Statistical features of large fluctuations in stochastic systems

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The fluctuation of transitional paths that describe the decay from a metastable state are studied with a space-time Monte Carlo algorithm. For a bistable stochastic system we characterize the statistical properties that describe the growth of large fluctuations. Interesting statistical features are discussed. In particular, we study the fluctuation enhancement (large non-Gaussian fluctuation) that occurs as the system escapes from a metastable state. The results are discussed in the context of a scaling theory for the decay from an unstable state. [S1063-651X(99)12202-5]

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I. INTRODUCTION

The occurrence of large fluctuations is fundamental to many physical processes, such as nucleation in phase transitions, chemical reactions, mutations in DNA sequences, and failures in electronic devices. A typical large fluctuation is one that enables a system to escape from a metastable state. Although such events are rare, they are responsible for a broad variety of physical processes.

The study of large fluctuations is difficult due to the rarity of the events. As such, there is little known regarding the statistics of these events. The only known insight into the study of large fluctuations goes back to the work of Onsager and Machlup [1]. For small noise Langevin dynamics, the distribution of transitional paths (trajectories that describe the growth of a fluctuation out of a stable state) is sharply peaked around a most probable or optimal path. For equilibrium systems, the optimal path for a transition to some fluctuational state is the time-reversed path of the decay of that fluctuation. Aside from this fundamental time reversibility of the optimal path for equilibrium dynamics, there are few known generic features for the growth of large fluctuations. For nongradient dynamical systems (nonequilibrium systems) the situation is far more nontrivial; recent studies have indicated interesting behavior (singularities) in the pattern of optimal paths [2,3].

There has been extensive work on the decay and relaxation of fluctuations to the equilibrium state. Starting from a Master equation level, the extensivity property (system size or small noise expansion) is used to derive equations for the most probable behavior [4]. For the decay of large fluctuations, such as the decay from an unstable state (saddle point), it is known that the system size expansion breaks down, and the most probable path is not meaningful [5]; this is also the case for the decay of metastable states [6]. Thus we can expect nontrivial (i.e., non-Gaussian) behavior in the statistical distribution of the transitional paths that describe large fluctuations from a locally stable state, i.e., fluctuations whereby the system makes a transition from a metastable state up to and over the free-energy barrier. This is precisely what we wish to study in this paper: the statistical properties of the transitional paths that describe the escape from a metastable state.

We introduce an efficient method to study large fluctuations in stochastic systems. The method, a space-time Monte Carlo (STMC) algorithm, was used in Ref. [7] in a study of the dynamic critical exponent in the Ising model. In this paper, we adapt the method for the purpose of characterizing the statistical properties of the transitional paths in the interesting regime where the barrier height is much larger than the noise strength. There was related work in Ref. [8], where the fluctuational paths were generated by an analog electric circuit system. The fluctuational state in this study was not very close to the saddle point; this is due to the difficulty in sampling large fluctuations in real time. The method we use in this paper allows us to study numerically the more inaccessible regime of fluctuations that drive the system all the way over the potential barrier in the limit of very small noise. The statistics of such processes are very difficult to study, and, to our knowledge, the work we present here is the first such study. Our goal is to search for some generic features that characterize the growth of large fluctuations, and in particular, to study the early stages of rare nucleation events in multicomponent systems. Indeed our primary motivation for devising the STMC method is the possibility of applying it to the study of rare nucleation events in physical systems. In this paper, to illustrate the method and approach, we study a simple bistable stochastic model.

Our main interest in this study is the fluctuation of the transitional paths that start at a (locally) stable or metastable state and grow up to some fluctuational state. For the model bistable system studied here, we study and characterize the statistical properties of the transitional paths in the limit of small noise. In particular, we quantify the large non-Gaussian fluctuations that result from the system transversing the potential barrier. The basic features of the data, such as an anomalous fluctuation and a fluctuation enhancement, will be discussed in analogy with Suzuki's scaling theory [5] for the decay from an unstable state.

In Sec. II we outline the STMC method and some relevant theoretical background. The model and the results are dis-

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cussed in Sec. III, followed by a brief summary and outline of future work in Sec. IV.

II. METHOD AND BACKGROUND

A. STMC

In order to study the statistics of rare events, one needs a method that can efficiently generate an ensemble of such events. The method we use is a space-time Monte Carlo algorithm. The principal idea is to study histories, whole space-time paths, in contrast to the usual approach, which is to update a spatial lattice. A common feature of the models we are interested in is that the probability for an entire history may be expressed in terms of an action function whose Lagrangian is a local function in the field variables $\phi(x,t)$ (and field derivatives), i.e., in the form

$$W \sim \exp[-S], \tag{2.1}$$

with $S=\int dt\, L(\phi(x,t),\dot{\phi}(x,t))$. This form of the probability weight on the path space is guaranteed for Markov processes, such as the Langevin dynamics considered in this work. We consider Langevin dynamics of the form (for simplicity the case of a scalar field and additive noise)

