Physical Review A, 1991

FINITE SIZE BEHAVIOR OF RELAXATION TIMES IN STOCHASTIC MODELS WITH ACCUMULATING FIXED POINTS

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PACS: 64.60.Ak, 05.90.+m.

ABSTRACT

We report numerical and analytical studies of the finite size time scales in a system with microscopic stochastic dynamics which in the bulk limit corresponds to an evolution equation with an accumulation point of critical fixed points. Our results suggest that the finite size behavior is dominated not by fluctuations but by the bottle-neck statistical weights at near-fixed-point conditions in a finite-size system.

1. Introduction

The detailed description of the emergence of macroscopic "hydrodynamic" equations from the underlying microscopic deterministic or stochastic dynamics is of importance in many fields. The scope and emphasis of discussion vary widely, ranging from conceptual questions of macroscopic irreversibility to more technical aspects of quantitative and qualitative characterization of the discreteness and finite-size effects. The present work falls in the latter category. Thus, we report numerical Monte Carlo studies, supplemented by analytical considerations, of the finite size behavior in a single-variable stochastic evolution model with an accumulation point of critical fixed points.

Single-variable stochastic models find applications in diverse fields ranging from excited electron-hole statistics in intrinsic semiconductors to models of chemical reactions, percolation, and evolution of epidemics.[1−7] The precise form of the dynamical rules depends on the phenomenon and model considered. In more generally oriented studies, however, one frequently concentrates on dynamical rules which have some particularly interesting features. Consider for instance the simplest "critical point" hydrodynamic evolution equation

$$\frac{d\tilde{\rho}}{dt} = -\tilde{\rho}^2 \tag{1.1}$$

Here $\tilde{\rho}$ is an average density variable, $0 \leq \tilde{\rho}(t) \leq 1$, and t denotes the time. The large-time behavior implied by (1.1) involves no exponential-relaxation time scales (which is the generic case) but is instead power-law, termed *critical*, $\tilde{\rho}(t\text{-large}) \sim t^{-1}$.

In the discrete, finite-size "microscopic" version, the dynamics is defined by the transition rules for the variable $n = 0, 1, \ldots, N$, where N is the total system size and n is the number of, e.g., wet sites in percolation or the number of sick individuals in a group of the total size N for epidemics, etc. The fluctuating density is then $\rho = n/N$. There have been very few systematic studies[1,5–6,8] in the framework of the modern scaling theories, of finite-size (e.g., finite population, N) effects which are particularly profound for critical or near critical stochastic models for which the leading relaxation times become infinite or very large as $N \to \infty$. Few results were also published[5,9–10] for stochastic models more complicated than single-variable.

The simplest critical-point dynamics (1.1) was recently studied[8] within the scaling description of the discrete, finite-N effects. In this work we report an investigation of a more complicated dynamics which corresponds to the bulk ($N = \infty$) evolution equation

$$\frac{d\tilde{\rho}}{dt} = -\tilde{\rho}^2 \sin^2\left(\frac{c}{\tilde{\rho}}\right) \tag{1.2}$$

where we will mostly consider the case

$$c = 1 \tag{1.3}$$

Thus, $\tilde{\rho} = 0$ is an accumulation point of critical fixed points which correspond to the zeros of the sine function, $\tilde{\rho} = c/(\pi k)$, $k = 1, 2, \ldots$. Note that (1.2) integrates to

$$\mathrm{cotan}\left[\frac{c}{\tilde{\rho}(0)}\right] - \mathrm{cotan}\left[\frac{c}{\tilde{\rho}(t)}\right] = ct \tag{1.4}$$

The flow diagrams for (1.1) and (1.2)-(1.3) are shown in Figure 1. The variation of $\tilde{\rho}(t)$ with time is always from right to left as t increases, with respect to the direction of the abscissa in Figure 1, for $\frac{d\tilde{\rho}}{dt} < 0$. The fixed points are at $\frac{d\tilde{\rho}}{dt} = 0$, and for (1.2) infinitely many of them accumulate at the origin. Thus, any initial value $\tilde{\rho}(0)$ in the interval $\left[\left((k+1)\pi\right)^{-1}, (k\pi)^{-1}\right)$ evolves in time to the fixed point value $\tilde{\rho}(\infty) = \big((k+1)\pi\big)^{-1}$. The initial values in the range $[\pi^{-1}, 1]$ evolve to π^{-1}.

