Spectral theory of metastability and extinction in a branching-annihilation reaction

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We apply the spectral method, recently developed by the authors, to calculate the statistics of a reaction-limited multistep birth-death process, or chemical reaction, that includes as elementary steps branching $A \to 2A$ and annihilation $2A \to 0$. The spectral method employs the generating function technique in conjunction with the Sturm-Liouville theory of linear differential operators. We focus on the limit when the branching rate is much higher than the annihilation rate and obtain accurate analytical results for the complete probability distribution (including large deviations) of the metastable long-lived state and for the extinction time statistics. The analytical results are in very good agreement with numerical calculations. Furthermore, we use this example to settle the issue of the "lacking" boundary condition in the spectral formulation.

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I. INTRODUCTION

The statistics of rare events, or large deviations, in chemical reactions and systems of birth-death type have attracted a great deal of interest in many areas of science including physics, chemistry, astrochemistry, epidemiology, population biology, cell biochemistry, etc. [1–14]. Large deviations become of vital importance when the discrete (noncontinuum) nature of a population of "particles" (molecules, bacteria, cells, animals, or even humans) drives it to extinction. A standard way of putting the discreteness of particles into theory is the master equation [1,2] which describes the evolution of the probability of having a certain number of particles of each type at time t. The master equation is rarely soluble analytically, and various approximations are in use [1,2]. One widely used approximation is the Fokker-Planck equation which usually gives accurate results in the regions around the peaks of the probability distribution, but fails in its description of large deviations—that is, the distribution tails [15–17]. Not much is known beyond the Fokker-Planck description. In some particular cases (especially, for single-step birth-death processes) complete statistics, including large deviations, were determined by applying various approximations directly to the pertinent master equation [10,12,14,17–23]. A different group of approaches employs the generating function formalism [1,5,8]; see below. Here the master equation is transformed into a linear partial differential equation (PDE) for the generating function, and this PDE is analyzed and solved by various techniques such as the method of second quantization [24–26] or the more recent time-dependent WKB approximation [16,27]. Recently, we combined the generating function technique with the Sturm-Liouville theory of linear differential operators and developed a *spectral theory* of rare events [28,29]. In this theory the problem of computing the complete statistics of (not necessarily single-step) birth-death systems reduces to solving an eigenvalue problem for a linear differential operator, the coefficients of which are determined by the reaction rates.

In this paper we apply the spectral method to the paradigmatic problem of branching $A+X \to 2X$ and annihilation $X+X \to E$, where A and E are fixed. This multistep single-species birth-death process describes, for example, chemical oxidation reactions [18,30]. If the branching rate is much higher than the annihilation rate (the case we will be mostly interested in throughout the paper), a long-lived metastable, or quasistationary, state exists where the two processes (almost) balance each other. Still, this long-lived state slowly decays with time, because a sufficiently large fluctuation ultimately brings the system into the absorbing state of no particles from which there is a zero probability of exiting. In this type of problems one is interested in the extinction time statistics and in the complete probability distribution, including large deviations, of the quasistationary state (formally defined as the limiting distribution conditioned on nonextinction). Turner and Malek-Mansour [18] calculated the mean extinction time in this system by solving a recursion equation for the extinction probability. More recently, Elgart and Kamenev [16] reexamined this problem in the light of their time-dependent WKB approximation for the generating function. Their insightful method readily yields an estimate of the mean extinction time, but only up to a (significant) preexponential factor. The quasistationary distribution for this system has not been previously found, and calculating it will be our objective. In the language of the spectral theory, the mean extinction time represents the inverse eigenvalue of the ground state, while the quasistationary distribution is derivable from the ground-state eigenfunction.

The paradigmatic branching-annihilation problem, considered in this paper, has an additional value, as it helps settle one unresolved issue of the spectral theory. In previous works [28,29] we considered reactions that conserve parity of the particles. Parity conservation provides an additional boundary condition for the PDE for the generating function which ensures a closed formulation of the problem already at the stage of the time-dependent PDE. The branching-annihilation process, considered in the present work, does *not* conserve parity. As we will show, the "lacking" boundary condition emerges here (and in a host of other problems of this type) only at the stage of the Sturm-Liouville theory.

Here is how we organize the rest of the paper. In Sec. II we apply the spectral method and reduce the governing master equations to a proper Sturm-Liouville problem. In Sec. III we employ a matched asymptotic expansion to approximately calculate the ground-state eigenvalue and eigenfunction and obtain the long-time asymptotics of the generating function. This asymptotics is used in Sec. IV to extract the quasistationary probability distribution and compare it with our numerical results. In Sec. V we calculate the mean extinction time and extinction probability distribution and compare these results with the previous work and with our numerics. Some final comments are presented in Sec. VI.

II. GENERATING FUNCTION AND SPECTRAL FORMULATION

We consider the branching and annihilation reactions

$$A \xrightarrow{\lambda} 2A \quad \text{and} \quad 2A \xrightarrow{\mu} 0,$$

where $\mu,\lambda>0$ are the rate constants. The (mean-field) rate equation for the number of particles $n(t)$, $dn/dt=\lambda n-\mu n^2$ predicts a nontrivial attracting steady state $n_s=\lambda/\mu\equiv\Omega$. Fluctuations invalidate this mean-field result due to the existence of an absorbing state at $n=0$. However, when $\Omega\gg 1$, there exists a long-lived fluctuating *metastable* (or quasistationary) state, which *slowly* decays in time, implying a slow growth of the extinction probability. The statistics of this quasistationary state and of the extinction times are in the focus of our attention here.

