Rare event statistics in reaction-diffusion systems

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We present an efficient method to calculate probabilities of large deviations from the typical behavior (rare events) in reaction-diffusion systems. This method is based on a semiclassical treatment of an underlying "quantum" Hamiltonian, encoding the system's evolution. To this end, we formulate the corresponding canonical dynamical system and investigate its phase portrait. This method is presented for a number of pedagogical examples.

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I. INTRODUCTION

Reaction-diffusion models have a vast area of applications [1,2] from the kinetics of chemical reactions [3], biological populations [4–6] and epidemics [7,8] to the dynamics of financial markets [9] and ecology [10]. The models describe the dynamics of a number of particles whose reactions are specified by a certain set of rules. The rules have a probabilistic nature and are most conveniently formulated on a lattice in a d-dimensional space. We shall restrict our attention to a wide subclass of such models, where the particles execute random walks (diffuse) on the lattice, while the reactions between them are purely local (on-site). Once the lattice, the reaction rules, and the initial conditions are specified, one is interested to find statistical characteristics of the system's subsequent evolution. This goal may be accomplished with various degrees of detailing and accuracy.

The most detailed information is contained in the probability distribution functions (PDF) of every possible microscopic state of the system. The PDF is a solution of an exponentially large system of Master equations, which specify the probabilities of transition between every two microscopic states of the system. The analytical solution of the Master equations is usually unrealistic and the information contained within them is excessive. Therefore, various approximation schemes are in order. The simplest one is the mean-field approximation, where a closed set of equations for average quantities (e.g., concentrations) is obtained by an approximate decoupling of higher moments. The mean-field theory describes a typical evolution of the system, if the fluctuations are weak in some way. The probability of small deviations from the mean-field predictions may be found with the help of the Fokker-Planck (FP) equation. It substitutes the discrete Master equation by a continuum (biased) diffusion equation in the space of concentrations. Analysis of the FP equation is usually complicated [1,2], moreover the approximation is reliable for small deviations only and fails to provide the probability of large deviations from the typical evolution.

Much attention was attracted recently to reaction-diffusion systems that are in a close proximity to dynamic phase transitions [11–13] (for recent reviews see, e.g., Refs. [14,15]). By fine-tuning one of the parameters, some systems may be brought to a point of quantitative change of their behavior (e.g., stable finite concentration versus extinction). In a vicinity of the transition, neither mean field nor FP can accurately predict the long-time scaling of the system's characteristics, such as particle concentration. The field-theoretical renormalization group (RG) methods were developed, and successfully applied, to a number of examples [16–19]. In particular, the directed percolation universality class was identified and studied as the most robust universality class for the dynamic phase transitions [14,20–22].

In the present work, we address a somewhat different set of questions. We consider a generic reaction-diffusion system that either does not exhibit, or is far enough from, the phase transition. A typical evolution scenario, and the probability of small deviations, are well described by the mean-field theory and the FP equation. We shall look, however, for the probability of *large* deviations from typical behavior. A "large" deviation may be loosely characterized as being of the same order as (or larger than) the typical value (as opposed to the "small" one, which is of the order of the square root of the typical value). Since the occurrence of such large deviations has a very small probability, they may be dubbed "rare events." Despite being rare, these "rare events" may be of great interest, especially if they have extreme consequences. Some examples are as follows: the proliferation of a virus after immunization (causing the death of a patient), large fluctuations in the number of neutrons in a nuclear reactor (causing explosion), etc. Clearly, in these and many other examples, one is interested to know rather precisely how improbable improbable events are.

Rare events in stochastic reaction-diffusion models, with thermal fluctuations described by white noise, were studied by many authors. For a review, see, e.g., [23]. For recent works, see [24,25]. It is assumed in this approach that the dynamics of the system is governed by the Langevin equation. In general, reaction-diffusion problems cannot be described by Langevin dynamics with a white additive noise. Usually, the noise happens to be colored (i.e., correlated with a reaction coordinate) and is not necessarily real [26]. The presence of the absorbing states does not allow the treatment of reaction-diffusion systems as Gaussian noise models. There exists no conventional Fokker-Planck equation in this case, and hence the calculus of the rare events is different. The escape rate from the metastable state to the absorbing state cannot be established following the well-developed Kramers theory [23].

Here we develop a rigorous, simple, and efficient method to calculate the rare event statistics in reaction-diffusion systems. To this end, we develop a Hamiltonian formulation of reaction-diffusion dynamics. Although the system is specified by a set of rules, rather than a Hamiltonian, one may nevertheless show that there is a certain canonical Hamiltonian associated with the system's dynamics. More precisely, the Master equation may be reformulated as a "quantum" (many-body) Schrödinger equation with some "quantum" Hamiltonian. This observation is not new and is sometimes referred to as Doi's operator technique [27,28]. In fact, its "quantum" version is the basis for the field-theoretical RG treatment of the dynamical phase transitions [16–19]. Here we notice that the *classical* (or rather semiclassical) dynamics of the very same Hamiltonian carries a lot of useful information about reaction-diffusion systems. In particular, it provides all the information about the rare event statistics. To extract this information, it is convenient to formulate the underlying Hamiltonian in classical terms (as a function of momenta and coordinates), rather than creation and annihilation operators, as is customary in the "quantum" approach [27–29].

A particularly convenient tool to visualize the system's dynamics is a phase portrait of the corresponding Hamiltonian. It consists of lines (or surfaces) of constant "energy" (the integral of motion naturally existing in a Hamiltonian system) in the space of canonical momenta and coordinates. The mean-field (typical) evolution corresponds to a particular manifold of zero energy, given by the fixed value of the canonical momenta, $p=1$. Rare events may be specified by certain initial and finite conditions in the phase space of the dynamical system, which, in general, do *not* belong to the mean-field manifold. The probability of the rare event is proportional to $\exp\{-S\}$, where S is the classical action on a unique trajectory, satisfying the specified boundary conditions. The problem is therefore reduced to finding an evolution of the *classical* dynamical system, whose quantized Hamiltonian encodes the Master equation. This task is substantially simpler than solving the full "quantum" Master equation. In fact, even the probability of small deviations is much more efficiently calculated in our semiclassical method than via solution of the FP equation (though the latter is also applicable). For large deviations, however, the FP approach leads to inaccurate results, while the semiclassical method provides a simple and accurate prescription. A similar strategy was recently applied for the calculation of the full current statistics of mesoscopic conductors [30–32].

In this paper, we develop the semiclassical method using a number of reaction-diffusion models as examples. We tried to keep the presentation self-contained and pedagogical. In Sec. II, we start from the model of binary annihilation in zero dimensions. In Sec. III, we complicate the model by including branching and discuss the extinction probability of a system having a stable population in the mean-field approximation. Section IV is devoted to the extension of the formalism to a d-dimensional space. As an example, we find an extinction probability of a finite cluster. In Sec. V, a population dynamics model with three reaction channels—reproduction, death, and emigration—is considered in a d-dimensional space. The model possesses a long-lasting metastable state with a fixed population that eventually escapes into the state of unlimited population growth. We show how the semiclassical method may be used to calculate the lifetime of such a metastable state. Finally, some conclusions and open problems are discussed in Sec. VI.

II. BINARY ANNIHILATION

The simplest reaction, which we use to introduce notations and set the stage for further discussions, is the binary annihilation process. It describes a chemical reaction, where two identical particles form an inert aggregate with the probability λ. This aggregate is not involved in further reactions: $A+A\xrightarrow{\lambda}\emptyset$. We start from the zero-dimensional version of the model, where every particle may react with every other. Such a reaction is fully described by the following Master equation:

$$\frac{d}{dt}P_n(t) = \frac{\lambda}{2}[(n+2)(n+1)P_{n+2}(t) - n(n-1)P_n(t)], \quad (1)$$

where $P_n(t)$ is the probability to find n particles at time t. The Master equation is to be supplemented with an initial distribution, e.g., $P_n(0)=e^{-n_0}n_0^n/n!$ for the Poisson distribution with the mean value n_0, or $P_n(0)=\delta_{n,n_0}$ for the fixed initial particle number. Let us now define the *generating function* as

$$G(p,t) \equiv \sum_{n=0}^{\infty} p^n P_n(t). \quad (2)$$

Knowing the generating function, one may find a probability of having (integer) n particles at time t as $P_n(t) = \partial_p^n G(p,t)|_{p=0}/n!$. If $n \gg 1$, it is more convenient to use an alternative representation,

$$P_n(t) = \frac{1}{2\pi i}\oint \frac{dp}{p} G(p,t) p^{-n}, \quad (3)$$

where integration is performed over a closed contour on the complex p plane, encircling $p=0$ and going through the region of analyticity of $G(p,t)$.