The reason for the particular choice (1.2) is mathematical: the dynamics described by this evolution equation extends the simpler dynamics (1.1) to having an infinite number of fixed points. Thus, (1.2) is not really favored on physical grounds, and in fact in most applications the function on the right-hand side of (1.2) would be rather a polynomial in $\tilde{\rho}$.

The outline of the next three sections is as follows. The microscopic transition rules and the associated notation and definitions are given in Section 2. Numerical results for the finite-size time scales are presented in Section 3. Finally, Section 4 is devoted to some qualitative and quantitative analytical considerations and to the concluding discussion.

2. Definition of the Microscopic Transition Rates

Discrete microscopic time evolution rules usually allow general changes in the occupation variable n in the range $n = 0, 1, \ldots, N$, on time scales of order 1. It proves convenient, however, to further discretize the time steps[1,8] in units of $\frac{1}{N^2} \ll 1$ and to consider only local changes $n \to n, n \pm 1$. On the time scales of order 1 such local steps can cumulatively represent rather general "bulk" ($N = \infty$) evolution equations. It turn out that for the discrete time steps $\Delta t = \frac{1}{N^2}$ the proper normalization of the transition rates is

$$\text{Rate}(n \to n-1) = N^{-1} A(n, N) \tag{2.1}$$

$$\text{Rate}(n \to n+1) = N^{-1} B(n, N) \tag{2.2}$$

$$\text{Rate}(n \to n) = 1 - N^{-1} \left[A(n, N) + B(n, N) \right] \tag{2.3}$$

where $A(n, N)$ and $B(n, N)$ are intensive-in-N, i.e., they approach definite limiting functions of

$$\rho \equiv \frac{n}{N} \tag{2.4}$$

as $N \to \infty$. In fact, we take $A = A(\rho)$, $B = B(\rho)$. Note that with the normalizations chosen, the variation of n for time steps $\Delta t = \frac{1}{N^2}$ is very slow: the changes (± 1) in the n value only occur a fraction of order $\frac{1}{N}$ of the attempts. This has important consequences for numerical implementation of the stochastic dynamics considered here, as will be described in Section 3.

The transition rules of the model studied in this work are defined as follows:

$$A = \left[(1-y)\rho + y\rho^2\right]\sin^2\left(\frac{c}{\rho}\right) \tag{2.5}$$

$$B = \left[(1-y)\rho(1-\rho)\right]\sin^2\left(\frac{c}{\rho}\right) \tag{2.6}$$

At $\rho = 0$, we take $A = B = 0$. The rates depend on a parameter $y \in [0,1]$, the significance of which will be discussed shortly. Note that we take $c = 1$ for most of this work. The choice of the value of c will be taken up in Section 4. The important property for now is that $c = 1$ is incommensurate with the period of the sine-squared function, i.e., with π. As a result, the finite-N evolution has no fixed points with $\rho > 0$. Of course, the point $\rho = 0\ \ (n = 0)$ is an absorbing state of the stochastic dynamics for finite N.

Generally, for transition rules (2.1)-(2.3), the Ω-expansion method of van Kampen[1] can be used to show that the bulk hydrodynamic equation is

$$\frac{d\tilde{\rho}}{dt} = B(\tilde{\rho}) - A(\tilde{\rho}) \tag{2.7}$$

where $\tilde{\rho}$ is the bulk average value of the density ρ. Note that the choice (2.5)-(2.6) yields (1.2) for any $y \in [0,1]$.

Usually, the corrections to the average equation (2.7) are due to fluctuations for finite N, and they can be calculated in some regimes by using the Ω-expansion or other approximation schemes,[1,11] or by numerical and scaling-analysis methods.[8] Indeed, for the rates leading, e.g., to (1.1), obtained if the sine-squared factors are dropped in (2.5)-(2.6), it was found[8] that pattern of fluctuations, unlike the bulk average behavior (1.1), is sensitive to the parameter y, both quantitatively and qualitatively.