The master equation for the probability $P_n(t)$ to find n particles at time t can be written as

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

$$\frac{d}{dt}P_0(t)=\mu P_2(t). \tag{1}$$

We introduce the generating function [1,2,8]

$$G(x,t)=\sum_{n=0}^{\infty}x^nP_n(t), \tag{2}$$

where x is an auxiliary variable. Once $G(x,t)$ is known, the probabilities $P_n(t)$ can be recovered from the Taylor expansion:

$$P_n(t)=\frac{1}{n!}\frac{\partial^nG(x,t)}{\partial x^n}\bigg|_{x=0}. \tag{3}$$

By virtue of Eqs. (2) and (3), $G(x,t)$ must be analytical, at all times, at $x=0$. Equations (1) and (2) yield a single PDE for $G(x,t)$ [16]:

$$\frac{\partial G}{\partial t}=\frac{\mu}{2}(1-x^2)\frac{\partial^2G}{\partial x^2}+\lambda x(x-1)\frac{\partial G}{\partial x}. \tag{4}$$

Conservation of probability yields one (universal) boundary condition for this parabolic PDE: $G(1,t)=1$ [31]. What is the second boundary condition? Note that $G(x=-1,t)$ must be bounded at all times, as it is equal to the difference between the sum of the probabilities to have an even number of particles and the sum of the probabilities to have an odd number of particles. Now, the *steady-state* solution of Eq. (4), $G_{st}(x)=G(x,t\to\infty)$, which obeys the equation

$$\frac{\mu}{2}(1-x^2)\frac{d^2G_{st}}{dx^2}+\lambda x(x-1)\frac{dG_{st}}{dx}=0, \tag{5}$$

must also be bounded at $x=-1$. Then Eq. (5) immediately yields a second boundary condition $G'_{st}(x)|_{x=-1}=0$, where the prime stands for the x derivative. Combined with $G_{st}(1)=1$, this condition selects the steady-state solution $G_{st}(x)=1$ describing an empty state.

Now let us introduce a new function $g(x,t)=G(x,t)-G_{st}(x)=G(x,t)-1$ [which obeys Eq. (4) with a homogenous boundary condition $g(x=1,t)=0$ and is bounded at $x=-1$] and look for separable solutions, $g_k(x,t)=e^{-\gamma_k t}\varphi_k(x)$. We obtain

$$(1-x^2)\varphi_k''(x)+2\Omega x(x-1)\varphi_k'(x)+2E_k\varphi_k(x)=0, \tag{6}$$

where $E_k=\gamma_k/\mu$. One boundary condition is of course $\varphi_k(1)=0$. The second boundary condition comes from the demand that $\varphi_k(x)$ be bounded at $x=-1$. Then Eq. (6) yields a homogenous boundary condition

$$2\Omega\varphi_k'(-1)+E_k\varphi_k(-1)=0, \tag{7}$$

for each $k=1,2,\ldots$. Notice that the eigenvalue E_k enters the boundary condition. Rewriting Eq. (6) in a self-adjoint form

$$[\varphi_k'(x)\exp(-2\Omega x)(1+x)^{2\Omega}]'+E_kw(x)\varphi_k(x)=0, \tag{8}$$

with the weight function

$$w(x)=\frac{2e^{-2\Omega x}(1+x)^{2\Omega}}{1-x^2}, \tag{9}$$

we arrive at an eigenvalue problem of the Sturm-Liouville theory [32]. Once the complete set of orthogonal eigenfunctions $\varphi_k(x)$ and the respective real eigenvalues E_k, $k=1,2,\ldots$, are calculated, one can write the exact solution of the time-dependent problem for $G(x,t)$:

$$G(x,t)=1+\sum_{k=1}^{\infty}a_k\varphi_k(x)e^{-\mu E_k t}, \tag{10}$$

where the amplitudes a_k are given by

$$a_k=\frac{\int_{-1}^{1}[G(x,t=0)-1]\varphi_k(x)w(x)dx}{\int_{-1}^{1}\varphi_k^2(x)w(x)dx}. \tag{11}$$

As all E_k are positive, Eq. (10) describes *decay* of initially populated states $k=1,2,\ldots$, so the system ultimately approaches the empty state $G(x,t\to\infty)=1$. Being mostly interested in the case of $\Omega\gg 1$, we note that while the eigenvalues of the "excited states" $E_2,E_3,\ldots$ scale like $O(\Omega)\gg 1$ [33], the "ground-state" eigenvalue E_1 is *exponentially* small [18]. Therefore, at sufficiently long times $\mu\Omega t=\lambda t\gg 1$, the contribution from the excited states to $G(x,t)$ becomes negligible, and we can write

$$G(x,t) = 1 + a_1\varphi_1(x)e^{-\mu E_1 t}. \quad (12)$$

So we need to calculate the ground-state eigenvalue E_1, the eigenfunction $\varphi_1(x)$, and the amplitude a_1. (Actually, the eigenvalue E_1 was calculated earlier [18], but we will rederive it here.) Note that, as E_1 is exponentially small, the boundary condition (7) for the ground state reduces, up to an exponentially small correction, to

