Journal of Statistical Physics, Vol. 60, Nos. 3/4, 1990

Solution Methods for Discrete-State Markovian Initial Value Problems

V. C. Boffi,[1,2] F. Malvagi,[1] and G. C. Pomraning[1]

Received September 6, 1989; final February 22, 1990

Solution methods, both numerical and analytical, are considered for solving the Liouville master equation associated with discrete-state Markovian initial value problems. The numerical method, basically a moment (Galerkin) method, is very general and is validated and shown to converge rapidly by comparison with an earlier reported analytical result for the ensemble-averaged transmission of photons through a purely scattering statistical rod. An application of the numerical method to a simple problem in the extended kinetic theory of gases is given. It is also shown that for a certain restricted class of problems, the master equation can be solved analytically using standard Laplace transform techniques. This solution generalizes the analytical solution for the photon transmission problem to a wider class of statistical problems.

KEY WORDS: Discrete-state Markov processes; Liouville master equation; Markov processes; master equation; random processes; stochastic processes.

1. INTRODUCTION

In a recent article, Vanderhaegen and Deutsch[1] (hereafter referred to as VD) considered the radiative equilibrium problem for a finite rod under the assumption that the rod is composed of two statistically mixed materials. The statistics of the mixing was taken as homogeneous (stationary) and Markovian, and the interaction coefficients (cross sections) between the radiation and each component of the mixture were assumed to be spatially independent. This boundary value problem was converted to an initial value problem via the invariant imbedding model[2]

[1] School of Engineering and Applied Science, University of California, Los Angeles, Los Angeles, California 90024-1597.

[2] Permanent address: Faculty of Engineering, University of Rome "La Sapienza," 00182 Rome, Italy.

0022-4715/90/0800-0445$06.00/0

(essentially a Riccati transformation), and the resulting statistical Markov initial value problem was treated using the Liouville master equation approach.[3] The master equation in this case is sufficiently simple that it can be solved analytically. From this solution, VD computed the quantity of interest, namely the ensemble-averaged transmission through the rod, by simple numerical integration. An independent analysis for this problem,[4] using an approach entirely different from the master equation, confirmed the results reported by VD.[1]

In this paper, we consider a very general class of initial value problems for a two-state Markovian mixture. In general, such problems are too complex to solve analytically, and accordingly we develop a numerical method for computing the ensemble average for any quantity of interest associated with the problem under consideration. The class of problems we consider is a general nonlinear scalar (single equation) binary mixture problem with nonstationary Markovian mixing, and the underlying formalism used is the Liouville master equation approach. The problem treated by VD falls within this class, and we use their analytical results to validate our general numerical approach. As will be evident from the details given in this paper, all of our considerations can be extended to treat matrix (more than one equation) initial value problems with M-state ($M > 2$), rather than binary ($M = 2$), Markovian statistics. These generalizations involve only additional algebraic, not conceptual, complexity. To make our meaning clear, "scalar" here means a single stochastic dependent variable in the dynamical description of the system, such as Eq. (2) where ρ as well as F are scalars. "Matrix" refers to a system of equations describing the dynamics; ρ and F in Eq. (2) would be K-component column vectors, and such a problem would constitute, in our language, a matrix problem of index (size) K. We note that K (the number of stochastic independent variables) and M (the number of discrete states) are independent, with $K \geqslant 1$ and $M \geqslant 2$.

The lowest order numerical approximation actually produces, for all problems, a very simple analytical result. This result may be useful for assessing in a very simple way the qualitative behavior of the solution for any problem in this stochastic class, in particular for short times. As an example of the use of our numerical method in higher order, we consider a simple stochastic problem drawn from the extended kinetic theory of gases.[5,6] This problem is sufficiently complex to preclude an analytical solution, but our numerical scheme is shown to give quite accurate results in relatively low order. We also show that for a certain subclass of the general class of problems under consideration, one can obtain exact analytical results for the solution of the master equation. This generalizes the analytical considerations of VD[1] to a larger class of problems than they considered, although the analytical techniques we use are quite dif-

ferent. They applied a Green's function technique to partial differential equations involving mixed derivatives, whereas we use traditional Laplace transform techniques on the hyperbolic master equation in its rudimentary form.

We are unaware of any work in the literature, other than the paper by Vanderhaegen and Deutsch, which deals with the solution of the master equation as considered in this paper. We would welcome communications giving references to any related work, including areas of application.

2. THE LIOUVILLE MASTER EQUATION FORMULATION

We consider a dynamical system which at any time t can be in one of two states. We label these states with indices 0 and 1. The specification of which state is present at any given time is taken as a statistical process, and is assumed to be Markovian. Specifically, if the system is in state i at time t, the probability of the system being in state $j \neq i$ at time $t + dt$ is assumed to be given by the no-memory statement

$$\text{Prob}(i \to j) = \frac{dt}{\lambda_i(t)}, \qquad i = 0, 1; \quad j \neq i \tag{1}$$

where the $\lambda_i(t)$ are prescribed functions of time. For any realization of the statistics, the dynamics of the system is taken as described by

$$\frac{d\rho(t)}{dt} + F(\rho, t) = 0, \qquad 0 \leqslant t < \infty \tag{2}$$

where F is a prescribed nonstochastic function of its arguments provided that the state of the system is specified. We let $F_i(\rho, t)$, $i = 0, 1$, be this function corresponding to state i. We assign a stochastic initial condition to Eq. (2) of the form

$$\rho(0) = \begin{cases} \hat{\rho}_0 & \text{if the system is in state 0 at } t = 0 \\ \hat{\rho}_1 & \text{if the system is in state 1 at } t = 0 \end{cases} \tag{3}$$

Associated with Eqs. (1) and (2) is the Liouville master equation[3,7] for the joint probability $P_i(\rho, t)$, defined such that $P_i\, d\rho$ is the probability that the system is in state i at time t, and that the stochastic solution lies between ρ and $\rho + d\rho$. We have the two coupled equations

$$\frac{\partial P_0}{\partial t} - \frac{\partial}{\partial \rho}(F_0 P_0) = \frac{P_1}{\lambda_1} - \frac{P_0}{\lambda_0} \tag{4}$$

$$\frac{\partial P_1}{\partial t} - \frac{\partial}{\partial \rho}(F_1 P_1) = \frac{P_0}{\lambda_0} - \frac{P_1}{\lambda_1} \tag{5}$$

The initial conditions on Eqs. (4) and (5) are

$$P_i(\rho, 0) = p_i(0)\,\delta(\rho - \hat{\rho}_i), \qquad i = 0, 1 \tag{6}$$

which expresses the nonstochastic nature of the solution if the system is in state i at $t = 0$. Here the $\hat{\rho}_i$ are the prescribed initial data according to Eq. (3), and $p_i(t)$ is the probability of the system being in state i at time t. This probability is given by

$$p_i(t) = \int_{-\infty}^{\infty} d\rho\, P_i(\rho, t) \tag{7}$$

Integration of Eqs. (4) and (5) over all ρ gives the (forward) Chapman–Kolmogorov equations

$$\frac{dp_0}{dt} = \frac{p_1}{\lambda_1} - \frac{p_0}{\lambda_0} \tag{8}$$

$$\frac{dp_1}{dt} = \frac{p_0}{\lambda_0} - \frac{p_1}{\lambda_1} \tag{9}$$

which relate the probabilities $p_i(t)$ to the Markov transition functions $\lambda_i(t)$. Equations (8) and (9) are easily solved to give

$$p_i(t) = p_i(0) \exp\left[-\int_0^t dt'' \frac{1}{\lambda(t'')} \right] + \int_0^t dt' \frac{1}{\lambda_j(t')} \exp\left[-\int_{t'}^t dt'' \frac{1}{\lambda(t'')} \right], \qquad j \neq i \tag{10}$$

where

$$\frac{1}{\lambda(t)} = \frac{1}{\lambda_0(t)} + \frac{1}{\lambda_1(t)} \tag{11}$$

The ensemble average of any function of the solution, say $G(\rho)$, is given by

$$\langle G(\rho) \rangle = \int_{-\infty}^{\infty} d\rho\, G(\rho)[P_0(\rho, t) + P_1(\rho, t)] \tag{12}$$

Thus, the key to obtaining complete results for this statistical problem is to obtain the solution for the $P_i(\rho, t)$ defined by Eqs. (4)–(6). The problem treated by VD[1] corresponds to

$$F_i(\rho, t) = a_i \rho^2; \qquad G(\rho) = \rho \tag{13}$$

where a_i is a constant. In an earlier paper,[8] Vanderhaegen considered the linear case

$$F_i(\rho, t) = a_i + b_i\rho; \qquad G(\rho) = \rho \tag{14}$$

We note that this linear case is particularly simple, since one can find the ensemble average of any nonnegative integral power of ρ without having to solve the partial differential equations for the $P_i(\rho, t)$ given by Eqs. (4)–(6). To see this, we define

$$p_i\langle\rho_i^n\rangle = \int_{-\infty}^{\infty} d\rho\, \rho^n P_i(\rho, t) \tag{15}$$

and it then follows that

$$\langle\rho^n\rangle = p_0\langle\rho_0^n\rangle + p_1\langle\rho_1^n\rangle \tag{16}$$

