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System size expansion for systems with an absorbing state

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The well-known van Kampen system size expansion, while of rather general applicability, is shown to fail to reproduce some qualitative features of the time evolution for systems with an absorbing state, apart from a transient initial time interval. We generalize the van Kampen ansatz by introducing a new prescription leading to non-Gaussian fluctuations around the absorbing state. The two expansion predictions are explicitly compared for the infinite range voter model with speciation as a paradigmatic model with an absorbing state. The new expansion, both for a finite size system in the large time limit and at finite time in the large size limit, converges to the exact solution as obtained in a numerical implementation using the Gillespie algorithm. Furthermore, the predicted lifetime distribution is shown to have the correct asymptotic behavior.

The time evolution of systems consisting of large number of discrete entities such as photons, nuclei, proteins, or organisms is often described by a master equation, a differential equation that, in most cases, cannot be solved analytically. The van Kampen system size expansion [1,2] is one of the techniques typically used to overcome such a limitation, although alternative approaches have been proposed [3]. This method allows one to account for the essential aspects of the problem and provides a very useful tool to approximate the temporal evolution. However, such an approach is able to characterize the fluctuations properly when the system has no boundaries or evolves far from them [4]. For instance, if a system is driven toward ultimate extinction, the van Kampen approximation is at best appropriate at short times.

When a system with no boundaries initially has a large number of particles, one expects that the macroscopic evolution is relatively less affected by fluctuations at least within a finite temporal scale. This general consideration leads to the rule of thumb that deviations from the collective behavior are of order $\sqrt{N}$, where N is the size of the system. More specifically, the population of the system, n, can be split into two contributions: a macroscopic part of order N, $N\phi(t)$, whose evolution is deterministic, and a random variable of order $\sqrt{N}$, $\sqrt{N}\xi$. This is the celebrated van Kampen ansatz, $n = N\phi(t) + \sqrt{N}\xi$, which approximates random jumps around the macroscopic part with Gaussian fluctuations and naturally introduces a small parameter for large N, $1/\sqrt{N}$, that can be used as an expansion parameter for the solution of the master equation. However, if the system has an absorbing state it will be driven toward a final absorption, for example, eventual extinction. Thus, sooner or later, the fluctuations could become comparable with the macroscopic part, despite starting off with a large number of individuals. This means that the validity of the van Kampen approximation may be limited

to a short initial time interval, and fluctuations may no longer be Gaussian.

As a paradigmatic example of a system with an absorbing state, we will consider the infinite range voter model with speciation, a simple model that can be handled analytically. By exploiting standard methods used for diffusion processes with absorbing boundaries, we will consider an improvement of the classical van Kampen technique. However, we will show that despite the modification, the new version fails to match numerical simulations, thus calling for a different approach. To provide a general context, we consider the following birth and death master equation, which is commonly encountered in population ecology:

$$\frac{d}{dt}P_n(t) = \left(\varepsilon_n^{-1} - 1\right)[T(n+1|n)P_n(t)] + \left(\varepsilon_n^{+1} - 1\right)[T(n-1|n)P_n(t)], \quad (1)$$

where $P_n(t)$ is the probability of observing the system in the state n at time t, and the shift operators $\varepsilon_n^{\pm 1}$ act on a function as $\varepsilon_n^{\pm 1} f(n) = f(n \pm 1)$. $T(i|j)$ is the transition probability from state j to state i. In ecology, the state n would correspond to a species abundance n. When populations are large, customarily birth and death transition rates turn out to be analytic functions of the density n/N, namely, $T(n \pm 1|n) = T_\pm(n/N)$, where N denotes the total number of individuals or particles. This naturally suggests a parameter to which fluctuations can be compared. Thus, in order to obtain the correct system–size expansion we introduce the following generalized van Kampen ansatz:

$$n = N\phi(t) + N^\alpha \xi \quad (2)$$

with $0 \leqslant \alpha < 1$. Under this assumption $n/N = \phi(t) + N^{\alpha-1}\xi$ and when $N \gg 1$ the transition rates can be expanded as power

series of $y = \xi N^{\alpha-1}$ according to

$$T_\pm(\phi + y) = \sum_{k=0}^{\infty} T_\pm^{(k)}(\phi) \frac{y^k}{k!}, \qquad (3)$$

where $T_\pm^{(k)}(z)$ is the kth derivative of $T_\pm(z)$. Since N is large the shift operators have the following representation:

$$\varepsilon_n^{\pm 1} \simeq 1 \pm \frac{1}{N^\alpha} \frac{\partial}{\partial \xi} + \frac{1}{2N^{2\alpha}} \frac{\partial^2}{\partial \xi^2} \pm \cdots. \qquad (4)$$