The point $p=1$ plays a special role in this formulation. First of all, the conservation of probability demands the fundamental normalization condition,

$$G(1,t) \equiv 1. \quad (4)$$

Secondly, the moments of the PDF, $P_n(t)$, may be expressed through derivatives of the generating function at $p=1$, e.g., $\langle n(t)\rangle \equiv \sum_n nP_n(t) = \partial_p G(p,t)|_{p=1}$.

In terms of the generating function, the Master equation (1) may be *identically* rewritten as

$$\frac{\partial G}{\partial t} = -\frac{\lambda}{2}(p^2-1)\frac{\partial^2 G}{\partial p^2}. \quad (5)$$

This equation is to be solved with some initial condition, e.g., $G(p,0)=\exp\{n_0(p-1)\}$ for the Poisson initial distribution or $G(p,0)=p^{n_0}$ for a rigidly fixed initial particle number. The solution should satisfy the normalization condition, Eq. (4), at any time. In addition, all physically acceptable solutions must have all p derivatives at $p=0$ non-negative.

One may consider Eq. (5) as the "Schrödinger" equation,

$$\frac{\partial}{\partial t}G = -\hat{H}G, \tag{6}$$

where the "quantum" Hamiltonian operator, $\hat{H}$, in the $\hat{p}$ ("momentum") representation is

$$\hat{H}(\hat{p},\hat{q}) = \frac{\lambda}{2}(\hat{p}^2 - 1)\hat{q}^2. \tag{7}$$

Here we have introduced the "coordinate" operator $\hat{q}$ as

$$\hat{q} \equiv -\frac{\partial}{\partial p}, \quad [\hat{p},\hat{q}] = 1. \tag{8}$$

The "Hamiltonian," Eq. (7), is normally ordered and not Hermitian. However, the last fact does not present any significant difficulties.

If the "quantum" fluctuations are weak (which in the present case is true as long as $\langle n(t)\rangle \gg 1$), one may employ the WKB approximation to solve the "Schrödinger"-Master equation. Using ansatz $G(p,t)=\exp\{-S(p,t)\}$ and expanding $S(p,t)$ to the leading order in $1/\lambda$, one obtains the classical Hamilton-Jacobi equation,

$$\frac{\partial S}{\partial t} = H\left(p, \frac{\partial S}{\partial p}\right) = \frac{\lambda}{2}(p^2 - 1)\left(\frac{\partial S}{\partial p}\right)^2. \tag{9}$$

Instead of directly solving the Hamilton-Jacobi equation, we will develop the Hamilton approach, which is much more convenient for finite-dimensional applications.

To this end, we employ the Feynman path-integral representation, which may be derived, introducing the resolution of unity at each infinitesimal time step and employing the normal ordering. As a result, one finds for the generating function

$$G(p,t) \lim_{M\to\infty} \int \prod_{k=0}^{M} \frac{dp_k dq_k}{2\pi} e^{-S[p_k,q_k]}, \tag{10}$$

where the discrete representation for the action $S[p_k,q_k]$ is given by

$$S = \sum_{k=1}^{M} [p_k(q_k - q_{k-1}) + H(p_k,q_{k-1})\delta t] + p_0 q_0 - p q_M - n_0(p_0 - 1) \tag{11}$$

and $\delta t = t/(M+1)$. The last term in this expression is specific to Poisson's initial conditions. If the initial number of particles is fixed to be n_0, and therefore $G(p,0)=p^{n_0}$, then the last term is changed to $n_0 \ln p_0$. The same path integral may be derived, of course, using Doi's operator algebra and coherent states. We summarize this derivation in Appendix A. The convergency of the path integral may be achieved by a proper rotation in the complex p_k and q_k planes.

In what follows, we are interested in the semiclassical treatment of this path integral. Varying the action with respect to p_k and q_k for $k=0,1,\ldots,M$, one obtains the classical equations of motion (in continuous notations),

$$\dot{q} = -\frac{\partial H}{\partial p} = -\lambda p q^2, \tag{12a}$$

$$\dot{p} = \frac{\partial H}{\partial q} = \lambda(p^2 - 1)q \tag{12b}$$

and the boundary conditions:

$$q(0) = n_0, \tag{13a}$$

$$p(t) = p, \tag{13b}$$

where p and t are the arguments of the generating function $G(p,t)$. Notice that, while the coordinate is fixed at an initial time (past), momentum is imposed at a finite time (future). These equations admit the integral of motion, which we call "energy": $\dot{E}=0$, where

$$E \equiv H(p(t),q(t)) = \frac{\lambda}{2}[p^2(t) - 1]q^2(t). \tag{14}$$

As a result, the action *on a classical trajectory* may be written as (in continuous notations)

$$S[p,q] = Et - \int_0^t q\dot{p}dt - n_0[p(0) - 1]. \tag{15}$$

To find the low moments, one needs to know $G(p,t)$ in the immediate vicinity of $p=1$. In this case, the Hamilton equations (12) with boundary conditions (13) may be solved with the *mean-field* ansatz,

$$\overline{p}(t) \equiv 1, \tag{16a}$$

$$\frac{d\overline{q}}{dt} = -\left.\frac{\partial H}{\partial p}\right|_{p=1} = -\lambda \overline{q}^2. \tag{16b}$$

The last equation constitutes the mean-field approximation for the reaction coordinate, $\overline{q} \equiv \overline{n} \approx \langle n \rangle$. The classical action, Eq. (15), is obviously nullified by the mean-field solution: $S[\overline{p},\overline{q}]=0$. This enforces the normalization, Eq. (4) (it is straightforward to show that the fluctuation determinant around the mean-field trajectory is unity). In fact, any legitimate Hamiltonian must satisfy the condition $H(1,q)=0$ to insure normalization. As a result, the mean-field solution, $\overline{p}=1$, is bound to have zero energy, $\overline{E}\equiv 0$.

However, the assumption that $p=1$ is *not* always a legitimate one. The probability of any event other than the mean-field prediction is automatically described by $p(t)=p$ different from unity. Rare events definitely belong to this category. For such cases, the mean-field ansatz, Eq. (16), is *not* applicable and one must go back to the full dynamical system, Eqs. (12) (provided the semiclassical approximation is justified). For example, let us imagine doing the contour integral, Eq. (3), by the stationary point method. Approximating, $G(p,t)=\exp\{-S(p,t)\}$, with the classical action, S, one finds the saddle-point condition, $n=-p\partial S/\partial p = p(t)q(t)$, since on the classical trajectory $\partial S/\partial p = -q(t)$. Therefore, if one is interested in n, which is different from the mean-field predic-

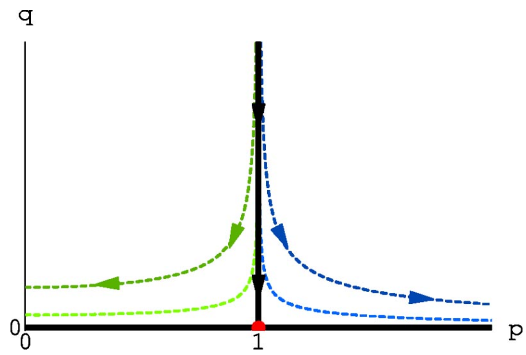

FIG. 1. The phase portrait of the binary annihilation process. Thick lines represent the solution of $H(p,q)=0$; the fat dot is a fixed point. Thinner lines represent dynamical trajectories with nonzero energy. Line $p=1$ gives the mean-field dynamics.

tion $\overline{q}(t)$, one must consider $p(t)=p$ to be different from unity.