$$\varphi_1'(-1) = 0. \quad (13)$$

III. GROUND-STATE CALCULATIONS

Throughout the rest of the paper we assume $\Omega \gg 1$. As E_1 is exponentially small, the last term in Eq. (6) is important only in a narrow boundary layer near $x=1$, and we can solve Eq. (6) for $\varphi_1(x) \equiv \varphi(x)$ by using a matched asymptotic expansion; see e.g., Ref. [34]. In the "bulk" region $-1 \le x < 1$ we can treat the last term in Eq. (6) perturbatively. In the zeroth order we put $E_1=0$ and arrive at the *steady-state* equation $(1+x)\varphi''(x) - 2\Omega x\varphi'(x) = 0$, whose (arbitrarily normalized) solution, bounded at $x=-1$, is $\varphi_b^{(0)}(x)=1$. Now we put $\varphi_b(x) = 1 + \delta\varphi_b(x)$, where $\delta\varphi_b(x) \ll 1$ and obtain in the first order

$$[\delta\varphi_b'(x)e^{-2\Omega x}(1+x)^{2\Omega}]' = -\frac{2E_1 e^{-2\Omega x}}{1-x^2}(1+x)^{2\Omega}. \quad (14)$$

Solving this equation, we obtain the bounded solution for $\varphi_b(x)$

$$\varphi_b(x) = 1 - 2E_1\int_0^x \frac{e^{2\Omega s}ds}{(1+s)^{2\Omega}}\int_{-1}^{s}\frac{(1+r)^{2\Omega}e^{-2\Omega r}}{1-r^2}dr. \quad (15)$$

This solution, which obeys the boundary condition (7), is almost constant in the entire region $-1 \le x < 1$ except in the boundary layer near $x=1$ (to be defined later on). To find the probabilities $P_n(t)$, we will need to calculate the derivatives of $\varphi_b(x)$ at $x=0$. As long as $1-x \gg 1/\Omega$, we can neglect the r^2 term in the denominator of the inner integral in Eq. (15) and obtain

$$\begin{aligned}\varphi_b(x) &\simeq 1 - 2E_1\int_0^x \frac{e^{2\Omega s}ds}{(1+s)^{2\Omega}}\int_{-1}^{s}(1+r)^{2\Omega}e^{-2\Omega r}dr \\ &= 1 - \frac{E_1}{\Omega}\left(\frac{e}{2\Omega}\right)^{2\Omega}\int_0^x \frac{e^{2\Omega s}}{(1+s)^{2\Omega}}\{\Gamma[2\Omega+1] \\ &\quad - \Gamma[2\Omega+1, 2\Omega(1+s)]\}ds, \end{aligned} \quad (16)$$

where $\Gamma(\alpha,z) = \int_z^\infty s^{\alpha-1}e^{-s}ds$ is the incomplete gamma function [35]. Using the expansion [36]

$$\Gamma(\alpha) - \Gamma(\alpha,z) = \sum_{j=0}^{\infty}\frac{(-1)^j z^{\alpha+j}}{j!\,(\alpha+j)}, \quad (17)$$

we can evaluate the integral in Eq. (16) and obtain

$$\varphi_b(x) \simeq 1 - \frac{E_1}{2\Omega^2}\sum_{j=0}^{\infty}\frac{\Gamma[2+j,-2\Omega] - \Gamma[2+j,-2\Omega(1+x)]}{j!\,(2\Omega+j+1)}. \quad (18)$$

One can check that the perturbative solution in the bulk is valid [that is, $\delta\varphi_b(x) \ll 1$] as long as $1-x \gg 1/\Omega$.

In the boundary layer $1-x \ll 1$ we can disregard, in Eq. (6), the (exponentially small) last term and arrive at the same equation as before: $(1+x)\varphi''(x) - 2\Omega x\varphi'(x) = 0$. The solution obeying the required boundary condition at $x=1$ is

$$\begin{aligned}\varphi_{bl}(x) &= \text{const} \times \int_1^x e^{2\Omega s}(1+s)^{-2\Omega}ds \\ &\simeq C\left[1 - e^{-2\Omega(1-\ln 2)}\frac{e^{2\Omega x}}{(1+x)^{2\Omega}}\right],\end{aligned} \quad (19)$$

where C is a yet unknown constant. To find E_1 and C we can match the asymptotes of the bulk and the boundary-layer solutions in the common region of their validity $1/\Omega \ll 1-x \ll 1$. Let us return to the first line of Eq. (16) and evaluate $\varphi_b(x)$ in this region. The inner integral receives the largest contribution from the vicinity of $r=0$, while the outer integral receives the largest contribution from the vicinity of $s=x$. Therefore, we can extend the upper limit of the inner integral to infinity and obtain (see Appendix A)

$$\begin{aligned}\varphi_b(x) &\simeq 1 - 2E_1\int_0^x \frac{e^{2\Omega s}ds}{(1+s)^{2\Omega}}\int_{-1}^{\infty}(1+r)^{2\Omega}e^{-2\Omega r}dr \\ &\simeq 1 - \frac{2E_1\sqrt{\pi}}{\sqrt{\Omega}}\int_0^x \frac{e^{2\Omega s}}{(1+s)^{2\Omega}}ds \\ &\simeq 1 - \frac{2E_1\sqrt{\pi}}{\Omega^{3/2}}\frac{e^{2\Omega x}}{(1+x)^{2\Omega}}.\end{aligned} \quad (20)$$

Now, by matching Eqs. (19) and (20), we obtain

$$E_1 = \frac{\Omega^{3/2}}{2\sqrt{\pi}}e^{-2\Omega(1-\ln 2)} \quad \text{and} \quad C = 1. \quad (21)$$

One can see that the ground-state eigenvalue E_1 is exponentially small in Ω. Equation (21) yields the mean extinction time $(\mu E_1)^{-1}$ (see Sec. V) which coincides with that obtained, by a different method, by Turner and Malek-Mansour [18].

