Expansion of moments of the Smoluchowski equation

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We derive a formal expansion in powers of t of the moments of the Smoluchowski equation in free space. The coefficients either are derived by an easily implemented recursion relation or can be expressed in terms of the functions appearing in the Smoluchowski equation and their derivatives. The formalism is shown to reproduce known exact results for several Smoluchowski equations with nonconstant coefficients.

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I. INTRODUCTION

There are many models in biology, chemistry, and physics whose analysis reduces to the problem of finding the solution to a Smoluchowski or Fokker-Planck equation with nonconstant coefficients [1,2]. In one dimension a Smoluchowski equation is typically of the form

$$\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}\left[D(x)\frac{\partial p}{\partial x}\right]-\frac{\partial}{\partial x}[v(x)p]=\mathcal{L}p\ , \tag{1}$$

where $p(x,t)$ is the probability density for the position of a diffusing particle at time t, $D(x)$ is a diffusion coefficient, $v(x)$ is a coefficient associated with convection, and $\mathcal{L}$ is the parabolic operator on the right-hand side. There are no general solutions of such equations other than a formal expansion derived by separating variables in Eq. (1). Such an expansion is not necessarily a numerically useful solution to Eq. (1). When diffusion can be regarded as being small in comparison to convection there are several techniques available for generating approximations to $p(x,t)$ in an unbounded space. These approximations are generally valid at sufficiently small times [1,3–5].

When there are absorbing boundaries it is possible to write down equations for moments of the first-passage time to absorption based on the adjoint operator [6]. In one dimension the resulting equations reduce to ordinary differential equations. The equation for the first moment can be solved explicitly and expressions for higher moments can be generated recursively. Quite recently van Kampen has presented an approximation to the solution to Eq. (1) in the presence of absorbing boundaries valid at sufficiently short times [7,8]. These techniques work because when the variables in Eq. (1) are separated, the space-dependent terms generate a set of eigenvalues and eigenfunctions which can be used to specify the behavior of $p(x,t)$. In this paper we present a systematic technique for generating short-time expansions of the moments associated with $p(x,t)$, provided that the moments can be expanded as a power series in the time. Such series can, for example, be applied to the analysis of the kinetics of the separation of DNA fragments in an electrophoretic gel.

II. DEVELOPMENT OF THE FORMALISM

Let us generate a purely formal short-time expansion to the solution of Eq. (1) subject to the initial condition

$$p(x,0)=\delta(x-x_0)\ . \tag{2}$$

We will assume that this solution can be written as the series

$$p(x,t)=\sum_{n=0}^{\infty}p_n(x)\frac{t_n}{n!}\ , \tag{3}$$

where, obviously, $p_0(x)=\delta(x-x_0)$. Successive terms in this series are obtained by substituting the expansion into Eq. (1). In this way we find that the p_n can be generated recursively from the relations

$$p_{n+1}=\mathcal{L}p_n \quad \text{or} \quad p_n=\mathcal{L}^n\{\delta(x-x_0)\}\ , \qquad n=0,1,2,\ldots\ . \tag{4}$$

It is trivially observable that Eq. (3) can only be a formal expression when the initial condition is a δ function, as indicated in Eq. (2), since in that case each time in the expansion will consist of either δ functions or derivatives of δ functions. However, the formal series is still useful in furnishing expansions in powers of the time of the spatial moments

$$\mu_k(t)\equiv\int_{-\infty}^{\infty}x^k p(x,t)dx, \quad k=0,1,2,\ldots \tag{5}$$

when these moments can indeed be expanded as a power series.