Multiplication of Eqs. (4) and (5) by ρ^n and integration over all ρ gives

$$\frac{d}{dt}\, p_0\langle\rho_0^n\rangle + np_0(a_0\langle\rho_0^{n-1}\rangle + b_0\langle\rho_0^n\rangle) = \frac{p_1\langle\rho_1^n\rangle}{\lambda_1} - \frac{p_0\langle\rho_0^n\rangle}{\lambda_0}, \quad n \geqslant 0 \tag{17}$$

$$\frac{d}{dt}\, p_1\langle\rho_1^n\rangle + np_1(a_1\langle\rho_1^{n-1}\rangle + b_1\langle\rho_1^n\rangle) = \frac{p_0\langle\rho_0^n\rangle}{\lambda_0} - \frac{p_1\langle\rho_1^n\rangle}{\lambda_1}, \quad n \geqslant 0 \tag{18}$$

The initial conditions on Eqs. (17) and (18) follow from Eq. (6) as

$$\langle\rho_i^n(0)\rangle = \hat{\rho}_i^n, \qquad i = 0, 1 \tag{19}$$

We see that Eqs. (17)–(19) can be solved sequentially. That is, the $n = 0$ equations are just a restatement of Eqs. (8) and (9), and the $n = 1$ equations are self-contained for $\langle\rho_i\rangle$, whose solution has been reported earlier[8,9] for a_i and b_i independent of time. At any higher level n, the equations for $\langle\rho_i^n\rangle$ depend only upon the $\langle\rho_i^{n-1}\rangle$, which are conceptually known from the prior consideration of the level $(n-1)$ equations. If one is only interested in the ensemble-averaged solution $\langle\rho\rangle$, it is not necessary to consider these higher-level n equations.

Such simplicity is not extant for a more general form of $F_i(\rho, t)$. In particular, it is much more difficult to treat the case considered by Vanderhaegen and Deutsch (VD)[1] as described by Eq. (13). In this case one must actually solve for the joint probability functions $P_i(\rho, t)$ and subsequently perform the numerical integration over ρ to obtain $\langle\rho\rangle$ or any other ensemble average. However, for this problem VD were able to obtain the $P_i(\rho, t)$ analytically in terms of Bessel functions by using a classic Green's function technique. Such an analytical solution is not possible for

general functions $F_i(\rho, t)$. This state of affairs leads us to the consideration of a general numerical method, valid for arbitrary $F_i(\rho, t)$, to obtain the $P_i(\rho, t)$. This is described in the next section of this paper, and the subsequent section gives a few numerical results based upon this method. Following these numerical considerations, we consider in an appendix a restricted class of functions $F_i(\rho, t)$ for which an analytical solution of Eqs. (4)–(6) can be found using standard Laplace transform methods. The VD case given by Eq. (13) falls into this class of problems which can be treated analytically.

3. THE NUMERICAL METHOD

We initially consider Eqs. (4)–(6) in slightly less than full generality. Specifically, we develop a numerical solution method for these equations under two simplifying assumptions. A completely general treatment will be given at the end of this section. The first simplification is that of stationary statistics, by which we mean that the Markov functions λ_i are constant, independent of time. In this case, Eq. (10) gives the simple result

$$p_i = \frac{\lambda_i}{\lambda_0 + \lambda_1} \tag{20}$$

To discuss the second simplification, we introduce the functions $\rho_0(t)$ and $\rho_1(t)$ as the solutions to the nonstochastic equations

$$\frac{d\rho_i(t)}{dt} + F_i(\rho_i, t) = 0, \qquad i = 0, 1 \tag{21}$$

with initial conditions

$$\rho_i(0) = \hat{\rho}_i, \qquad i = 0, 1 \tag{22}$$

The physical significance of $\rho_i(t)$ is that it represents the dynamics of the problem for the statistical realization corresponding to the system being in state i for all times $0 \leqslant t < \infty$. Our second simplification in this initial development is the assumption that the solution $\rho(t)$ for a given (but arbitrary) realization of the statistics is bounded according to

$$\rho_0(t) \leqslant \rho(t) \leqslant \rho_1(t) \tag{23}$$

That is, the statistical realization corresponding to the system being in state 0 for all times forms a lower bound on the solution for any other realization, and the statistical realization corresponding to the system being in state 1 for all times forms an upper bound on the solution for any other

realization. This situation is often encountered in practice and is the case for the previously reported analytical solutions corresponding to Eq. (13)[1,4] and Eq. (14).[8,9] If Eq. (23) is true, it must be the case that

$$P_i(\rho, t) = 0, \qquad \rho < \rho_0(t), \quad \rho > \rho_1(t) \tag{24}$$

Thus, the joint probability functions have compact support over an interval which is time dependent. We remark that although Eq. (23) is often the case in practice, it is in general a very restrictive assumption. At the end of this section, we generalize our considerations so that Eq. (23) is not required.

To proceed with the development of the numerical scheme for solving Eqs. (4)–(6), we first note that if the system is in state i at $t=0$, there is a probability given by $\exp(-t/\lambda_i)$ of the system being in state i for all times in the interval $(0, t)$. Further, the probability of the system being in state i at $t=0$ is just p_i as given by Eq. (20). Finally, if the system is in state i for $(0, t)$, the solution for $P_i(\rho, t)$ will contain a Dirac delta function with argument $\rho - \rho_i(t)$. These observations suggest a change of variable from $P_i(\rho, t)$ to $Q_i(\rho, t)$ according to the equation

$$\begin{aligned} P_i(\rho, t) = {} & p_i \exp(-t/\lambda_i)\, \delta[\rho - \rho_i(t)] \\ & + Q_i(\rho, t)\, H[\rho_1(t) - \rho]\, H[\rho - \rho_0(t)] \end{aligned} \tag{25}$$

where $H(z)$ is the Heaviside (unit step) function. The Heaviside functions were introduced in Eq. (25) because of the compact support indicated in Eq. (24). Use of Eq. (25) in Eqs. (4) and (5) gives

$$\frac{\partial Q_0}{\partial t} - \frac{\partial}{\partial \rho}(F_0 Q_0) = \frac{Q_1}{\lambda_1} - \frac{Q_0}{\lambda_0} \tag{26}$$

$$\frac{\partial Q_1}{\partial t} - \frac{\partial}{\partial \rho}(F_1 Q_1) = \frac{Q_0}{\lambda_0} - \frac{Q_1}{\lambda_1} \tag{27}$$

These two coupled equations for $Q_i(\rho, t)$ hold in the time-dependent interval $\rho_0(t) < \rho < \rho_1(t)$. Using Eq. (25) in Eq. (6), we deduce the homogeneous initial conditions

$$Q_i(\rho, 0) = 0 \tag{28}$$

The change of dependent variables given by Eq. (25) also yields jump conditions, which are the driving terms for the solution, at $\rho = \rho_0(t)$ and $\rho = \rho_1(t)$. These are given by

$$Q_0(\rho_1, t) = \frac{p_1 \exp(-t/\lambda_1)}{\lambda_1 [F_0(\rho_1, t) - F_1(\rho_1, t)]} \tag{29}$$

$$Q_1(\rho_0, t) = \frac{p_0 \exp(-t/\lambda_0)}{\lambda_0[F_0(\rho_0, t) - F_1(\rho_0, t)]} \tag{30}$$

Equations (29) and (30) arise from an examination of the change of variables from $P_i(\rho, t)$ to $Q_i(\rho, t)$ at the interval edges $\rho_0(t)$ and $\rho_1(t)$. However, they can also be obtained from the normalization condition on the $P_i(\rho, t)$ given by Eq. (7). In the special case of stationary statistics, Eqs. (7) and (25) combine to give the normalization conditions on the $Q_i(\rho, t)$ as

$$\int_{\rho_0(t)}^{\rho_1(t)} d\rho\, Q_i(\rho, t) = p_i[1 - \exp(-t/\lambda_i)] \tag{31}$$

If we integrate Eqs. (26) and (27) over ρ in the interval $\rho_0(t) < \rho < \rho_1(t)$ and subsequently make use of Eq. (31), we again arrive at the jump conditions given by Eqs. (29) and (30). Thus, given the differential equations which the $Q_i(\rho, t)$ satisfy, namely Eqs. (27) and (28), the set of two jump conditions given by Eqs. (29) and (30) and the set of two normalization conditions given by Eq. (31) are not independent. Either of these two sets can be disregarded without losing any information.