In the case of the binary annihilation, the mean-field prediction is a solution of the equation $\partial_t \overline{q} = -\overline{q}^2$, hence $\overline{q}(t) \equiv \overline{n}(t) = n_0/(1+n_0\lambda t) \approx (\lambda t)^{-1}$ for $1<(\lambda t)^{-1} \ll n_0$. We are looking for a probability to find $n \neq \overline{n}(t) = (\lambda t)^{-1}$ particles at time $t \gg (\lambda n_0)^{-1}$. The phase portrait of the dynamical system, Eqs. (12), is plotted in Fig. 1. Dynamical trajectories for a given energy, E, are given by $q=\sqrt{2E\lambda^{-1}/(p^2-1)}$. Since $q(0)=n_0 \gg 1$, one finds $p(0)=1+2E/(\lambda n_0^2) \approx 1$. Substituting this trajectory into Eq. (12b), and integrating it between $p(0)\approx 1$ and $p(t)=p$, one finds $E=-\arccos^2 p/(2\lambda t^2)$. The corresponding classical action, Eq. (15), is given by

$$S(p,t) = \frac{1}{2}\overline{n}(t)\arccos^2 p. \tag{17}$$

This action solves the Hamilton-Jacobi equation (9) and is nullified at the mean-field trajectory, $p=1$. As a result, the generating function is given by $G(p,t) \approx \exp\{-S(p,t)\}$ with the classical action, Eq. (17).

We are now in the position to find the rare event statistics: namely, we are looking for the probability to find n particles after time t, that is, $P_n(t)$, where n is significantly different from the mean-field prediction $\overline{n} = (\lambda t)^{-1}$. To this end, one may perform integration, required by Eq. (3), in the stationary point approximation to obtain the probability distribution

$$P_n(t) = \mathcal{N} \exp\left\{ -\overline{n}\left(\frac{1}{2}\arccos^2 p_s + \frac{n}{\overline{n}} \ln p_s \right) \right\}, \tag{18}$$

where $p_s = p_s(n/\overline{n})$ is the solution of the saddle-point equation: $p_s(p_s^2-1)^{-1/2} \arccos p_s = n/\overline{n}$. In limiting cases, the exponent takes the form

$$-\ln P_n(t) \approx \begin{cases} \frac{\pi^2}{8}\overline{n} - n \ln \frac{\pi \overline{n}}{2n}, & n \ll \overline{n}; \\ \frac{3}{4}(n-\overline{n})^2/\overline{n}, & |n-\overline{n}| \ll \overline{n}; \\ \frac{1}{2}n^2/\overline{n} - n \ln 2, & n \gg \overline{n}. \end{cases} \tag{19}$$

The logarithm of the PDF is plotted in Fig. 2 versus $n/\overline{n}$ for a fixed $\overline{n}=\overline{n}(t)$. The corresponding exponent, resulting from the solution of the Fokker-Planck equation, is shown in the same plot for comparison. The two exponents coincide for small deviations from the mean-field result, $|n/\overline{n}-1| \ll 1$. For larger deviations (rare events), $n/\overline{n} \sim O(1)$, the Fokker-Planck results are significantly off the correct ones. Finally, the normalization factor $\mathcal{N} = \sqrt{3/(4\pi \overline{n})}$ is simply determined by the immediate vicinity of the maximum of the distribution, $|n-\overline{n}| \ll \overline{n}$.

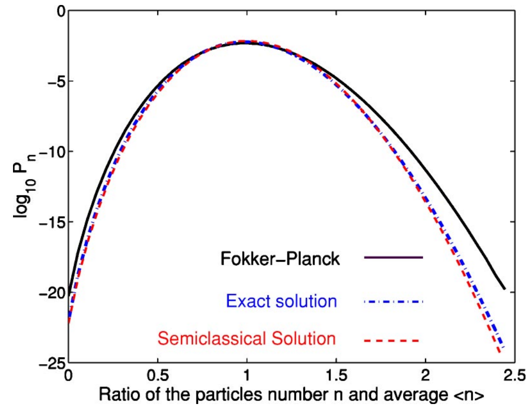

FIG. 2. The logarithm of the PDF $P_n(t)$ as a function of $n/\overline{n}(t)$ at a fixed time t. The semiclassical result, Eq. (18), is a dashed line; the exact solution produced by the numerical simulation of the Master equation (1) is a dashed-dotted line; the numerical solution of the FP equation, $\dot{P}=\lambda\{[(n^2-n)P]''+(n^2P)'\}$, is a full line.

III. BRANCHING AND ANNIHILATION

Let us consider now a more interesting example of binary annihilation with branching. The model consists of the two reactions: annihilation $A+A \xrightarrow{\lambda} \varnothing$ and branching $A \xrightarrow{\sigma} 2A$. The Master equation is written as

$$\frac{d}{dt}P_n(t) = \frac{\lambda}{2}[(n+2)(n+1)P_{n+2}(t) - n(n-1)P_n(t)] + \sigma[(n-1)P_{n-1}(t) - nP_n(t)]. \tag{20}$$

One may check that the corresponding Hamiltonian takes the form

$$\hat{H}(\hat{p},\hat{q}) = \frac{\lambda}{2}(\hat{p}^2-1)\hat{q}^2 - \sigma(\hat{p}-1)\hat{p}\hat{q}. \tag{21}$$

As expected, it satisfies the normalization condition, $H(1,q)=0$. The classical equations of motion are

$$\dot{q} = -\lambda p q^2 + \sigma(2p-1)q, \tag{22a}$$

$$\dot{p} = \lambda(p^2-1)q - \sigma(p-1)p, \tag{22b}$$

with the same boundary conditions as in the previous example, Eqs. (13). The classically conserved energy is $E = H(p(t),q(t))$. The mean-field ansatz, $\overline{p}(t)\equiv 1$, leads to the mean-field equation for the reaction coordinate, $\overline{q} \approx \langle n \rangle$,

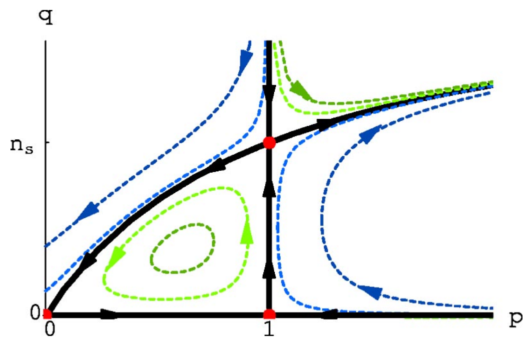

FIG. 3. The phase portrait of the branching annihilation process. Thick lines are lines of zero energy, $H(p,q)=0$. Fat dots are fixed points.

$$\frac{d\overline{q}}{dt} = -\lambda\overline{q}^2 + \sigma\overline{q}. \tag{23}$$

This equation possesses two stationary states, namely, the active state $\overline{q}=\sigma/\lambda \equiv n_s$ and the passive state $\overline{q}=0$. Below we show that the active state is *not* actually thermodynamically stable (in the 0d system) and in a finite time decays into the passive one.

To proceed with the discussion of the rare event statistics, we need a phase portrait of the system. It contains three lines of zero energy: the mean-field line $p=1$, the empty system line $q=0$, and the nontrivial line $q=2n_s p/(1+p)$. These lines determine the topology of the phase diagram, Fig. 3, where the arrows show the positive time direction. According to the mean-field equation (23), from any initial state with $n_0 \neq 0$, the system reaches the active state with n_s particles during the time $t \approx \sigma^{-1}$. Hereafter, we assume that $n_s=\sigma/\lambda \gg 1$. We shall look for a probability to find $n \neq n_s$ particles after a time $t \gg \sigma^{-1}$.