For the purpose of deriving this expansion we define the sequence

$$\rho_{k,n}=\int_{-\infty}^{\infty}x^k p_n(x)dx, \quad k,n=0,1,2,\ldots\ , \tag{6}$$

which, together with Eq. (5), furnishes the expansion

$$\mu_k(t)=\sum_{n=0}^{\infty}\rho_{k,n}\frac{t_n}{n!}\ . \tag{7}$$

We can find yet another formal representation for the $\rho_{k,n}$, which can be written in terms of integrals with

respect to the $p_n(x)$. It is convenient to introduce the notation

$$\langle g(x)\rangle_n=\int_{-\infty}^{\infty} g(x)p_n(x)dx \tag{8}$$

in terms of which we can write $\rho_{k,n}=\langle x^k\rangle_n$. This notation, together with the recursion relation in Eq. (4), allows us to represent $\rho_{k,n}$ in the form

$$\rho_{k,0}=x_0^k,$$
$$\rho_{k,n}=k\langle (k-1)x^{k-2}D(x)+x^{k-1}[v(x)+D'(x)]\rangle_{n-1}\ ,$$
$$n\geq 1\ . \tag{9}$$

The fact that $D'(x)$ and $v(x)$ appear on an equal footing in this equation follows from the consideration that in writing the relation between a one-dimensional Fokker-Planck equation and the Smoluchowski equation a gradient in the diffusion function induces a net velocity. In particular, the coefficients $\rho_{1,n}$ and $\rho_{2,n}$ can be expressed in terms of the equivalent velocity $V(x)=v(x)+D'(x)$ as

$$\rho_{1,n}=\langle V(x)\rangle_{n-1}\ ,$$
$$\rho_{2,n}=2\left\{\left\langle\frac{d}{dx}[xD(x)]\right\rangle_{n-1}+\langle xv(x)\rangle_{n-1}\right\}\ . \tag{10}$$

Equation (9) can be converted into a convenient recurrence relation for the $\rho_{k,n}$ regarded as a function of n. We will use two different forms of such recurrence relations. Assume first that $D(x)$ and $v(x)$ can be expanded as power series in x around $x=0$, i.e.,

$$u(x)=\sum_{j=0}^{\infty} v_jx^j,\quad D(x)=\sum_{j=0}^{\infty} D_jx^j\ . \tag{11}$$

Then Eq. (9) is equivalent to the recursion relation

$$\rho_{k,n}=k\sum_{j=0}^{\infty}(k-1+j)D_j\rho_{j+k-2,n-1}$$
$$+k\sum_{j=0}^{\infty} v_j\rho_{j+k-1,n-1},\quad n\geq 1\ , \tag{12}$$

which is most convenient for computer implementation. A second recurrence relation for $\rho_{k,n}$ can be found by regarding it as a function of x_0. An integration by parts shows that $\rho_{k,n}$ can also be generated recursively by

$$\rho_{k,n+1}(x_0)=D(x)\frac{d^2\rho_{k,n}(x)}{dx^2}+V(x)\frac{d\rho_{k,n}(x)}{dx}\bigg|_{x=x_0}\ . \tag{13}$$

It is instructive to consider two examples in which all of the steps can be carried out in closed form. One of these is the Ornstein-Uhlenbeck equation, which we write as

$$\frac{\partial p}{\partial t}=\varepsilon\frac{\partial^2 p}{\partial x^2}+\frac{\partial}{\partial x}(xp)\ , \tag{14}$$

for which the solution is known to be

$$p(x,t)=\frac{1}{\sqrt{2\pi\varepsilon(1-e^{-2t})}}\exp\left\{-\frac{(x-x_0e^{-t})^2}{2\varepsilon(1-e^{-2t})}\right\}\ , \tag{15}$$

which allows an easy calculation of the moments. The expansion in Eq. (12) takes on a simple form because there are few values of the coefficients that differ from zero. Specifically we have $v_1=1$ and $v_j=0$, $j\neq 1$; $D_0=\varepsilon$ and $D_j=0$, $j>0$. When applied to this particular example Eq. (12) becomes

$$\rho_{k,0}=x_0^k,\quad k\geq 0$$
$$\rho_{k,n}=\varepsilon k(k-1)\rho_{k-2,n-1}-k\rho_{k,n-1},\quad n\geq 1\ . \tag{16}$$

The first two of the $\rho_{k,n}$ are readily found to be

$$\rho_{1,n}=(-1)^nx_0\ ,$$
$$\rho_{2,0}=x_0^2,\quad \rho_{2,n}=(-1)^{n+1}2^n(\varepsilon-x_0^2),\quad n\geq 1\ . \tag{17}$$

These results allow us to sum the series for the moments in closed form in Eq. (7) to find

$$\mu_1(t)=x_0e^{-1},\quad \mu_2(t)=2\varepsilon(1-e^{-2t})+x_0^2e^{-2t}\ , \tag{18}$$

which are readily shown to be in agreement with a direct calculation based on Eq. (15). One finds similar results in terms of the formalism indicated in Eq. (13).

