Approximation of the Linear Boltzmann Equation by the Fokker-Planck Equation

R. F. PAWULA

Department of the Aerospace and Mechanical Engineering Sciences, University of California, San Diego, La Jolla, California

and

*Institute for Radiation Physics and Aerodynamics**

In general, transformation of the linear Boltzmann integral operator to a differential operator leads to a differential operator of infinite order. For purposes of mathematical tractability this operator is usually truncated at a finite order and thus questions arise as to the validity of the resulting approximation. In this paper we show that the linear Boltzmann equation can be properly approximated *only* by the first two terms of the Kramers-Moyal expansion; i.e., the Fokker-Planck equation, with the retention of a *finite number* of higher-order terms leading to a logical inconsistency.

I. INTRODUCTION

FREQUENTLY, in the study of relaxation phenomena described by the linearized Boltzmann (master) equation, the Boltzmann integral operator is approximated by a differential operator.[1–10] The differential operator is obtained by terminating the Kramers-Moyal expansion at a finite number of terms, with the lowest-order approximation (the first two terms) being the Fokker-Planck operator. Intuitively, one is tempted to expect that the degree of approximation is directly related to the number of terms retained in the expansion. However, even if the expansion can be made in terms of a small parameter (such as the mass ratio of a light to a heavy particle) difficulties arise when terms of order greater than two are retained. For example, additional boundary conditions must somehow be prescribed for the solution of the resulting partial differential equation. Furthermore, if the solution represents a distribution function, then terms must be retained in such a way as to render a non-negative answer. Although these well-known difficulties can to some extent be overcome,[8] the general procedure of passing from an integral operator to a differential operator has eluded mathematical justification.[7]

As a result of investigating generalizations of the Fokker-Planck-Kolmogorov equations to non-Markov processes,[11] we have obtained a partial solution to the above problem. As is shown in Sec. III, if one assumes that terms above a given order are zero in the Kramers-Moyal expansion, this assumption implies that *all* terms above second order are zero.

It is to be emphasized that the passage from the linear Boltzmann equation to the Kramers-Moyal expansion is not free from mathematical criticism. One must *assume* the existence of certain partial derivatives, the convergence properties of certain series, and the interchange of certain limits. For example, if a distribution function (probability density function) contains a Dirac δ function and is otherwise analytic, we cannot expect the Kramers-Moyal expansion to yield the δ function *even if an infinite number of terms are retained.*[12] In the following, *we assume* that the linear Boltzmann equation is equivalent to the Kramers-Moyal expansion as given by Moyal.[13]

II. THE LINEAR BOLTZMANN EQUATION AND THE KRAMERS-MOYAL EXPANSION

For the sake of clarity, we confine our attention to a one-dimensional random process $x(t)$ which can take on a continuous range of values as a function of the continuous time parameter t. $x(t)$ might represent, for example, the position, speed, or energy of a gas particle. Let $P(x,t)$ denote the probability density function of the random variable $x(t)$ at time t and let $P(x,t|x_0,t_0)$ denote the transition probability density function, i.e., the conditional probability density function of $x(t)$ at time t given that $x(t)=x_0$ at time $t=t_0$. $P(x,t)$ then satisfies the linearized Boltzmann equation

$$\frac{\partial P(x,t)}{\partial t}=\lim_{\Delta\to 0}\frac{1}{\Delta}\int_{-\infty}^{\infty}[P(x',t)P(x,t+\Delta|x',t) -P(x,t)P(x',t+\Delta|x,t)]dx'. \quad (1)$$

* This research was supported in part by the Advanced Research Projects Agency (Project DEFENDER) and was monitored by the U. S. Army Research Office (Durham) under Contract No. DA-31-124-ARO-D-257.

[1] H. A. Kramers, Physica **7**, 284 (1940).

[2] J. E. Moyal, J. Roy. Stat. Soc. (London) **B11**, 150 (1949).

[3] J. Keilson and J. E. Storer, Quart. Appl. Math. **10**, 243 (1952).

[4] A. Siegel, J. Math. Phys. **1**, 378 (1960).

[5] M. Lax, Rev. Mod. Phys. **32**, 25 (1960).

[6] N. G. van Kampen, Can. J. Phys. **39**, 551 (1961).

[7] K. Anderson and K. E. Shuler, J. Chem. Phys. **40**, 633 (1963).

[8] H. Akama and A. Siegel, Physica **31**, 1493 (1965).

[9] N. G. van Kampen, in *Fluctuation Phenomena in Solids*, edited by R. E. Burgess (Academic Press Inc., New York, 1965), p. 139.