Equations (15) and (19) yield the ground-state eigenfunction

$$\varphi_1(x) \simeq \begin{cases}\varphi_b(x) & \text{for } 1-x \gg 1/\Omega, \\ \varphi_{bl}(x) & \text{for } 1-x \ll 1.\end{cases} \quad (22)$$

Now we use Eq. (11) to calculate the amplitude a_1 entering Eq. (12). Let the initial number of particles be n_0, so $G(x,t=0) = x^{n_0}$. Evaluating the integrals, we notice that (i) the main contributions come from the bulk region $1-x \gg 1/\Omega$ and (ii) it suffices to take the eigenfunction $\varphi_b(x)$ in the zeroth order: $\varphi_b^{(0)}(x) \simeq 1$. Furthermore, when $n_0 \gg 1$, the term x^{n_0} under the integral in the numerator is negligible compared to 1. So, for $n_0 \gg 1$, the numerator and denominator are approximately equal to each other up to a minus sign. Therefore, $a_1 \simeq -1$ (and independent of n_0) which completes our solution (12) for times $\mu t \gg \Omega^{-1}$.

IV. STATISTICS OF THE QUASISTATIONARY STATE AND ITS DECAY

What is the average number of particles $\bar{n}(t)$ and the standard deviation $\sigma(t)$ at times $\mu t \gg \Omega^{-1}$? Using Eqs. (2) and (12) with $a_1 = -1$, we obtain

$$\bar{n}(t) = \sum_{n=0}^{\infty} n P_n(t) = \partial_x G|_{x=1} = \Omega e^{-\mu E_1 t}. \tag{23}$$

Furthermore,

$$\begin{aligned}\sigma^2(t) = \overline{n^2} - \bar{n}^2 &= \sum_{n=0}^{\infty} n^2 P_n(t) - \left(\sum_{n=0}^{\infty} n P_n(t)\right)^2 \\ &= [\partial_{xx}^2 G + \partial_x G - (\partial_x G)^2]|_{x=1} \\ &= \left[\frac{3\Omega}{2} + \Omega^2 (1 - e^{-\mu E_1 t})\right] e^{-\mu E_1 t},\end{aligned} \tag{24}$$

where we have used for $\varphi_1(x)$ its boundary layer asymptote $\varphi_{bl}(x)$, Eq. (19), with $C=1$. At *intermediate* times $\Omega^{-1} \ll \mu t \ll E_1^{-1}$ one obtains a weakly fluctuating quasistationary (metastable) state. Here the average number of particles,

$$\bar{n} \simeq \Omega, \tag{25}$$

coincides with the attracting point of the mean-field theory, while the standard deviation

$$\sigma \simeq \left(\frac{3\Omega}{2}\right)^{1/2} \tag{26}$$

coincides with that obtained from the Fokker-Planck approximation; see Appendix B. Note that $\sigma(t)$ from Eq. (24) is a nonmonotonic function. This stems from the fact that the quasistationary probability distribution around $n \simeq \Omega$ decays in time, whereas the extinction probability $P_0(t)$ grows. At times $\mu E_1 t \ll 1$ the standard deviation $\sigma \simeq \sqrt{3\Omega/2}$ corresponds to the unimodal quasistationary distribution around $n \simeq \Omega$, whereas at $\mu E_1 t \gg 1$, $\sigma \to 0$ corresponds to the unimodal Kronecker δ distribution at $n=0$. At intermediate times $\mu E_1 t \simeq 1$, the distribution is distinctly bimodal. The maximum standard deviation $\sigma_{max} \simeq \Omega/2$ is obtained for $e^{-\mu E_1 t} \simeq 1/2$. Figure 1 shows the $\bar{n}(t)$and $\sigma(t)$ dependences.

Let us now proceed to calculating the complete probability distribution $P_n(t)$ of the (slowly decaying) quasistationary state, conditional on nonextinction. For $n=0$ we obtain

$$P_0(t) = G(x=0,t) = 1 - e^{-\mu E_1 t} \tag{27}$$

which, at $\mu E_1 t \ll 1$, is much less than unity. For $n \geq 1$ Eqs. (3) and (12) yield

$$P_n(t) = -\frac{1}{n!} \frac{d^n \varphi_b(x)}{dx^n}\bigg|_{x=0} e^{-\mu E_1 t}, \tag{28}$$

where $\varphi_b(x)$ should be taken from Eq. (16). After some algebra (see Appendix C), we obtain, for $n \geq 1$,