Substituting Eqs. (2), (3), and (4) into Eq. (1) and defining the new probability distribution Π as $\Pi(\xi, t) \propto P_n(t)$, one can collect terms proportional to different powers of N. In the limit of large N the leading order provides the usual macroscopic law defined by the following deterministic equation:

$$\frac{d}{d\tau} \phi = T_+(\phi) - T_-(\phi), \qquad (5)$$

where $\tau = t/N$ and we assume that $T_+(\phi) - T_-(\phi)$ is not identically zero. Working out the next-to-leading orders, one eventually obtains a differential equation that up to the second derivative reads:

$$\frac{\partial}{\partial \tau} \Pi = N^0 [T_-^{(1)}(\phi) - T_+^{(1)}(\phi)] \frac{\partial}{\partial \xi}(\xi \Pi) + \frac{1}{2} N^{1-2\alpha} [T_-(\phi) $$
$$+ T_+(\phi)] \frac{\partial^2}{\partial \xi^2} \Pi + \frac{1}{2} N^{-\alpha} [T_-^{(1)}(\phi) + T_+^{(1)}(\phi)]$$
$$+ \frac{\partial^2}{\partial \xi^2}(\xi \Pi) \sum_{k=2}^{\infty} [T_-^{(k)}(\phi)$$
$$- T_+^{(k)}(\phi)] \frac{N^{(k-1)(\alpha-1)}}{k!} \frac{\partial}{\partial \xi}(\xi^k \Pi) + \sum_{k=2}^{\infty} [T_-^{(k)}(\phi)$$
$$+ T_+^{(k)}(\phi)] \frac{N^{k(\alpha-1)-2\alpha+1}}{k!} \frac{\partial^2}{\partial \xi^2}(\xi^k \Pi), \qquad (6)$$

where the time dependence of ϕ is given by Eq. (5). The right-hand side of this equation contains two series that are negligible with respect to the first three terms when N is large, which are proportional to N^0, $N^{1-2\alpha}$, and $N^{-\alpha}$, respectively. If we assume that both $T_-^{(1)}(\phi) - T_+^{(1)}(\phi)$ and $T_-(\phi) + T_+(\phi)$ are different from zero in order to avoid the trivial result of vanishing fluctuations, one has to set $\alpha = 1/2$ in Eq. (6) Accordingly, in the limit $N \to \infty$ we recover the standard van Kampen equation

$$\frac{\partial}{\partial \tau} \Pi = [T_-^{(1)}(\phi) - T_+^{(1)}(\phi)] \frac{\partial}{\partial \xi}(\xi \Pi)$$
$$+ \frac{1}{2} [T_-(\phi) + T_+(\phi)] \frac{\partial^2}{\partial \xi^2} \Pi, \qquad (7)$$

which is a linear Fokker-Planck equation whose solution is a nonstationary Gaussian distribution.

However, for systems with absorbing boundaries at $n = 0$ and large temporal scales, the term proportional to $N^{1-2\alpha}$, $T_-(\phi) + T_+(\phi)$, approaches zero, while the one proportional to $N^{-\alpha}$, $T_-^{(1)}(\phi) + T_+^{(1)}(\phi)$, does not. This is because when $\phi \to 0$, $T_-(\phi) \pm T_+(\phi)$ are proportional to ϕ (in the case of a simple absorbing state). In this case the van Kampen prescription is no longer valid, and we need to set $\alpha = 0$ in the limit of large N. For these systems fluctuations are progressively

more important in the long run because $N\phi(\tau) \ll \xi$. Thus, the differential equation governing the fluctuations is well approximated by the following Fokker-Planck equation:

$$\frac{\partial}{\partial \tau} \Pi = [T_-^{(1)}(0) - T_+^{(1)}(0)] \frac{\partial}{\partial \xi}(\xi \Pi)$$
$$+ \frac{1}{2} [T_-^{(1)}(0) + T_+^{(1)}(0)] \frac{\partial^2}{\partial \xi^2}(\xi \Pi). \qquad (8)$$