$$\dot{\phi}=F(\phi,t)+\epsilon\eta, \tag{2.2}$$

where η is the zero mean Gaussian white noise with variance $\langle \eta(x,t)\eta(x',s)\rangle=\delta(t-s)\delta(x-x')$, and ϵ^2 is the overall strength of the noise. The probability weight on the path space for model (2.2) is given by [9,10]

$$W\sim\exp\left[-\frac{1}{\epsilon^2}S_0-S_1\right], \tag{2.3}$$

where S_0 is the Onsager-Machlup action [1],

$$S_0=\tfrac{1}{2}\int(\dot{\phi}-F)^2 dx\, dt, \tag{2.4}$$

and the term higher order in the noise is given by $S_1=\frac{1}{2}\int\partial_\phi F\, dx\, dt$ [11].

In the STMC algorithm, the objective is to generate histories over some time-interval T with probability weight W. This is achieved in the usual manner by the Metropolis algorithm [12], i.e., by imposing the detailed balance condition

$$\frac{P(\phi(x,t)\to\phi'(x,t))}{P(\phi'(x,t)\to\phi(x,t))}=\exp\left(S(\phi(x,t))-S(\phi'(x,t)\right), \tag{2.5}$$

where $P(\phi(x,t)\to\phi'(x,t))$ denotes the transition probability between two *space-time* configurations, and the "Hamiltonian" in Eq. (2.5) is the action functional defined on the path space as $H=S\sim-\ln W$. The detailed balance condition guarantees that after many iterations or MC steps (a MC step here refers to an update over the whole space-time volume), the probability of a path is sampled according to $W\sim\exp[-S]$.

The boundary conditions on the space-time lattice of the form $\phi(t=0)=\phi_I,\phi(t=T)=\phi_F$, allows us to study the fluctuation of the field ϕ conditioned on an initial and future time constraint. Thus we can study the statistical quantity $\rho(\phi,t|\phi_F,T;\phi_I,0)$ $(t\in[0,T])$, which can describe the effect a future time constraint has on the present. Schulman considered such a quantity recently to clarify the issue of time-reversibility in thermodynamics and cosmology [13]. For the purpose of studying rare transitions out of a metastable state ϕ_m to some fluctuational state $\phi_{\rm fl}$, one generates an ensemble of trajectories with the boundary conditions $\phi_I=\phi_m$ (metastable state), and $\phi_F=\phi_{\rm fl}$, where the fluctuational state $\phi_{\rm fl}$ is the equilibrium state (or a saddle point state, a critical droplet, etc.).

The notion of introducing a Hamiltonian defined on the path space has been discussed [14,15] for discrete space-time models (probabilistic cellular automata). For discrete space-time models [where we denote by $s(t)$ the (spin) configuration of the system at time t], the weight becomes

$$W=\prod_t P(s(t)|s(t-1))=\prod_{i,t} p_{it}(s_i(t)|s(t-1),x_i(t-1)), \tag{2.6}$$

where $P(s(t)|s(t-1))$ denotes the transition probability between two spatial configurations at adjacent time slices, i labels the spatial lattice site, p_{it} denotes the individual site transition rate, and $x_i(t)$ denotes the set of spins (e.g., nearest neighbors) on which p_{it} depends. Note that by the structure of the weight W, the dynamics of the system is one in which the spatial spin configuration is updated simultaneously (in parallel), in contrast to the usual MC where the update is done sequentially (i.e., after each spin flip). It is important to notice that because of the parallel update structure, if the single site transition rate satisfies detailed balance with respect to some Hamiltonian, the same detailed balance condition may not hold for $P(s(t)|s(t-1))$. In particular, for the case where p_{it} is the Glauber transition rate $p_{it}=0.5(1-\tanh(\Delta H/2k_bT))$, for say an Ising system, the detailed balance condition with respect to the Ising Hamiltonian is not satisfied for $P(s(t)|s(t-1))$ [14]. One can strictly impose the detailed balance condition by introducing the two-step Domany algorithm [16]. However, the STMC algorithm is somewhat tedious to code, and the two-step update scheme does not seem to be a very natural dynamics.

In this paper, we study a continuum model, where the above issue of detailed balance does not arise (except for discretization corrections, see below). For Langevin models of the form $\dot{\phi}=F+\epsilon\eta$, one can express the action functional (2.3) to first order in the time discretization as [10,17] (suppressing the space dependence)

$$S=\frac{dt}{2\epsilon^2}\sum_i\left\{\frac{\phi(t_i)-\phi(t_{i-1})}{dt}-\alpha F(\phi_i)-\beta F(\phi_{i-1})\right\}^2 + dt\,\alpha\sum_i \partial_{\phi_{i-1}}F(\phi_{i-1}), \tag{2.7}$$

where $dt=t_i-t_{i-1}$, $\phi(t_i)=\phi_i$, and $\alpha+\beta=1$, $0\leqslant\alpha,\beta\leqslant 1$. The family of actions parametrized by α and β arises from the equivalent ways of discretizing a continuous function. The different choices of α and β result in correction terms of order $dt\sqrt{d}t$.

