ABSTRACT: The purpose of the paper is to give a pedagogical introduction to the multiple time-scale technique, on the example of the high friction limit of the Kramers equation. We begin with a discussion of the standard perturbation technique as presented in van Kampen’s reference book $VK$, which will be shown to fail in the long-time limit. Application of the multiple time-scale technique avoids these difficulties and leads to a uniform expansion in powers of the inverse of the friction. Analogy with the Chapman-Enskog expansion is discussed.

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I. INTRODUCTION

From a pedagogical point of view, the theory of Brownian motion is of fundamental interest in a graduate course on Statistical Mechanics. Starting with quite simple assumptions, a microscopic stochastic model - namely the Langevin model - can be introduced to describe the thermal motion of the suspended Brownian particles. It is noteworthy that this simple treatment contains already all the basic features of non-equilibrium thermodynamics, such as diffusive motion, fluctuation-dissipation theorem, Einstein relation between mobility and diffusion and the Green-Kubo relation for the diffusion coefficient $V_K$.

A complete description requires however a more precise characterization of the stochastic processes involved in Brownian motion, culminating in the Fokker-Planck evolution equation for the probability distribution of the Brownian particle $V_K,DGM$. Two levels of description can be used. First, if both the velocity and position of the particle are considered, the probability distribution $P(r,v,t)$ evolves according to the Kramers equation

$$\left[ \frac{\partial}{\partial t} + v \cdot \nabla r + \frac{F(r)}{M} \cdot \nabla v \right] P(r,v,t) = \xi \nabla v \cdot \left\{ \left( v + \frac{k_B T}{M} \nabla v \right) P(r,v,t) \right\}$$

where $M$ denotes the mass of the Brownian particle, $\xi$ the friction, $k_B T$ the bath temperature and $F(r)$ an external force field. This description was first given by Klein $Klein^{21}$ and Kramers $Kramers^{40}$. On the other hand, if only the spatial evolution of the particle is considered, one may rather use the Smoluchowski equation, governing the time evolution of the probability density $\rho(r,t)$ in configuration space :

$$\frac{\partial}{\partial t} \rho(r,t) = \frac{1}{M \xi} \nabla r \cdot \left\{ k_B T \nabla r - F(r) \right\} \rho(r,t)$$

This description, first put forward by Smoluchowski $Smolu^{16}$, predates that of Kramers and Klein.

However it took a long time to clarify the link between both descriptions. Kramers $Kramers^{40}$ already pointed out that the Smoluchowski description should be obtained from the Kramers equation in the high-friction limit. This can indeed be intuitively understood : if the friction is high, the velocity relaxes after a short time, of order $1/\xi$, and the evolution on larger time scales is only determined by the spatial distribution. However, a rigorous perturbative derivation of the Smoluchowski equation from the Kramers one was given by Wilemski only in 1976 $Wilemski^{76}$. Another systematic expansion procedure was later suggested by Titulaer $Titulaer^{78}$. The latter is closely related to the Chapman-Enskog perturbation scheme to solve the Boltzmann equation $Cercignani$. This method is indeed
natural in the present case, in view of the formal analogy between the collisional terms occurring in the Boltzmann and in the Kramers equations. In both equations, the right-hand side characterizes the effect of collisions on the time evolution of the distribution function. The singular nature of the expansion is due to the presence of the small parameter $1/\xi$ (replaced by the Knudsen number in the case of the Boltzmann equation) multiplying the time derivative in the Kramers equation. This makes a straightforward application of the perturbation theory impossible. In his reference textbook $VK$ (pp. 234-236), van Kampen proposes an alternative, pedagogical method, which is closer in spirit to the Hilbert perturbation scheme $Cercignani$. This procedure leads indeed to the Smoluchowski equation. The purpose of this paper is to show that this pedagogical approach is however incomplete and leads to inconsistencies in the expansion procedure. In section II, we will show that hidden secular terms are present in this description, which diverge as time goes to infinity. These terms make the asymptotic expansion non-uniform in the small parameter $1/\xi$. In section III, we propose an alternative approach, based on the multiple-time scale method. This procedure eliminates the secular divergences and construct a uniform expansion in the small parameter (the inverse friction in our case) $Nayfeh$. The multiple time-scale method allows one to recover quite easily all the features of the Chapman-Enskog procedure of Titulaer $Titulaer$78. Moreover, it gives a clear interpretation of the contribution of all orders in $1/\xi$ in the time derivative, as it is formally introduced in the Chapman-Enskog expansion $Cercignani$.

