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Random walk in a quasicontinuum

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A continuous-time random walk on a spatial lattice described by the Kramers-Moyal expansion has a continuum limit described by a Fokker-Planck equation. It is often desirable to know corrections to quantities computed in the continuum limit, but truncation of the Kramers-Moyal expansion at any level other than the Fokker-Planck either breaks down or yields unphysical results. Here we introduce an alternative approximation to the Kramers-Moyal expansion which circumvents the problems of a naive truncation and correctly incorporates the first-order corrections due to the discrete lattice.

I. INTRODUCTION

Continuous-time Markovian random walks in a discrete state space have many applications in the physical sciences,[1] but they are often difficult to treat analytically and numerically since the evolution of the probability distribution is given in terms of the Kramers-Moyal expansion (KME)—a partial differential equation of infinite order.[2,3] A well-defined continuum limit can be formulated by truncation of the KME at second order, yielding the Markov diffusion approximation described by a Fokker-Planck equation (FPE). This limit corresponds to taking the lattice spacing to zero while some characteristic transition rate diverges as the inverse square of the lattice spacing, and it gives a qualitatively correct picture only for large times, and for distances of order $\sqrt{t}$.[4-6]

Much recent work has gone into determining the corrections to quantities computed in the diffusion approximation for diffusion across interfaces,[7] and especially for first-passage times.[8-11] Formally the nth term in the KME is of order h^n, where h is the lattice spacing, and it seems sensible to work with a partial differential equation of finite order by truncating the KME at some given level, but there are two main problems with this approach. First, truncation at alternate even orders results in a "bad" equation yielding solutions which certainly blow up, due to the "wrong" sign of the highest-order differential operator. Of course, any such higher-order truncation also necessitates the specification of more boundary conditions. Second, truncation at any order greater than the second will result in a transition density which takes unphysical negative values, according to the theorem of Pawula.[4,12] This limitation is acceptable for some purposes, but the region in which Pawula's theorem applies with the most vengeance is exactly that region in which the diffusion approximation is the weakest: at short times.

There is a different approach to this problem, however, which was recently introduced in the context of a dense nonlinearly vibrating lattice.[13,14] In the present context this simple approach, which we call the "quasicontinuum" approximation (QCA), incorporates the lowest-order corrections due to the discreteness of the lattice while circumventing the problems associated with a naive truncation of the KME outlined above. It results in a well-posed mathematical problem and yields a positive, normalized probability density as its solution which corrects in a meaningful way the continuum Fokker-Planck description. The rest of this paper is organized as follows. In Sec. II we develop the quasicontinuum approximation to the KME in a general setting, most importantly proving the positivity of the quasicontinuum probability density. As an example of this approach, in Sec. III we consider the exactly soluble free random walk on a lattice and compare the exact solution, the diffusion approximation (DA), and the QCA. In Sec. IV we summarize our results and point out some areas for future development.

II. THE QUASICONTINUUM APPROXIMATION

The probability distribution for a continuous-time Markov process, $u(x,t)$, obeys the KME

$$\partial_t u(x,t)=\sum_{n=1}^{\infty}(-\partial_x)^n D^{(n)}(x)u(x,t) ,\qquad u(x,0)=u_0(x) , \tag{1}$$

where we assume time homogeneity and $D^{(n)}(x)$ is the KME coefficient defined by

$$D^{(n)}(x)=\lim_{\tau\to 0}\tau^{-1}(1/n!)\times\int dx'(x'-x)^n P(x',t+\tau\,|\,x,t) , \tag{2}$$

with $P(x',t+\tau\,|\,x,t)$ the transition density of the process (the density at x' at $t+\tau$ given a δ distribution at x at t). For processes taking values on a discrete lattice with spacing h (with meaningful initial conditions) the solution $u(x,t)$ is a sum of weighted δ functions located at the points $x=nh$. For simplicity, in the following we restrict ourselves to the isotropic case, where $D^{(n)}=0$ for n odd, and the case of uniformly bounded and nonvanishing diffusion, i.e., $D^{(n)}>0$ for n even.

The diffusion approximation is obtained by truncating the KME after the second term resulting in the FPE

$$\partial_t u=\partial_x^2 D^{(2)}u . \tag{3}$$

The solution of the FPE is a well-behaved analytic function (for $t > 0$). Truncation after the fourth term, naively incorporating corrections to the solution of the FPE to order h^2, yields the "unstable" equation

$$\partial_t u = (\partial_x^2 D^{(2)} + \partial_x^4 D^{(4)})u \ . \tag{4}$$

The positive fourth spatial derivative generally leads to a blowup of the solution; consequently an initial-value problem for Eq. (4) is ill posed. The next higher truncations lead to a better behaved equation, but Pawula's theorem ensures that the approximate transition density is *negative* somewhere.