To solve these differential equations for the $Q_i(\rho, t)$ numerically, we recast them into a weak form by taking moments in the ρ variable. We first treat Eq. (26) for $Q_0(\rho, t)$ and consider an infinite set of functions $w_m^{(0)}(\rho, t)$, $m \geqslant 1$, which are linearly independent and form a complete set in ρ for each time t. We multiply Eq. (26) by $w_m^{(0)}(\rho, t)$ and integrate over $\rho_0(t) < \rho < \rho_1(t)$. This infinite set of moment equations is equivalent to Eq. (26) in information since the $w_m^{(0)}(\rho, t)$ form a complete set. To be precise, there are very mild smoothness conditions on the functions F_i in Eqs. (26) and (27) for this equivalence to be extant, but these conditions are almost always satisfied in physical problems. However, the equivalence (or not) between Eq. (26) and the infinite set of moment equations is not crucial to our development. In obtaining numerical results, we by necessity deal only with a finite number of moment equations and, as will become clear shortly, our method can be considered as a Galerkin (weighted residual) numerical scheme. A bit of algebraic manipulation on these moment equations gives the result

$$\begin{aligned}
&\frac{d}{dt}\int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho)\, Q_0(\rho) - w_m^{(0)}(\rho_1)\, Q_0(\rho_1)\frac{d\rho_1}{dt} + w_m^{(0)}(\rho_0)\, Q_0(\rho_0)\frac{d\rho_0}{dt} \\
&\quad = \int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho)\left[\frac{Q_1(\rho)}{\lambda_1} - \frac{Q_0(\rho)}{\lambda_0}\right] \\
&\qquad + \int_{\rho_0}^{\rho_1} d\rho\left[Q_0(\rho)\frac{\partial w_m^{(0)}(\rho)}{\partial t} + w_m^{(0)}(\rho)\frac{\partial}{\partial \rho}[F_0(\rho)\, Q_0(\rho)]\right], \quad m \geqslant 1
\end{aligned} \tag{32}$$

In writing Eq. (32), we have not indicated the time dependence of all quantities, to simplify the notation somewhat. Using Eq. (21) to eliminate $d\rho_i/dt$ in Eq. (32) gives the slightly simpler form

$$\frac{d}{dt}\int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho)\, Q_0(\rho) + [F_1(\rho_1) - F_0(\rho_1)]\, w_m^{(0)}(\rho_1)\, Q_0(\rho_1)$$
$$+ \int_{\rho_0}^{\rho_1} d\rho \left[F_0(\rho) \frac{\partial w_m^{(0)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(0)}(\rho)}{\partial t} \right] Q_0(\rho)$$
$$= \int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho) \left[\frac{Q_1(\rho)}{\lambda_1} - \frac{Q_0(\rho)}{\lambda_0} \right], \qquad m \geqslant 1 \tag{33}$$

Finally, using the jump condition given by Eq. (29) in Eq. (33), we find

$$\frac{d}{dt}\int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho)\, Q_0(\rho) + \int_{\rho_0}^{\rho_1} d\rho \left[F_0(\rho) \frac{\partial w_m^{(0)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(0)}(\rho)}{\partial t} \right] Q_0(\rho)$$
$$= \int_{\rho_0}^{\rho_1} d\rho\, w_m^{(0)}(\rho) \left[\frac{Q_1(\rho)}{\lambda_1} - \frac{Q_0(\rho)}{\lambda_0} \right] + \frac{p_1}{\lambda_1} w_m^{(0)}(\rho_1) \exp(-t/\lambda_1), \quad m \geqslant 1 \tag{34}$$

We treat Eq. (27) for $Q_1(\rho, t)$ in a similar manner, using a complete set of weight functions $w_m^{(1)}(\rho, t)$, $m \geqslant 1$. We find, again using Eq. (21) and the jump condition given by Eq. (30),

$$\frac{d}{dt}\int_{\rho_0}^{\rho_1} d\rho\, w_m^{(1)}(\rho)\, Q_1(\rho) + \int_{\rho_0}^{\rho_1} d\rho \left[F_1(\rho) \frac{\partial w_m^{(1)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(1)}(\rho)}{\partial t} \right] Q_1(\rho)$$
$$= \int_{\rho_0}^{\rho_1} d\rho\, w_m^{(1)}(\rho) \left[\frac{Q_0(\rho)}{\lambda_0} - \frac{Q_1(\rho)}{\lambda_1} \right] + \frac{p_0}{\lambda_0} w_m^{(1)}(\rho_0) \exp(-t/\lambda_0), \quad m \geqslant 1 \tag{35}$$

In summary, the moment equations (34) and (35) are a weak form of the differential equations (26) and (27), and incorporate the jump conditions given by Eqs. (29) and (30).

To proceed, we expand the functions $Q_i(\rho, t)$ in specified functions $\phi_n^{(i)}(\rho, t)$ according to

$$Q_0(\rho, t) = \sum_{n=1}^{\infty} c_n^{(0)}(t)\, \phi_n^{(0)}(\rho, t) \tag{36}$$

$$Q_1(\rho, t) = \sum_{n=1}^{\infty} c_n^{(1)}(t)\, \phi_n^{(1)}(\rho, t) \tag{37}$$

where the $\phi_n^{(i)}(\rho, t)$, $n \geqslant 1$, represent a complete set of linearly independent functions in ρ for any time t for each index $i = 0, 1$, and the $c_n^{(i)}(t)$ are expansion coefficients to be determined. Without loss of generality, we assume that the expansion functions $\phi_n^{(i)}(\rho, t)$ have been made orthogonal to the weight functions $w_m^{(i)}(\rho, t)$, and further that these functions are normalized such that

$$\int_{\rho_0(t)}^{\rho_1(t)} d\rho\, w_m^{(i)}(\rho, t)\phi_n^{(i)}(\rho, t) = \delta_{mn}, \qquad i = 0, 1 \tag{38}$$

where δ_{mn} is the Kronecker delta symbol. Inserting Eqs. (36) and (37) into Eqs. (34) and (35) and making use of Eq. (38), we find the coupled ordinary differential equations for the expansion coefficients given by

$$\frac{dc_m^{(0)}(t)}{dt} + \frac{1}{\lambda_0} c_m^{(0)}(t) + \sum_{n=1}^{\infty} A_{mn}^{(0)}(t)\, c_n^{(0)}(t) = \sum_{n=1}^{\infty} B_{mn}^{(1)}(t)\, c_n^{(1)}(t) + S_m^{(0)}(t), \qquad m \geqslant 1 \tag{39}$$

$$\frac{dc_m^{(1)}(t)}{dt} + \frac{1}{\lambda_1} c_m^{(1)}(t) + \sum_{n=1}^{\infty} A_{mn}^{(1)}(t)\, c_n^{(1)}(t) = \sum_{n=1}^{\infty} B_{mn}^{(0)}(t)\, c_n^{(0)}(t) + S_m^{(1)}(t), \qquad m \geqslant 1 \tag{40}$$

Here the matrix elements $A_{mn}^{(i)}(t)$ and $B_{mn}^{(i)}(t)$ are given by

$$A_{mn}^{(i)}(t) = \int_{\rho_0}^{\rho_1} d\rho \left[F_i(\rho) \frac{\partial w_m^{(i)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(i)}(\rho)}{\partial t} \right] \phi_n^{(i)}(\rho) \tag{41}$$

$$B_{mn}^{(i)}(t) = \frac{1}{\lambda_i} \int_{\rho_0}^{\rho_1} d\rho\, w_m^{(j)}(\rho)\, \phi_n^{(i)}(\rho), \qquad j \neq i \tag{42}$$

and the source components $S_m^{(i)}(t)$ are defined by

$$S_m^{(i)}(t) = (p_j/\lambda_j)\, w_m^{(i)}(\rho_j) \exp(-t/\lambda_j), \qquad j \neq i \tag{43}$$

Once again, to simplify the notation we have not indicated the time variable of the functions on the right-hand sides of Eqs. (41)–(43). For Eqs. (36) and (37) to satisfy the zero initial conditions given by Eq. (28), we must have

$$c_m^{(0)}(0) = c_m^{(1)}(0) = 0 \tag{44}$$

which constitute the initial conditions on Eqs. (39) and (40).

The infinite set of moment-expansion equations developed here are exact and generally, in accord with the discussion above Eq. (32), their solution is equivalent to the solution of the differential equations for the $Q_i(\rho, t)$. To form a numerical approximation scheme, we replace the upper summation limits in Eqs. (39) and (40) by a finite integer N and use these moment equations only for the indices $1 \leqslant m \leqslant N$. This gives $2N$ ordinary differential equations for the expansion coefficients $c_m^{(0)}(t)$ and $c_m^{(1)}(t)$, $1 \leqslant m \leqslant N$. These equations can be solved numerically by any one of a number of standard solvers. The accuracy of the Nth-order approximation obviously depends upon N, and one would expect greater accuracy as N increases. The accuracy for a given value of N will also depend upon the choice of the expansion functions $\phi_n^{(i)}(\rho, t)$ as well as the choice of the weight functions $w_m^{(i)}(\rho, t)$. In particular, if one chooses the expansion functions $\phi_n^{(i)}(\rho, t)$ to reflect any *a priori* knowledge one has concerning the ρ dependence of $Q_i(\rho, t)$, one would expect good results for low N and fast convergence as N increases. In the numerical applications we consider in the next section, we have not attempted to optimize the expansion and weight functions in any way; we have used simple polynomials in ρ for both the expansion and weight functions, and we observe reasonably fast convergence as a function of N.

