# Quasicontinuum Fokker-Planck equation

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Building on the work [C. R. Doering, P. S. Hagan, and P. Rosenau, Phys. Rev. A **36**, 985 (1987)] we present a regularized Fokker-Planck equation for discrete-state systems with more accurate short-time behavior than its standard, Kramers-Moyal counterpart. This regularization leads to a quasicontinuum Fokker-Planck equation with several key features: it preserves crucial aspects of state-space discreteness ordinarily lost in the standard Kramers-Moyal expansion; it is well posed, and it is more amenable to analytical and numerical tools currently available for continuum systems. In order to expose the basic idea underlying the regularization, it suffices for us to focus on two simple problems—the chemical reaction kinetics of a one-component system and a two-dimensional symmetric random walk on a square lattice. We then describe the path to applying this approach to more complex, discrete-state stochastic systems.

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## I. INTRODUCTION

Stochastic, discrete-state models abound in the description of a variety of both naturally occurring and engineered systems. In cell biology, for example, biochemical processes often involve only a small number of relevant molecules and/or occur at spatially distinct locations. As a result, these processes demand a *discrete* description—discrete in physical and/or state space [1]. Examples include cell signaling [2] random walks and bubble dynamics on DNA [3], gene expression [4], molecular motors [5], and ratchets [6] with distinct potential wells, and diffusion of cancer cells [7].

When modeling such systems over long time intervals and/or over large spatial/state-space scales, one can often safely ignore the effects of discreteness. (See [8] for exceptions). Such an approximation gives rise to the standard Fokker-Planck equation via the Kramers-Moyal expansion truncated at second order. See [9] for a complete description.

However, if one would like to investigate short-time or short-distance behavior, the second-order truncation is insufficient. In this paper, we address this issue by extending the work of Rosenau [10] and more specifically that described in Doering *et al.* [11]. In particular, we bridge the gap between a general discrete state-space system and its Fokker-Planck limit via a regularization process. This regularized, or so-called quasicontinuum Fokker-Planck equation, accurately treats coarse-grained descriptions over large regions of phase space yet still retains some key features of original discrete system. The price for this improvement, furthermore, is not significant—the usual local drift and diffusion operators are replaced with bounded, nonlocal counterparts, with little increase in computational complexity and effort of analysis.

We begin with the master equation which tracks the probability that the system is in a specific, discrete state $\mathbf{s}$

$$P(\mathbf{s},t+dt) = P(\mathbf{s},t) + \sum_{\mathbf{s}'\neq\mathbf{s}} T(\mathbf{s}'\to\mathbf{s})P(\mathbf{s}',t)dt - \sum_{\mathbf{s}\neq\mathbf{s}'} T(\mathbf{s}\to\mathbf{s}')P(\mathbf{s},t)dt. \quad (1)$$

for all allowed $\mathbf{s}$. Here $T(\mathbf{s}'\to\mathbf{s})$ is the rate at which the system transitions from the state $\mathbf{s}$ to the state $\mathbf{s}'$. The quantity $P(\mathbf{s},t)$ may represent the probability of having a specified number $\mathbf{s}$ of particles of a given type at time $t$, or the probability that a particle is at a specified site $\mathbf{s}$ on a discrete lattice, or the probability that a queue has length $s$, etc.

The solution of this coupled set of equations Eq. (1) contains information about all single-time statistics of the process under investigation. Unfortunately, these solutions are rarely available in closed form and can be quite costly to obtain numerically. See the following references for work in the domain of biochemically reacting systems [12–17]. A promising alternative to straightforward discretization of the master equation has been developed by Munsky and Khammash [18–21].

