moment, so the statistical error is bigger. The dynamic critical exponent also can be attained from the finite-size scaling (10). By searching for a time rescale factor $(2/3)^z$ for $L=2000$ such that the cumulant of $L=2000$ has the best match to that of $L=3000$, we attain $z=1.578(3)$. In order to estimate the exponent $1/\nu$, the left-hand side of Eq. (8) is replaced by a difference. The difference of rates should not be too small otherwise the fluctuation would overwhelm any information. With $r=0.335\,241$ and $0.337\,241$, i.e., $\Delta\tau=0.002$, we attain $1/\nu=0.572(1)$.

Similar scaling behaviors are observed for the synchronous rule. The process started from $n(0)=1/L$ with $L=10\,000$ is simulated for $r=0.472\,244$, $0.472\,444$, and $0.472\,644$ with 120×10^3 samples for each. In the time range 1000–50 000 we attain the critical point $r_{csyn}=0.472\,403(39)$. As expected, the exponents for the synchronous rule and the sequential rule are the same within the errors since two dynamic rules belong to the same universal class.

IV. CHARACTERISTIC FUNCTION

The time development of $n(t)$ at the critical point for $n(0)$ between $1/L_1$ and 1 is shown in Fig. 2 with $L_1=2000$. One sees that the adsorption phase and desorption phase are not clearly separated. The dash line is corresponding to $n_0=1/L_1$ with the slop η. The vacancy fraction of the dash line has been amplified by 20 times in order to make it visible in the figure. As $n(0)$ increases, the increase of $n(t)$ becomes slower and finally crosses over to decrease. The decrease is guided by the power-law relaxation from $n(0)=1$.

For $n(0)$ not small nor close to 1, there is no power law. However, the observations are compact to a generalized scaling relation (6). Assuming the existence of a characteristic function $\phi(n_0,b)$, we try to match the results of $L_2=b^{-1}L_1$ with $b=2$ to those of L_1. The time of the smaller lattice is rescaled by a factor b^z. One also needs to rescale the amplitudes properly. For instance, for $n(t)$ the rescaled factor is $b^{-\beta/\nu}$, for R^2 it is $b^{3-\beta/\nu}$. The amplitude of $U(t)$ needs no rescaling. In Fig. 2, the solid curves are $n(t)$ of $L_1=2000$ while the crosses are rescaled results of $L_2=1000$. The function ϕ for $b=2$ is plotted as an inset. The uncertainty of ϕ is bigger as n_0 is close to 1 since then $n(t)$ is not sensitive to n_0 and hard to be distinguished from the relaxation of $n_0=1$. However the error is bound since $\phi\leqslant 1$.

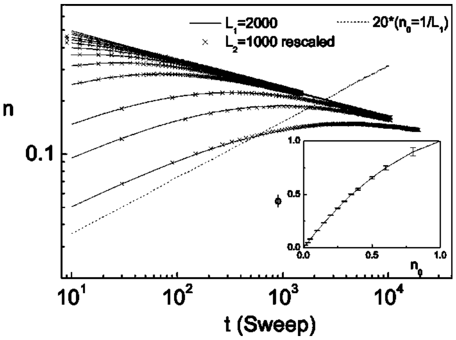

FIG. 2. The solid lines are $n(t)$ of the sequential rule of $L_1=2000$ at r_{cseq} with $n_0=0.015$, 0.03, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5, 0.6, and 1, respectively, from the bottom to top. The crosses are rescaled results of $L_2=1000$ with $n_0'=0.025$, 0.049, 0.082, 0.161, 0.233, 0.304, 0.370, 0.424, 0.500, and 0.552 from the bottom to top. The dash line is $n(t,n_0=1/L_1)$, which is enlarged 20 times for comparison. The inset is the characteristic function $\phi(n_0,b)$ for $b=2$.

For a given n_0 of certain L, ϕ as a function of b can be determined by searching for a $n_0'=\phi(n_0,b)$ in the lattice $L'=bL$ such that the rescaled $b^{-\beta/\nu}n(b^{-z}t,n_0',b^{-1}L)$ collapses into that of lattice L. An instance of $n_0=0.1$ is shown in Fig. 3 where $n(t)$ of $L=2000$ is compared with that of $L'=2250$, 1750, 1500, 1250, and 750. The resulted $\phi(n_0=0.1,b)$ is given as an inset.