This numerical method actually produces a very simple and clean analytical result in lowest order. Specifically, we set $N=1$, choose unit weight functions, i.e.,

$$w_1^{(0)}(\rho, t) = w_1^{(1)}(\rho, t) = 1 \tag{45}$$

and choose expansion functions which are independent of ρ. Enforcing Eq. (38), this implies

$$\phi_1^{(0)}(\rho, t) = \phi_1^{(1)}(\rho, t) = \frac{1}{\rho_1(t) - \rho_0(t)} \tag{46}$$

We then find that Eqs. (39)–(43) reduce to the two equations

$$\frac{dc_1^{(0)}(t)}{dt} + \frac{c_1^{(0)}(t)}{\lambda_0} = \frac{c_1^{(1)}(t)}{\lambda_1} + \frac{p_1 \exp(-t/\lambda_1)}{\lambda_1} \tag{47}$$

$$\frac{dc_1^{(1)}(t)}{dt} + \frac{c_1^{(1)}(t)}{\lambda_1} = \frac{c_1^{(0)}(t)}{\lambda_0} + \frac{p_0 \exp(-t/\lambda_0)}{\lambda_0} \tag{48}$$

The solution to these two equations subject to the zero initial conditions given by Eq. (44) is easily verified to be

$$c_1^{(i)}(t) = p_i[1 - \exp(-t/\lambda_i)] \tag{49}$$

Thus, in this lowest order approximation, we have, using Eqs. (46) and (49) in Eqs. (36) and (37),

$$Q_i(\rho, t) = \frac{p_i[1 - \exp(-t/\lambda_i)]}{\rho_1(t) - \rho_0(t)} \tag{50}$$

Use of Eq. (50) in Eq. (25) then gives the $P_i(\rho, t)$, and subsequent use of these $P_i(\rho, t)$ in Eq. (12) with $G(\rho) = \rho$ gives an explicit analytical approximation for the ensemble-averaged solution $\langle \rho(t) \rangle$. This is given by

$$\langle \rho(t) \rangle = p_0 \rho_0(t) \exp(-t/\lambda_0) + p_1 \rho_1(t) \exp(-t/\lambda_1)$$
$$+ \tfrac{1}{2}[\rho_0(t) + \rho_1(t)][1 - p_0 \exp(-t/\lambda_0) - p_1 \exp(-t/\lambda_1)] \tag{51}$$

where $\rho_0(t)$ and $\rho_1(t)$ are the nonstochastic solutions defined by Eqs. (21) and (22). We note from Eq. (51) that all of the influence of the functions $F_i(\rho, t)$ is indirect, influencing the solution for $\langle \rho(t) \rangle$ only through the $\rho_i(t)$. One can easily show that Eq. (51) gives the true behavior for $\langle \rho(t) \rangle$ for small time. More generally, although Eq. (51) is the result of the lowest order ($N = 1$) approximation using very simple expansion and weight functions, it may be useful in assessing in a qualitative way the overall dynamical behavior of the system. We examine, through numerical examples, the behavior of our approximation scheme for higher values of N in the next section, and there we will also see numerically the accuracy of the $N = 1$ result expressed analytically by Eq. (51).

Before leaving this section, however, we recall that the analysis just given involved two simplifying assumptions, namely: (1) stationary statistics, and (2) simple bounds on $\rho(t)$ as expressed by Eq. (23). We now briefly indicate the development of the numerical method in the general case, without making these two simplifying assumptions. We begin by discussing the bounds on $\rho(t)$; i.e., we seek the analog of Eq. (23) in the general case. We note that one, or perhaps more than one, of the realizations of the statistics will give, at a given time t, a maximum result for $\rho(t)$. At a second time, one or more different realizations (or perhaps the same realizations as for the first time) will also give a maximum result for $\rho(t)$. We denote this upper bound on $\rho(t)$ by $U(t)$. Similarly, at any given time one or more statistical realizations will give the smallest possible value for $\rho(t)$. We denote this lower bound on $\rho(t)$ by $L(t)$. Thus, for an arbitrary realization of the statistics we have

$$L(t) \leqslant \rho(t) \leqslant U(t) \tag{52}$$

The bounding functions satisfy the equations

$$\frac{dU(t)}{dt} + F_u(U, t; T) = 0, \qquad 0 \leqslant t \leqslant T \tag{53}$$

$$\frac{dL(t)}{dt} + F_l(L, t; T) = 0, \qquad 0 \leqslant t \leqslant T \tag{54}$$

The initial condition on Eqs. (53) and (54) is, in each case, either $\hat{\rho}_0$ or $\hat{\rho}_1$ [see Eq. (3)], depending upon the state of the system at $t = 0$. The function $F_u(U, t; T)$ is, at any time t, either $F_0(U, t)$ or $F_1(U, t)$, chosen such that the function $U(t)$ is the maximum value, over all realizations, of $\rho(t)$ at $t = T$. That is, it is this function F_u which reflects the particular realization of the statistics which maximizes $\rho(t)$ at $t = T$. Similarly, the function $F_l(L, t; T)$ is, at any time t, either $F_0(L, t)$ or $F_1(L, t)$, and this function reflects the particular realization of the statistics which minimizes $\rho(t)$ at $t = T$. In view of Eq. (52), we have

$$P_i(\rho, t) = 0, \qquad \rho < L(t) \quad \text{and} \quad \rho > U(t) \tag{55}$$

We assume that the functions $U(t)$, $L(t)$, $F_u(U, t; T)$, and $F_l(L, t; T)$ can be found and hence we take them as known. In our final result, the functions F_u and F_l do not appear. Thus, it is really only necessary that the bounding functions $L(t)$ and $U(t)$ be known explicitly. We remark that in general the functions $L(t)$ and $U(t)$ are difficult to determine. However, in many problems they can be found from simple physical considerations. These functions determine the region of support (in ρ) of the functions $P_i(\rho, t)$, and our numerical method makes use of this compact support.

Considering now the solution of Eqs. (4)–(6) in the general case, which allows the Markov functions λ_i to depend upon time, we note that if the system is in state i at $t = 0$, the probability of the system being in state i for the interval $(0, t)$ is given by

$$\text{Prob} = \exp(-\tau_i) \tag{56}$$

where

$$\tau_i = \int_0^t dt'/\lambda_i(t') \tag{57}$$

Further, the probability of the system being in state i at $t = 0$ is just $p_i(0)$, and if the system is in state i for $(0, t)$, the joint probability $P_i(\rho, t)$ will contain a Dirac delta function with argument $\rho - \rho_i(t)$, where $\rho_i(t)$ is

defined by Eqs. (21) and (22). These observations together with Eq. (55) lead us to introduce the change of variables

$$P_i(\rho, t) = p_i(0) \exp(-\tau_i)\, \delta[\rho - \rho_i(t)] + Q_i(\rho, t)\, H[U(t) - \rho]\, H[\rho - L(t)] \tag{58}$$

We find that within the interval $L(t) < \rho < U(t)$ the $Q_i(\rho, t)$ satisfy the coupled equations

$$\frac{\partial Q_0}{\partial t} - \frac{\partial}{\partial \rho}(F_0 Q_0) = \frac{Q_1}{\lambda_1} - \frac{Q_0}{\lambda_0} + \frac{p_1(0)}{\lambda_1} \exp(-\tau_1)\, \delta(\rho - \rho_1) \tag{59}$$

$$\frac{\partial Q_1}{\partial t} - \frac{\partial}{\partial \rho}(F_1 Q_1) = \frac{Q_0}{\lambda_0} - \frac{Q_1}{\lambda_1} + \frac{p_0(0)}{\lambda_0} \exp(-\tau_0)\, \delta(\rho - \rho_0) \tag{60}$$

with initial conditions

$$Q_i(\rho, 0) = 0 \tag{61}$$

We note the appearance of delta-function terms in Eqs. (59) and (60) which were not present in the previous analysis [see Eqs. (26) and (27)]. We comment more on this point later. The change of variables given by Eq. (58) also leads to boundary terms at $\rho = L(t)$ and $\rho = U(t)$ given by

$$[F_0(L) - F_l(L)]\, Q_0(L) = 0 \tag{62}$$

$$[F_0(U) - F_u(U)]\, Q_0(U) = 0 \tag{63}$$

$$[F_1(L) - F_l(L)]\, Q_1(L) = 0 \tag{64}$$

$$[F_1(U) - F_u(U)]\, Q_1(U) = 0 \tag{65}$$

In writing Eqs. (62)–(65), we have only indicated the ρ variable in all functions for simplicity of notation. We note that at any time t, each of the functions F_l and F_u is either F_0 or F_1. Thus, two of the four equations (62)–(65) are identities. The remaining two equations constitute nontrivial conditions on the $Q_i(\rho, t)$.