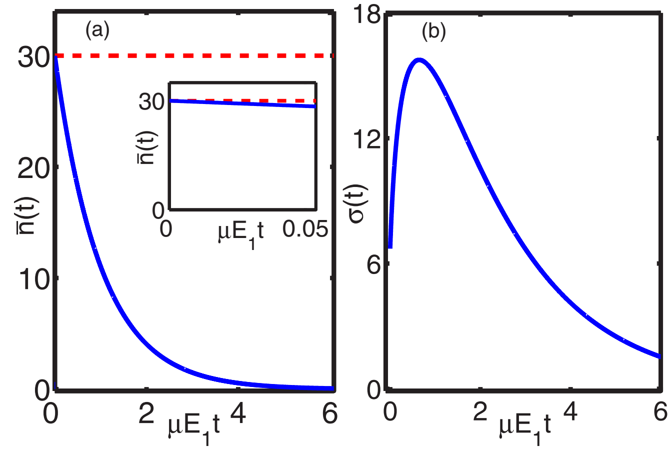

FIG. 1. (Color online) (a) The average number of particles as a function of time at $\mu t \gg 1/\Omega$ as described by Eq. (23) (solid line) compared with the prediction from the rate equation $\bar{n}(t) \simeq \Omega$ (dashed line), for $\Omega = 30$. The inset shows a blowup at intermediate times $\Omega^{-1} \ll \mu t \ll E_1^{-1}$ where the curves almost coincide. (b) The standard deviation from Eq. (24) versus time for the same Ω.

$$P_n(t) = \frac{2E_1}{n} \frac{(2\Omega)^{n-1} e^{2\Omega} \Gamma(2\Omega)}{\Gamma(2\Omega + n)} {}_1F_1(2\Omega, n + 2\Omega, -2\Omega) e^{-\mu E_1 t}, \tag{29}$$

where ${}_1F_1(a,b,x)$ is the Kummer confluent hypergeometric function [35]. To avoid excess of accuracy, we need to find the large Ω asymptotics of Eq. (29). To that aim we use the identity [35]

$${}_1F_1(2\Omega, n + 2\Omega, -2\Omega) = \frac{\Gamma(n + 2\Omega)}{\Gamma(2\Omega)\Gamma(n)} \times \int_0^1 e^{-2\Omega s} s^{2\Omega - 1} (1 - s)^{n-1} ds \tag{30}$$

and consider separately two cases $n \gg 1$ and $n = O(1)$.

For $n \gg 1$, the integral in Eq. (30) can be evaluated by the saddle point method [34]. Denoting $\Phi(s) = -2\Omega s + 2\Omega \ln(s) + n \ln(1-s)$ we obtain

$$P_n(t) \simeq \frac{2E_1}{n!} \frac{\sqrt{2\pi}(2\Omega)^{n-1} e^{2\Omega}}{\sqrt{2\Omega(1 - s_*)^2 + n s_*^2}} e^{-2\Omega[s_* - \ln(s_*)] + n \ln(1 - s_*) - \mu E_1 t}, \tag{31}$$

where $s_* = 1 + q - (q^2 + 2q)^{1/2}$ is the solution of the saddle point equation $\Phi'(s) = 0$ and $q = n/(4\Omega)$. Equation (31) can be simplified in three limiting cases. In the high-n tail $n \gg \Omega \gg 1$, we have $s_* \simeq 2\Omega/n \ll 1$ and

$$P_n(t) \simeq \frac{2^{2\Omega - 3/2}}{\sqrt{\pi n}} \left(\frac{2\Omega}{n}\right)^{n + 2\Omega} e^{n - 2\Omega - 6\Omega^2/n - \mu E_1 t}. \tag{32}$$

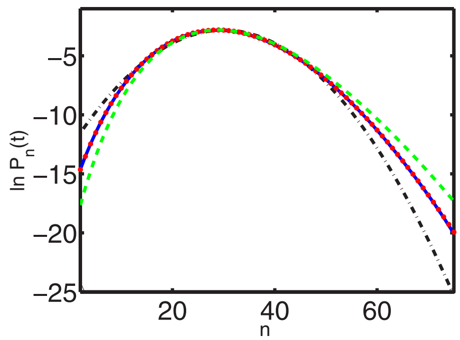

FIG. 2. (Color online) The natural logarithms of the analytical result (31) for the quasistationary distribution (dots), of the distribution obtained by a numerical solution of the (truncated) master equation (1) (solid line), of the stationary solution (B2) of the Fokker-Planck equation (dashed line), and of the Gaussian distribution (34) (dash–dotted line), for $\Omega=30$ and $\mu E_1 t \ll 1$.

In the low-n tail $1 \ll n \ll \Omega$, we have $s_* \simeq 1-\sqrt{n/(2\Omega)}$ and

$$P_n(t) \simeq \frac{2^{2\Omega-2}}{\sqrt{\pi n}}\left(\frac{2\Omega}{n}\right)^{n/2+1/2} e^{n/2-2\Omega-\mu E_1 t}. \tag{33}$$

Finally, for $|n-\Omega| \ll \Omega$, $s_* \simeq 1/2-(n-\Omega)/(6\Omega)$, and we obtain

$$P_n(t) \simeq (3\pi\Omega)^{-1/2} e^{-(n-\Omega)^2/(3\Omega)-\mu E_1 t}. \tag{34}$$

For $\mu E_1 t \ll 1$ this result describes a normal distribution with mean Ω and variance $3\Omega/2$, in agreement with Eqs. (25) and (26) and with the predictions from the Fokker-Planck equation; see Appendix B.