II. THE HILBERT EXPANSION

In this section, we first reproduce and then discuss the expansion procedure as given in van Kampen’s reference book, in order to point out the limitation of this “Hilbert” perturbation scheme. We will restrict ourselves to the one-dimensional case to simplify the analysis.

First, we introduce new dimensionless variables

$$\tau = t \frac{v_T}{\ell}; \quad V = \frac{v}{v_T}; \quad X = \frac{x}{\ell}; \quad F = \frac{F}{Mv_T^2}$$  \hspace{1cm} (3.a)

and a dimensionless friction

$$\xi_d = \xi \frac{\ell}{v_T}$$  \hspace{1cm} (3.b)

where $v_T = \sqrt{k_BT/M}$ is the thermal velocity and $\ell$ is a characteristic length scale of the system (such as the Brownian particle diameter). The Kramers equation then takes the
following form
\[ \frac{\partial}{\partial V} \left( V + \frac{\partial}{\partial V} \right) P(X, V; \tau) = \frac{1}{\xi_d} \left[ \frac{\partial}{\partial \tau} + V \frac{\partial}{\partial X} + F(X) \frac{\partial}{\partial V} \right] P(X, V; \tau) \] (4)

Let us insert into (4) the “naive” expansion
\[ P = P^{(0)} + \xi_d^{-1} P^{(1)} + \xi_d^{-2} P^{(2)} + \ldots \] (5)

By identifying terms of the same order, we find the following equations
\[ \mathcal{L}_{FP} P^{(0)} = 0 \]
\[ \mathcal{L}_{FP} P^{(1)} = \left[ \frac{\partial}{\partial \tau} + V \frac{\partial}{\partial X} + F(X) \frac{\partial}{\partial V} \right] P^{(0)} \]
\[ \mathcal{L}_{FP} P^{(2)} = \left[ \frac{\partial}{\partial \tau} + V \frac{\partial}{\partial X} + F(X) \frac{\partial}{\partial V} \right] P^{(1)} \] (6)

where we introduced a “Fokker-Planck” operator \( \mathcal{L}_{FP} \) defined as
\[ \mathcal{L}_{FP} = \frac{\partial}{\partial V} \left( V + \frac{\partial}{\partial V} \right) \] (7)

The zeroth order equation imposes a maxwellian velocity distribution
\[ P^{(0)}(X, V; \tau) = \Phi(X; \tau) e^{-1/2V^2} \] (8)

and the function \( \Phi \) has to be determined.

The first order term then gives
\[ \mathcal{L}_{FP} P^{(1)} = \frac{\partial \Phi}{\partial \tau} e^{-1/2V^2} + V \left\{ \frac{\partial \Phi}{\partial X} - F \Phi \right\} e^{-1/2V^2} \] (9)

By integrating both sides over \( V \), one obtains a “solubility condition”
\[ \frac{\partial \Phi}{\partial \tau} = 0 \] (10)

This can be understood in terms of linear algebra. The eigenfunctions of \( \mathcal{L}_{FP} \) are the functions \( H_n(V/\sqrt{2}) \exp(-V^2/2) \), where \( H_n \) is the \( n \)-th Hermite polynomial. Since the Maxwellian is associated with a null eigenvalue, the orthogonality between the eigenfunctions imposes that all terms multiplying the maxwellian on the right hand-side (r.h.s.) of equations like (9) must be vanish. This is precisely the “solubility condition” (10).
Equation (9) can now be solved to yield

\[ P^{(1)}(X, V; \tau) = -V \left\{ \frac{\partial \Phi}{\partial X} - F \Phi \right\} e^{-1/2V^2} + \Psi(X; \tau) e^{-1/2V^2} \]  
(11)

where \( \Psi \) has to be determined.