As a middle-ground approach between faithfulness to discrete dynamics offered by the master equation and the computational benefits offered by the Fokker-Planck, we construct a quasicontinuum approximation a la [11] to the discrete-state master equation. The quasicontinuum approach is appealing since it retains the structure/language of a continuum description. As such, it is amenable to the arsenal of computational methods for time-dependent PDE's including Galerkin [22], Adaptive Mesh, and variational approaches. The quasicontinuum Fokker-Planck equation also inherits a trace of the original discrete process and moreover can be constructed to capture the time-dependent, higher-order (beyond second order) fluctuations.

In order to illustrate the motivation for and the mechanics of the regularization, it is sufficient for us to focus on two relatively simple problems—(1) the reaction kinetics of a one-component chemical system and (2) a two-dimensional,

 

symmetric random walk on a square lattice. This extends regularization the procedure beyond the original work [11] to systems with nonuniform drift (potential) and to higher-dimensional state spaces. In Sec. II we describe the master equation, the Kramers-Moyal expansion, and its associated regularization. In Sec. III we apply the method to the aforementioned reaction kinetics example. We then apply the regularization method to a random walk in two spatial dimensions in Sec. IV. Our results are summarized in Sec. V where we also conclude with a discussion of future directions and both the potential and limitations of the approach.

## II. KRAMERS-MOYAL EXPANSION AND REGULARIZATION

The regularization method we use in this paper is described in a number of works (see for example [11,23–26]) but the sake of completeness, we outline it again here.

Consider a the time evolution of a symmetric random walker on a one-dimensional lattice. Let $n$ index the lattice site $n=\ldots-2,-1,0,1,2\ldots$, $h$ be the constant distance between sites, and $\sigma$ be the jump rate; i.e., the probability of jumping from one site to a neighboring site per unit time. The master equation (1) for this process takes the particularly simple form

$$P(n,t+dt) = P(n,t) + \sigma P(n+1,t) - 2\sigma P(n,t) + \sigma P(n-1,t). \tag{2}$$

The standard path from the master equation to a coarse-grained description is via the Kramers-Moyal expansion [9,27]. The discrete index $n$ is replaced by the density variable $x=n/\Omega$, where $\Omega$ is the system volume. We then expand the distribution function

$$\partial_t P(x,t) = \sum_{k=1}^{\infty} (-\partial_x)^k D^{(k)}(x) P(x,t), \tag{3}$$

where the coefficients $D^{(k)}$ are given by moments of the transition rates,

$$D^{(k)}(x) = \lim_{\tau\to 0} \frac{1}{\tau}\frac{1}{k!}\int dx'(x'-x)^k P(x',t+\tau|x,t). \tag{4}$$

For our one-dimensional random walk example we obtain

$$D^{(odd)} = 0;\ D^{(2)} = h^2;\ D^{(4)} = \frac{h^4}{12};\ D^{(6)} = \frac{2h^6}{6!}, \tag{5}$$

and the Kramer-Moyal expansion gives

$$P_t(x,t) = \sigma\left[P_{xx}(x,t) + \frac{h^2}{12}P_{4x}(x,t) + \frac{2h^4}{6!}P_{6x}(x,t) + \ldots\right] \tag{6}$$

supplemented with initial conditions

$$P(x,0) = P_0(x). \tag{7}$$

The usual truncation of the Kramers-Moyal expansion at second order, i.e., the standard Fokker Planck equation, exactly captures the time dependence of the second moments of the distribution for all times, but higher-order moments are only approximated. For late times, the quality of this approximation improves, but for short times there can be considerable disagreement.

This disagreement stems from the fact that at the level of Fokker-Planck equation all traces of discreteness are washed away. We shall therefore go beyond that level in order to retain some of the effects of a discrete-state space [11]. However, to this end one cannot simply use the expansion above—Eq. (6) has to be regularized.