[10] C. F. Eaton and L. H. Holway, Jr., Phys. Rev., **143**, 48 (1966).

[11] R. F. Pawula, IEEE Trans. Inform. Theory **13**, 33 (1967).

[12] This statement is made without proof and is based upon the fact that a number of regularity assumptions must be imposed in transforming the Boltzmann operator to a differential operator. However, Siegel and Kohlberg [A. Siegel and I. Kohlberg, Bull. Am. Phys. Soc. **8**, 30 (1963)] have shown in a special case that the eigenvalues of the differential operator converge to the eigenvalues of the integral operator.

[13] See Ref. 2, p. 197, Eqs. (8.1.15) and (8.1.16).

We now assume that the right-hand side of this equation can be expanded in the Kramers-Moyal expansion; viz.,

$$\frac{\partial P(x,t)}{\partial t}=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[A_n(x,t)P(x,t)], \tag{2}$$

where the derivate moments A_n are given by

$$A_n(x,t)=\lim_{\Delta\to 0}\frac{1}{\Delta}\int_{-\infty}^{\infty}(x'-x)^n P(x',t+\Delta|x,t)dx'. \tag{3}$$

It is common to *assume* that the limit and integration operations in (1) and (3) can be interchanged and to define a transition probability density per unit time as

$$B(x,x')=\lim_{\Delta\to 0}\frac{P(x,t+\Delta|x',t)}{\Delta}. \tag{4}$$

The limit in this definition of $B(x,x')$ is to be interpreted in the physical, rather than in the mathematical, sense. By this we mean, for example, that if $x(t)$ were some property of a gas particle, that we might require that Δ always be much larger than a characteristic interaction time between gas particles (see, for example, the discussion by Uhlenbeck[14]). However, even for a well-behaved process such as a continuous Gaussian process, $B(x,x')$ is poorly behaved mathematically, consisting of Dirac δ functions and their derivatives. We thus choose to retain the form (1) for the linearized Boltzmann equation and (3) for the derivate moments. In Sec. IV, we discuss the implications of the limit and integration interchanges.

In general, (2) is an infinite-order partial differential equation which, for purposes of mathematical tractability, we desire to truncate at a finite number of terms.

III. THE TRUNCATION LEMMA

In this section we consider conditions under which (2) reduces to a partial differential equation of finite order. These conditions follow directly from the following:

Lemma: If A_n, as defined by (3), exists for all n, and if $A_n=0$ for some even n, then $A_n=0$ for all $n\geq 3$.

Usually the derivate moments A_n will be nonzero for all values of n. However, this lemma tells us that if we *assume* $A_n=0$ for some even n, that we are in actuality assuming A_n to be zero for all $n\geq 3$. Thus we conclude that it is logically inconsistent to retain more than two terms in the Kramers-Moyal expansion unless *all* of the terms are retained.

The proof of a generalized form of the above lemma is given in Ref. 11 and is reproduced here as a matter of completeness. From (3), we have

$$A_n=\lim_{\Delta\to 0}\frac{1}{\Delta}\int_{-\infty}^{\infty}(x'-x)^{(n-1)/2}(x'-x)^{(n+1)/2}\times P(x',t+\Delta|x,t)dx'. \tag{5}$$

Assuming n odd and $n\geq 3$, and applying the Schwarz inequality to (5), we obtain

$$A_n^2\leq A_{n-1}A_{n+1} \qquad n \text{ odd } n\geq 3. \tag{6}$$

In a similar way, it follows that

$$A_n^2\leq A_{n-2}A_{n+2} \qquad n \text{ even, } n\geq 4. \tag{7}$$

Setting $n=r-1$, $r+1$ in (6) and $n=r-2$, $r+2$ in (7), where r is an even integer, we obtain the four equations

$$A_{r-2}^2\leq A_{r-4}A_r,\quad r\geq 6 \tag{8}$$

$$A_{r-1}^2\leq A_{r-2}A_r,\quad r\geq 4 \tag{9}$$

$$A_{r+1}^2\leq A_rA_{r+2},\quad r\geq 2 \tag{10}$$

$$A_{r+2}^2\leq A_rA_{r+4},\quad r\geq 2. \tag{11}$$

If $A_n<\infty$ for all n and if $A_r=0$ for some even $r\geq 6$, then (8)–(11) show that A_{r-2}, A_{r-1}, A_{r+1}, A_{r+2} must be zero. By repeated application of this argument it follows that $A_n=0$ for all $n\geq r$. Going in the other direction and taking cognizance of the limits on r in (8)–(11), it follows that $A_n=0$ for all $n\geq 3$.