The QCA introduced herein is obtained as follows. Keeping in mind that $D^{(4)}(x)$ is of order h^2 when the diffusion limit is approached, Eq. (4) above is, to order h^4, equivalent to

$$\partial_t u = \partial_x^2 D^{(2)}[1-(1/D^{(2)})\partial_x^2 D^{(4)}]^{-1} u \ , \tag{5}$$

where the inverse of the term in brackets is taken in the operator sense. This is a nonlocal equation, like the original KME, but the length scale of the nonlocality is limited to order h. The most important point is that the QCA is positivity preserving: When the initial condition is a positive probability distribution, then the solution remains a positive probability distribution for all times. The proof of this relies intimately on the maximum principle[15] for elliptic operators and requires that we restrict the magnitude of the length scales implied in the variations of $D^{(2)}(x)$ and $D^{(4)}(x)$ with respect to the lattice spacing, as is necessary to obtain a meaningful diffusion limit.

To realize the scaling of $D^{(2)}$ and $D^{(4)}$ explicitly, we write

$$r(x) = h^2 D^{(2)}(x)/D^{(4)}(x) \ , \tag{6}$$

where $r(x)$ is bounded and bounded away from zero, and its first and second derivatives are bounded, uniformly in h as $h \to 0$. Introducing the Green's function $K(x,x')$ satisfying

$$[r(x) - h^2\partial_x^2]K(x,x') = \delta(x-x') \ , \tag{7}$$

and the function $w(x,t)$ defined by

$$w(x,t) = \int dx' K(x,x')D^{(2)}(x')u(x',t) \ , \tag{8}$$

the QCA evolution Eq. (5) may be rewritten

$$\partial_t u = -(r^2 D^{(4)}/h^4)u + [(r^2/h^2) + r'' + 2r'\partial_x \ln w]w \ . \tag{9}$$

The maximum principle for elliptic operators ensures that $K(x,x')$ is a well-behaved *positive* function, and hence when $u \geq 0$ (but not identically 0), $w > 0$. Assuming positive normalized initial data for u, at the first time $t = t^*$, at which $u(x,t^*) = 0$, its time derivative is

$$\partial_t u = [(r^2/h^2) + r'' + 2r'\partial_x \ln w]w \ . \tag{10}$$

Since $w > 0$, it is sufficient to show that the term in brackets is positive, because then u increases at that point. To establish the result, we must bound $\partial_x \ln w$. In particular,

$$|\partial_x w(x,t)| \leq \int dx' |\partial_x K(x,x')| D^{(2)}(x')u(x',t) \ , \tag{11}$$

and the derivative of $K(x,x')$ is bounded by $K(x,x')$ as

$$|\partial_x K(x,x')| \leq (r_s^{1/2}/h)K(x,x') \ , \tag{12}$$

where r_s is the supremum of $r(x)$. This result follows simply from the defining equation for K and its known regularity and positivity properties. Hence, $\partial_x \ln w$ is bounded uniformly by $(r_s^{1/2}/h)$, and the term brackets in Eq. (10) satisfies

$$[(r^2/h^2) + r'' + 2r'\partial_x \ln w] \geq (r_i^2/h^2) - \|r''\|_\infty - 2\|r'\|_\infty (r_s^{1/2}/h) \ , \tag{13}$$

where r_i is the infimum of $r(x)$ and $\|\cdots\|_\infty$ denotes the supremum of the absolute value. As long as

$$h < r_i^2/[\|r'\|_\infty r_s^{1/2} + (\|r'\|_\infty^2 r_s + r_i\|r''\|_\infty)^{1/2}] \ , \tag{14}$$

the term in brackets is bounded above 0 and the result is established. Note that in the case of constant $r(x)$ this implies no restriction on the lattice spacing.

The fact that the QCA preserves the normalization of $u(x,t)$ is immediate from its form whenever the probability current $-\partial_x D^{(2)}\{1-(1/D^{(2)})\partial_x^2 D^{(4)}\}^{-1}u$ vanishes at the boundaries of the state space.