The conundrum of this expansion is noted by observing that to include the effects due to discreteness, one has to go beyond the second order. But the expected correction due to fourth order rather than improving the situation, yields an ill-posed problem. At sixth order the ill posedness is removed, but the positivity of $P$ is then lost. If non-negativity of the distribution function $P>0$ is required for all times $t>0$, then this series simply cannot be truncated at arbitrary order. By Pawula's theorem [28], non-negativity demands that one keep *either* only the first and second terms *or* the full, infinite set of them. This is best seen in Fourier space. With the usual identification of $\partial_x \to ik$ we have

$$\hat{P}_t(x,t) = -\sigma\left(k^2 - \frac{h^2}{12}k^4 + \frac{2h^4}{6!}k^6 + \cdots\right)\hat{P}, \tag{8}$$

where $\hat{P}$ is the Fourier transform of $P$.

To resolve the difficulty we note that Eq. (8) is a truncated expansion of the following:

$$\hat{P}_t(x,t) = -\sigma\frac{4\sin^2(kh/2)}{h^2}\hat{P}. \tag{9}$$

But this expansion is precisely the source of the difficulty. While the exact discrete operator as given in Eq. (9) is bounded from below and above, its truncated, polynomial expansion is unbounded, leading to the apparent difficulties. This is resolved if instead we use a Pade representation which honors the boundedness. We thus approximate

$$\frac{4\sin^2(kh/2)}{h^2} \sim \frac{k^2}{1+\frac{h^2k^2}{12}}, \tag{10}$$

which is bounded from above and below and approximates the original expression up to fourth order. Of course, the Pade used is not unique; many others could be devised approximating the original expression to a desired degree of accuracy. Its utility is twofold—first it is simple; second, though per se this operator is nonlocal, see below, being a ratio of two polynomials its action can be made local by simply multiplying Eq. (3) by the denominator. This at once leads to

$$P_t = \sigma P_{xx} + \frac{h^2}{12}P_{xxt} \tag{11}$$

(where subscripts indicate partial differentiation) which is not only well posed, but also restores a number of features lost in the standard Fokker-Planck description.

The last term on the right-hand side introduces explicitly the effect of discreteness. The basic properties of this equation were presented in [10]. Its fundamental effect is to slow the initial spread. Thus the Green's function response to a Dirac delta function source is not smoothed immediately. Instead, there is a delay which causes the initial delta to persist for a while. The instant smoothing is often mentioned in the literature as the main shortcoming of the Fokker Planck process. The presented regularization resolves this difficulty at once.

Often the localization of the nonlocal Pade in Eq. (10) is inconvenient (when more than just few terms are present in the equation) or in the higher dimensional case, utterly impossible. In such cases one has to address the Pade approximant as is. In our case since the denominator in nothing but a transform of Cauchy operator this is a trivial task leading to

$$\partial_t P^{Reg}(x,t) = -\partial_x Q(x,t);$$

$$Q(x,t) = -\int_{-\infty}^{\infty} \exp\left(-\left|\frac{\xi}{12}\right|\right) P_x^{Reg}(x-\xi,t)d\xi. \tag{12}$$

The net effect of regularization as seen here is to replace the constant diffusion coefficient with an effective, nonlocal one which bounds the probability flux resulting from potentially large gradients in the distribution. In this case (where $D^{(2)}$ and $D^{(4)}$ are constant), we can rewrite Eq. (12) as

$$\partial_t P^{Reg}(x,t) = \partial_x D_* \star \partial_x P^{Reg}(x,t), \tag{13}$$

and $f \star g$ denotes the convolution of $f$ with $g$. The probability flux $Q(x,t)$ takes the form

$$Q(x,t) = -D_* \star \partial_x P(x,t). \tag{14}$$

The interpretation is clear in $k$ space where

$$D_*(k) = \frac{1}{1+h^2k^2/12} \tag{15}$$

and

$$\partial_t \hat{P}^{Reg}(k,t) = -k^2 \hat{D}_*(k) \hat{P}^{Reg}(k,t). \tag{16}$$

The merit of this representation will be evident in the next section when we turn to higher dimensions.