Note that the above lemma *does not* guarantee that the Fokker-Planck equation will be a good approximation to the linear Boltzmann equation. We should in general expect to obtain different solutions from each equation. The lemma merely leads to the conclusion that the probability density function of a random process cannot be correctly described by a finite number, greater than two, of terms of the Kramers-Moyal expansion.

If the derivate moment inequalities (8)–(11) are ignored, the equation resulting from a finite number, say n, of terms of the Kramers-Moyal expansion can, in principle, be solved to yield a function $Q_n(x,t)$. This function will in certain cases approach $P(x,t)$ as $n\to\infty$. However, the approximations $Q_n(x,t)$ may possess undesirable properties. Using a rearrangement of terms of the Kramers-Moyal expansion called Siegel's *CD* expansion, Kohlberg and Siegel[15] have found, for example, that approximate solutions for $P(x,t)$ are not always non-negative.

Although we have restricted ourselves to the simplest case of a one-dimensional random variable $x(t)$ and a marginal probability density function $P(x,t)$, the above lemma is true under much broader conditions. The

[14] G. E. Uhlenbeck, in *Probability and Related Topics in Physical Sciences*, edited by M. Kac (Interscience Publishers, Ltd., London, 1959), Appendix I, p. 183.

[15] I. Kohlberg and A. Siegel, Boston University report, 1965 (unpublished).

general one-dimensional case and the multidimensional case are discussed in detail in Ref. 11.

IV. USE OF A TRANSITION PROBABILITY DENSITY PER UNIT TIME

Let us assume that the limit defining the transition probability per unit time exists in some appropriate sense so that the linearized Boltzmann equation can be written as

$$\frac{\partial P(x,t)}{\partial t}=\int_{-\infty}^{\infty} P(x',t)B(x,x')dx' -P(x,t)\int_{-\infty}^{\infty} B(x',x)dx', \quad (12)$$

and the Kramers-Moyal expansion as

$$\frac{\partial P(x,t)}{\partial t}=\sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\frac{\partial^n}{\partial x^n}[a_n(x,t)P(x,t)], \quad (13)$$

where the derivate moments a_n are given by

$$a_n(x,t)=\int_{-\infty}^{\infty} (x'-x)^n B(x',x)dx'. \quad (14)$$

Since $B(x',x)$ is non-negative it follows that if $a_n(x,t)$ vanishes for some even n, then $B(x',x)$ must be zero for almost all x'. Thus for well-behaved $B(x',x)$, for example, as in the Keilson-Storer[3] model, the Kramers-Moyal expansion apparently becomes meaningless if an even derivate moment vanishes.[16] Thus for well-behaved $B(x',x)$ we conclude that no even derivate moment can vanish and that approximate solutions obtained from a finite number of terms of the Kramers-Moyal expansion will not necessarily represent probability density functions of random processes.

[16] This conclusion has been pointed out to the author by Professor J. Keilson of the University of Rochester.

If, on the other hand, the transition probability density $B(x',x)$ is allowed to contain certain singularities, then we are led to the results of Sec. III. For example, if

$$B(x',x)=\tfrac{1}{4}\delta''(x-x'), \quad (15)$$

then the Kramers-Moyal expansion becomes

$$\frac{\partial P(x,t)}{\partial t}=\frac{1}{4}\frac{\partial^2 P(x,t)}{\partial x^2}, \quad (16)$$

which for the initial condition $P(x,0)=\delta(x)$ has the solution

$$P(x,t)=(\pi t)^{-1/2}\exp[-x^2/t] \quad t\geq 0. \quad (17)$$

V. DISCUSSION

The derivate moment inequalities presented in Sec. III have led to the conclusion that the linear Boltzmann integral operator cannot properly be approximated by a finite number, greater than two, of terms of the Kramers-Moyal expansion. Although it is possible to construct approximate solutions by ignoring these inequalities, the validity of these approximations has not yet, to the author's knowledge, been established.

In our above treatment we have avoided a number of fundamental questions, such as the continuity of the random processes under consideration, the ability of a continuous random process to approximate a discontinuous random process, the validity of interchanging limiting operations, etc. These questions, as well as the all important problem of establishing error bounds on approximate solutions to the linear Boltzmann equation, remain areas for further investigation.

ACKNOWLEDGMENTS

The author is indebted to Dr. Kurt E. Shuler of the National Bureau of Standards for helpful discussions and for pointing out to the author a number of pertinent references. Thanks also are extended to Professor A. Siegel of Boston University for critical and informative comments on the original version of this manuscript.