For the case where $F=-\partial_\phi H$ (as in the model studied in this paper), the detailed balance condition with respect to H is satisfied to order $dt\sqrt{d}t$, i.e.,

$$\frac{P(\phi(t)\rightarrow\phi'(t+dt))}{P(\phi'(t)\rightarrow\phi(t+dt))}=\exp[H(\phi)-H(\phi')+O(dt\sqrt{d}t)]. \tag{2.8}$$

B. Small noise limit

In the limit of zero noise $\epsilon\rightarrow 0$, the average or most probable path $\phi_o(t)$ is obtained by minimizing the Onsager-Machlup action (2.4). Consider a zero-dimensional bistable system, where the stable states ($\phi_{\rm eq}$ or ϕ_m) are separated by a saddle point ϕ_s. For gradient dynamics ($F=-\partial_\phi H$), the optimal path is

$$\dot{\phi}_o(t)=-F(\phi_o(t)) \tag{2.9}$$

for the growth of a fluctuation, (i.e., say for the transition $\phi_{\rm eq}\rightarrow\phi_{\rm fl},\phi_{\rm fl}<\phi_s$), and

$$\dot{\phi}_o(t)=F(\phi_o(t)) \tag{2.10}$$

for the decay ($\phi_{\rm fl}\rightarrow\phi_{\rm eq},\phi_{\rm fl}>\phi_s$). The optimal path that connects one attractor to another is given by connecting the above two solutions separated by an infinite time span where the system sits at the saddle point ϕ_s.

We are interested in studying the *fluctuation* of the transitional paths. The quantity of interest is

$$\chi(t)=\langle\phi^2(t)\rangle-\langle\phi(t)\rangle^2, \tag{2.11}$$

where $\langle\ \rangle$ denotes an ensemble average. At the Gaussian level, χ is determined by the inverse of the fluctuation operator $\mathcal{L}$, which is obtained by expanding the action functional (2.4) to second order around the optimal path $\phi_0(t)$,

$$\mathcal{L}=(F''F+F'F')-\partial_t^2, \tag{2.12}$$

where $F'=\partial_{\phi_o(t)}F(\phi_o(t))$.

As mentioned in Sec. I, the small noise expansion breaks down for the decay from an unstable or metastable state, and thus the zero noise theory is a singular limit. This singularity is related to the breaking of the time translational symmetry. Consider the kinklike trajectory $\phi_o(t)$ connecting ϕ_m at $t=0$ to ϕ_s at $t=T$. The position of the kink can occur anywhere along the time axis, and is a Goldstone mode (in the limit $T\rightarrow\infty$). For large T, the zero noise path exhibits a turning point near the saddle point where $\dot{\phi}_o\approx 0$. This feature leads to an infinite variance, since the fluctuation operator $\mathcal{L}$ has the solution $\mathcal{L}\dot{\phi}_o(t)=0$, and due to the turning point at ϕ_s (note that $\dot{\phi}_o=0$ at the stable or metastable states), $\dot{\phi}_o(t)$ is a zero eigenvalue of the fluctuation operator. This zero eigenvalue signals the breakdown of the Gaussian (small noise) approximation.

Our main interest in this paper is in the fluctuations of the transitional paths $\phi_m\rightarrow\phi_{\rm eq}$, which are characterized by the statistical quantity $\rho(\phi,t|\phi_{\rm eq},T;\phi_m;0)$. For gradient dynamical models the system passes through the saddle point in the decay process ($\phi_m\rightarrow\phi_{\rm eq}$), and thus, as discussed above, the variance (2.11) at the Gaussian level diverges (the small noise expansion breaks down). The way to regularize the variance is to introduce the notion of collective coordinates, in this case the collective coordinate being the position of the kink. There has been work on using the method of collective coordinates for the decay from an unstable state in stochastic models [18]. However, we are not aware of any work on directly calculating the expression $\rho(\phi,t|\phi_{\rm eq},T;\phi_m;0)$, in particular for the regime of interest where $\phi(t)$ is not close to either ϕ_m or $\phi_{\rm eq}$.

III. RESULTS AND DISCUSSION

The simulations were performed for the model (note that we now use the notation $\phi=x$)

$$\dot{x}=F=rx-x^3+h+\epsilon\eta, \tag{3.1}$$

where $r>0$, and the noise strength parameter is ϵ^2. For $h=0$, we have $x_m=-x_{\rm eq}=-\sqrt{r}$ and $x_s=0$. The Metropolis algorithm is used to update the (temporal) lattice. The lattice was updated by selecting a point, perturbing it, finding the difference in the action S between the two configurations, and accepting the move using the Metropolis algorithm. As in usual MC simulations, we can choose different ways to update the configurations and different sampling functions (aside from the Metropolis one) to improve statistics and increase efficiency. However, in this paper, for simplicity, the ‘‘proposal’’ moves are local moves (i.e., the field variable at a given site is deviated by a random amount on some interval).