III. THE FREE RANDOM WALK

As an example of the QCA we consider the free random walk on a lattice with lattice spacing h, with an initial distribution concentrated at the origin.[1] The initial condition for the KME, the DA, and the QCA is thus taken to be $u(x,0) = \delta(x)$. (With this initial condition the solutions are the Green's functions for the linear equations, in terms of which the solutions for arbitrary initial conditions may be expressed.) The KME may be written

$$\partial_t u(x,t) = 2\mu \sum_{n=1}^{\infty} (2n)!^{-1} h^{2n} \partial_x^{2n} u(x,t) \ , \tag{15}$$

where μ is the transition rate of the walker to each of its nearest-neighbor lattice sites. The exact solution is

$$u^E(x,t) = \sum_{n=-\infty}^{\infty} p_n(t)\delta(x-nh) \ ,$$
$$p_n(t) = e^{-2\mu t} \sum_{m=0}^{\infty} (\mu t)^{2m+|n|}/m!(m+|n|)! \ . \tag{16}$$

The DA is

$$\partial_t u = D\partial_x^2 u \ , \tag{17}$$

where we have defined the diffusion coefficient $D = \mu h^2$, and the solution is

$$u^D(x,t) = (4\pi D t)^{-1/2} \exp(-x^2/4Dt) \ . \tag{18}$$

The QCA is

$$\partial_t u = D\partial_x^2 (1-\varepsilon\partial_x^2)^{-1} u, \ \varepsilon = h^2/12 \ . \tag{19}$$

The nature of the QCA density is best seen in terms of its Fourier transform

$$u^Q(k,t) = \exp[-k^2 Dt/(1+\varepsilon k^2)]$$
$$= \exp(-Dt/\varepsilon) + \{\exp[(Dt/\varepsilon)/(1+\varepsilon k^2)] - 1\} . \quad (20)$$

Since the second term above decays as k^{-2} as $k \to \infty$, it is an integrable function of k and its inverse Fourier transform is a continuous function of x by the Riemann-Lebesgue lemma. Thus the QCA density is the sum of a δ function at the origin weighted by $\exp(-Dt/\varepsilon)$ and a continuous function of x and t (for $t > 0$). This makes sense from a physical point of view since the random walker will have some probability of being at the origin at all times, and from a mathematical point of view since the exact density which is being approximated is a sum of δ functions. This decomposition of the density also shows that the QCA is not merely the replacement of one random walk on the lattice with another, as might be inferred from the nonlocal nature of the problem. An explicit expression for the QCA density is obtained from Eq. (20) via the inverse Fourier transform

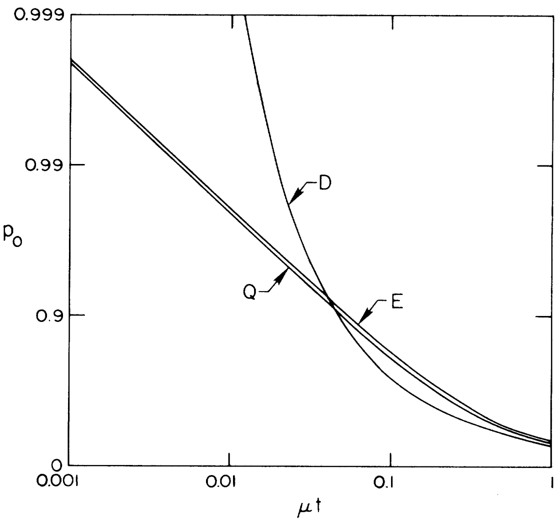

FIG. 1. Probability of finding the random walker at the origin vs dimensionless time for the exact process (E), the diffusion approximation (D), and the quasicontinuum approximation (Q).

$$u^Q(x,t) = \exp(-Dt/\varepsilon)\delta(x) + (Dt/\varepsilon)\exp(-Dt/\varepsilon)(2\varepsilon^{1/2})^{-1}\exp(-|x|/\varepsilon^{1/2})$$
$$\times \sum_{n=0}^{\infty} (Dt|x|/\varepsilon^{3/2})^n (2^n n!)^{-1} \sum_{m=0}^{\infty} (Dt/4\varepsilon)^m (2m+n+1)!/[(m+n+1)!(m+n)!m!] . \quad (21)$$

To compare these densities we consider short times on the dimensionless time scale μt, and in Fig. 1 plot the probability, $p_0(t)$, that the walker is at the origin (i.e., between $-h/2$ and $h/2$) as a function of time. As is evident from the figure, the QCA probability is a far better approximation to the true probability for short times. In fact, while $p_0(t)$ is analytic in t as $t \to 0$ for the exact and QCA densities, it is nonanalytic in the DA. To compare the long-distance behavior of the densities at short times, we consider various moments. All three densities have the same time-dependent second moment ($\langle x^2\rangle^E = \langle x^2\rangle^Q = \langle x^2\rangle^D = 2Dt$) and the QCA density gives the exact fourth moment [$\langle x^4\rangle^E = \langle x^4\rangle^Q = 3(2Dt)^2 + 12\varepsilon(2Dt)$ while $\langle x^4\rangle^D = 3(2Dt)^2$]. The QCA moments are always correct to $O(\varepsilon^2)$, while the DA is only good to $O(\varepsilon)$. At short times this is especially apparent, as shown in Fig. 2 where we plot the sixth moment for the three densities. This shows that at short times the wings of the DA density are much smaller than those for the exact density, while the QCA density has slightly more weight in the wings than the exact density. As $t \to \infty$, both the DA and the QCA asymptotically approach the exact result, at both short and long distances.