Of particular interest, of course, is the probability of going to the passive state, namely $n=0$, during a large time t. According to the definition of the generating function, Eq. (2), this probability is given by $G(0,t)$. We are interested, therefore, in the trajectory which starts at some initial coordinate $q_0=n_0$ (and arbitrary momentum) and ends at $p_M=0$ (and arbitrary coordinate) after time t. In a long time limit, $t \to \infty$, such a trajectory approaches the lines of zero energy. The system first evolves along the mean-field trajectory, $p=1$, towards the active state, $q=n_s$, and then goes along the nontrivial line, $q=2n_s p/(1+p)$, towards the passive state $p=q=0$, cf. Fig. 3. The action is zero on the mean-field part of the evolution, while it is

$$S_0 = -\int_1^0 \frac{2n_s p}{1+p} dp = n_s 2(1-\ln 2) \tag{24}$$

along the nontrivial line.

According to the standard semiclassical description of tunneling [33], to find an escape probability, one has to sum up the contributions of all classical trajectories with an arbitrary number of bounces from $(1,n_s)$ to (0, 0) and back. Each bounce brings the factor $\sigma t e^{-S_0}$, where the prefactor reflects the fact that the center of the bounce may take place at any time without changing the action (zero mode). Since the distant (in time) bounces interact with each other only exponentially weakly, the escape attempts are practically uncorrelated. As a result, the probability to find an empty system, $P_0(t)=G(0,t)$, is

$$P_0(t) = 1 - e^{-t/\tau}, \tag{25}$$

where the decay time τ is given by

$$\tau = \sigma^{-1}\exp\{+S_0\}. \tag{26}$$

The semiclassical calculation is valid as long as $S_0 \gg 1$ and thus the decay time is much longer than the microscopic time, $\tau \gg \sigma^{-1}$.

IV. DIFFUSION

We turn now to the discussion of finite-dimensional systems. To characterize a microscopic state, one needs to specify the number of particles at every site of the lattice: $\{n_1,\ldots,n_N\}$, where $N \sim L^d$ is the total number of sites. The probability of a given microscopic state may be written as $P_{n_1,\ldots,n_N}(t)$ and the corresponding generating function is

$$G(p_1,\ldots,p_N,t) \equiv \sum_{n_1,\ldots,n_N} p_1^{n_1}\cdots p_N^{n_N} P_{n_1,\ldots,n_N}(t). \tag{27}$$

Assuming that the reaction rules are purely local (on-site), while the motion on the lattice is diffusive, one finds that the Hamiltonian takes the form

$$\hat{H}(\hat{p}_1,\ldots,\hat{p}_N,\hat{q}_1,\ldots,\hat{q}_N) = \sum_i [\hat{H}_0(\hat{p}_i,\hat{q}_i) + D\,\boldsymbol{\nabla}\hat{p}_i\cdot\boldsymbol{\nabla}\hat{q}_i], \tag{28}$$

where $\hat{H}_0(\hat{p},\hat{q})$ is a zero-dimensional on-site Hamiltonian given, for example, by Eqs. (7) or (21); D is a diffusion constant and $\boldsymbol{\nabla}$ is the lattice gradient. To shorten notations, we pass to the continuous d-dimensional variable x and introduce the fields $p(x)$ and $q(x)$. The generating function becomes a generating functional, $G(p(x),t)$. The latter may be written as a functional integral over canonically conjugated fields $p(x,t)$ and $q(x,t)$, living in $(d+1)$-dimensional space, with the action

$$S[p,q] = \int_0^t dt \int d^dx[H_0(p,q) + D\,\boldsymbol{\nabla}p\cdot\boldsymbol{\nabla}q - q\dot{p}]. \tag{29}$$

The initial term, e.g., the Poisson term, $\int d^dx n_0(x)[1-p(x,0)]$, should also be added to the action. The corresponding classical equations of motions are

$$\dot{q} = D\boldsymbol{\nabla}^2 q - \frac{\delta H_0}{\delta p}, \tag{30a}$$

$$\dot{p} = -D\boldsymbol{\nabla}^2 p + \frac{\delta H_0}{\delta q}. \tag{30b}$$

These equations are to be solved with the following boundary conditions:

$$q(x,0) = n_0(x), \tag{31a}$$

$$p(x,t) = p(x), \tag{31b}$$

where $n_0(x)$ is an initial space-dependent concentration and $p(x)$ is the source field in the generating functional $G(p(x),t)$. The mean-field approximation is obtained by putting $p(x,t)=1$ and is described by the reaction-diffusion equation,

$$\partial_t \overline{q} = D\nabla^2 \overline{q} - \left.\frac{\delta H_0(p,\overline{q})}{\delta p}\right|_{p=\overline{p}=1}, \tag{32}$$

that is the subject of numerous studies.

Equations (30) admit the integral of motion: $E = \int d^d x [H_0(p,q) + D\nabla p \nabla q]$. In some cases (see below), an additional infinite sequence of integrals of motion may be found, making the classical problem, Eqs. (30), analytically solvable. In a general case, these equations must be solved numerically. We notice, however, that such a numerical problem is orders of magnitude simpler than the numerical solution of the Master and even the FP equations, or direct modeling of the stochastic system. Below, we discuss a fast, efficient algorithm for the numerical solution of Eqs. (30) with the boundary conditions Eqs. (31). Moreover, a lot of insight may be gained by investigating the phase portrait of the zero-dimensional Hamiltonian, $H_0(p,q)$, which allows to make some semiquantitative predictions without a numerical solution.

To illustrate how the method works, we consider the branching annihilation problem of Sec. III [H_0 is given by Eq. (21)] on a compact d-dimensional cluster—the "refuge" [34]—denoted as $\mathcal{R}$. Outside of the refuge, there is a very high mortality rate, $A \to \emptyset$, which is eventually taken to infinity. This dictates the boundary condition

$$q(\partial\mathcal{R},t) = 0, \tag{33}$$

where $\partial\mathcal{R}$ is the boundary of the cluster $\mathcal{R}$. It is convenient to pass to the dimensionless time $\sigma t \to t$ and coordinates $x/\xi \to x$, where $\xi \equiv \sqrt{D/\sigma}$. We also introduce the rescaled fields $q(x,t) = n_s \varphi(x,t)$ (where $n_s = \sigma/\lambda$) and $p(x,t) = 1 - \hat{\varphi}(x,t)$. In these notations, the semiclassical equations, Eq. (30), take the symmetric form

$$\partial_t \varphi = \nabla^2 \varphi + \varphi - \varphi^2 + \hat{\varphi}\varphi^2 - 2\hat{\varphi}\varphi, \tag{34a}$$

$$-\partial_t \hat{\varphi} = \nabla^2 \hat{\varphi} + \hat{\varphi} - \hat{\varphi}^2 + \varphi\hat{\varphi}^2 - 2\varphi\hat{\varphi}. \tag{34b}$$

Consider first the mean-field ($\hat{\varphi}=0$) evolution, described by the equation

$$\partial_t \varphi = \nabla^2 \varphi + \varphi - \varphi^2 \tag{35}$$

and subject to the boundary condition $\varphi(\partial\mathcal{R},t)=0$. For the small concentrations, $\varphi \ll 1$, the last term may be omitted and the solution takes the form

$$\varphi(x,t) = \sum_{n=0}^{\infty} \alpha_n e^{(1-\lambda_n)t} Y_n(x), \tag{36}$$

where $Y_n(x)$ are normalized eigenfunctions of the Laplace operator in the region $\mathcal{R}$ with zero boundary conditions and eigenvalues $-\lambda_n < 0$; coefficients α_n depend on an initial condition. Therefore, if the smallest eigenvalue, λ_0, is larger than unity (the cluster is small enough), any initial distribution evolves towards the empty system. The characteristic lifetime of the system is thus

$$\tau = \sigma^{-1}(\lambda_0 - 1)^{-1}, \quad \lambda_0 > 1. \tag{37}$$

If $\lambda_0 < 1$ (the cluster is larger than some critical size), the mean-field evolution, Eq. (35), leads to a stable nonvanishing concentration $\varphi_0(r)$, which is given by the solution of the equation $\nabla^2\varphi_0 + \varphi_0 - \varphi_0^2 = 0$ with zero boundary conditions. It is clear, however, that such a solution is actually a metastable state of the system. Namely, after a long enough time, the system will find itself in the empty (passive) state. Our task is to find the system's lifetime, τ, for the metastable case, $\lambda_0 < 1$. According to our previous discussions, the lifetime is expected to be exponentially long,

$$\tau = \sigma^{-1} e^{S_d}, \quad \lambda_0 < 1, \tag{38}$$

where S_d is the action along the semiclassical trajectory, which solves Eqs. (34a) and (34b) with the initial condition $\varphi(x,0) = \varphi_0(x)$ and the final condition $\hat{\varphi}(x,t_e)=1$. The extinction time, t_e, is to be sent to infinity. Indeed $\partial S_d/\partial t_e = E(t_e) \leqslant 0$, and thus the longer the extinction time, the smaller the action. In practice, however, the action almost saturates at modest values of t_e.