The data presented for the model system were found with the choice $\alpha=\beta=0.5$ in Eq. (2.7), which corresponds to the Stratonovich discretization. We do not expect the qualitative features of the result to be sensitive to the choice of α and β. Some data were checked for the case $\alpha=1,\beta=0$ (Ito discretization) to confirm this. Data were also taken for a smaller dt, and no qualitative change was observed. The time increment for the simulations reported below was $dt=0.05$, and the extent of the time axis T was chosen to be sufficiently larger than the typical time scale for the transition, which decreases with r. For a given simulation, roughly about 10^7 or 10^8 (for very small noise) MC steps (recall that a MC step refers to an update over the temporal lattice of size T) were used to relax the system, and then the statistics were obtained by averaging over another $\approx 5\times 10^7(10^8)$ MC steps.

Figure 1 shows the typical behavior for the average path and the fluctuation $\chi(t)$ for the transition $x_m\rightarrow x_{\rm eq}$. For each sample path, statistics were obtained for the process from time $t=0$ (first time slice of the lattice) up to the time where the system crosses a given point $x_{\rm fl}$. Since the transition from $x_m\rightarrow x_{\rm fl}$ can occur anywhere along the temporal lattice, we monitor the time when the process hits $x_{\rm fl}$, and accumulate statistics to the left of this time. We are interested in the behavior of the process as it nucleates (i.e., as it makes it all the way over to the equilibrium state); therefore we choose

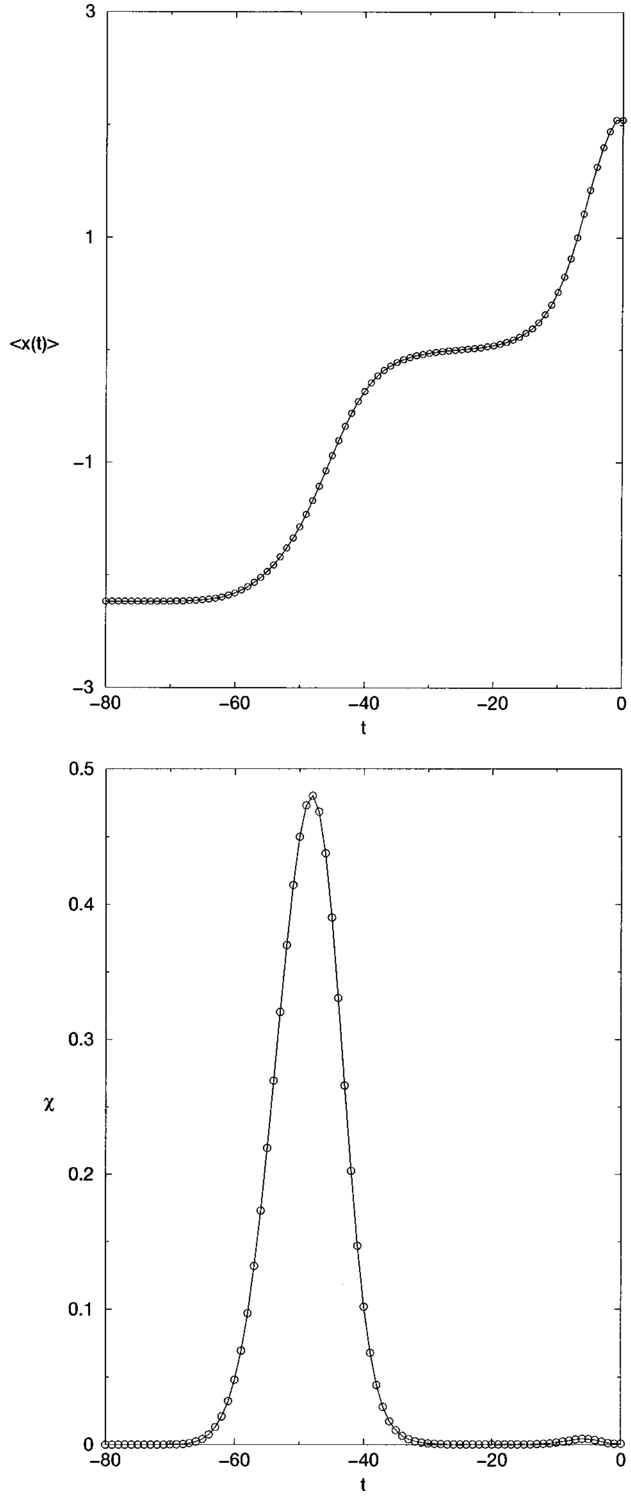

FIG. 1. For $r=5$, $h=0$, and $\epsilon^2=0.001$: (a) is average path $\langle x(t)\rangle$, and (b) the variance $\chi(t)$. The time $t=0$ is when the sample paths pass the fluctuational state, i.e., $x(t=0)=x_{\mathrm{fl}}=0.9x_{\mathrm{eq}}$. The boundary conditions on the lattice are $x_F=x_{\mathrm{eq}}, x_I=x_m=-x_{\mathrm{eq}}$ (for $h=0$). In (b) the scale of the fluctuation well away from the peak is of order ϵ^2, which is too small to see in the figure.

