Matrix Continued Fraction Solutions of the Kramers Equation and Their Inverse Friction Expansions

H. Risken*
Department of Physics and Optical Sciences Center, University of Arizona, Tucson, Arizona, USA

H.D. Vollmer and M. Mörsch
Abteilung für Theoretische Physik der Universität, Ulm, Federal Republic of Germany

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The distribution function in position and velocity space for the Brownian motion of particles in an external field is determined by the Kramers equation, i.e., by a two variable Fokker-Planck equation. By expanding the distribution function in Hermite functions (velocity part) and in another complete set satisfying boundary conditions (position part) the Laplace transform of the initial value problem is obtained in terms of matrix continued fractions. An inverse friction expansion of the matrix continued fractions is used to show that the first Hermite expansion coefficient may be determined by a generalized Smoluchowski equation. The first terms of the inverse friction expansion of this generalized Smoluchowski operator and of the memory kernel are given explicitly. The inverse friction expansion of the equation determining the eigenvalues and eigenfunctions is also given and the connection with the result of Titulaer is discussed.

1. Introduction

The distribution function \( W(x, v, t) \) in position and velocity space for the Brownian motion of particles in an external potential \( f(x) \) is determined by the following two variable Fokker-Planck equation or Kramers equation [1, 2]

\[
W(x, v, t) = L_K(x, v) W(x, v, t),
\]

\[
L_K(x, v) = -\frac{\partial}{\partial x} v + \frac{\partial}{\partial v} \left( \gamma v + \frac{f'(x)}{m} \right) + \frac{\gamma k T}{m} \frac{\partial^2}{\partial v^2}.
\]

In (1.2) \( \gamma \) is the friction constant, \( m \) the mass of the particles, \( T \) the temperature of the surrounding heat bath, \(-f'(x) = -df/dx\) is the external force due to the potential \( f(x) \) and \( W \) is the time derivative \( \partial W/\partial t \). A general analytic solution of the two variable Fokker-Planck equation (1.1) and (1.2) is only known for linear forces [2].

In the present paper the Laplace transform of the general initial value problem is given in terms of matrix continued fractions. This general solution is valid for arbitrary position dependent friction constants and potentials. All the occurring matrix continued fractions may be evaluated numerically as was done for the problem of stationary Brownian motion in periodic potentials with an external constant force [3, 4]. The analytic convergence of similar matrix continued fractions was proved recently [5]. Furthermore the high friction expansion is obtained by expanding the matrix continued fractions. As will be shown for the high friction limit the distribution function in position only, i.e.,

\[
c_0(x, t) = \int W(x, v, t) dv,
\]

will for certain initial conditions obey an equation of the Smoluchowski type

\[
c_0(x, t) = L_0(t) c_0(x, t),
\]

where the generalized Smoluchowski operator depends on the time and in general contains derivatives with respect to \( x \) of the order >2. The first three terms of the inverse friction expansion of this Smo-
luchowski operator are explicitly given. For large times they agree with the result of Wilemski [6] and Titulaer [7], the first order term being the Smoluchowski operator

\[
L_0 = \frac{\partial}{\partial x} \frac{1}{m \gamma} \left( \frac{\partial}{\partial x} + f' \right).
\]

(1.5)

It will also be shown that the solution \( c_0(x, t) \) obeys a generalized master equation [8, 9]

\[
\frac{d}{dt} c_0(x, t) = \int_0^t K_0(t - \tau) c_0(x, \tau) d\tau.
\]

(1.6)

The first three expansion terms of the memory kernel \( K_0 \) are also given explicitly.

The present paper is organized as follows: In Chap. 2 the general initial value problem of a tridiagonal vector recurrence relation is obtained in terms of matrix continued fractions, thereby extending our recent investigation [10].

Next in Chap. 3 we expand the velocity part of the distribution function into Hermite functions as is usually done [3, 4, 7, 11-16]. After making a Laplace transform for the time dependence, one is lead to an infinite set of coupled differential equations for the position dependent expansion coefficients, previously derived by Brinkman [11]. Using a further expansion of these position dependent coefficients and a suitable vector notation these equations are cast into a tridiagonal vector recurrence relation. By applying the results of Chap. 2, the Laplace transform of the general initial value problem of the Kramers equation is found. For \( f'(x) = \text{const} \) and \( \gamma(x) = \text{const} \) one of the continued fractions is evaluated analytically. This leads to a solution of the Kramers equation given by Resibois [17], Dufty [18] and Mazo [19].

2. Solutions of Tridiagonal Recurrence Relations

In a recent paper [10], we have investigated the solutions of the one sided tridiagonal vector recurrence relation\( ^* \left( c_n = 0 \text{ for } n < 0 \right) \)

\[
\hat{c}_n(t) = P_n \hat{c}_{n+1}(t) + Q_n \hat{c}_n(t) + R_n \hat{c}_{n-1}(t).
\]

(2.1)

In (2.1) \( c_n \) are column vectors having \( M \) components and \( P_n, Q_n, R_n \) are time independent \( M \times M \) matrices. In order to derive the general solution of the initial value problem of the Kramers equation, the general solution of the initial value problem of (2.1) is needed. This general solution may be written in the form

\[
c_n(t) = \sum_{m=0}^{\infty} G_{n,m}(t) c_m(0),
\]

(2.2)

where the initial condition of the Greens function is given by \( (I \text{ is the unit matrix}) \).

\[
G_{n,m}(0) = I \delta_{nm}.
\]

(2.3)

Performing the Laplace transform

\[
\tilde{G}_{n,m}(s) = \int_0^\infty G_{n,m}(t) e^{-st} dt,
\]

(2.4)

the \( \tilde{G}_{n,m} \) have to obey the following inhomogeneous recurrence relations

\[
P_n \tilde{G}_{n+1,m} + (Q_n - s I) \tilde{G}_{n,m} + R_n \tilde{G}_{n-1,m} = -I \delta_{nm}.
\]

(2.5)

Next we introduce the two matrices \( S_n(s) \) and \( T_n(s) \) which connect \( G_{n,m} \) and \( \tilde{G}_{n+1,m} \):

\[
\tilde{G}_{n,m} = S_n \tilde{G}_{n+1,m},
\]

(2.6)

\[
G_{n,m} = T_n G_{n+1,m}.
\]

(2.7)

Inserting (2.6) and (2.7) into (2.5) and neglecting for the moment the inhomogeneous term, we easily derive the recurrence relations \( (T_{n-1} = 0) \).

\( ^* \) In order to obtain similar expressions for the up and down iteration (see (2.11) and (2.12)) we have used a slightly different notation in the present paper (\( P_{n+1} \) of [10] is replaced by \( P_n \)).