In general, the problem cannot be solved analytically and one needs to resort to numerical approaches. The following iteration scheme rapidly converges to the desired solution: one first fixes the momenta to be $\hat{\varphi}_1(x,t)=1$ at any time and solves Eq. (34a) with the initial condition $\varphi(x,0)=\varphi_0(x)$ by forward iteration from $t=0$ to $t=t_e$. The result of this procedure, $\varphi_1(x,t)$, is kept fixed during the next step, which is the solution of Eq. (34b) with the condition $\hat{\varphi}(x,t_e)=1$ by the backward iteration from $t=t_e$ to $t=0$. This way, one finds $\hat{\varphi}_2(x,t)$, which is kept fixed while the next approximation $\varphi_2(x,t)$ is obtained by the forward iteration of Eq. (34a). Repeating successively forward and backward iterations, the algorithm rapidly converges to the required solution. The action $S_d = S_d(t_e)$ is then calculated according to Eq. (29). Finally, one has to check that $S_d(t_e)$ does not decrease significantly upon increasing t_e.

The action, S_d, for a one-dimensional cluster of size $2R$ is plotted in Fig. 4 as a function of R. The critical radius $R_c = \pi/2$ (in units of ξ) is found from the condition $\lambda_0=1$. For $R<R_c$, there is no metastable state and thus $S_d=0$, while the cluster lifetime is given by Eq. (37). For $R>R_c$, the lifetime is given by Eq. (38), with the numerically calculated S_d plotted in Fig. 4. The asymptotic behavior of the action S_d for $R \gg R_c$ ($\lambda_0 \ll 1$) and $R - R_c \ll R_c$ ($1-\lambda_0 \ll 1$) may be readily found analytically.

For $R \gg R_c$ ($\lambda_0 \ll 1$), the concentration throughout the bulk of the cluster is practically uniform, apart from a surface

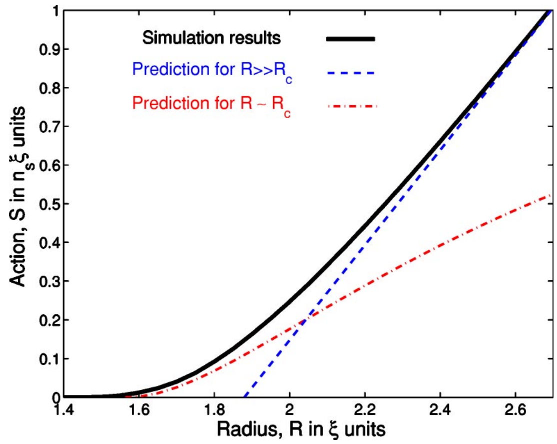

FIG. 4. The semiclassical action (in units of $\xi^d n_s$) for the extinction of a one-dimensional cluster is shown as a function of the cluster's radius R (in units of ξ), full line; the large radius approximation, Eq. (39), is shown by the dashed line; the near-critical, $\pi/2 \lesssim R$, approximation, Eq. (45), is shown by the dashed-dotted line.

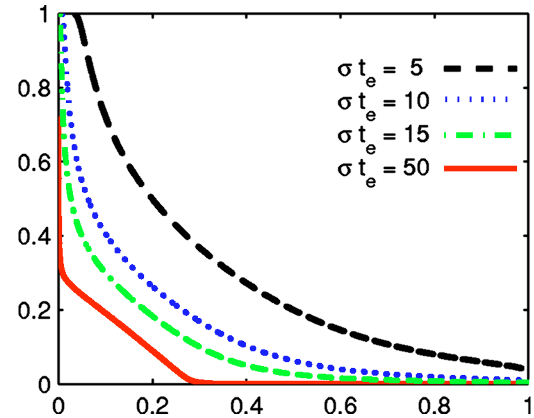

FIG. 5. Trajectories on the $(\hat{\varphi}, \varphi)$ plane are shown for the center point of the 1D cluster, $x=0$. The horizontal axis is $\hat{\varphi}$ variable and the vertical axis is φ. Different curves are distinguished by their escape time, marked in dimensionless units σt_e. $\epsilon\eta Y_0(0)=0.3$.

layer of thickness ξ. One may therefore apply the results of the zero-dimensional problem, Eq. (24), to find

$$S_d = 2(1-\ln 2) n_s \xi^d (\mathcal{V} - c\mathcal{S}), \tag{39}$$

where $\mathcal{V}$ and $\mathcal{S}$ are the cluster's dimensionless volume and surface area correspondingly and c is a numerical constant, which we shall not evaluate here. For the 1D case, the corresponding line is plotted in Fig. 4 by the dashed line.

We turn finally to the clusters that are only slightly larger than the critical size: $\epsilon \equiv 1-\lambda_0 \ll 1$ [e.g., for a spherical cluster with the radius R one finds $\epsilon = 1-(R_c/R)^2$, where R_c is a critical radius, found from $\lambda_0 = 1$]. In this case, only the zeroth eigenfunction $Y_0(x)$ is the unstable direction of the linearized mean-field equation. The full nonlinear mean-field equation (35) possesses, therefore, the stable solution $\varphi_0(x)$, that is expected to be of order ϵ. One may thus look for this solution in the following form:

$$\varphi_0(r) = \epsilon[\eta Y_0(x) + \epsilon \varphi_1(x)], \tag{40}$$

where $\varphi_1(x)$ is orthogonal to $Y_0(x)$. One can now substitute this trial solution in Eq. (35), keeping only the leading (second) order of ϵ terms, and project on Y_0, using its orthogonality to φ_1. As a result, the coefficient η is found to be

$$\eta^{-1} = \int_{\mathcal{R}} d^d r Y_0^3(r). \tag{41}$$

The metastable solution of Eq. (34) in the leading order in ϵ is therefore $\varphi_0(x) = \epsilon\eta Y_0(x)$ and $\hat{\varphi}_0(x) = 0$. To find the optimal escape trajectory, let us parametrize deviations from this metastable state as

$$\varphi(x,t) = \epsilon\eta Y_0(x) + \sum_{n=0}^{\infty} \alpha_n(t) Y_n(x), \tag{42a}$$

$$\hat{\varphi}(x,t) = \sum_{n=0}^{\infty} \beta_n(t) Y_n(x), \tag{42b}$$

where $\alpha_n(t)$ and $\beta_n(t)$ are assumed to be small. One can now substitute these deviations into the dynamical equations (34) and linearize them with respect to α_n, β_n. It is easy to see then that in the leading order in ϵ only α_0 and β_0 should be retained. They evolve according to

$$\frac{d}{dt}\begin{pmatrix}\alpha_0 \\ \beta_0\end{pmatrix} = \epsilon\begin{pmatrix}-1 & -2 \\ 0 & 1\end{pmatrix}\begin{pmatrix}\alpha_0 \\ \beta_0\end{pmatrix} + O(\epsilon^2). \tag{43}$$