$x_{\mathrm{fl}}\approx 0.9x_{\mathrm{eq}}$. In practice, once x_{fl} is well over the barrier ($x_{\mathrm{fl}} \gg x_s$), the statistics do not depend too much on the exact location of x_{fl}.

Since we can regard the system as sitting at the metastable state for a long time (for small noise), we can think of the initial time as being at $t=-\infty$. As mentioned above, for each sample path in the ensemble we can reference $t=0$ to be the time where the system reaches ϕ_{fl}. Thus the STMC algorithm allows us to measure the statistical quantity $\rho(x,t|x_{\mathrm{fl}},0;x_m,-\infty)$ $(t<0)$, termed the prehistory probability in Ref. [8]. The effect of the final time boundary condition on the lattice, $x_F=x_{\mathrm{eq}}$, is irrelevant if x_{fl} is well over the barrier and the noise ϵ^2 is small.

Some interesting features to be noted in Fig. 1 are the flat region at the saddle point ($\langle x\rangle=0$), which increases as the noise decreases, and the peak in χ that occurs in the growth of the fluctuation [i.e., the region $\langle x(t)\rangle<x_s$]. The location of the peak occurs around $\langle x\rangle=1.4$, which is close to the spinodal point ($=\sqrt{r/3}$); away from this peak the fluctuation is of order ϵ^2. Also, though not visible on the scale of Fig. 1, the fluctuation quickly relaxes from $\chi=0$ at the end points of the lattice (due to the fixed field constraint at the ends of the lattice) to the correct value [given by $\chi=\epsilon^2/2F'(x_{m,\mathrm{eq}})$] in the metastable and equilibrium states, respectively. Finally, for a STMC simulation with the boundary conditions $x_F=x_f<x_s, x_I=x_m$, we find a strong dependence of χ on x_{fl}; χ increases considerably with x_{fl} for $x_{\mathrm{fl}}<x_s$.

In order to analyze the general features of the data, we consider the problem of the decay from an unstable state for small noise Langevin dynamics. We know that the extensivity property breaks down and the small noise behavior in this regime is described by a scaling theory [5]. In particular, there is an extensive region where $\delta \gg \epsilon^{2\mu}$, and a scaling regime where $\delta<\epsilon^{2\mu}$; δ denotes the deviation of the initial state from the unstable (saddle point) state, and the positive exponent $\mu=\frac{1}{2}$ for our model system. The fluctuation in the extensive regime scales as ϵ^2, and is characterized by an anomalous fluctuation that scales with δ as $A\sim 1/\delta^2$ [A is the peak value of $\chi(t)$ as the system decays to equilibrium]. In the scaling regime, the zero noise limit is a singular limit. The decay of the system in the scaling regime is characterized by an initial stage with time scale $T_o\sim-\ln(\epsilon^2)$, where the system diffuses around the saddle point state (with fluctuation of order ϵ^2), and a second non-Gaussian stage where a fluctuation enhancement [$\chi(t)\sim 1$] occurs as the system makes the transition to the final state.

It is reasonable to expect a similar situation in the growth of a large fluctuation from a stable (or metstable) state. If the fluctuation grows up to and over the saddle point, then, as discussed in Sec. II B, the extensivity assumption breaks down, and large non-Gaussian fluctuations should occur. In this case, we may expect some features of the scaling regime of Suzuki's theory to apply. On the other hand, for transitional paths that end at the point $x_{\mathrm{fl}}=x_s-\delta$, $\delta>0$ (i.e., fluctuations that do not make it over the potential barrier) we can expect an anomalous fluctuation to occur if $\delta \gg \epsilon$.

In order to study the anomalous fluctuation, we performed STMC simulations with the boundary conditions on the lattice: $x_F=x_f=x_s-\delta$ and $x_I=x_m$. The anomalous fluctuation relation strictly holds for $\delta \gg \epsilon$. Thus we should have $|x_m|$ sufficiently larger than x_s, so that we can satisfy $\delta \gg \epsilon$, for not unreasonably small noise levels. Nonetheless, for the system parameters studied here, one can clearly see the scaling $A\sim 1/\delta^2$ in Fig. 2. The peak value of χ is also ob-