This equation is different from Eq. (7) owing to the linear diffusion term, which results in the fluctuations being no longer Gaussian distributed. Furthermore, if we do not provide Eq. (7) with an absorbing boundary condition for the solution, fluctuations could lead to negative values for n. In contrast, Eq. (8) has a natural boundary at $\xi = 0$ that prevents fluctuations, and thus n, from becoming negative. Similar considerations also hold when transition rates have more general algebraic behaviors in the vicinity of the absorbing state.[1] Interestingly, Eq. (8) can be exactly solved [5], its solution being

$$\Pi(\xi, \tau | \xi_0, 0) = \frac{\mu}{D} \frac{1}{1 - e^{-\mu\tau}} \exp\left[-\frac{\frac{\mu}{D}(\xi + \xi_0 e^{-\mu\tau})}{1 - e^{-\mu\tau}} \right]$$
$$\times \left(\frac{\xi}{\xi_0} e^{\mu\tau} \right)^{-\frac{1}{2}} I_1\left(\frac{\frac{2\mu}{D} \sqrt{\xi_0 \xi e^{\mu\tau}}}{e^{\mu\tau} - 1} \right), \qquad (9)$$

where $\mu = T_-^{(1)}(0) - T_+^{(1)}(0)$ is supposed to be positive, $D = [T_-^{(1)}(0) + T_+^{(1)}(0)]/2$, $I_1(z)$ is the modified Bessel function of the first kind, and ξ_0 is the value of ξ when $\tau = 0$. It is worth noting that although the solution is absorbing, one gets $\lim_{\xi \to 0} \Pi(\xi, \tau | \xi_0, 0) \neq 0$.

The theory we have developed so far can be applied straightforwardly to many different absorbing systems. In particular, we now focus on the infinite range voter model with speciation, a particular case of the more general voter model, which is of interest in opinion formation problems [6–8] as well as in biological [9,10] and ecological contexts [11,12].

The modified version of the voter model we investigate is characterized by a parameter, the speciation rate ν, that averts the collapse of the whole system into a trivial monodominant state characterized by $\phi = 1$. Specifically, let us consider a system composed of N elements, all of them mutually interacting and belonging to possibly different species. If we now focus on a specific species, we can remap all elements with two labels: the label X_1 for the elements of the selected species, the label X_0 for the rest. Finally, at each time step we randomly choose and update a pair of elements according to the following interaction rules:

$$X_1 + X_0 \xrightarrow{1} X_0 + X_0, \qquad (10)$$

$$X_0 + X_1 \xrightarrow{1-\nu} X_1 + X_1, \qquad (11)$$

$$X_1 + X_1 \xrightarrow{\nu} X_1 + X_0. \qquad (12)$$

An individual of the species of the first term on the left-hand side is envisaged to be replaced by an individual of the second

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[1]Suppose that $f_\pm(x)$ are two analytic functions such that $f_\pm(0) = 1$, $\lambda_\pm$ two constants rates, $l_+ \geqslant l_- > 1$ and that $T(n \pm 1|n) = \lambda_\pm(n/N)^{l_\pm} f_\pm(n/N)$ for $n/N \ll 1$. In this case in Eq. (8) both the drift and diffusion terms are proportional to ξ^{l_-}.
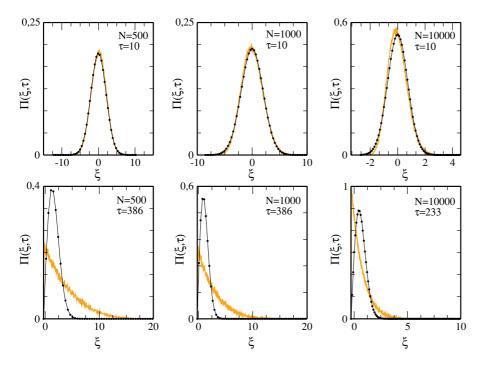
FIG. 1. (Color online) Probability distribution for the fluctuations ξ at different times and with different parameters specified in the top right of the panels. The noisy lines are the results of numerical solutions obtained by averaging over 10^6 stochastic realizations; the solid-dotted lines represent the Gaussian solution modified for absorbing boundaries given by (16). Fluctuations are approximately Gaussian distributed only for relatively short times, while for large τ the Gaussian assumption breaks down. In all cases $\nu = 0.01$ and $n_0 = 300$.

term on the left-hand side except for speciation, which occurs with a probability ν as in the third rule. The factors above the arrow denote the probability of the event indicated in the equation.