For a simple stable fixed point at $\tilde{\rho} = \rho^*$, one can expand $\frac{d\tilde{\rho}}{dt} \simeq (\rho^* - \tilde{\rho})/\tau$, so that the approach to the fixed point value has a characteristic time scale $\tau > 0$. For critical fixed points, the leading term in the expansion vanishes ($\tau = \infty$). One of the most remarkable finite-N effects is that in the microscopic system various definitions of the time scales characterizing the dynamics near a critical fixed point yield finite values, usually diverging as powers of N, as $N \to \infty$. For the quadratic fixed point at $\tilde{\rho} = 0$, with dynamics (1.1), it was found[8] that this divergence, and more generally the form of fluctuation effects, depend on the value of y. Three time scales considered, the "first passage" time to reach $n = 0$, the evolution operator spectral-gap time scale (studied[8] only for $y = 1$; results for $y = 0$ are available for a nearly identical model[6]), and the time scale defined by the limits of applicability of the Ω-expansion, — all suggested the following pattern. The finite-N time scales varied smoothly with N, and diverged $\sim \sqrt{N/(1-y)}$ for fixed $0 \leq y < 1$, as $N \to \infty$, crossing over to the divergence $\sim N$ at $y = 1$. The crossover was further described by a scaling form which will not be discussed here.

The oscillating sine-squared factors added in the rates (2.5)-(2.6) incorporate a new effect. Indeed, the infinite sequence of the fixed points present in the bulk, exist for finite N only as approximate fixed points corresponding to small, "bottle-neck" transition rates at certain n values. (Recall that we take c incommensurate with π.) Thus the finite-N time scales can be large both due to fluctuations near $\rho = 0$ and due to these bottle-neck rates. In fact, the standard expansion methods[1,11] are hardly useful here beyond the leading bulk result (2.7). We will mostly rely on numerical results reported in Section 3; some analytical considerations will be offered in Section 4. Our conclusion will be that the "bottle-neck" effects are dominant.

3. First Passage Times: Numerical Results

Perhaps the most profound difference between the finite-N dynamics, defined by (2.5)-(2.6) with (1.3), and its macroscopic limit (1.2), is that the fixed points at $\rho = 1/(\pi k)$, $k = 1, 2, \ldots < \infty$ are not exact for finite N. As a result, any finite-N evolution starting from an arbitrary initial value $n(0)$ and advancing according to (2.1)-(2.3), will eventually end up in the only finite-N absorbing state, that at $n = 0$. One obvious definition of the "largest" time scales for the finite-N system is therefore via the distribution of the times it takes to reach $n = 0$.

Since the full distribution is difficult to calculate with reasonable accuracy, our numerical studies were focused on its first and second moments, denoted T_1 and T_2, respectively (the precise definitions are given later in this section). Let us outline the numerical procedure employed. A *time-driven* mechanism of simulation would be advancing time by regular step increments $\Delta t = \frac{1}{N^2}$. At each step one would decide whether the sample process experiences increment $n \to n + 1$, decrement $n \to n - 1$ or stays the same $n \to n$. This easy-to-code time-driven procedure was used, e.g., in Ref. 8. However, we observed that the transitions rates of *changes* $n \to n \pm 1$ at each given n are quite small, see (2.1)-(2.6). In the time-driven scheme, most of the time steps the computer would advance simulated time without a change to the process. Thus, we devised a different *event-driven* simulation mechanism wherein the computer efforts are spent only on the processing of actual events,[12] and the simulated time is advanced by typically not equal time intervals, — from event to event. The computations of these, — potentially much longer than Δt time intervals, — is done in the following way: the probability for a change in n to occur exactly at the kth time step ($k = 1, 2, \ldots$) is $P(1 - P)^{k-1}$, where

$$P = [A(n) + B(n)]/N \tag{3.1}$$

see (2.1)-(2.2). The weights $P(1-P)^{k-1}$ sum up to 1. Given the current n value (the initial n value was selected at random) at each step of the event-driven algorithm, we sample a random number uniformly distributed on (0,1). It is compared to the partial sums