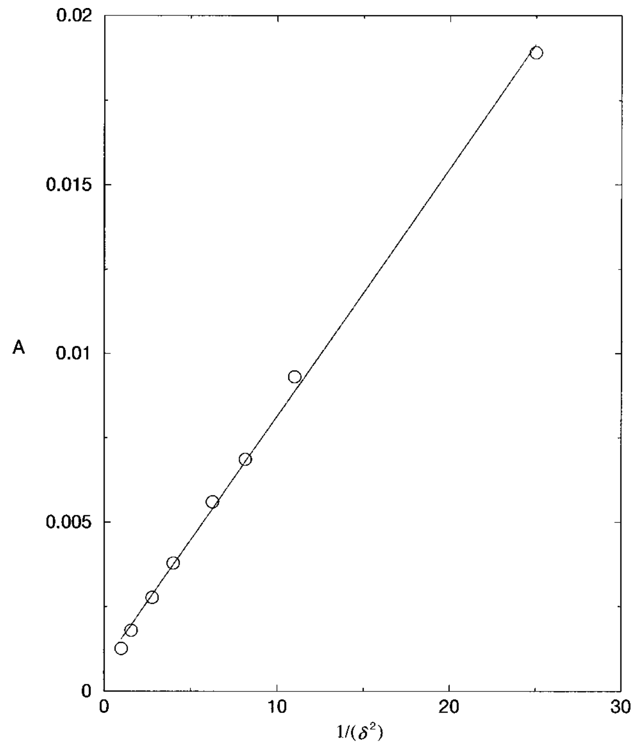

FIG. 2. The anomalous fluctuation A [the peak value of $\chi(t)$] as a function of $1/\delta^2$ for $\epsilon^2=0.01$, $h=0$, and $r=5$. The boundary conditions on the lattice are $x_F=x_s-\delta=-\delta\,(\delta>0)$ and $x_I=x_m=-x_{\rm eq}$.

served to occur at the expected time scale $\ln(1/\delta^2)$ [5]. The anomalous feature is a direct result of the detailed balance condition (2.8). We can demonstrate this in the following fashion [13].

As mentioned above, the statistical quantity we are measuring with the STMC algorithm is the prehistory probability distribution, which can be written as (recall that $t<0$)

$$\rho_h(x,t|x_{\rm fl},0;x_m,-\infty)=\frac{p(x_{\rm fl},0|x,t)p(x,t|x_m,-\infty)}{p(x_{\rm fl},0|x_m,-\infty)}, \tag{3.2}$$

where the Markov property has been used. The quantity $p(b,t|a,0)$ is the transition probability which can be expressed as

$$p(b,t|a,0)=\int\prod_{i=0,N-1}dx_i\,P(x_i,t_i\to x_{i+1},t_{i+1}), \tag{3.3}$$

where $t_0=0,t_N=t,x_0=a,x_N=b$, and P is the transition probability from $t_i\to t_{i+1}=t_i+dt$. From the detailed balance condition [Eq. (2.8)], which is satisfied to first order in dt (we can ignore the $dt\sqrt{dt}$ corrections), the above expression becomes

$$p(b,t|a,0)=p(a,t|b,0)\frac{\exp(-H(b))}{\exp(-H(a))}. \tag{3.4}$$

Thus we have, for expression (3.2),

$$\rho_h(x,t|x_{\rm fl},0;x_m,-\infty)\sim p(x,0|x_{\rm fl},t)=p(x,-t|x_{\rm fl},0), \tag{3.5}$$

where the relation $p(a,t;x_m,-\infty)\sim\exp(-H(a))$ (for state a in the basin of attraction of x_m) has been used, and time-translational symmetry for the second equality. The right hand side of Eq. (3.5) is the transition probability that describes the *decay* from an initial state $x_{\rm fl}$. Hence the prehistory probability distribution is simply the transition probability for the corresponding decay process. Therefore the increase in the fluctuation of the form $\sim 1/\delta^2$ (for $\delta\gg\epsilon$), for the transition $x_m\to x_s-\delta$, is the anomalous fluctuation feature [5] observed in the decay from the initial state $x_s-\delta$. A behavior of the form $1/(x_s-x_{\rm fl})^2$ for the fluctuation was observed in Ref. [8] for the model (3.1), but the connection to Suzuki's scaling theory was not recognized.

We note that the above result is not strictly applicable to spatially extended or microscopic systems. This is because the fluctuational state of interest for these systems will typically be a coarse-grained one, i.e., the state x would denote quantities averaged over the system configuration (observables such as the average magnetization and energy, or a Fourier mode, etc.), while x_m and $x_{\rm fl}$ would be microconfiguration states. The Markov property used in Eq. (3.2) (as well as the detailed balance condition) are conditions imposed on the (microscopic) configurations, and do not generally hold for a transition from a microconfiguration to a coarse-grained (or macro) state. Nonetheless, we can still expect some related feature to persist in more general (spatial extended) systems. In particular, in the decay of the metastable state ($x_m\to x_{\rm eq}$), it is likely that some type of anomalous fluctuation (i.e., say an increase or peak in the fluctuation before or close to the saddle point state) should occur. This was observed in a quasilinear spin model in Ref. [19], and in our preliminary simulations of a spatially extended version of Eq. (3.1). A spatially extended system will be investigated in a future work.