To develop the numerical scheme, we take moments of Eqs. (59) and (60) with respect to weight functions $w_m^{(i)}(\rho, t)$, $m \geqslant 1$, just as we did earlier. Omitting the algebraic details, we find, making use of Eqs. (53), (54), and (62)–(65), the weak form of the equations for $Q_i(\rho, t)$ given by

$$\frac{d}{dt}\int_L^U d\rho\, w_m^{(0)}(\rho)\, Q_0(\rho) + \int_L^U d\rho \left[F_0(\rho) \frac{\partial w_m^{(0)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(0)}(\rho)}{\partial t} \right] Q_0(\rho)$$
$$= \int_L^U d\rho\, w_m^{(0)}(\rho) \left[\frac{Q_1(\rho)}{\lambda_1} - \frac{Q_0(\rho)}{\lambda_0} \right] + S_m^{(0)}, \qquad m \geqslant 1 \tag{66}$$

$$\frac{d}{dt}\int_L^U d\rho\, w_m^{(1)}(\rho)\, Q_1(\rho) + \int_L^U d\rho \left[F_1(\rho)\frac{\partial w_m^{(1)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(1)}(\rho)}{\partial t}\right] Q_1(\rho)$$

$$= \int_L^U d\rho\, w_m^{(1)}(\rho)\left[\frac{Q_0(\rho)}{\lambda_0} - \frac{Q_1(\rho)}{\lambda_1}\right] + S_m^{(1)}, \qquad m \geqslant 1 \tag{67}$$

where we have defined

$$S_m^{(i)}(t) = \frac{p_j(0)}{\lambda_j(t)}\, w_m^{(i)}(\rho_j)\exp(-\tau_j), \qquad j \neq i \tag{68}$$

To proceed, we expand the functions $Q_i(\rho, t)$ just as before according to Eqs. (36) and (37), with the limits of integration on the normalization conditions given by Eq. (38) now taken as $L(t)$ and $U(t)$. We arrive at the coupled ordinary differential equations for the expansion coefficients $c_m^{(i)}(t)$ given by

$$\frac{dc_m^{(0)}(t)}{dt} + \frac{1}{\lambda_0(t)}\, c_m^{(0)}(t) + \sum_{n=1}^{\infty} A_{mn}^{(0)}(t)\, c_n^{(0)}(t)$$

$$= \sum_{n=1}^{\infty} B_{mn}^{(1)}(t)\, c_n^{(1)}(t) + S_m^{(0)}(t), \qquad m \geqslant 1 \tag{69}$$

$$\frac{dc_m^{(1)}(t)}{dt} + \frac{1}{\lambda_1(t)}\, c_m^{(1)}(t) + \sum_{n=1}^{\infty} A_{mn}^{(1)}(t)\, c_n^{(1)}(t)$$

$$= \sum_{n=1}^{\infty} B_{mn}^{(0)}(t)\, c_n^{(0)}(t) + S_m^{(1)}(t), \qquad m \geqslant 1 \tag{70}$$

The matrix elements $A_{mn}^{(i)}(t)$ and $B_{mn}^{(i)}(t)$ in Eqs. (69) and (70) are given by

$$A_{mn}^{(i)}(t) = \int_L^U d\rho \left[F_i(\rho)\frac{\partial w_m^{(i)}(\rho)}{\partial \rho} - \frac{\partial w_m^{(i)}(\rho)}{\partial t}\right] \phi_n^{(i)}(\rho) \tag{71}$$

$$B_{mn}^{(i)}(t) = \frac{1}{\lambda_i(t)}\int_L^U d\rho\, w_m^{(j)}(\rho)\, \phi_n^{(i)}(\rho), \qquad j \neq i \tag{72}$$

Equations (69) and (70) are to be solved subject to the initial conditions

$$c_m^{(0)}(0) = c_m^{(1)}(0) = 0 \tag{73}$$

The Nth-order approximation follows by replacing the upper summation limits in Eqs. (69) and (70) by a finite integer N and using these moment equations for the restricted set of indices $1 \leqslant m \leqslant N$. This completes the development of our numerical scheme to solve Eqs. (4)–(6) in the most general case.

We note the similarity of our equations in the general case to those we obtained earlier in a more restricted setting. Specifically, Eqs. (68)–(73) are the generalizations of Eqs. (43), (39)–(42), and (44), respectively. If we set $L(t)=\rho_0(t)$, $U(t)=\rho_1(t)$, and take the Markov functions λ_i to be independent of time, our general equations (68)–(73) reduce identically to Eqs. (39)–(44). However, it might also be noted that the structure of the intermediate equations preceding our final result is different in the general case than in the simplified case. In particular, Eqs. (59) and (60) contain delta-function inhomogeneous terms, whereas Eqs. (26) and (27) do not. Further, Eqs. (62)–(65) represent homogeneous boundary conditions, whereas Eqs. (29) and (30) are inhomogeneous. The delta functions in Eqs. (59) and (60) in the general case take the place, and form the equivalent driving terms for the solution, of the inhomogeneous boundary conditions given by Eqs. (29) and (30) in the simplified cases. This equivalence between the inhomogeneous delta-function terms and the inhomogeneous boundary conditions is evident from the close correspondence of our final equations in the general and simplified cases.

It is clear that the delta functions in Eqs. (59) and (60) will lead to a discontinuity in the solution for $Q_0(\rho, t)$ at $\rho=\rho_1(t)$ and a similar discontinuity in the solution for $Q_1(\rho, t)$ at $\rho=\rho_0(t)$. This suggests that a more rapidly converging numerical solution method would be one based upon separate smooth expansions on either side of the discontinuity, with appropriate jump conditions connecting the expansions at the point of discontinuity. Such a scheme is easily developed by a straightforward extension of the analysis given here, but the details are algebraically cumbersome and will not be pursued in this paper. This two-expansion scheme in the limit of $L(t)=\rho_0(t)$ and $U(t)=\rho_1(t)$ reduces to the single-expansion method already discussed, since in this limit the locations of the delta functions coincide with the ends of the support interval of the $Q_i(\rho, t)$.

4. NUMERICAL RESULTS

In this section we give representative numerical results using the expansion method just described. We first apply our method to a problem considered earlier[1,4] which describes the transmission of photons through a purely scattering statistical rod. This problem is one for which $\rho(t)$ decreases monotonically with time for any realization of the statistics, and corresponds to $F_i=a_i\rho^2$, with the constants $a_i>0$, in the notation of Eqs. (2) and (21). The second problem we consider corresponds to $F_i=a_i\rho^{1/2}$, with $a_i<0$. For any realization of the statistics, this problem leads to a solution for $\rho(t)$ which increases monotonically with time. Both of these problems have an analytical solution for the $P_i(\rho, t)$ as outlined in the

appendix, and we use these analytical results to assess the convergence of our numerical method as a function of N, the order of the approximation. The final example we consider is a simple problem arising in extended kinetic theory,[5,6] for which no analytical results are available.

All three of these problems share the common characteristic that $\rho_0(t)$ and $\rho_1(t)$ bound $\rho(t)$ for any realization of the statistics, i.e.,

$$L(t) = \rho_0(t); \qquad U(t) = \rho_1(t) \tag{74}$$

Further, in all three cases we use very simple expansion and weight functions, namely polynomials in ρ orthogonal on the time-dependent interval (L, U). Specifically, we choose the weight functions to be

$$w_m^{(i)}(\rho, t) = P_{m-1}(x), \qquad m \geqslant 1 \tag{75}$$

where P_m denotes the mth-order Legendre polynomial, and

$$x = \frac{2\rho - L(t) - U(t)}{U(t) - L(t)} \tag{76}$$

The change of variables from ρ to x given by Eq. (76) transforms the ρ interval (L, U) to $-1 \leqslant x \leqslant 1$, the natural interval for Legendre polynomials. We choose the expansion functions as similar polynomials according to

$$\phi_n^{(i)}(\rho, t) = P_{n-1}(x)/N_{n-1}(t), \qquad n \geqslant 1 \tag{77}$$

where $N_n(t)$ is a normalization factor introduced to ensure that Eq. (38) is satisfied, and is given by

$$N_n(t) = \frac{U(t) - L(t)}{2n+1}, \qquad n \geqslant 0 \tag{78}$$

Finally, in all three examples we consider stationary statistics, i.e., the Markov functions λ_i are taken as independent of time, and we choose the initial condition to be nonstochastic (independent of the state i at $t = 0$). By a proper scaling of the dependent variable ρ, we can thus use, without loss of generality, a unit initial condition, i.e.,

$$\rho(0) = \hat{\rho}_0 = \hat{\rho}_1 = 1 \tag{79}$$

The numerical procedure is as follows. For given functions $F_i(\rho, t)$, Eqs. (21) and (22) are solved to obtain $L(t)$ and $U(t)$ [see Eq. (74)]. One then computes the source terms $S_m^{(i)}(t)$ from Eq. (68) using the weight

functions given by Eq. (75), and computes the matrix elements $A_{mn}^{(i)}(t)$ and $B_{mn}^{(i)}(t)$ from Eqs. (71) and (72) using the expansion and weight functions given by Eqs. (75) and (77). For general $F_i(\rho, t)$, the evaluation of these matrix elements will require numerical integration. The system of equations given by Eqs. (69) and (70) for $1 \leqslant m \leqslant N$ is then solved numerically using any standard package (we used a Gear package) for numerical integration of a set of coupled initial value first-order ordinary differential equations. From the computed values of $c_n^{(i)}(t)$, one reconstructs the $Q_i(\rho, t)$ according to Eq. (36), replacing the upper summation limit by N, and then finds the $P_i(\rho, t)$ from Eq. (58). Any desired ensemble average then follows from Eq. (12) via numerical integration. In our three examples, we took $\langle \rho(t) \rangle$, the ensemble-averaged solution, as the quantity of interest and thus chose $G(\rho) = \rho$ in Eq. (12). It might be noted that in computing $\langle \rho(t) \rangle$ using polynomial expansion functions according to Eq. (77), $\langle \rho(t) \rangle$ is entirely determined by the first two expansion coefficients $c_n^{(i)}(t)$ for $n = 1$ and 2. Specifically, we have

$$\langle \rho(t) \rangle = p_0 \rho_0(t) \exp(-\tau_0) + p_1 \rho_1(t) \exp(-\tau_1) + \tfrac{1}{2}\{[\rho_1(t) + \rho_0(t)]\, k_1(t) + [\rho_1(t) - \rho_0(t)]\, k_2(t)\} \tag{80}$$

where

$$k_n(t) = c_n^{(0)}(t) + c_n^{(1)}(t), \qquad n = 1, 2 \tag{81}$$

The $c_n^{(i)}(t)$ for $n \geqslant 2$ do not enter into the expression for $\langle \rho(t) \rangle$, since ρ is orthogonal to $P_n(x)$ on the interval (L, U) for $n \geqslant 2$. Of course, the $c_n^{(i)}(t)$ for $n = 1, 2$ are coupled to the higher n values according to Eqs. (69) and (70).