$$S_K = \sum_{k=1}^{K} \left[P(1-P)^{k-1}\right] = 1 - (1-P)^K \tag{3.2}$$

Depending on which interval $[S_K, S_{K+1})$ the random number was in, the time was advanced by the appropriate $K\Delta t$. The n value was then changed by $+1$ or -1, with probabilities $B/(A+B)$ and $A/(A+B)$, respectively, by generating another random number and comparing it to these two weights. The process was repeated with the new n value until $n = 0$ was reached. The comparison of random numbers to the partial sums (3.2) required a careful consideration of roundoff errors. The random number generator was the Kirkpatrick-Stoll R250.

The trajectories generated by the new event-driven procedure are statistically indistinguishable[12] from those generated by the time-driven procedure, while the speed of simulation is at least two orders of magnitude higher. Even with the efficient numerical procedure, the simulations required nontrivial CPU resources. Thus, we had two types of runs. For N values from 1 to 100, we calculated $T_{1,2}$ averaged over 160000 realizations, i.e., different, randomly selected initial values of n, and different random number sequences for the time evolution, as just described. For these N values, the calculations were done for $y = 0.0, 0.1, 0.2, \ldots, 1.0$. For $N = 101$ to 700, we averaged over only 40000 realizations, and these longer runs were limited to $y = 0, \frac{1}{2}, 1$. As a measure of the CPU time, we quote that the long run for $y = \frac{1}{2}$ took about 3.5 CPU *days* on the IBM RS/6000 workstation, model 320.

We denote by $T(i)$ the first passage times obtained in the different runs, where $i = 1, 2, \ldots, I$, with $I = 160000$ or 40000, as described above. The moments were defined as follows:

$$T_1 = I^{-1} \sum_{i=1}^{I} T(i) \tag{3.3}$$

$$T_2^2 = I^{-1} \sum_{i=1}^{I} T^2(i) \tag{3.4}$$

Let us first consider the results for $y = 0$ which are presented in Figures 2 and 3, for the first and second moment, respectively. These figures are drawn on a semilogarithmic scale. The $T_{1,2}$ values do not vary smoothly with N. In fact, they fluctuate widely, sometimes by orders of magnitude, for adjacent N values. This "local" variation is difficult to quantify. There is, however, also a superimposed overall upward trend with increasing N which seems to be well represented by $T_{1,2} \sim N$. Note that the data in Figures 2 and 3 were plotted as $T_{1,2}/N$ to emphasize this proportionality. The case $y = 0$ for the simpler model (1.1), without the oscillatory factors in the rates, was studied extensively,[6,8] by numerical transfer matrix and Monte Carlo methods, because it corresponds to the critical point of the mean-field directed percolation. As mentioned already, the time scales varied smoothly with N and increased $\sim \sqrt{N}$ for large N. Obviously, the present, multiple-fixed-point model is quite different. Here the time scales show behavior which can be represented as

$$T \simeq N\Theta(N) \tag{3.5}$$

where $\Theta(N)$ varies widely and shows no apparent regularities as N increases (at least in the range up to $N = 700$ covered by our numerical study).

The second moment, T_2, behaves similarly to the first moment, T_1, and is generally somewhat larger. This observation applies for all y. Thus, we only discuss the first moment for other y values. The results of the two other computer runs up to $N = 700$ are shown in Figures 4 and 5, where $y = \frac{1}{2}$ and 1, respectively. They are qualitatively similar to those for $y = 0$. The data follow the pattern summarized by (3.5). The runs up to $N = 100$ for the intermediate y values (data not shown here) also confirm the conclusion that there is no qualitative variation of the behavior for $y \in [0, 1]$. This is in contrast to the model (1.1) for which there was a qualitative crossover in the y-dependence at $y = 1$, as described earlier.[8]

The conclusion of our numerical study is that the model with the accumulating bulk fixed points at $\rho = 0$ is qualitatively different from that with a single fixed point at $\rho = 0$. Furthermore, for a single-fixed-point model the finite-size effects were dominated by fluctuations and could be quantified to a certain extent by using the large-N expansions and scaling ideas.[1,8,11] For the new, multiple-fixed-point model the finite-N time scales seem to be dominated by the bottle-neck weights due to small transition rates when the discretized ρ values are close to the bulk fixed point values. This conclusion is suggested by the irregularity of the N-dependence, and will be further confirmed in the next section.