The matrix on the right-hand side has two eigenvectors, (1,0) and $(1,-1)$, with the eigenvalues -1 and 1 correspondingly. The first eigenvector describes deviation in the mean-field direction, $\hat{\varphi}=0$, and leads to the restoring force back to the metastable state. The second one gives the most unstable direction, which describes the way the system escapes towards the empty state. The corresponding trajectory on the $(\hat{\varphi}, \varphi)$ plane is plotted in Fig. 5 for the center point of the 1D cluster, $x=0$. Different lines correspond to a few values of t_e. For $t_e \to \infty$, the energy, E, approaches zero and the trajectory approaches the $(1,-1)$ direction that leads from the metastable point $(0, \epsilon\eta Y_0)$ to a symmetric metastable point $(\epsilon\eta Y_0, 0)$. [The existence of the latter follows directly from the symmetry of Eqs. (34).] For $\epsilon \ll 1$, the small deviation analysis describes the entire transition between the two metastable points that takes place, therefore, along the straight line,

$$\varphi(x,t) = \epsilon\eta Y_0(x) - \hat{\varphi}(x,t), \tag{44}$$

on the $(\hat{\varphi}, \varphi)$ plane. Further evolution takes place along the $\varphi=0$ direction. As a result, in the limit $t_e \to \infty$, and therefore $E \to 0$, the semiclassical escape action is given by the area of the straight triangle, with the height $\epsilon\eta Y_0(x)$, integrated over the cluster, cf. Eq. (29),

$$S_d = -\int_{\mathcal{R}} d^d x \int q dp = n_s \xi^d \int_{\mathcal{R}} d^d x \int \varphi d\hat{\varphi} = \frac{1}{2}(\eta\epsilon)^2 n_s \xi^d. \tag{45}$$

For the 1D cluster [$\epsilon = 1-(\pi/2R)^2$ and $\eta^2 = 9\pi^3/128$], Eq. (45) is shown in Fig. 4 by a dashed-dotted line. (For a circular cluster in 2D, $R_c = 2.4$ and $\eta^2 = 9.4$, while for a spherical 3D cluster, $R_c = \pi$ and $\eta^2 = 51.7$.) One may observe that the large and small cluster asymptotic results, Eqs. (39) and (45) correspondingly, provide a reasonable approximation for the exact numerical calculation of the semiclassical action, S_d. Finally, the probability of the system staying in the metastable state is $P(t) = \exp\{-t/\tau\}$, where the lifetime τ is given by Eq. (38).

V. RUNAWAY SYSTEMS

In this section, we consider a qualitatively different system that exhibits a runaway behavior, characterized by unlimited proliferation of the number of particles. The simplest example is given by the population dynamics model, consisting of three reactions: binary reproduction, death, and emigration, characterized by probabilities λ, σ, and μ correspondingly. The schematic way to write it is $A+A \xrightarrow{\lambda} 3A$, $A \xrightarrow{\sigma} \emptyset$, and $\emptyset \xrightarrow{\mu} A$. The Master equation for the zero-dimensional system has the form

$$\frac{dP_n}{dt} = \lambda\left[\frac{(n-1)(n-2)}{2}P_{n-1} - \frac{n(n-1)}{2}P_n\right] + \sigma[(n+1)P_{n+1} - nP_n] + \mu[P_{n-1} - P_n]. \tag{46}$$

The corresponding zero-dimensional Hamiltonian is

$$\hat{H}_0(\hat{p},\hat{q}) = \frac{\lambda}{2}(\hat{p}^2 - \hat{p}^3)\hat{q}^2 + \sigma(\hat{p}-1)\hat{q} + \mu(1-\hat{p}) \tag{47}$$

and the classical equations of motions are

$$\dot{q} = -\lambda\left(p - \tfrac{3}{2}p^2\right)q^2 - \sigma q + \mu, \tag{48a}$$

$$\dot{p} = \lambda(p^2 - p^3)q + \sigma(p-1). \tag{48b}$$

As always, the mean-field equation of motion for the reaction coordinate $\overline{q} \approx \langle n\rangle$ is obtained by the ansatz $p=1$ and takes the form

$$\frac{d\overline{q}}{dt} = \frac{\lambda}{2}\overline{q}^2 - \sigma\overline{q} + \mu. \tag{49}$$

According to the mean-field equation, there are two qualitatively different scenarios of the system's evolution. They are distinguished by the parameter

$$\delta^2 \equiv 1 - \frac{2\lambda\mu}{\sigma^2}. \tag{50}$$

If $\delta^2 < 0$, the right-hand side of Eq. (49) is strictly positive and the reaction coordinate always grows to infinity. This is the scenario, where the population proliferates indefinitely. Alternatively, for $\delta^2 > 0$ the system possesses two stationary

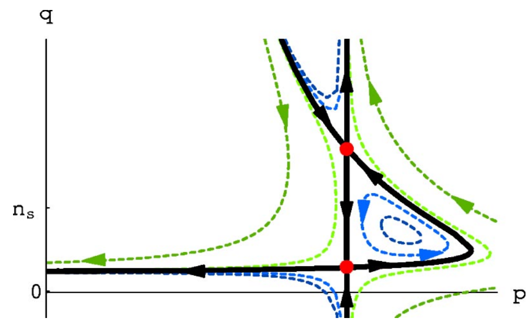

FIG. 6. The phase portrait of the runaway process, Eq. (46). Thick lines represent the solution of $H(p,q)=0$. The fat dots are fixed points. $\delta^2 = 1/2$.

concentrations: $n_{\mp} = n_s(1 \mp \delta)$, where $n_s = \sigma/\lambda$. The point $\overline{q} = n_-$ is the stable one, while $\overline{q} = n_+$ is unstable. In this case (the only one we discuss hereafter), the mean field predicts that for the range of initial concentrations $0 < n_0 < n_+$ the system evolves towards the stable population n_-. If the initial concentration exceeds n_+, the system runs away and the population diverges.

If one goes beyond the mean-field treatment, however, one realizes that the state n_- is actually a *metastable* one. To see this fact, and calculate the lifetime of the metastable state, it is convenient to draw the phase portrait, Fig. 6. It has two lines of zero energy: the mean-field line, $p=1$, and the nontrivial line $\lambda p^2 q^2/2 - \sigma q + \mu = 0$. These two lines intersect at the mean-field stable points $p=1, q=n_{\mp}$ and determine the topology of the phase diagram. It is clear from the phase portrait that the point $p=1, q=n_-$ is not stable once motion with $p \neq 1$ (non-mean-field) is allowed. More precisely, there is a non-mean-field path that brings the system from the point $q=n_-$ to the point $q=n_+$. Once the point $q=n_+$ is reached, the system may continue to evolve according to the mean field towards indefinite population growth. Repeating the calculations, similar in spirit to the calculations of the decay time in Sec. III, one finds for the lifetime of the metastable state, $q=n_-$,

$$\tau \approx \sigma^{-1}\exp\{+S_0\}, \tag{51}$$

where S_0 is the classical action along the nontrivial line of zero energy between points $(1, n_-)$ and $(1, n_+)$. Calculating the integral, one finds $S_0 = f(n_+) - f(n_-)$, where $f(x) \equiv x - \sqrt{8\mu/\lambda}\arctan(x\sqrt{\lambda/2\mu})$.

Two limiting cases are of particular interest: (i) the "near-critical" system, $0 < \delta^2 \ll 1$ and (ii) the system with almost no immigration, $\mu \to 0^+, \delta \to 1^-$. In the former case, the two mean-field stationary points approach each other, making the escape from the metastable state relatively easy. Expanding the f function up to the third order, one finds $S_0 = 2n_s\delta^3/3 \ll n_s$. As expected, the action is small and correspondingly the lifetime is short (notice that the quasiclassical picture applies as long as $S_0 > 1$). In the latter case, the two mean-field stationary points tend to $n_- \to 0$ and $n_+ \to 2n_s$. If the immigration is absent, $\mu = 0$, the mean-field stable point, $n_- = 0$, coincides with the empty state of the system. The empty state is absolutely stable since no fluctuations are possible. Naively, one may expect that in this limit the lifetime of the metastable state (and thus S_0) diverges. This is *not* the case, however. The calculation shows $S_0 \to 2n_s$. As a result, even a negligibly small probability of immigration, μ, leads to a finite probability of unlimited population expansion. (Strictly speaking, one also needs to show that the preexponential factor does not go to zero once $\mu \to 0$.)