Now we turn to the case of $n=O(1)$. Then it is always $n \ll \Omega$. Here it is convenient to rewrite the integral in Eq. (30) as

$$\int_0^1 e^{\Psi(s)} s^{-1}(1-s)^{n-1} ds, \tag{35}$$

where $\Psi(s)=2\Omega(\ln s - s)$. The function $\Psi(s)$ has its maximum exactly at $s=1$, the upper integration limit. The largest contribution to the integral comes from the small region $O(1/\sqrt{\Omega})$ near $s=1$. Therefore, it suffices to expand $\Psi(s)$ up to the second order in $(s-1)^2$, replace the factor s^{-1} by 1, and extend the lower integration limit to $-\infty$. The result is

$$e^{-2\Omega}\int_{-\infty}^1 e^{-\Omega(s-1)^2}(1-s)^{n-1} ds = \frac{e^{-2\Omega}\,\Gamma(n/2)}{2\Omega^{n/2}}. \tag{36}$$

Therefore, for $n=O(1)$, we obtain

$$P_n(t) \simeq \frac{2E_1(4\Omega)^{n/2-1}\Gamma(n/2)}{n!} e^{-\mu E_1 t}, \tag{37}$$

which, for $n \gg 1$, coincides with that given by Eq. (33).

Figure 2 compares our analytical result (31) with (i) a numerical solution of the (truncated) master equation (1) with $(d/dt)P_n(t)$ replaced by zeros and $P_0=0$, (ii) the prediction from the Fokker-Planck equation for this problem [Eq. (B2) of Appendix B], and (iii) the Gaussian distribution (34) for $\mu E_1 t \ll 1$. In the central part all the distributions coincide.

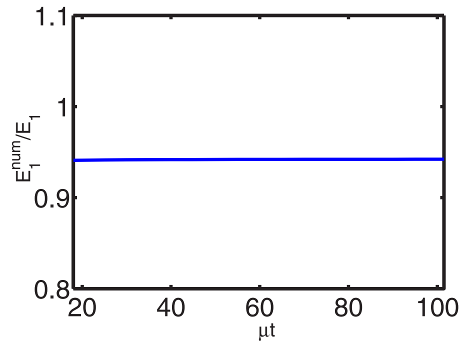

FIG. 3. (Color online) Shown is the ratio of the numerical ground-state eigenvalue E_1^{num} from Eq. (38) and the approximate analytical value of E_1 from Eq. (21), for $\Omega=20$ and $n_0=100$. The deviation from 1 is about 5.6%—that is, within error $O(1/\Omega)$.

The Fokker-Planck approximation strongly underpopulates the low-n tail and overpopulates the high-n tail. On the contrary, the Gaussian approximation strongly overpopulates the low-n tail and underpopulates the high-n tail. Our analytical solution (31) is essentially indistinguishable from the numerical result, even at small values of n. Actually, it is in good agreement with the numerics already for $\Omega=O(1)$, and the agreement improves further as Ω increases.

We also computed the ground-state eigenvalue by solving Eq. (4) numerically with the boundary conditions $G(1,t)=1$, $\partial_x G(-1,t)=0$ and the initial condition $G(x,t=0)=x^{n_0}$. At times $\mu t \gg 1/\Omega$, the numerical ground-state eigenvalue E_1^{num} can be found from the following expression:

$$E_1^{num} = -\frac{1}{\mu t}\ln[1-G^{num}(0,t)], \tag{38}$$

where $G^{num}(x,t)$ is the numerical solution for $G(x,t)$ and the result in Eq. (38) should be independent of time. A typical example is shown in Fig. 3, and a good agreement with the theoretical prediction (21) is observed.

V. STATISTICS OF THE EXTINCTION TIMES

The quantity $P_0(t)$, given by Eq. (27), is the probability of extinction at time t. The extinction probability density is $p(t)=dP_0(t)/dt$. Using Eq. (27), we obtain the exponential distribution of the extinction times:

$$p(t) \simeq \mu E_1 e^{-\mu E_1 t} \quad \text{at } \lambda t \gg 1. \tag{39}$$

The average time to extinction is, therefore,

$$\bar{\tau} = \int_0^\infty t p(t) dt \simeq (\mu E_1)^{-1} = \frac{2\sqrt{\pi}}{\mu\Omega^{3/2}} e^{2\Omega(1-\ln 2)}. \tag{40}$$

This is in full agreement with the result of Turner and Malek-Mansour [18] and in disagreement with the prediction from the Fokker-Planck approximation, given by Eq. (B5), and with the prediction from the Gaussian approximation, given by Eq. (B7); see Appendix B.

Figure 4 compares the analytical result (27) for $P_0(t)$ with the extinction probability $P_0^{num}(t)=G^{num}(0,t)$ found by solv-

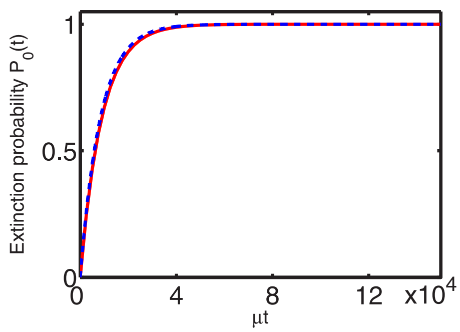

FIG. 4. (Color online) Shown are the extinction probability $P_0(t)$ [Eq. (27)] (dashed line) and the numerical solution of Eq. (4) (solid line) at $x=0$, for $\Omega=20$ and $n_0=100$.

ing Eq. (4) numerically as described at the end of the previous section, and a very good agreement is observed.