## III. BIOCHEMICAL REACTION

We now consider one of the simplest examples of reaction kinetics [29]. Reactant A is created (from the vacuum) at a rate $k$ and decays at a rate $qA$; i.e., proportional to the number of A molecules present: This could, for example, be model of mRNA production and decay, or it could represent particle number fluctuations in a well-mixed vessel which is coupled to a particle bath through a membrane.

$$\varnothing \rightarrow^{k} A \quad A \rightarrow^{qa} \varnothing \tag{17}$$

Using the standard Kramers-Moyal expansion procedure [9], we obtain the following terms:

$$D^{(1)} = k - qx; \quad D^{(2)} = \frac{k+qx}{2}; \quad D^{(3)} = \frac{k-qx}{6};$$

$$D^{(4)} = \frac{k+qx}{24}. \tag{18}$$

More generally, if $n$ is even, then

$$D^{(n)} = \frac{k+qx}{n!} \tag{19}$$

and, if $n$ is odd, then

$$D^{(n)} = \frac{k-qx}{n!}. \tag{20}$$

This gives rise to the following evolution equation:

$$\partial_t P(x,t) = -\partial_x[(k-qx)P(x,t)] + \partial_{xx}\left[\frac{k+qx}{2}P(x,t)\right] - \partial_{xxx}\left[\frac{k-qx}{6}P(x,t)\right] + \partial_{xxxx}\left[\frac{k+qx}{24}P(x,t)\right] + \ldots \tag{21}$$

The standard Fokker-Planck equation results from retaining only first two terms is on the right-hand side.

As with the previously described random walker, we use the regularization procedure to circumvent a truncation of the moment expansion. We sum all of the odd terms in the expansion to obtain $\sinh(\partial_x)P$. In Fourier space this becomes $\sin(k)P$ and is replaced with the bounded expression $k/(1+k^2/6)$. The new, bounded operator exactly reproduces moments up to a specified order (in this case fourth). For the even terms, a similar procedure is applied, yielding $k/(1+k^2/12)$. This leads to the complete, regularized Fokker-Planck equation,

$$\partial_t P^{RFP} = \partial_x\left[\frac{1}{1-6\partial_x^2}(A_-(x)P^{RFP})\right] + \frac{1}{2}\partial_{xx}\left[\frac{1}{1-12\partial_x^2}(A_+(x)P^{RFP})\right], \tag{22}$$

where $A_\pm = qx \pm k$.

In real space/number space we have

$$\partial_t P^{RFP}(x,t) = \partial_x \int_{-\infty}^{\infty} \exp\left(-\left|\frac{x-\xi}{6}\right|\right) A_-(\xi) P^{RFP}(\xi,t)d\xi + \partial_{xx}\int_{-\infty}^{\infty} \exp\left(-\left|\frac{x-\xi}{12}\right|\right) A_+(\xi) P^{RFP}(\xi,t)d\xi \tag{23}$$

with a no-flux boundary condition at the origin.

To demonstrate the quantitative improvement, we compare the short-time solutions of the Fokker-Planck [Eq. (21) with the first two terms on the right-hand side)] and the Regularized Fokker-Planck equation (23) with the behavior of the fully discrete process. We compare the evolution of the discrete process to solutions of the FP and RFP with initial conditions $P(x,0) = P^{RFP}(x,0) = \delta(x-5)$, namely, a system initially with $n=5$ molecules of type $A$. We then investigate the time evolution of various low-order moments of this distribution, $m_1 = \langle x \rangle$ and $m^j = \langle (x-m_1)^j \rangle$.