We consider now a finite-dimensional generalization of this population dynamics model. The physics of the phenomena, discussed here, is as follows: if a critically large cluster "tunnels" into the runaway state, both diffusion and reaction dynamics work to expand the cluster and flip the entire system into the runaway mode. The situation is similar to nucleation of a critical domain in the supercooled state of a system close to a first-order phase transition. To simplify the algebra, we shall consider only the case of the "near-critical" system, $0<\delta^2 \ll 1$, where the apparatus turns out to be rather similar to that of the theory of the first-order phase transitions.

As discussed above, the finite-dimensional generalization of the Hamiltonian is $H[p,q]=\int d^d x [H_0(p,q)+D\nabla p \nabla q]$. For $\delta \ll 1$, it is convenient to make a change of variables $(p,q)\to(\hat{\varphi},\varphi)$, as $p=1+\hat{\varphi}$ and $q=n_s(1+\varphi)$, where $\varphi \sim \delta$, while $\hat{\varphi}\sim\delta^2$. Substituting it into the reaction part of the Hamiltonian, Eq. (47), and keeping terms up to δ^4, one obtains $H_0(\hat{\varphi},\varphi)=\sigma n_s[\hat{\varphi}(\delta^2-\varphi^2)/2-\hat{\varphi}^2]$. As a result, the d-dimensional action, Eq. (29), for the conjugated fields $\hat{\varphi}(x,t)$ and $\varphi(x,t)$ takes the form

$$S = n_s \xi^d \int_0^t dt \int d^d x \left[\hat{\varphi}\left(\dot{\varphi} - \nabla^2 \varphi + \frac{\delta^2 - \varphi^2}{2} \right) - \hat{\varphi}^2 \right], \tag{52}$$

where we have introduced the dimensionless time $\sigma t \to t$ and coordinate $x/\xi \to x$, where $\xi = \sqrt{D/\sigma}$. The functional integration over the field $\hat{\varphi}$ should be understood as running along the imaginary axis. The field theory with the action, Eq. (52), may be considered as a Martin-Sigia-Rose [35] representation of the following Langevin equation:

$$\frac{\partial \varphi}{\partial t} = \nabla^2 \varphi - \frac{\partial V}{\partial \varphi} + \zeta(x,t), \tag{53}$$

where $\zeta(x,t)$ is a Gaussian noise with the correlator

$$\langle \zeta(x,t)\zeta(x',t')\rangle = \frac{2}{n_s \xi^d}\delta(x-x')\delta(t-t') \tag{54}$$

and the potential is $V(\varphi)=-\varphi^3/6+\delta^2\varphi/2$. This potential has a metastable minimum at $\varphi=-\delta$ and an unstable maximum at $\varphi=\delta$. The barrier height is $V(\delta)-V(-\delta)=2\delta^3/3$ and therefore the lifetime of the zero-dimensional ($d=0$) system is expected to be given by the activation exponent [with $(n_s\xi^d)^{-1}$ playing the role of temperature] $\sim \exp\{n_s 2\delta^3/3\}$, in agreement with Eq. (51).

To discuss the lifetime of the finite-dimensional system, we shall not use the Langevin approach, but rather return to the action, Eq. (52), and write down the classical equations of motion,

$$\partial_t \varphi = \nabla^2 \varphi - \frac{\partial V}{\partial \varphi} + 2\hat{\varphi}, \tag{55a}$$

$$\partial_t \hat{\varphi} = -\nabla^2 \hat{\varphi} + \hat{\varphi}\frac{\partial^2 V}{\partial \varphi^2}. \tag{55b}$$

The energy density, corresponding to these two equations, is defined as $E(x,t)=-\hat{\varphi}(\nabla^2\varphi-\partial V/\partial\varphi+\hat{\varphi})$. The global energy, $E=\int d^d x E(x,t)$, is, of course, conserved. However, in the present case if $E(x,0)=0$, it keeps holding *locally* at any time: $E(x,t)=0$. Indeed, the energy density vanishes if either $\hat{\varphi}=0$ or $\hat{\varphi}=-\nabla^2\varphi+\partial V/\partial\varphi=2\hat{\varphi}-\partial_t\varphi$, and thus $\hat{\varphi}=\partial_t\varphi$, where we have employed Eq. (55a). It is easy to check that in both cases Eq. (55b) is satisfied automatically. Therefore, the evolution with zero-energy density is described by either $\partial_t\varphi=\nabla^2\varphi-\partial V/\partial\varphi$, which is the mean-field equation, or by $\partial_t\varphi=-\nabla^2\varphi+\partial V/\partial\varphi$, which gives the motion along the nontrivial line of zero energy.

Notice that the last equation happens to be the time-reversed version of the mean field [36]. If one starts, thus, from the stationary solution $\varphi=-\delta$ and perturbs it infinitesimally, then the perturbation grows until it reaches the stable configuration, satisfying

$$\nabla^2 \varphi - \frac{\partial V}{\partial \varphi} = 0. \tag{56}$$

The critical domain is given, therefore, by a localized solution of Eq. (56). Since the energy along the nucleation dynamics is zero, the action to nucleate the critical domain is given by $S_d=n_s\xi^d\int d^d x\int dt\hat{\varphi}\partial_t\varphi=n_s\xi^d\int d^d x\int dt(-\nabla^2\varphi+\partial V/\partial\varphi)\partial_t\varphi$. Performing the time integration in this expression, one finds for the action

$$S_d = n_s \xi^d \int d^d x \left(\frac{1}{2}(\nabla \varphi_d)^2 + V(\varphi_d) - V(-\delta) \right), \tag{57}$$

where $\varphi_d=\varphi_d(x)$ is a stationary localized solution of Eq. (56), which is an extremum of the functional (57). As a result, the problem of the dynamical escape from the metastable configuration is reduced to the static Landau theory of the first-order transitions. As far as we know, such reduction is not a general statement, but rather is a consequence of the assumption $\delta \ll 1$ and the resulting *local* energy conservation, $E(x,t)=0$. In a general situation, one still has to solve a considerably more complicated problem of dynamic equations (48) for $\varphi(x,t)$ and $\hat{\varphi}(x,t)$.

From the scaling analysis of Eq. (56), one finds that $\varphi \sim \delta$ in the core of the critical domain. Employing this fact, one finds that the characteristic spatial scale of the domain is given by $\delta^{-1/2} \gg 1$ (distance is measured in units of $\xi = \sqrt{D/\sigma}$). Therefore, the action cost to create the critical domain is

$$S_d = c_d n_s \xi^d \delta^{3-d/2}, \tag{58}$$

where c_d is a numerical factor of the order of 1: $c_0=2/3, c_1=24/5$. This result suggests that for $d>6$, the state with finite population density $n=n_s(1-\delta)$ is stable, while for $d<6$ the state is metastable. The concentration of critical domains is given by $\xi^{-d}\exp\{-S_d\}$ and the typical distance between them is $\xi\exp\{S_d/d\}$. They grow diffusively until the entire system is flipped over to the runaway state in time $\tau \sim \sigma^{-1}\exp\{2S_d/d\}$. The semiclassical calculation is applicable as long as $S_d > 1$ and therefore δ is not too small. For very small δ, the escape is driven by the fluctuations rather than the semiclassical dynamics.

VI. CONCLUSIONS

Rare events play an important role in a variety of systems in nature; the immediate practical application may be a stochastic evolution in virology [45]. The process of evolution is a consequence of the interplay of mutation and selection on a population of organisms, leading to an observable change in its genetic makeup. Because of their simple genomes, viruses make good models for studying and testing evolutionary theory. "Rare" events are thought to be responsible for processes such as creating new populations with properties altered dramatically, such as evasion of the immune response or resistance to antiviral therapy.

The examples, considered above, are meant to illustrate the general technique to calculate the probability of rare events in reaction-diffusion systems. The technique is based on the existence of the many-body "quantum" Hamiltonian, which fully encodes the microscopic Master equation. The very same Hamiltonian, in its second quantized representation, serves as a starting point for field-theoretical treatments of dynamic phase transitions in the reaction-diffusion system [11–19]. For our present purposes, we have deliberately chosen to work with systems that are away from a possible continuous phase-transition point. Namely, we focus on the parts of the phase diagram where the mean-field considerations suggest a nonvanishing population of particles (or at least transiently nonvanishing population). In such cases, the "quantum" fluctuations are small and one may treat the underlying "quantum" dynamics in a semiclassical way.