VI. FINAL COMMENTS

We calculated, at intermediate and long times, the complete probability distribution, including the quasistationary distribution of the long-lived metastable state, and the extinction time statistics in a (non-single-step) branching-annihilation reaction. To this end we employed the spectral method, recently developed by the authors [28,29]. We also used this example to illustrate how the "lacking" boundary condition of the spectral method emerges in the theory.

The spectral method reduces the problem of finding the statistics to that of finding the ground-state eigenvalue and eigenfunction of a linear differential operator emerging from the generating function formalism. The quasistationary distribution that we have calculated analytically is in excellent agreement with numerics. The two widely used "rival" approximations—the Fokker-Planck approximation and its reduced version, the Gaussian approximation—perform well only in the peak region of the quasistationary distribution. They both fail in the tails of the distribution and, as a result, cause exponentially large errors in the estimates of the mean extinction time.

It is worth reiterating that, for *single*-step birth-death systems, the quasistationary distribution can be found directly from a recursion equation for P_n, obtained by putting $P_0=0$, assuming a zero flux into the empty state, and replacing $(d/dt)P_n(t)$ by zeros in Eq. (1); see, e.g., [12]. For *multi*-step systems such recursion equations are not generally soluble analytically.

In conclusion, the spectral method is a powerful tool for calculating the quasistationary distributions and extinction time statistics of a host of multistep birth-death processes possessing a metastable state and an absorbing state.

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APPENDIX A

Here we will derive the result given by Eq. (20). First, we calculate the inner integral

$$I_1 = \int_{-1}^{\infty} (1+r)^{2\Omega} e^{-2\Omega r} dr = \left(\frac{e}{2\Omega}\right)^{2\Omega} \Gamma(2\Omega). \qquad \text{(A1)}$$

As $\Omega \gg 1$, we can use the large-argument asymptotics of the Γ function and obtain

$$I_1 \simeq \sqrt{\frac{\pi}{\Omega}}. \qquad \text{(A2)}$$

Second, at $\Omega \gg 1$, the integral

$$I_2 = \int_0^x \frac{e^{2\Omega s}}{(1+s)^{2\Omega}} ds \equiv \int_0^x e^{2\Omega \Upsilon(s)} ds, \qquad \text{(A3)}$$

where $\Upsilon(s)=s-\ln(1+s)$, receives the largest contribution in the vicinity of $s=x$ (remember that $1-x \ll 1$). Then, expanding $\Upsilon(s)$ around $s=x$, we obtain

$$\Upsilon(s) = x - \ln(1+x) + \frac{x}{1+x}(s-x) + \cdots . \qquad \text{(A4)}$$

Extending the lower integration limit to $-\infty$ and evaluating the remaining elementary integral we obtain, in the leading order,

$$I_2 \simeq \frac{e^{2\Omega x}}{\Omega(1+x)^{2\Omega}}. \qquad \text{(A5)}$$

APPENDIX B

What are the predictions from the Fokker-Planck (FP) approximation for the quasistationary distribution and the mean extinction time of the branching-annihilation problem? The FP description introduces an (in general, uncontrolled) approximation into the exact master equation (1) by assuming $n \gg 1$ and treating the discrete variable n as a continuum variable. The FP equation can be obtained from Eq. (1) by a Kramers-Moyal "system size expansion" [1,2] (in our case, expansion in the small parameter $\Omega^{-1} \ll 1$). Using this prescription, we obtain after some algebra

$$\frac{\partial P(n,t)}{\partial t} = \frac{\mu}{2}\left\{ -\frac{\partial}{\partial n}[2n(\Omega-n)P(n,t)] + \frac{1}{2}\frac{\partial^2}{\partial n^2}[2n(2n+\Omega)P(n,t)] \right\}. \qquad \text{(B1)}$$

The quasistationary distribution of the metastable state corresponds to the (zero-flux) steady-state solution of the FP equation. In the leading order in $1/\Omega$ we obtain

$$P_{st}(n) \simeq (3\pi\Omega)^{-1/2} e^{\Omega - n + (3/2)\Omega \ln[(2n+\Omega)/(3\Omega)]}, \qquad \text{(B2)}$$

where only the central (Gaussian) part of the distribution contributes to the normalization. In fact, the distribution (B2) is accurate only in the peak region $|n-\Omega| \ll \Omega$ (see Sec. IV), where it reduces to a Gaussian distribution with mean Ω and variance $3\Omega/2$:

$$P_{Gauss}(n) = (3\pi\Omega)^{-1/2} e^{-(n-\Omega)^2/(3\Omega)}. \tag{B3}$$

Were the FP equation (B1) valid for all n, one could use it to find the mean time to extinction τ_{FP} (conditional on nonextinction prior to reaching the quasistationary state) by a standard calculation; see, e.g., Ref. [1]. This calculation would yield

$$\tau_{FP} \simeq 2\int_0^{\Omega} e^n \left(1+\frac{2n}{\Omega}\right)^{-3\Omega/2} dn \int_n^{\infty} \frac{e^{-k}\left(1+\frac{2k}{\Omega}\right)^{3\Omega/2}}{\mu k(2k+\Omega)} dk. \tag{B4}$$

As $\Omega \gg 1$, the inner integral receives its main contribution from the vicinity of $k=\Omega$. The outer integral receives its main contribution from the vicinity of $n=0$. Therefore, one can use the saddle point method for the inner integral and a Taylor expansion for the outer one. The result is

$$\tau_{FP} \simeq \sqrt{\frac{\pi}{3}} \frac{1}{\mu\Omega^{3/2}} e^{\Omega[(3/2)\ln 3-1]}. \tag{B5}$$

Comparing it with Eq. (40), one can see that the FP approximation gives a poor estimate of the mean extinction time, as it introduces an exponentially large error.