As shown in Fig. 1(a), there is a plateau region where the system diffuses around the saddle point state with fluctuation $\chi\sim\epsilon^2$. The time scale T_o, characterizing this region where $\langle x\rangle\sim x_s$ increases as $\epsilon\to 0$, and the Suzuki scaling result $T_o\sim-\ln\epsilon^2$ is, in fact, observed in our simulations (with $x_{\rm fl}=x_s+\delta$, for $\delta\gg\epsilon$). This behavior of the plateau region is interesting, but the divergence as $\epsilon\to 0$ is expected to be a feature of the low dimensionality of the system. For microscopic models, (microscopic) fluctuations persist in the thermodynamic limit $\epsilon^2\sim 1/V\to 0$, and hence one would expect T_o to remain finite.

Because of the plateau feature around x_s with fluctuation size $\sim\epsilon^2$, it is not meaningful to set $x_{\rm fl}=x_s$ in the prehistory distribution. ρ_h is operationally well defined for $|x_{\rm fl}-x_s|$ sufficiently greater than ϵ. If we set $x_{\rm fl}=x_s-\delta$ (for positive δ with $\delta\sim\epsilon$), then from the discussion above we have that [see Eq. (3.5)] $\rho_h(x,t|x_{\rm fl},0;x_m,-\infty)\sim p(x,-t|x_{\rm fl},0)$, which means that at least at the boundary of Suzuki's scaling theory ($\delta\sim\epsilon$), the statistical properties of the decay is the same as the growth.

However, we are more interested in the decay of the metastable state, i.e., transitional paths that go all the way over the barrier. In this case we need $x_{\rm fl}-x_s\gg\epsilon$ (we choose $x_{\rm fl}\sim 0.9x_{\rm eq}$ in our simulations), and the quantity ρ_h is more

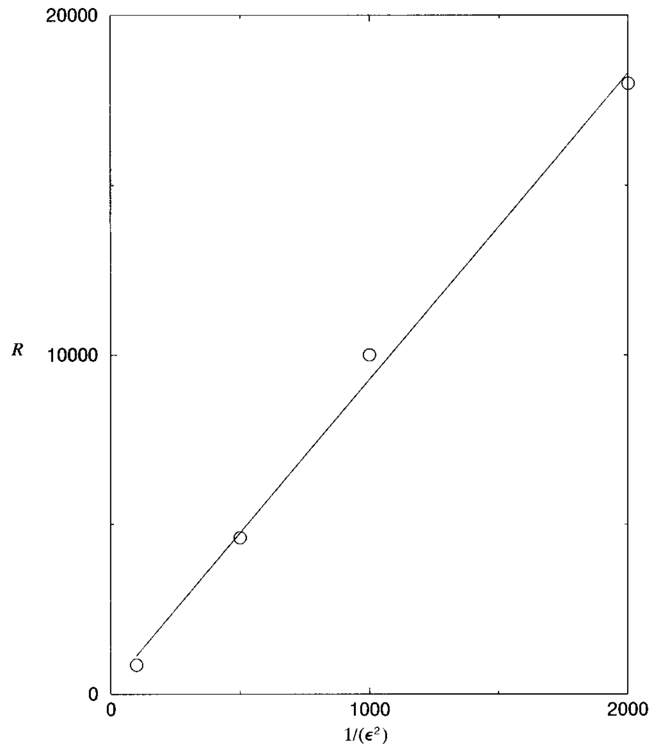

FIG. 3. The fluctuation enhancement R as a function of $1/\epsilon^2$, for $r=5$ and $h=0$. The noise levels shown in the figure are $\epsilon^2=0.0005, 0.001, 0.005$, and 0.01. This linear behavior persists to noise levels up to $\epsilon^2 \sim 0.05$.

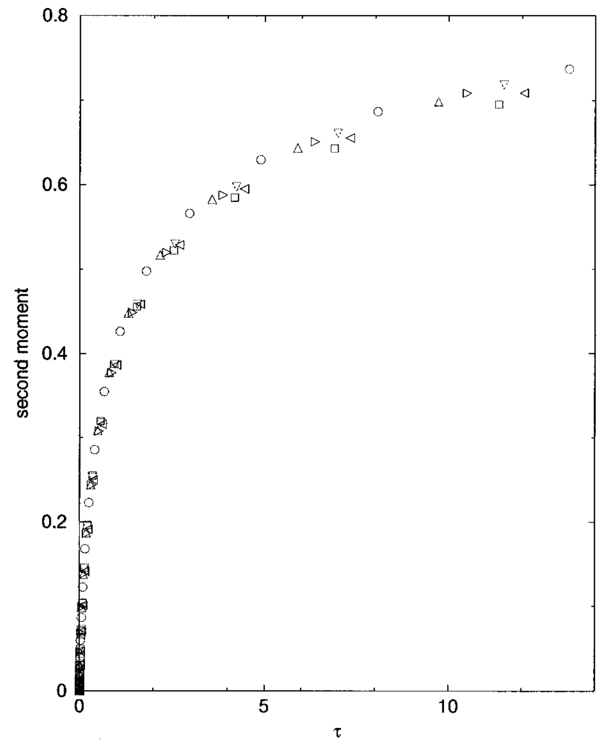

FIG. 4. The second moment $\langle x^2 \rangle$ for $r=5$ and $h=0$ as a function of the rescaled time τ [Eq. (3.6)] at various noise levels: $\epsilon^2=0.0005$ (circle), 0.001 (square), 0.002 (triangle up), 0.005 (triangle left), 0.01 (triangle down), and 0.02 (triangle right).