Table I gives numerical results for the problem originally considered by Vanderhaegen and Deutsch,[1] namely

$$F_i(\rho) = a_i \rho^2 \tag{82}$$

with a_0 and a_1 both positive constants. This leads to a monotonically decreasing solution for $\rho(t)$ as time increases. This table gives $\langle \rho(t) \rangle$ for various times t corresponding to the Nth-order, $1 \leqslant N \leqslant 10$, approximation. The exact results were computed from a numerical integration according to Eq. (12) with $G(\rho) = \rho$ using the analytical results for the $P_i(\rho, t)$ given in the appendix. We see that the numerical scheme converges very rapidly to the exact result for small times, while higher N is needed to obtain accurate results for longer times. In particular, we see that the $N = 1$ result, expressed analytically by Eq. (51), is quite accurate for $t < 1$, but the accuracy deteriorates substantially for longer times. We also observe that

Table I. $\langle \rho(t) \rangle$ for $F_i = a_i \rho^2$, with $a_0 = 9.1$, $a_1 = 0.1$, $\lambda_0 = 0.1$, $\lambda_1 = 1.0$

	$\langle \rho(t) \rangle$						
N	$t = 0.1$	$t = 0.5$	$t = 1$	$t = 5$	$t = 10$	$t = 50$	$t = 100$
1	0.94091	0.77894	0.63951	0.34606	0.25544	0.84430	0.46003
2	0.94052	0.78627	0.63972	0.20971	0.11450	0.03289	0.01775
3	0.94052	0.78705	0.64304	0.21343	0.10243	0.02073	0.01095
4	0.94052	0.78710	0.64341	0.21877	0.10828	0.01834	0.00899
5	0.94052	0.78710	0.64344	0.21988	0.11118	0.01969	0.00921
6	0.94052	0.78710	0.64344	0.21994	0.11172	0.02132	0.01016
7	0.94052	0.78710	0.64344	0.21991	0.11167	0.02210	0.01090
8	0.94052	0.78710	0.64344	0.21990	0.11161	0.02221	0.01118
9	0.94052	0.78710	0.64344	0.21989	0.11159	0.02209	0.01115
10	0.94052	0.78710	0.64344	0.21989	0.11158	0.02198	0.01104
Exact	0.94052	0.78710	0.64344	0.21989	0.11158	0.02193	0.01093

for large times the numerical results as a function of N oscillate noticeably around the exact solution as convergence is approached for large N. This is undoubtedly due to the fact that the exact solution for $Q_i(\rho, t)$ is a relatively smooth function of x for small times, but develops an increasingly sharp peak as time increases. This behavior for $Q_0(\rho, t)$ is shown graphically in Fig. 1, which was constructed from the exact analysis given in the appendix. The curves in Fig. 1 have been normalized at each time to a unit area under the curve. This large-time peak is obviously not well represented by a Legendre expansion of low order, thus accounting for the slower rate of convergence as time increases. A more sophisticated

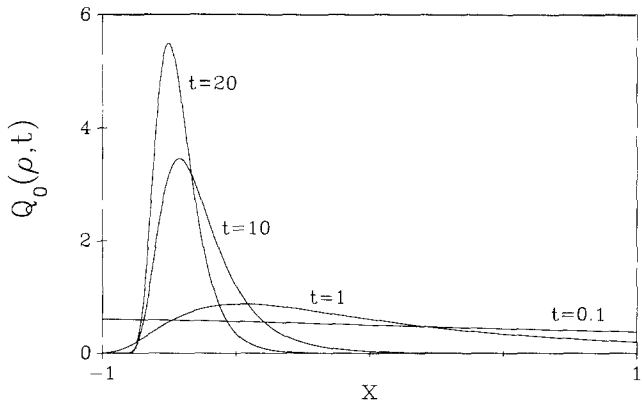

Fig. 1. $Q_0(\rho, t)$, normalized to unit area, for Table I conditions.

choice of the expansion functions, tailored to have the capability of representing this peak, should improve the long-time convergence.

The second case we consider is

$$F_i(\rho) = a_i \rho^{1/2} \tag{83}$$

where a_0 and a_1 are both negative constants. In this case the solution for $\rho(t)$ for any realization of the statistics will grow without bound as time increases. This case is also amenable to the analytical treatment in the appendix, and Table II compares results from our numerical scheme with the exact analytical results. We again observe rapid convergence for small times, followed by slower convergence for intermediate times, and oscillatory convergence for long times. Figure 2 shows $Q_1(\rho, t)$, again normalized to unit area, for various times as computed from the analytical results in the appendix. We again see a very pronounced sharp maximum for long times. Just as in the previous case, this behavior for the $Q_i(\rho, t)$ explains the observed slower convergence rate for long times. In this case, however, the maximum seems to be at $x = -1$ for all times, whereas in the previous case the maximum, while near $x = -1$, was in the interior of the interval $-1 \leqslant x \leqslant 1$.

The final case we consider is the stochastic problem corresponding to

$$F_i = a_i \rho + \rho^2 \tag{84}$$

with a_0 and a_1 both positive constants. In extended kinetic theory,[5,6] the dependent variable ρ is the particle density in an infinite, source-free,

Table II. $\langle \rho(t) \rangle$ for $F_i = a_i \rho^{1/2}$, with $a_0 = -0.1$, $a_1 = -9.1$, $\lambda_0 = 1.0$, $\lambda_1 = 0.1$

	$\langle \rho(t) \rangle$						
N	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 1$	$t = 5$	$t = 10$	$t = 20$
1	1.0094	1.1267	3.2237	10.986	28.109	108.22	423.40
2	1.0094	1.1059	1.6446	2.5019	19.462	67.571	254.42
3	1.0094	1.1059	1.6373	2.4258	15.275	49.516	180.10
4	1.0094	1.1059	1.6365	2.4102	13.647	41.845	147.11
5	1.0094	1.1059	1.6364	2.4066	12.909	37.961	129.38
6	1.0094	1.1059	1.6364	2.4058	12.560	35.863	119.07
7	1.0094	1.1059	1.6364	2.4056	12.398	34.720	112.91
8	1.0094	1.1059	1.6364	2.4056	12.329	34.120	109.27
9	1.0094	1.1059	1.6364	2.4056	12.305	33.836	107.23
10	1.0094	1.1059	1.6364	2.4056	12.302	33.374	106.07
Exact	1.0094	1.1059	1.6364	2.4056	12.354	34.273	109.73

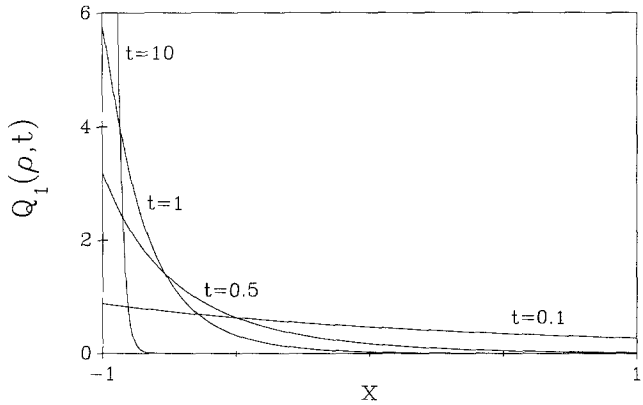

Fig. 2. $Q_1(\rho, t)$, normalized to unit area, for Table II conditions.

homogeneous medium whose density varies stochastically in time between two states 0 and 1. The constant a_i, which is positive, is then the absorption coefficient for removal of particles by the background material when in state i, and the quadratic term in Eq. (84) accounts for the removal of particles due to particle–particle collisions. The nonstochastic constant (the particle–particle cross section) multiplying the ρ^2 term has been set to unity by a proper choice of the time scale. For this problem, no analytical results are available, and Table III shows the convergence of the numerical scheme as N, the order of the approximation, is increased. Once again, we see very rapid convergence for short times and somewhat slower convergence for long times.

In summary, the numerical scheme suggested in this paper appears to work quite well for all cases we have tested, including several not reported here. Presumably, better convergence behavior could be achieved for long

Table III. $\langle \rho(t) \rangle$ for $F_i = a_i \rho + \rho^2$, with $a_0 = 9.1$, $a_1 = 0.1$, $\lambda_0 = 0.1$, $\lambda_1 = 1.0$

	$\langle \rho(t) \rangle$						
N	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 1$	$t = 2$	$t = 5$	$t = 10$
1	0.98139	0.84534	0.49792	0.30938	0.16345	0.06183	0.02513
2	0.98140	0.84767	0.50775	0.30241	0.13045	0.01919	0.00186
3	0.98140	0.84767	0.50793	0.30263	0.13000	0.01745	0.00098
4	0.98140	0.84767	0.50793	0.30265	0.12999	0.01736	0.00093
5	0.98140	0.84767	0.50793	0.30265	0.12999	0.01736	0.00092
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
10	0.98140	0.84767	0.50793	0.30265	0.12999	0.01736	0.00092

times by using expansion functions other than polynomials which can better represent the peaked behavior of the $Q_i(\rho, t)$ for long times. We hope to report results in this direction in the future.