A second, slightly less trivial model is based on an exact solution to the equation

$$\frac{\partial p}{\partial t}=\frac{1}{2}\frac{\partial^2 p}{\partial x^2}-\frac{\partial}{\partial x}[\tanh(x)p] \tag{19}$$

provided by Hongler [9]. He has shown that the solution to this equation is

$$p(x,t)=\frac{1}{\sqrt{2\pi}}\frac{\cosh x}{\cosh x_0}\exp\left\{-\frac{1}{2}-\frac{(x-x_0)^2}{2t}\right\}\ . \tag{20}$$

From this, one can calculate expressions for the first two moments of x exactly as

$$\mu_1(t)=x_0+(\tanh x_0)t\ ,$$
$$\mu_2(t)=x_0^2+[1+2x_0\tanh x_0]t+t^2\ . \tag{21}$$

Here we see that the first two moments are polynomials. On combining the expression for the velocity $v(x)=\tanh x$ and $D=\frac{1}{2}$ with Eq. (13) we find that our formalism exactly reproduces the expressions in this last equation since $\rho_{2,2}=1$ so that $\rho_{2,n}\equiv 0$ for $n>2$. In consequence, the second moment is quadratic in t. The last example suggests that our procedure will be especially useful when the moments are polynomials in the time.

We have seen in the framework of two examples that even though successive approximants to $p(x,t)$ can be expressed in terms of generalized functions and are therefore not very useful in a practical sense, they are able to furnish perfectly reasonable expressions for the spatial

moments. While our discussion has been based on the one-dimensional Smoluchowski equation in Eq. (1), it is clear that the extension to higher dimensions is a matter of detail only, requiring only more complicated calculations, but no new ideas.

Finally, we mention the possibility of developing an analogous, but slightly more complicated, theory for the survival probability for a system described by a Smoluchowski equation with a first-order distributed reaction term, i.e.,

$$\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}\left[D(x)\frac{\partial p}{\partial x}\right]=\frac{\partial}{\partial x}[v(x)p]-k(x)p \tag{22}$$

in the absence of boundaries. A number of investigators have analyzed properties of the survival probability [10–13]

$$S(t)\equiv\int_{-\infty}^{\infty}p(x,t)dx \tag{23}$$

using various approximations (which depend on whether diffusion or reaction is the dominant effect). While there are no rigorous mathematical analyses that bear on the validity of the different expansions, they all seem to be useful at sufficiently short times only. At least in theory, the present approach allows a direct calculation of $S(t)$ at short times without the necessity of introducing approximations as in all previous analyses, provided only that $D(x)$, $v(x)$, and $k(x)$ can be expanded in a Taylor series.

Although the validity of the expansion given here is obviously restricted to short times, it is also true that the accuracy of approximations based on diffusive effects being small relative to convective effects [3,4] is similarly restricted. These generally give incorrect results for the stationary solution when such a solution exists. In these it is difficult either to estimate the period of time during which the approximate solutions yield accurate results or to prolong this period.

A clear distinction exists between our expansion, which makes no assumptions about the relative contributions from diffusion and convection, and the expansions of [3,4]. This distinction appears in the lowest-order term, which contains only the point x_0 rather than the deterministic trajectories that appear in those expansions. This distinction allows us to make a crude estimate of the time period during which the lowest-order terms in the polynomial expansion can be expected to yield accurate results. On using the expansion in Eq. (9) one finds that the expansion of the moments to first order in the dimensionless time is

$$\mu_k(t)=x_0^k\left\{1+k\left[k-1+\frac{V(x_0)x_0}{D(x_0)}\right]\frac{D(x_0)t}{x_0^2}+\cdots\right\}, \tag{24}$$

where higher-order terms in powers of t contain higher derivatives of the functions $D(x)$ and $V(x)$ evaluated at x_0. Thus, for $k=1$, the term proportional to t is small provided that $t\ll x_0/V(x_0)$, while for higher-order moments the condition is $t\ll x_0^2/D(x_0)$. These conditions are in accord with the intuitively reasonable consideration that when both diffusion and convection are small in the neighborhood of the initial point, the diffusing particle tends to remain for a long period in that neighborhood.