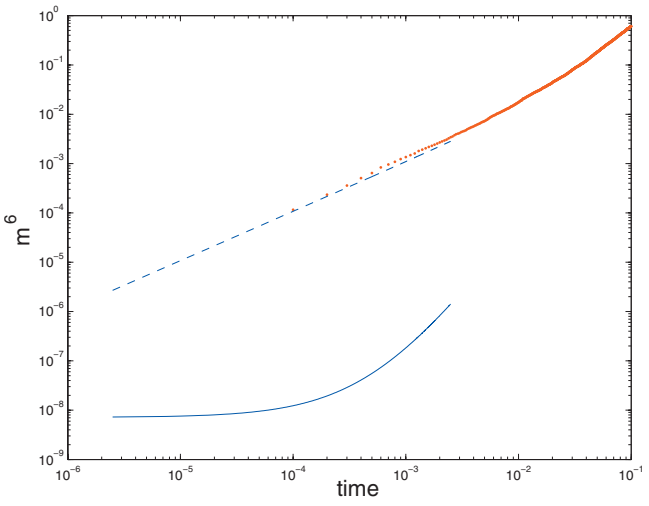


FIG. 1. (Color) Evolution of the sixth moment as a function of time for the exact process (red), the regularized FPE (dashed line) and the FPE (solid line).

By construction, the first and second moments are identical for the discrete process, the FP equation and the RFP equation. However, beyond the second moment, the FP and discrete process begin to disagree. The RFP, which uses information about the fourth moment, is identical to the discrete process. Moreover, there is good agreement for the sixth moment as well [see Fig. 1].

## IV. TWO-DIMENSIONAL RANDOM WALK

Next we consider the symmetric random walk on a the two-dimensional square lattice. We assume the jump rate to nearest-neighbor sites in both $x$ and $y$ directions is $\mu$. The Kramers-Moyal expansion for this process gives

$$D^{(1)} = D^{(3)} = 0 \quad D^{(2)} = \frac{\mu}{2} \quad D^{(4)} = \frac{\mu}{24}. \tag{24}$$

Keeping terms up to second order leads to the following Fokker-Planck/Diffusion equation:

$$\partial_t P^{FP} = \mu(\partial_{xx} + \partial_{yy}) P^{FP}. \tag{25}$$

Applying the same set of techniques as in the previous section, we obtain the associated regularized FP equation

$$\partial_t P^{RFP} = \frac{1}{2}\partial_{xx}\left[\frac{1}{1-12\partial_x^2} P^{RFP}\right] + \frac{1}{2}\partial_{yy}\left[\frac{1}{1-12\partial_y^2} P^{RFP}\right], \tag{26}$$

where each of the terms in brackets can be understood in the operator sense via the Fourier transform as in one dimension.

Consider the lattice random walk with the single walker initially ($t=0$) located the origin $x=0$, $y=0$. The analogous initial condition for both FP and RFP have the Dirac function $P^{FP}(x,y,0) = P^{RFP}(x,y,0) = \delta(x)\delta(y)$. We compare the moments for short times for all three processes. A short-time expansion for the moments $\langle x^\alpha y^\beta \rangle(t)$ can be worked out exactly combinatorially for the discrete process, and the moments $\langle x^\alpha y^\beta \rangle(t)$ for the FP and RFP can be worked out analytically.

TABLE I. Moments of the RFP and the original, discrete process.

| Process | $\langle x^2 \rangle$ | $\langle x^4 \rangle$ | $\langle x^6 \rangle$ |
|---|---|---|---|
| Discrete | $\frac{t}{2}$ | $\frac{3}{4}t^2 + \frac{t}{2}$ | See figure |
| FP | $\frac{t}{2}$ | $\frac{3}{4}t^2$ | $\frac{15}{8}t^3$ |
| Regularized FP | $\frac{t}{2}$ | $\frac{3}{4}t^2 + \frac{t}{2}$ | $\frac{15}{8}t^3 + \frac{15}{4}t^2 + \frac{5}{4}t$ |

The results are given in Table I. As can be seen, the moments of the RFP and the original, discrete process are identical up to fourth order. A comparison of the sixth order moment is given in Fig. 2. Despite the fact that the agreement for the sixth order moment was not demanded in the regularization, the fit is nevertheless quite impressive. A more complicated Pade approximation could have been constructed to match moments higher than fourth, but the complexity of the resulting equation would likely not have been worth the gains in accuracy.