5. CONCLUDING REMARKS

A numerical method, based upon a moments-expansion technique, has been developed in Section 3 for solving the Liouville master equation description of discrete-state Markovian initial value problems. This description is given by Eqs. (4)–(6), and involves general functions $F_i(\rho, t)$ which determine the dynamics of the system. Numerical results for three cases—(1) $F_i(\rho, t) = a_i\rho^2$, $a_i > 0$; (2) $F_i(\rho, t) = a_i\rho^{1/2}$, $a_i < 0$; and (3) $F_i(\rho, t) = a_i\rho + \rho^2$, $a_i > 0$—have been reported and discussed in Section 4. For cases 1 and 2, the numerical results were shown to converge to the exact answers which were constructed using standard Laplace transform techniques as discussed in the appendix for the class of dynamic functions given by $F_i(\rho, t) = a_i F(\rho)$. Further validation of the numerical method comes from comparison of the results for case 1 with results available in the literature.[1,4]

Future investigations in this general area will concentrate on two items, namely (1) the improvement of the convergence rate of the numerical method for large times by utilizing expansion functions more appropriate than simple polynomials, and (2) the extension of the analytic treatment to a wider class of functions than given by Eq. (A.14), to include, in particular, case 3 and other problems drawn from extended kinetic theory.[5,6]

APPENDIX. ANALYTICAL SOLUTION OF THE LIOUVILLE MASTER EQUATION

In this appendix we show that the coupled equations satisfied by $P_0(\rho, t)$ and $P_1(\rho, t)$ can be solved analytically for a certain class of functions $F_i(\rho, t)$. The equations to be considered are

$$\frac{\partial P_0}{\partial t} - \frac{\partial}{\partial \rho}(F_0 P_0) = \frac{P_1}{\lambda_1} - \frac{P_0}{\lambda_0} \tag{A.1}$$

$$\frac{\partial P_1}{\partial t} - \frac{\partial}{\partial \rho}(F_1 P_1) = \frac{P_0}{\lambda_0} - \frac{P_1}{\lambda_1} \tag{A.2}$$

with initial conditions

$$P_i(\rho, 0) = p_i(0)\,\delta(\rho - \hat{\rho}_i), \qquad i = 0, 1 \tag{A.3}$$

The state probabilities $p_i(t)$ are related to the $P_i(\rho, t)$ according to

$$\int_{-\infty}^{\infty} d\rho\, P_i(\rho, t) = p_i(t) \tag{A.4}$$

For this integral to exist, $P_i(\rho, t)$ must vanish for $\rho = \pm\infty$, and hence the characteristics (if any) emanating from $\rho = \pm\infty$ have a zero boundary condition. In our analysis, we restrict ourselves to the case of stationary statistics; that is, λ_0 and λ_1 are constant, independent of time. In this case, the probabilities p_i are also independent of time and given by [see Eq. (20)]

$$p_i = \frac{\lambda_i}{\lambda_0 + \lambda_1} \tag{A.5}$$

Thus, in the case we consider, the integral on the left-hand side of Eq. (A.4) is a constant, independent of time, and this constant is given by Eq. (A.5).

If we also restrict ourselves to functions F_i which are independent of time, we can Laplace transform Eqs. (A.1) and (A.2) with respect to time to obtain

$$\left(s + \frac{1}{\lambda_0}\right)\tilde{P}_0 - \frac{\partial}{\partial\rho}(F_0\tilde{P}_0) = \frac{\tilde{P}_1}{\lambda_1} + p_0\delta(\rho - \hat{\rho}) \tag{A.6}$$

$$\left(s + \frac{1}{\lambda_1}\right)\tilde{P}_1 - \frac{\partial}{\partial\rho}(F_1\tilde{P}_1) = \frac{\tilde{P}_0}{\lambda_0} + p_1\delta(\rho - \hat{\rho}) \tag{A.7}$$

Here s is the transform variable and $\tilde{P}_i(\rho, s)$ is the Laplace transform of $P_i(\rho, t)$. In writing Eqs. (A.6) and (A.7), we have assumed a nonstochastic initial condition, i.e.,

$$\hat{\rho}_0 = \hat{\rho}_1 = \hat{\rho} \tag{A.8}$$

This was done for algebraic simplicity in the considerations to follow, but the more general case $\hat{\rho}_0 \neq \hat{\rho}_1$ can also be treated. The inhomogeneous equations (A.6) and (A.7) can be replaced with the homogeneous equations

$$\left(s + \frac{1}{\lambda_0}\right)\tilde{P}_0 - \frac{\partial}{\partial\rho}(F_0\tilde{P}_0) = \frac{\tilde{P}_1}{\lambda_1}, \qquad \rho \neq \hat{\rho} \tag{A.9}$$

$$\left(s + \frac{1}{\lambda_1}\right)\tilde{P}_1 - \frac{\partial}{\partial\rho}(F_1\tilde{P}_1) = \frac{\tilde{P}_0}{\lambda_0}, \qquad \rho \neq \hat{\rho} \tag{A.10}$$

subject to the discontinuity requirement

$$F_i(\hat{\rho})[\tilde{P}_i(\hat{\rho}^-, s) - \tilde{P}_i(\hat{\rho}^+, s)] = p_i, \qquad i = 0, 1 \tag{A.11}$$

Further, Laplace transformation of Eq. (A.4), with p_i independent of time, gives

$$\int_{-\infty}^{\infty} d\rho\, \tilde{P}_i(\rho, s) = \frac{p_i}{s} \tag{A.12}$$

In writing Eq. (A.11), we have assumed that the $F_i(\rho)$ are continuous at $\rho = \hat{\rho}$, but generalization to discontinuous $F_i(\rho)$ is straightforward.

We use Eq. (A.9) to eliminate $\tilde{P}_1(\rho, s)$ in Eq. (A.10). The result is

$$\frac{\partial}{\partial\rho}\left[F_1 \frac{\partial}{\partial\rho}(F_0\tilde{P}_0)\right] - \left(s+\frac{1}{\lambda_1}\right)\frac{\partial}{\partial\rho}(F_0\tilde{P}_0)$$
$$-\left(s+\frac{1}{\lambda_0}\right)\frac{\partial}{\partial\rho}(F_1\tilde{P}_0) + s\left(s+\frac{1}{\lambda_0}+\frac{1}{\lambda_1}\right)\tilde{P}_0 = 0, \qquad \rho \neq \hat{\rho} \tag{A.13}$$

Equation (A.13) is a second-order differential equation in ρ with, for general $F_i(\rho)$, variable coefficients. As such, a general solution is not available. If, however, we restrict our further considerations to the subclass

$$F_i(\rho) = a_i F(\rho) \tag{A.14}$$

then Eq. (A.13) is amenable to an analytical solution. That is, we treat the case when F_0 and F_1 have a common ρ dependence and differ only by a multiplicative constant. In this case the change of variables

$$r(\rho) = \int_{\hat{\rho}}^{\rho} \frac{d\rho'}{F(\rho')}; \qquad \tilde{R}_0(r, s) = F(\rho)\,\tilde{P}_0(\rho, s) \tag{A.15}$$

reduces Eq. (A.13) to the constant-coefficient equation given by

$$a_0 a_1 \frac{\partial^2 \tilde{R}_0}{\partial r^2} - \left[(a_0+a_1)s + \frac{a_0}{\lambda_1} + \frac{a_1}{\lambda_0}\right]\frac{\partial \tilde{R}_0}{\partial r}$$
$$+ s\left(s+\frac{1}{\lambda_0}+\frac{1}{\lambda_1}\right)\tilde{R}_0 = 0, \qquad r \neq 0 \tag{A.16}$$

The general solution of Eq. (A.16) is readily found to be

$$\tilde{R}_0(r, s) = A_0(s)\exp[\alpha(s)r] + B_0(s)\exp[\beta(s)r] \tag{A.17}$$

where A_0 and B_0 are integration constants, and α and β are given by

$$2a_0 a_1 \gamma(s) = (a_0+a_1)s + \frac{a_0}{\lambda_1} + \frac{a_1}{\lambda_0}$$
$$\pm\left[(a_0-a_1)^2 s^2 + 2(a_0-a_1)\left(\frac{a_0}{\lambda_1}-\frac{a_1}{\lambda_0}\right)s + \left(\frac{a_0}{\lambda_1}+\frac{a_1}{\lambda_0}\right)^2\right]^{1/2} \tag{A.18}$$

For concreteness, we take $\gamma = \alpha$ as corresponding to the plus sign in Eq. (A.18), and $\gamma = \beta$ is associated with the minus sign. From Eq. (A.18) it is easily deduced that $\alpha, \beta > 0$ for $a_0, a_1 > 0$ and $\alpha, \beta < 0$ for $a_0, a_1 < 0$. When a_0 and a_1 have different signs, the signs of α and β depend upon the parameters λ_0 and λ_1 as well as the value of the Laplace transform variable s.