In the following section we compare our expansion of the moments with that obtained from the van Kampen size expansion using an exactly solvable equation

III. APPLICATION TO CONVECTION-DOMINATED EXPANSIONS

As has already been mentioned, there are at least two systematic perturbation schemes available for generating solutions to Eq. (1) in the weak-noise limit, i.e., when $D(x)$ is small in a suitable dimensionless sense [3,4]. In this section we examine the accuracy of moments generated by these methods in the limit of short times for the Lamm equation [14], showing that the term to lowest order in ε in the first and second moments is already in error.

The dimensionless form of the Lamm equation can be written

$$\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}\left[x\left[\varepsilon\frac{\partial p}{\partial x}-p\right]\right],\quad x\geq 0\ . \tag{25}$$

This can be solved in closed form, but it is also possible to generate differential equations for the moments directly by multiplying both sides by x^n and integrating. We find in this way that the first and second moments are given by

$$\begin{aligned}\mu_1(t)&=x_0e^t+\varepsilon(e^t-1)\ ,\\ \mu_2(t)&=x_0^2e^{2t}+4\varepsilon(x_0+\varepsilon)e^t(e^t-1)-2\varepsilon^2(e^{2t}-1)\ .\end{aligned} \tag{26}$$

Both of these expressions are readily expanded in a power series in t and it is easily verified that our formalism gives results in agreement with the expanded version of this equation.

The van Kampen procedure for finding an approximate solution to Eq. (1) presumes that $D(x)$ is small in some sense. This assumption will be made explicit by writing the diffusion coefficient as $D(x)=\varepsilon\mathcal{D}(x)$, where ε is a small dimensionless constant and $\mathcal{D}(x)$ and $v(x)$ are assumed to be $O(1)$. Let $X(t)$ be the solution to the noise-free equation of motion $\dot{X}=v(X)$. The van Kampen approximation is obtained by replacing the spatial variable by y, which is related to x by $x=X(t)+y\sqrt{\varepsilon}$. The lowest-order approximation to the solution in the van Kampen expansion is then obtained as the solution to an Ornstein-Uhlenbeck equation having the form

$$\frac{\partial p_0}{\partial t}=a(t)\frac{\partial^2 p_0}{\partial y^2}-b(t)\frac{\partial}{\partial y}(yp_0)\ , \tag{27}$$

in which

$$a(t)=\mathcal{D}(X(t)),\quad b(t)=\left.\frac{dv}{dx}\right|_{x=X(t)}\ . \tag{28}$$

The solution to Eq. (27) is a Gaussian, which for the Lamm equation in Eq. (25) is

$$p_0(x,t)=\frac{e^{-t}}{\sqrt{4\pi\varepsilon(1-e^{-t})}}\exp\left[-\frac{(xe^{-t}-x_0)^2}{4\varepsilon(1-e^{-t})}\right], \tag{29}$$

from which the first moment is found to be

$$\mu_{1,vK}(t)=x_0e^t,$$
$$\mu_{2,vK}(t)=x_0^2e^{2t}+2\varepsilon e^t(e^t-1). \tag{30}$$

We see that, in contrast to the exact results given in Eq. (26), the expression for the first moment has no term proportional to ε, although the lowest-order term is given correctly, while in the second moment there is no term proportional to ε^2. At short times both approximate moments give incorrect results in the term that is $O(\varepsilon t)$. We have not checked whether the inclusion of higher approximations to the van Kampen formalism also produces proper corrections to the moments, but presumably this will be the case. A similar conclusion holds for the approximation scheme developed in [4]. Thus the only reliable way to generate moments at short times is based on the expansion method of Sec. II, when the forms of $D(x)$ and $v(x)$ are such as to validate the use of the method.

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