We stress that the semiclassical treatment is *not* equivalent to that of the mean field. The latter requires a very special assumption about dynamics of the canonical momenta, namely, $p(x,t)=1$. This assumption may be justified, as long as one is interested in a typical system's behavior (even this is not guaranteed if the system possesses metastable states, as in our last example). In such cases, the problem is reduced to a partial differential equation for the reaction coordinates, $q(x,t)$, only. However, if questions about atypical, rare events are asked, the mean-field assumption, $p(x,t)=1$, must be abandoned. As a result, one has to deal with the canonical pair of Hamilton equations for reaction coordinates, $q(x,t)$, and momenta, $p(x,t)$. The degree of deviation from the mean-field line, $p=1$, is specified (through proper initial and finite boundary conditions) by the concrete sort of the rare event of interest. Finally, the probability of the rare event is proportional to the exponentiated action along the classical trajectory, satisfying specified boundary conditions.

We found it especially useful to work with the phase portrait of the corresponding dynamical system on the (p,q) plane. The emerging structures are fairly intuitive and can tell a great deal about the qualitative behavior of the system even before any calculations. On one hand, the Hamiltonians underlying the Master equations of reaction systems are typically *not* of the type traditionally considered in the theory of dynamical systems. For example, they usually *cannot* be cast into the familiar form $H(p,q)=p^2/2+A(q)p+V(q)$. On the other hand, they possess some universal features, such as $H(1,q)=0$, or, if there is an empty absorbing state, $H(p,0)=0$, etc. These features dictate a specific topology of the phase portrait. It would be extremely interesting to explore this class of Hamiltonians from the point of view of the mathematical theory of dynamical systems [37]. A question of particular interest is a possible, exact integrability of the resulting Hamiltonian equations (especially in $d=1$) [38].

There are a number of issues that are not addressed in the present paper and require further investigation. Let us mention some of them. (i) Throughout the paper we have discussed rare event probability with exponential accuracy. In some cases, this is not enough and one would like to know the preexponential factor rather precisely. This requires a calculation of the fluctuation determinant on top of the nontrivial classical trajectory. This task is relatively straightforward for the $d=0$ systems, where it may be addressed by writing down "quantum" corrections to the Hamilton-Jacobi equation and treating them iteratively (in the way it is usually done in the single-particle WKB method). For extended systems, the task is reduced to the spectral problem of a certain matrix differential operator. At present, we are not aware of a general recipe to solve it. One may show, however, that on any mean-field trajectory, $p(x,t)=1$, the fluctuation determinant is equal to unity. The simplest way of doing it is to use the discrete representation of the functional integral, Eq. (10), and notice that the quadratic fluctuation matrix has a triangular structure with unities on the main diagonal (and, hence, unit determinant). Unfortunately, this is not the case away from the mean field, $p\neq 1$.

(ii) We have restricted ourselves to systems with a single sort of species only. It is straightforward to generalize the technique to any number of species, K. The difficulty is that the phase portrait becomes a $2K$-dimensional construction, which is not easy to visualize. Correspondingly, the mean-field line becomes a K-dimensional hyperplane. Moreover, some qualitatively new physics may arise, such as stable oscillatory limiting cycles on the mean-field hyperplane. A paradigm of such behavior is a Lotka-Volterra [39] system: $A+B\xrightarrow{\lambda}2A$; $A\xrightarrow{\sigma}\varnothing$ and $B\xrightarrow{\mu}2B$. An example of a rare event may be an "escape" from the periodic limiting cycle on the A-B mean-field plane into the empty state in a finite-size system. Finding an optimal "reaction path" for such an escape is not an obvious matter, however.

(iii) We have not treated long-range interactions and (local or nonlocal) constraints. The simplest ("fermionic") constraint is that of a maximum single occupancy of each lattice site. It was shown recently that such a constraint may be incorporated into the "bosonic" formulation [40], leading to a new class of the interesting Hamiltonians. Studying rare event statistics for such hard-core particles (by studying classical dynamics of the corresponding Hamiltonians) is a very interesting subject.

(iv) There is a close resemblance between the formalism presented here for essentially classical systems and the

Keldysh technique for nonequilibrium quantum statistics [41]. The semiclassical solutions with $p \neq 1$, considered here, correspond to saddle-point configurations of the Keldysh action with a different behavior on the forward and backward branches of the time contour. Although examples of such saddle points were considered in the literature [42,43], it would be interesting to learn more about possible applications of the present technique for true quantum problems.

ACKNOWLEDGMENTS

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APPENDIX A: OPERATOR TECHNIQUE

We give here a brief account of the operator technique [27–29,44] for completeness. Define the ket-vector $|n\rangle$ as the microscopic state with n particles. Let us also define the vector

$$|\Psi(t)\rangle \equiv \sum_{n=0}^{\infty} P_n(t)|n\rangle. \tag{A1}$$

Notice that the weight, P_n, is the probability rather than the amplitude. It is convenient to introduce the creation and annihilation operators with the following properties:

$$a^\dagger|n\rangle = |n+1\rangle, \tag{A2a}$$

$$a|n\rangle = n|n-1\rangle. \tag{A2b}$$

As a byproduct, one has $a|0\rangle = 0$. One may immediately check that such operators are "bosonic":

$$[a,a^\dagger] = 1. \tag{A3}$$

As for any pair of operators satisfying Eq. (A3), one may prove the identity

$$e^a f(a,a^\dagger) = f(a,a^\dagger+1)e^a, \tag{A4}$$

where f is an arbitrary operator-value function. In these notations, the whole set of the Master equations may be recast into a single "imaginary time" Schrödinger equation

$$\frac{d}{dt}|\Psi(t)\rangle = -\hat{H}|\Psi(t)\rangle, \tag{A5}$$

where $\hat{H}$ is the "Hamiltonian" operator. One may check that the Hamiltonian of the binary annihilation process, Eq. (1), has the form

$$\hat{H} = \frac{\lambda}{2}[(a^\dagger)^2 - 1]a^2, \tag{A6}$$

where the first term in brackets on the right-hand side is the "out" term and the second is the "in" term.

One may formally solve the Schrödinger equation: $|\Psi(t)\rangle = \exp\{-\hat{H}(a^\dagger,a)t\}|\Psi(0)\rangle$. An initial state, $|\Psi(0)\rangle$, is specified as, e.g., $|\Psi(0)\rangle = e^{-n_0(a^\dagger-1)}|0\rangle$ for the Poisson initial distribution, or $|\Psi(0)\rangle = (a^\dagger)^{n_0}|0\rangle$ for the fixed particle number. The generating function Eq. (2) is given by

$$G(p,t) = \langle 0|e^{pa}e^{-\hat{H}(a^\dagger,a)t}|\Psi(0)\rangle. \tag{A7}$$

The normalization, $G(1,t=0)=1$, is guaranteed by the identity $\langle 0|e^a|n\rangle = 1$ for any n [this fact may be checked using Eq. (A4)] and the constraint $\Sigma_n P_n(0) = 1$. The normalization is kept intact at any time if $\langle 0|e^a\hat{H}(a^\dagger,a) = 0$. Since the coherent state $\langle 0|e^a$ is an eigenstate of the creation operator, $\langle 0|e^a a^\dagger = \langle 0|e^a$, one arrives at the conclusion that any legitimate Hamiltonian must obey

$$\hat{H}(a^\dagger = 1, a) = 0. \tag{A8}$$

For instance, the Hamiltonian of the binary annihilation, Eq. (A6), indeed satisfies this condition.

One may now employ the standard bosonic coherent state technique to write the generating function, Eq. (A7), as the functional integral. The result coincides identically with Eq. (10) of the main text. One notices, thus, the formal correspondence between the operators $a^\dagger$ and a, and operators $\hat{p}$ and $\hat{q}$ correspondingly.

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