Returning to the variable $\tilde{P}_0$ and ρ, we write Eq. (A.17) as

$$F(\rho)\tilde{P}_0(\rho, s) = \begin{cases} A_0^+(s)\exp[\alpha(s)\, r(\rho)] + B_0^+(s)\exp[\beta(s)\, r(\rho)], & \rho > \hat{\rho} \\ A_0^-(s)\exp[\alpha(s)\, r(\rho)] + B_0^-(s)\exp[\beta(s)\, r(\rho)], & \rho < \hat{\rho} \end{cases} \tag{A.19}$$

where we have divided the ρ space into two regions, one to the left $(-)$ and one to the right $(+)$ of the discontinuity at $\rho = \hat{\rho}$. In complete analogy, we find that $\tilde{P}_1$ is given by

$$F(\rho)\,\tilde{P}_1(\rho, s) = \begin{cases} A_1^+(s)\exp[\alpha(s)\, r(\rho)] + B_1^+(s)\exp[\beta(s)\, r(\rho)], & \rho > \hat{\rho} \\ A_1^-(s)\exp[\alpha(s)\, r(\rho)] + B_1^-(s)\exp[\beta(s)\, r(\rho)], & \rho < \hat{\rho} \end{cases} \tag{A.20}$$

Equations (A.19) and (A.20) contain eight constants, $A_0^{\pm}$, $B_0^{\pm}$, $A_1^{\pm}$, $B_1^{\pm}$, which must be determined. Consistency between Eqs. (A.9) and (A.10) requires that

$$A_1^{\pm}(s) = \lambda_1 \left[a_0 \alpha(s) + s + \frac{1}{\lambda_0} \right] A_0^{\pm}(s) \tag{A.21}$$

$$B_1^{\pm}(s) = \lambda_1 \left[a_0 \beta(s) + s + \frac{1}{\lambda_0} \right] B_0^{\pm}(s) \tag{A.22}$$

Applying the jump conditions given by Eq. (A.11) yields

$$a_i[A_i^-(s) + B_i^-(s) - A_i^+(s) - B_i^+(s)] = p_i, \qquad i = 0, 1 \tag{A.23}$$

Finally, demanding that Eqs. (A.19) and (A.20) satisfy the integral conditions given by Eq. (A.5) yields

$$\{\exp[\alpha(s) r_+] - 1\} \frac{A_i^+(s)}{\alpha(s)} + \{\exp[\beta(s) r_+] - 1\} \frac{B_i^+(s)}{\beta(s)} + \{1 - \exp[\alpha(s) r_-]\} \frac{A_i^-(s)}{\alpha(s)} + \{1 - \exp[\beta(s) r_-]\} \frac{B_i^-(s)}{\beta(s)} = \frac{p_i}{s}, \quad i = 0, 1 \tag{A.24}$$

Here r_- and r_+ are defined as

$$r_- = \int_{\hat{\rho}}^{\rho_{\min}} \frac{d\rho}{F(\rho)}; \qquad r_+ = \int_{\hat{\rho}}^{\rho_{\max}} \frac{d\rho}{F(\rho)} \tag{A.25}$$

where $\rho_{\min}$ and $\rho_{\max}$ form the edges of the largest interval $(\rho_{\min}, \rho_{\max})$ for which the change of variables from ρ to r given by Eq. (A.15) is invertible. This implies that $F(\rho)$ cannot change sign in this interval, and for concreteness we take $F(\rho) \geqslant 0$. For the first two examples in Section 4 of the text, $\rho_{\min} = 0$ and $\rho_{\max} = \infty$. The third example in that section is not in the class defined by Eq. (A.14). Equations (A.21)–(A.25) constitute eight conditions for the eight constants $A_i^{\pm}$ and $B_i^{\pm}$, $i = 0, 1$. Making use of the identities

$$\left(\frac{\alpha}{s} - \frac{1}{a_0}\right)(a_0\beta - s) = \left(\frac{\beta}{s} - \frac{1}{a_0}\right)(a_0\alpha - s) = \frac{1}{\lambda_0}\left(\frac{1}{a_1} - \frac{1}{a_0}\right) \tag{A.26}$$

$$\left(\frac{\alpha}{s} - \frac{1}{a_1}\right)(a_1\beta - s) = \left(\frac{\beta}{s} - \frac{1}{a_1}\right)(a_1\alpha - s) = \frac{1}{\lambda_1}\left(\frac{1}{a_0} - \frac{1}{a_1}\right) \tag{A.27}$$

one can easily verify that the solution for these constants is

$$A_0^-(s) = -\left[\frac{\exp(\alpha r_+)}{\exp(\alpha r_+) - \exp(\alpha r_-)}\right] g_0(s) \tag{A.28}$$

$$B_0^-(s) = \left[\frac{\exp(\beta r_+)}{\exp(\beta r_+) - \exp(\beta r_-)}\right] h_0(s) \tag{A.29}$$

$$A_0^+(s) = -\left[\frac{\exp(\alpha r_-)}{\exp(\alpha r_+) - \exp(\alpha r_-)}\right] g_0(s) \tag{A.30}$$

$$B_0^+(s) = \left[\frac{\exp(\beta r_-)}{\exp(\beta r_+) - \exp(\beta r_-)}\right] h_0(s) \tag{A.31}$$

where

$$g_0(s) = \frac{p_0\alpha(a_0\beta - s)}{a_0(\alpha - \beta)s} \tag{A.32}$$

$$h_0(s) = \frac{p_0\beta(a_0\alpha - s)}{a_0(\alpha - \beta)s} \tag{A.33}$$

The constants $A_1^{\pm}$ and $B_1^{\pm}$ are obtained from Eqs. (A.28)–(A.33) by interchanging the state indices 0 and 1.

At this point the Laplace transforms $\tilde{P}_i(\rho, s)$ are fully determined, and we only need to invert these transforms to obtain the joint probability

functions $P_i(\rho, t)$. In the general case, we have been unable to analytically find this inverse. However, in most physical cases it happens that either $r_- = -\infty$ or $r_+ = \infty$ or both. This is the case for the first two examples in Section 4. The constants then simplify as shown in Table IV; we have omitted the state index on the entries in this table. In all of these cases, analytical inversion is possible. We give explicit results only for the case $\alpha, \beta > 0$, but the other three cases are treated in a completely analogous fashion. Considering $P_0(\rho, t)$ for the $\alpha, \beta > 0$ case with $A_i^{\pm} = B_i^{\pm} = 0$, we have

$$\tilde{P}_0(\rho, s) = \begin{cases} -\dfrac{g_0(s)}{F(\rho)} \exp[\alpha(s)\, r(\rho)] + \dfrac{h_0(s)}{F(\rho)} \exp[\beta(s)\, r(\rho)], & \rho < \hat{\rho} \\ 0, & \rho > \hat{\rho} \end{cases} \tag{A.34}$$

with r, α, β, g_0, and h_0 given by Eqs. (A.15), (A.18), (A.32), and (A.33). Equation (A.34) is easily inverted using any relatively complete Laplace inversion table. In particular, we used Eqs. (70), (72), and (74) on pages 254 and 255 of ref. 10. The result is given by

$$P_0(\rho, t) = \frac{p_0 \exp[r(\rho)/(a_0\lambda_0)]}{a_0(a_0 - a_1)\, F(\rho)} \left\{ \delta(\theta_0) + \left[\frac{a_0 a_1 \theta_1}{\lambda_0 \lambda_1} [I_2(u) - I_0(u)] + \frac{a_0}{\lambda_0} I_o(u) \right] H(\theta_0)[1 - H(\theta_1)] \exp\left[\left(\frac{a_1}{\lambda_0} - \frac{a_0}{\lambda_1} \right) \theta_0 \right] \right\} \tag{A.35}$$

where $H(z)$ is the Heaviside (unit step) function, $\delta(z)$ is the Dirac delta function, $I_i(z)$ is the usual modified Bessel function, and

$$\theta_0 = \frac{a_0 t + r(\rho)}{a_0(a_0 - a_1)}; \qquad \theta_1 = \frac{a_1 t + r(\rho)}{a_1(a_0 - a_1)} \tag{A.36}$$

$$u = \left[\frac{2a_0 a_1 |\theta_0 \theta_1|}{\lambda_0 \lambda_1} \right]^{1/2} \tag{A.37}$$

Table IV. The Constants $A^{\pm}$ and $B^{\pm}$ When r_- or r_+ Is Unbounded

	$\alpha, \beta > 0$	$\alpha, \beta < 0$	$\alpha > 0, \beta < 0$	$\alpha < 0, \beta > 0$
A^-	$-g$	0	$-g$	0
B^-	h	0	0	h
A^+	0	g	0	g
B^+	0	$-h$	$-h$	0

The results for $P_1(\rho, t)$ can be obtained from $P_0(\rho, t)$ by interchange of the state indices 0 and 1.

The exact results reported in Table I and Fig. 1 were computed from Eq. (A.35) and the corresponding result for $P_1(\rho, t)$. The exact results reported in Table II and Fig. 2 were computed from formulas analogous to these for the case $\alpha, \beta < 0$ with $A_i^- = B_i^- = 0$.

ACKNOWLEDGMENTS

This work was partially supported by the U.S. Department of Energy under grant DE-FG03-89ER14016. The work of F.M. was also partially supported by the Los Alamos National Laboratory.

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