4. Analytical Considerations and Discussion

In an ensemble of systems evolving according to the stochastic dynamics (2.1)-(2.3), it is convenient to put the probabilities of the various n values at time t in a column vector $\mathcal{V}$ of size $N+1$ the entries of which are labeled by $n = 0, 1, \ldots, N$. The appropriate probability vector for $t + \Delta t = t + \frac{1}{N^2}$ is then obtained by applying (left-multiplying) the matrix of the transition rates (2.1)-(2.3) on the vector at t:

$$\mathcal{V}_{t+\Delta t} = \mathcal{M}\mathcal{V}_t \tag{4.1}$$

The transfer matrix, or evolution operator, $\mathcal{M}$, has elements

$$\mathcal{M} = \begin{pmatrix} 1 & \mathrm{R}(1\to 0) & 0 & \ldots & & \\ 0 & \mathrm{R}(1\to 1) & \mathrm{R}(2\to 1) & 0 & \ldots & \\ 0 & \mathrm{R}(1\to 2) & \mathrm{R}(2\to 2) & \mathrm{R}(3\to 2) & 0 & \ldots \\ \vdots & 0 & \mathrm{R}(2\to 3) & \mathrm{R}(3\to 3) & \mathrm{R}(4\to 3) & 0 \\ & \vdots & 0 & \ddots & \ddots & \ddots \end{pmatrix}_{(N+1)\times(N+1)} \tag{4.2}$$

where R abbreviates for "Rate;" see (2.1)-(2.3). This tridiagonal, stochastic matrix has the largest eigenvalue $\lambda_0 = 1$, corresponding to the "stationary" evolution in the absorbing state $n = 0$. All other eigenvalues are less than 1 in absolute value; some may form complex-conjugate pairs although typically a large number of the leading eigenvalues are real. The time scales ξ_m associated with the spectral gaps are obtained by the identification

$$\left(\frac{\lambda_m}{\lambda_0}\right)^{t/\Delta t} = \mathrm{e}^{-t/\xi_m} \tag{4.3}$$

where we assumed for simplicity that $\lambda_{m>0}$ is real. For the present case, we have

$$\xi_m = -\frac{1}{N^2 \ln \lambda_m} \tag{4.4}$$

For the mean-field directed percolation model,[6] which is nearly identical with the model (1.1) at $y = 0$, as formulated here, with no sine-squared factors in the transition rates, the time scales ξ_m had a physical interpretation of the longitudinal percolation correlation lengths, and the largest such length was studied numerically quite extensively.[6] With oscillating rates, the numerical methods employed[6] become unstable to roundoff errors, and no results for large N values can be obtained. Analytical progress can be made, however, for the special case $y = 1$.

Indeed, for $y = 1$ the transition rate for $n \to n+1$ vanishes; see (2.6). Thus the lower off-central diagonal in (4.2) consists of zeros. As a result, $\mathcal{M}$ is an upper-diagonal matrix, and the eigenvalues are given by the diagonal elements:

$$\lambda_m = 1 - \frac{m^2}{N^3} \sin^2\left(\frac{cN}{m}\right) \tag{4.5}$$

where $m = 0, 1, 2, \ldots, N$, and we used (2.3)-(2.5).