The characteristic function $\phi(n_0,b)$ is universal in the sense that it is not only valid for various quantities but also for different dynamic rules of the same universal class. For instance, with the same value of $\phi=n_0'$ corresponding to each n_0 that has been found in Fig. 2 for the sequential rule,

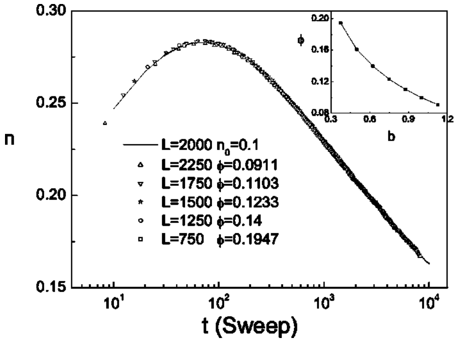

FIG. 3. The rescaled vacancy fraction $b^{-\beta/\nu}n(b^{-z}t,\phi(n_0,b),b^{-1}L)$ with $n_0=0.1$ and $L=2000$ for various b at the critical point. The sequential dynamic rule is adopted. The inset is the characteristic function $\phi(n_0,b)$ with $n_0=0.1$.

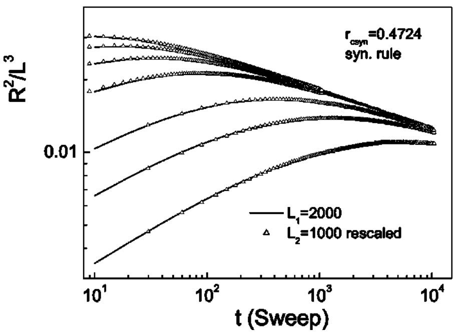

FIG. 4. $R^2(t)/L^3$ vs time is plotted. The synchronous dynamic rule is adopted. The solid line has $L_1=2000$, while the triangles are rescaled results of $L_2=1000$. The correspondence between n_0 for L_1 and n_0' for L_2 is the same as in Fig. 2. n_0 from the bottom to top are 0.015, 0.03, 0.05, 0.1, 0.15, 0.2, and 0.25.

the rescaled $R^2(t)/L_2^3$ of $L_2=1000$ matches to that of $L_1=2000$, as shown in Fig. 4 for the synchronous rule.

V. DISCUSSIONS AND CONCLUSIONS

The one-dimensional adsorption-desorption process is simulated with both sequential and synchronous dynamic rules. By fitting the power laws of various observables for either $n_0=1/L$ or 1, we attain the critical points and the critical exponents. The critical point for the sequential rule is found to be $r_{cseq}=0.336\,24(1)$, while $r_{csyn}=0.472\,40(4)$ for the synchronous one. Our critical points are bigger than that $r=0.303$ of the previous Monte Carlo simulation and series expansions via time-independent perturbation theory. By the coherent anomaly method theory, Marque [13] attained $r=0.337$ that is closer to our one for the sequential rule. The results of critical exponents confirm the universality and the hyperscaling relations. Our best estimations for the exponents from $n_0=1/L$ are $\eta=0.3137(28)$, $\delta=0.1594(14)$, and $z=1.578(9)$. Those from $n_0=1$ are $\beta/\nu z=0.1597(5)$, $1/z=0.631(2)$, and $1/\nu=0.572(1)$. They are consistent with the best analytical results [14] that we have known.

We generalized the dynamic scaling for finite n_0 by introducing a characteristic function of n_0 and the scaling factor b. This function not only describes the crossover of all observables but also should be universal for different dynamic rules. That is confirmed by the sequential and the synchronous dynamic rules. n_0 could be viewed as a relevant parameter that is running from zero to one according to the characteristic function $\phi(n_0,b)$. The power laws only appear at vicinity of two fixed points of the function, i.e., $n_0=0$ and $n_0=1$. All initial states considered here have zero correlation length. When there is a nonzero initial correlation, the picture would change.

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