Let us denote by n the number of X_1 individuals, so that $N - n$ is the total number of elements of type X_0. According to (10)–(12) the only transitions allowed are those from n to $n \pm 1$, and the corresponding transition probabilities read

$$T(n-1|n) = (1-\nu)\frac{n}{N}\frac{N-n}{N-1} + \nu\frac{n}{N}, \tag{13}$$

$$T(n+1|n) = (1-\nu)\frac{N-n}{N}\frac{n}{N-1}, \tag{14}$$

where the initial states are on the right and final states on the left. Since $T(\pm 1|0) = 0$, once the population of X_1 dies out, the selected species cannot be reintroduced into the system. Thus, this model has a continual turnover of species: New species appear at rate ν, but eventually they go extinct. This implies that $n = 0$ is an absorbing state. On the contrary, when the population of X_1 reaches the maximum value N, transitions to $N + 1$ are not allowed since $T(N+1|N) = 0$, while $T(N-1|N) = \nu$. As a consequence, $n = N$ is a reflecting boundary. In the following we will focus on the time evolution of the system when n is kept finite as N becomes larger and larger.[2]

If we apply the generalized expansion described in the previous section, we find that the macroscopic law according to Eq. (5) is $\dot{\phi} = -\nu\phi$, thus $\phi(\tau) = \phi_0 e^{-\nu\tau}$ with $\tau = t/(N-1)$. The van Kampen equation corresponding to Eq. (7) reads

$$\frac{\partial}{\partial \tau}\Pi = \nu\frac{\partial}{\partial \xi}(\xi\Pi) + f(\tau)\frac{\partial^2}{\partial \xi^2}\Pi, \tag{15}$$

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[2]The master equation (1) with the transition rates as given by Eqs. (13) and (14) can be analytically solved in the infinite size limit. However, the explicit solution can be numerically evaluated only at small n.

where $f(\tau) = 1/2[(2-\nu)\phi_0 e^{-\nu\tau} + 2(\nu-1)\phi_0^2 e^{-2\nu\tau}]$. Its solution is

$$\Pi(\xi,\tau) = \frac{e^{\nu\tau}}{\sqrt{4\pi\eta(\tau)}}\exp\left[-\frac{(\xi e^{\nu\tau})^2}{4\eta(\tau)}\right],$$

with $\eta(\tau) = (2-\nu)\phi_0(e^{\nu\tau}-1)/(2\nu) - (1-\nu)\phi_0^2\tau$.

In order to account for the absorbing boundary, we added a time-dependent constraint on ξ, so that n in Eq. (2) varies between 0 and N. To guarantee this latter condition, we imposed $\xi_{\min} \leqslant \xi \leqslant \xi_{\max}$, where $\xi_{\min} = -\sqrt{N}\phi_0 e^{-\nu\tau}$ and $\xi_{\max} = \sqrt{N}(1 - \phi_0 e^{-\nu\tau})$. In correspondence to $n = 0$, $\xi = \xi_{\min}$ is an absorbing boundary, while $\xi = \xi_{\max}$, which corresponds to $n = N$, is a reflecting boundary. The final solution accounting for the absorbing boundary reads

$$\Pi_{\mathrm{abs}}(\xi,\tau) = \frac{e^{\nu\tau}}{\sqrt{4\pi\eta(\tau)}}\left\{\exp\left[-\frac{(\xi e^{\nu\tau})^2}{4\eta(\tau)}\right]\right.$$
$$\left. - \exp\left[-\frac{(\xi e^{\nu\tau} + 2\sqrt{N}\phi_0)^2}{4\eta(\tau)}\right]\right\}. \tag{16}$$

This solution has a delta peak at $\xi = 0$ (or $n = N\phi_0$) for $\tau \to 0$ and vanishes at $\xi = -\sqrt{N}\phi_0 e^{-\nu\tau}$.

We now turn to Eq. (8), which now reads

$$\frac{\partial}{\partial \tau}\Pi(\xi,\tau) = \nu\frac{\partial}{\partial \xi}(\xi\Pi) + \frac{2-\nu}{2}\frac{\partial^2}{\partial \xi^2}(\xi\Pi),$$

where we have used that $T_-^{(1)}(0) - T_+^{(1)}(0) = \nu$ and $T_-^{(1)}(0) + T_+^{(1)}(0) = 2 - \nu$ [see Eqs. (13) and (14)].