An interesting question arises: which of the eigenvalues (with $m > 0$) is the largest for a given N, yielding the largest time scale ξ? More generally, one could consider the distribution of the ξ values for each N. We haven't attempted the mathematical analysis of this rather complicated problem in the number theory. Indeed, it is obvious that the answer depends on how close c is to a number commensurate with π. By a numerical test up to $N = 10^4$ we found that for our preferred choice $c = 1$ the largest ξ value is obtained for $m = 1$. However, for other c values this need not be the case. As indicated, the proximity to a number commensurate with π seems to be decisive. For instance, for $c = 1.570800$ the largest eigenvalue is obtained with $m = 1$, for $N = 2, 3, \ldots, 100$, as one can easily check numerically. However, for $c = 1.570796$, which is closer to $\pi/2$, the largest eigenvalue up to $N = 100$ is obtained for $m = m_{max} > 1$ for several N values: 6, 10, 12, 20, 24, 30, 36, 40, 42, 48, 50, 54, 60, 66, 70, 72, 78, 80, 84, 90, 96, 100. The corresponding m_{max} values are 3, 5, 3, 5, 3, 15, 9, 5, 3, 3, 25, 9, 15, 11, 35, 9, 13, 5, 3, 3, 3, 25.

As mentioned, we haven't attempted a mathematical explanation of the patterns observed. A conclusion for the case $c = 1$ is that at least up to $N = 10^4$, the largest time scale is given by the analytical expression

$$\xi_1(N) = -\left[N^2 \ln\left(1 - N^{-3}\sin^2 N\right)\right]^{-1} \tag{4.6}$$

Note that for $N \gg 1$, one can use

$$\frac{\xi_1(N)}{N} \simeq \frac{1}{\sin^2 N} \tag{4.7}$$

The result (4.6) is plotted for $N = 1$ to 700 in Figure 6, and it should be compared with the first-passage time shown in Figure 5. The physical interpretation of the transfer matrix time scales ξ_m for $y = 1$ is less interesting than that of the first-passage times considered in Section 3. Indeed, while the first-passage times provide an overall characteristic time of the stochastic dynamics, the largest transfer matrix times in this case ($y = 1$) simply translate to the time scales the "bottle-neck" transition rates at densities $\rho = \frac{m}{N}$. The largest such time scale is given by (4.6) and is obtained at the lowest possible discrete ρ value, $\frac{1}{N}$ (for $c = 1$).

However, as far as general features of the increase of the time scales as $N \to \infty$ go, the transfer matrix results do yield a useful insight. Indeed, the overall trend $\sim N$ is seen, and one can write a representation (3.5) for $\xi_1(N)$. The corresponding varying function $\Theta(N) \simeq (\sin N)^{-2}$, which is actually plotted in Figure 6, on a semilogarithmic plot, shows an interesting pattern which is not exact and probably reflects the incommensurability of $c = 1$ with π. The pattern is self-similar in that it is observed "rescaled" in plots for much larger N values. It is not clear to what extent this visually observed semi-regular behavior can be utilized to quantify the results for the first-passage times, e.g., Figure 5, which look much more irregular.

In summary, the main conclusions of our work are that for accumulating fixed points, the finite-N time scales are dominated by the bottle-neck near-fixed-point transition rates. Large fluctuations in the time scale values result, for adjacent N, and they are difficult to quantify in general. The overall trend $\sim N$ in the finite-N time scales was found numerically and confirmed analytically for a special case. A weak dependence on the values of the parameter y suggests that the rôle of fluctuations, which are important at isolated fixed points, is secondary in our case.

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FIGURE CAPTIONS

Figure 1. The "flow diagram" corresponding to (1.2)-(1.3), solid line, and to (1.1), broken line.

Figure 2. The average (first-moment) passage time, T_1, to $n = 0$. These numerical data were obtained for $y = 0$; see Section 3.

Figure 3. The second-moment-average passage time, T_2, to $n = 0$. These numerical data were obtained for $y = 0$, in the same computer run that yielded the data shown in Figure 2.

Figure 4. The average (first-moment) passage time, T_1, to $n = 0$. These numerical data were obtained for $y = \frac{1}{2}$.

Figure 5. The average (first-moment) passage time, T_1, to $n = 0$. These numerical data were obtained for $y = 1$.

Figure 6. The largest transfer matrix time scale for $y = 1$; see (4.6). Note that the value for $N = 355$, $\xi_1(355)/355 \simeq 10^{9.04}$ is outside the ordinate limits (chosen to facilitate comparison with Figure 5).