The central (Gaussian) part of the quasistationary distribution, $|n-\Omega| \ll \Omega$, Eq. (B3), can be *correctly* obtained by keeping only leading-order terms, in the small parameter $|n-\Omega|/\Omega \ll 1$, in the FP equation:

$$\frac{\partial P(n,t)}{\partial t} = \frac{\mu}{2}\left\{-\frac{\partial}{\partial n}[2\Omega(\Omega-n)P(n,t)] + \frac{1}{2}\frac{\partial^2}{\partial n^2}[6\Omega^2 P(n,t)]\right\}. \tag{B6}$$

Indeed, the zero-flux steady-state solution of this equation yields the Gaussian distribution (B3).

Finally, what would be the prediction for the mean extinction time from the *reduced* FP description—that is, the one in terms of Eq. (B6)? Here one would obtain

$$\tau_{gauss} \simeq 2\int_0^{\Omega} e^{n^2/(3\Omega)-2n/3} dn \int_n^{\infty} \frac{e^{2k/3-k^2/(3\Omega)}}{3\mu\Omega^2} dk \simeq \frac{\sqrt{3\pi}}{\mu\Omega^{3/2}} e^{\Omega/3}, \tag{B7}$$

which again gives an exponentially large error as compared with the accurate result (40).

APPENDIX C

Here we calculate the nth derivative of $\varphi_b(x)$, given by Eq. (16), at $x=0$. The first derivative is

$$\varphi_b'(x) = -\frac{E_1}{\Omega}\left(\frac{e}{2\Omega}\right)^{2\Omega} \frac{e^{2\Omega x}}{(1+x)^{2\Omega}} \times \{\Gamma[2\Omega+1] - \Gamma[2\Omega+1, 2\Omega(1+x)]\}. \tag{C1}$$

Let us introduce two auxiliary functions

$$f(x) = \frac{\{\Gamma[2\Omega+1] - \Gamma[2\Omega+1, 2\Omega(1+x)]\}}{(1+x)^{2\Omega}},$$

$$h(x) = e^{2\Omega x}. \tag{C2}$$

Using Eqs. (C1) and (C2), we can write the nth derivative of $\varphi_b(x)$ [that is, the $(n-1)$th derivative of $\varphi_b'(x)$] at $x=0$ as

$$\left.\frac{d^n\varphi_b(x)}{dx^n}\right|_{x=0} = -\frac{E_1}{\Omega}\left(\frac{e}{2\Omega}\right)^{2\Omega} \sum_{k=0}^{n-1} \frac{(n-1)!}{k!\,(n-k-1)!} \times f^{(k)}(x)\big|_{x=0}\, h^{(n-1-k)}(x)\big|_{x=0}, \tag{C3}$$

where $f^{(k)}(x)$ is the kth derivative of $f(x)$ and the same notation is used for $h(x)$.

After some algebra, we find that the kth derivative ($k \geq 1$) of $f(x)$ at $x=0$ is [35,36]

$$\left.\frac{d^k f(x)}{dx^k}\right|_{x=0} = (-1)^k 2\Omega[\Gamma(2\Omega+k) - \Gamma(2\Omega+k, 2\Omega)]. \tag{C4}$$

Now, the kth derivative of $h(x)$ at $x=0$ is

$$\left.\frac{d^k h(x)}{dx^k}\right|_{x=0} = (2\Omega)^k. \tag{C5}$$

Using Eqs. (28) and (C3)–(C5), we obtain for $n \geq 1$

$$P_n(t) = e^{-\mu E_1 t}\frac{2E_1}{n}\left(\frac{e}{2\Omega}\right)^{2\Omega} \sum_{k=0}^{n-1} \frac{(-1)^k (2\Omega)^{n-k-1}}{k!\,(n-k-1)!} \times [\Gamma(2\Omega+k) - \Gamma(2\Omega+k, 2\Omega)]. \tag{C6}$$

Actually, for $n=1$ one has

$$P_1(t) \simeq (\pi/\Omega)^{1/2} E_1 [1 + O(\Omega^{-1/2})],$$

and the subleading term $O(\Omega^{-1/2})$ has been neglected in Eq. (C6). Finally, using Eq. (17) and changing the order of summation in Eq. (C6), we obtain the following result for $n \geq 1$:

$$P_n(t) = \frac{2E_1}{n} \frac{(2\Omega)^{n-1} e^{2\Omega} \Gamma(2\Omega)}{\Gamma(2\Omega+n)}\, {}_1F_1(2\Omega, n+2\Omega, -2\Omega) e^{-\mu E_1 t}, \tag{C7}$$

where ${}_1F_1(a,b,x)$ is the Kummer confluent hypergeometric function [35]. To avoid excess of accuracy, we need to work with the large-Ω asymptotics of this result; see Sec. IV.

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