## V. CONCLUDING NOTES

The essential message presented in this paper is the following: the conventional Fokker-Planck equation is insufficient to describe the short-time behavior of general, discrete-state systems. By using a regularization scheme originally proposed in [11], one can correct this shortcoming applied to more general systems than the simple one-dimensional random walker presented there. Moreover, this regularization results in the same level of complexity as the ordinary Fokker-Planck equation in that the resulting operator is continuous in both space and time.

Our approach introduces a new equation which improves the FP description at short times and blends into FP in the long time limit, providing an all-inclusive description over all time scales. This is a new and improved fundamental

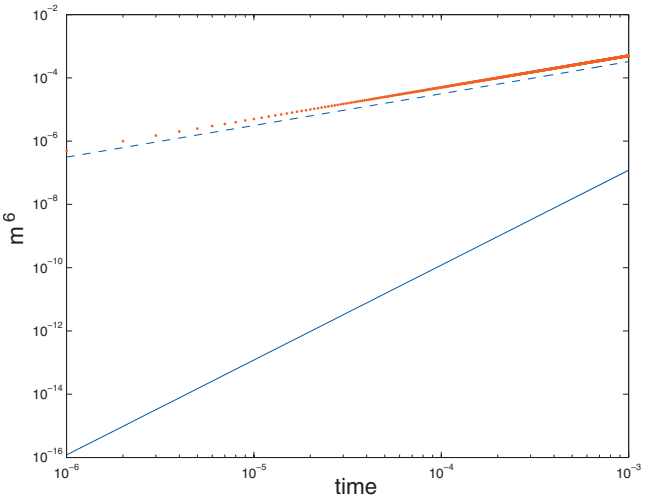


FIG. 2. (Color) Time dependence of the sixth moment for the two-dimensional process. Discrete process (red), regularized FPE (dashed line) and FPE (solid line).

description and not merely a numerical algorithm. Hence our approach has an advantage both over numerical algorithms, which may work well for short-time simulations, but may have difficulty capturing the long time behavior, and over the FP which is inadequate until later times.

We have derived and solved regularized FP equations for two representative cases—the short-time behavior of a single component reaction kinetics and a two-dimensional, lattice random walk. In particular, we have demonstrated that the solutions of these regularized equations better track the statistics of high order moments than the solutions to the standard FP equation. As a by-product we note that the regularization, while perhaps appearing formidable in its real space, convolutional form, actually helps ameliorate stiffness issues by virtue of its gradient smoothing effect.

We have purposely dealt with two very simple in examples in order to illustrate our specific approach for regularization. Extensions to a class of more complex systems where reactions occur only in *one* variable at a time are straightforward. A key question toward more general applicability is: can one develop regularized FPEs for systems in which transitions change several variables at once (e.g., reactions where $A \to A+1$ and $B \to B-1$ simultaneously and or $A \to A-1$ and $B \to B+1$ simultaneously). By a coordinate rotation we believe this case can be handled as well. For systems which evolve by changes both along coordinate axes *and* along diagonals, the straightforward application of the ideas presented here will no longer be possible, thought improvements to short-time behavior may still result from a "partial" regularization.

Several other questions arise: what continuous state Langevin processes also gives rise to these same regularized FP equations? What is the most general class of reaction/transition rates to which one can apply the regularization procedure?

Areas of future application include queueing systems moving beyond the diffusion/heavy traffic limit [30], filtering/optimal estimation where the regularized FP would replace the Kushner-Stratnovich equation [31,32] and Kushner-Stratonovich-Pardoux' [33] equations. This approach can be used for state/parameter estimation from short-time data. We also believe that the quasicontinuum approach can bridge discrete and continuum domains in coupled particle-continuum hybrid solvers for the simulation of multiscale systems.

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