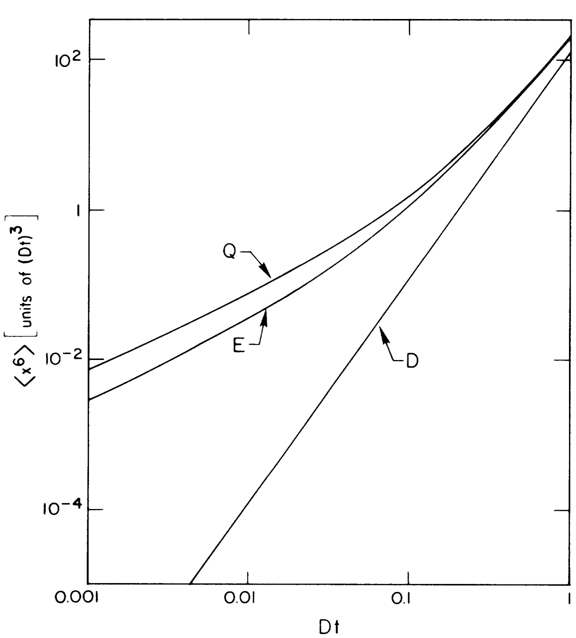

FIG. 2. Time-dependent sixth moment vs Dt for the case $\varepsilon = 0.1$ for the exact process (E), the diffusion approximation (D), and the quasicontinuum approximation (Q).

IV. SUMMARY AND DISCUSSION

The quasicontinuum approximation to the KME presented in this Communication offers a new and meaningful technique for dealing with corrections to the diffusion equation in close-to-continuum conditions. The example above shows that it effectively incorporates corrections due to the presence of the lattice in the short-time regime where the diffusion approximation is especially suspect. Its usefulness is apparent in this regime where no other approximation (known to us) that incorporates only the information in $D^{(4)}$ is valid.

Although the QCA is nonlocal, it can be cast into a local form by considering the new variable

$$v(x,t)=\int dx'[1-(1/D^{(2)})\partial_x^2 D^{(4)}]^{-1}(x,x')u(x',t) \ , \tag{22}$$

which satisfies the equation

$$\partial_t v(x,t)=\partial_x^2 D^{(2)}(x)v(x,t) + [1/D^{(2)}(x)]\partial_t\partial_x^2 D^{(4)}(x)v(x,t) \ . \tag{23}$$

If working with local equations is desired, Eq. (23) may be utilized and the QCA recovered (locally) by way of

$$u(x,t)=[1-(1/D^{(2)})\partial_x^2 D^{(4)}]v(x,t) \ . \tag{24}$$

The approach presented here can be generalized in several directions, two of which will be mentioned here: (a) random walks on multidimensional lattices, and (b) random walks with drifts. For example, in the case of constant drift and diffusion coefficients it is easy to show that the KME

$$\partial_t u(x,t)=2\mu\sum_{n=1}^{\infty}(2n)!^{-1}h^{2n}\partial_x^{2n}u(x,t) - v\sum_{n=0}^{\infty}(2n+1)!^{-1}h^{2n+1}\partial_x^{2n+1}u(x,t) \tag{25}$$

has the strictly positive QCA (written in local form)

$$\partial_t u = -f\partial_x(1+\varepsilon\partial_x^2)u + D\partial_x^2 u + \varepsilon\partial_t\partial_x^2 u \ , \tag{26}$$

where $D=\mu h^2$, $\varepsilon=h^2/12$, and $f=vh$, if and only if $h<3^{1/2}D/|f|$. Finally, it should be noted that the QCA developed here defines a Markov stochastic process in its own right. The sample paths for the exact process are well understood (piecewise-constant functions with isolated discontinuities) as are those of the diffusion process (Brownian paths—continuous but nowhere differentiable). It would be quite interesting to know more detail about the quasicontinuum sample paths characterizing the low-order lattice effects neglected in the Brownian paths.

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