nontrivial (it now involves the transition probability for the transition over the potential barrier). The interesting feature in the data [see Fig. 1(b)] is the peak in χ that occurs well before the saddle point. This peak is the non-Gaussian fluctuation that we generally expect due to the slowing down of the system as it crosses the saddle point. In order to quantify the large non-Gaussian fluctuations, very long runs were required to obtain reliable statistics. In particular, for very small noise, sufficiently long runs were necessary to allow the plateau region (flat region at the saddle point) to relax. In Fig. 3, we show the peak of χ as a function of the noise strength. Here the quantity R is taken as the ratio of the peak value of χ to the value in the metastable state. A fluctuation enhancement that scales according to $R \sim 1/\epsilon^2$ can clearly be seen in data. Similar scaling is observed for nonzero h, with a smaller slope (which should vanish when h is large enough to remove the potential barrier).

In Fig. 4 we show the scaling of the second moment $\langle x^2(t) \rangle$ as a function of a rescaled time

$$\tau = \epsilon^2 \exp(-2rt), \tag{3.6}$$

where $t=0$ is taken to be the center of the plateau region. The nonlinear time transformation (3.6) is same scaling function [for model (3.1)] used in Suzuki's theory for decay of unstable states [5]. Although there is some error due to the precise location of $t=0$, one can see that the collapse of the curves for different ϵ values is fairly good, at least for $\langle x^2(t) \rangle < 0.7 x_m^2$, which is the expected regime of validity (the scaling theory for the decay [5] is not valid for the late stage where the system approaches equilibrium).

Finally, as shown in Fig. 1(b), once the system is over the saddle point, the fluctuation is of order $\sim \epsilon^2$ and the system decays according to the most probable path $\dot{x}=F$ (the zero noise path). This is the case except for a much smaller peak (which does seem to be a fluctuation enhancement effect) in the fluctuation as the system decays to equilibrium; the small peak occurs close to $t \approx -5$ in Fig. 1(b). The statistics near the second peak are more sensitive to the final time constraint, and it is difficult to say whether the smaller peak is an enhancement that scales like $1/\epsilon^2$ (albeit with a much smaller magnitude and prefactor) as $\epsilon \to 0$. This strong asymmetry in the size of the fluctuation before and after the saddle point is an interesting feature. It is important to note that the statistics for the decay ($x_s \to x_{eq}$) part of the transition $x_m \to x_{eq}$, being conditioned on the final time, is different from the usual study of the decay of fluctuations, which are conditioned on the initial time.

IV. SUMMARY AND FUTURE WORK

In this paper we have studied the statistical properties of the transitional paths that describe the growth of very large fluctuations out of a metastable state. We have introduced a useful numerical method to quantify the statistics of these rare events, and demonstrated the method for a bistable stochastic system. Various interesting statistical features were studied and discussed, and the close connection to Suzuki's theory has been pointed out. In particular, we have demonstrated that there is a fluctuation enhancement that scales like $1/\epsilon^2$ (for $\epsilon \to 0$) as the system escapes over the potential barrier.

It would be of interest to consider various extensions of this work. One would be to consider a nongradient dynamical system, say by adding a time-dependent field to the Langevin dynamics. In this case, there is no known relation between the average growth of the fluctuation and the decay, and the features of the optimal paths are more complex [2,3]. We can easily perform a quantitative study with the numerical method used in this paper. In particular, the effect of the broken detailed balance condition on some of the features discussed in this study should be investigated.

Another possible application is the case of colored noise, i.e., dynamics of form (2.2), with the noise correlation

$$\langle \eta(t)\,\eta(s)\rangle \sim \frac{\epsilon^2}{\tau}\exp[-|t-s|/\tau]. \tag{4.1}$$

This stochastic process can be cast as a path integral with a local action functional [20]; the action contains a second time derivative term in the variable x [i.e., $S=\int L(x,\dot{x},\ddot{x})dt$]. The STMC algorithm can therefore be applied to this system (boundary conditions on the lattice must now be specified for both x and $\dot{x}$), and the statistical properties of the barrier crossing, as studied in this paper, can be investigated.

A more interesting and relevant avenue of study is that of a spatially extended model. Using the STMC scheme we can numerically study the configurational structure of the system in the very early stages of nucleation. Of course, in this case, the crucial problem is how large a time axis is required. One would need to study nucleation events where the time scale for the transition time is not too large, and the final state would have to be suitably prepared to be a desired rare configuration (i.e., a critical droplet), in order to minimize the size of the time axis in the $d+1$ volume. Needless to say, the study would necessarily have to be more qualitative for spatially extended systems. We hope to report on such a study in the near future.

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