In order to test the validity of the methods, we performed extensive numerical simulations of Eqs. (10)–(12) through the Gillespie algorithm [13], which allows one to produce time series that exactly recover the solution of the master equation (1) with the rates in Eqs. (13) and (14). Figure 1 shows typical results of the stochastic simulations and their comparison with the absorbing van Kampen solution in Eq. (16). For short times the first three profiles overlap well, but as time increases, the
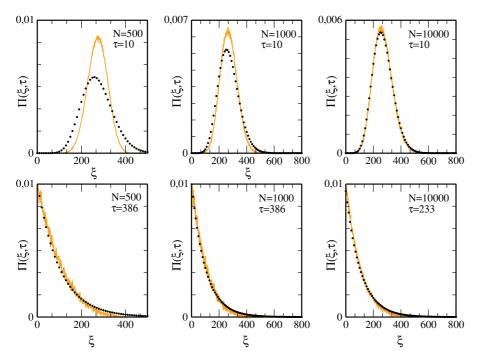
FIG. 2. (Color online) Comparison between the numerical simulations of the rules in Eqs. (10)–(12) and the theoretical predictions of the probability distribution in Eq. (9) at different times and systems sizes, according to the parameters specified in the top right of the panels. The noisy lines are the numerical profiles obtained by averaging over 10^6 stochastic simulations. While initially fluctuations are approximately Gaussian, in the sequel they are non-Gaussian and peak at zero. In all cases $\nu = 0.01$ and $n_0 = 300$.

probability distribution does not match the numerical simulation, as shown in the last three panels. Furthermore, the agreement does not improve on increasing the size of the system. In contrast, Fig. 2 shows the solution in Eq. (9) with $\mu = \nu$ and $D = (2 - \nu)/2$. Increasing N, while keeping τ fixed, improves the matching as shown in the first three panels. As expected Eq. (9) converges to the numerical profiles as τ increases.

As illustrated in both figures, in the presence of an absorbing state, the system is characterized by at least two temporal scales, τ_1 and τ_2, which make fluctuations evolve according to Eq. (7) for $\tau < \tau_1$ and Eq. (8) for $\tau > \tau_2$. It is possible to estimate roughly the two scales by observing that one should expect the generalized van Kampen ansatz to work until the fluctuations are of the same magnitude as the macroscopic part, namely, $N\phi(\tau) \simeq N^\alpha \sigma(\tau)$, where $\sigma(\tau)$ is the variance of ξ. When $\alpha = 1/2$, this condition translates into $N\phi_0 e^{-\nu\tau} \simeq \sqrt{2N\eta(\tau)}$, which gives $\tau_1 \simeq 1/(3\nu)\ln[n_0\nu/(2-\nu)]$ for $\nu\tau \gg 1$. For the expansion with $\alpha = 0$, we have $N\phi_0 e^{-\nu\tau} \simeq e^{-\nu\tau}\sqrt{(2-\nu)n_0/\nu(e^{\nu\tau}-1)}$, which gives $\tau_2 \simeq 1/\nu \ln[\nu n_0/(2-\nu)+1]$. Note that $\tau_1 < \tau_2$. The mentioned

condition of validity of the classic van Kampen expansion is confirmed by numerical simulations (data not shown).

Finally, for systems with absorbing boundaries, it is interesting to calculate an analytical expression for the survival probability $P_S(\tau)$ [14]. In our case, we get the exact expression $P_S(\tau) = 1 - [(1-e^{-\nu\tau})/(1-(1-\nu)e^{-\nu\tau})]^{n_0}$, which, in the scaling limit $\nu \to 0$ with $\nu\tau$ fixed, simplifies to $f(\nu\tau)/t$ with $f(z) = zn_0/(e^z - 1)$. Amazingly, the same result is also obtainable using Eq. (9), with $P_S(\tau) = \int d\xi \, \Pi(\xi,\tau|\xi_0,0)$.

Summarizing, in the presence of systems with absorbing states, one has to generalize the standard van Kampen ansatz in order to monitor the temporal evolution at large times. As time elapses, fluctuations become more and more important and are no longer Gaussian. However, they still can be analytically treated and lead to the general solution given by Eq. (9).

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