By inserting this solution into (6), one obtains

\[ \mathcal{L}_{FP} P^{(2)} = \left\{ \frac{\partial \Psi}{\partial \tau} - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) \right\} e^{-1/2V^2} + \left\{ \frac{\partial \Psi}{\partial X} - F \Psi \right\} V e^{-1/2V^2} \]

\[ - \left\{ F \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) \right\} (1 - V^2) e^{-1/2V^2} \]  
(12)

where the terms have been grouped into Hermite polynomials \( H_n(V/\sqrt{2}) \). According to the solubility condition, the first term in the r.h.s. of (12) must be set to zero, so that

\[ \frac{\partial \Psi}{\partial \tau} - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) = 0 \]  
(13)

Following van Kampen, one can then collect the results to obtain the distribution function to order \( 1/\xi_d^2 \):

\[ P(X, V; \tau) = e^{-1/2V^2} \left[ \Phi(X) - \xi_d^{-1} V \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) + \xi_d^{-1} \Psi(X; \tau) + \mathcal{O}(\xi_d^{-2}) \right] \]  
(14)

After integrating over the velocity, one obtains the spatial probability density \( \rho(X; \tau) \) as

\[ \rho(X; \tau) = \sqrt{2\pi} \left[ \Phi(X) + \xi_d^{-1} \Psi(X; \tau) + \mathcal{O}(\xi_d^{-2}) \right] \]  
(15)

and eq. (13) then yields the (dimensionless) Smoluchowski equation

\[ \frac{\partial \rho(X, \tau)}{\partial \tau} = \frac{1}{\xi_d} \frac{\partial}{\partial X} \left( \frac{\partial \rho(X, \tau)}{\partial X} - F(X) \rho(X, \tau) \right) \]  
(16)

However, a careful inspection of eq. (13) shows that \( \Psi \) diverges as time goes to infinity. Indeed, eq. (10) shows that \( \Phi \) is independent of time. Then, the first term in (13) does not depend on time either and the function \( \Psi \) is proportional to time \( \tau \)

\[ \Psi(X; \tau) \sim \tau \]  
(17)

The standard expansion (5) of the solution thus leads to secular divergences and cannot be correct in the long time limit. In other words, a naive expansion is not uniformly convergent for small \( 1/\xi_d \). The limit of time going to infinity cannot be inverted with the limit of friction going to infinity, so that taking small corrections in \( 1/\xi_d \) into account
leads to an upper bound for the time $\tau$. In fact, this procedure implicitly expands time dependent terms like $\tau/\xi_d$ as $\xi_d^{-1}$ terms, and secular divergences appear in the long-time limit.

III. THE MULTIPLE TIME-SCALE APPROACH

In the limit $\xi^{-1} \rightarrow 0$, the Kramers argument presented above indicates a time-scale separation. There is first a very short period ($t \sim \xi^{-1}$) during which the velocity of the Brownian particle thermalizes. Then the dynamical evolution is controlled by the time-dependence of the spatial distribution on longer time-scales. This separation of time-scales in the limit $\xi^{-1} \rightarrow 0$ suggests the application of the multiple time-scale analysis. This method replaces the physical distribution function $P(X,V;\tau)$ by an auxiliary function, $P(X,V;\tau_0,\tau_1,\tau_2,\ldots)$, depending on several time-scales. Accordingly, the time derivative in the physical evolution equation (4) is replaced by the sum of time derivatives on each time-scale,

$$\frac{\partial}{\partial \tau} \rightarrow \frac{\partial}{\partial \tau_0} + \xi_d^{-1} \frac{\partial}{\partial \tau_1} + \xi_d^{-2} \frac{\partial}{\partial \tau_2} + \ldots \quad (18)$$

The auxiliary distribution function $P(X,V;\tau_0,\tau_1,\tau_2,\ldots)$ is then expanded in powers of the small parameter $\xi_d^{-1}$ and inserted into the evolution equation, where terms of the same order are identified. The physical solution of the system is eventually obtained by restricting the different time variables to the so-called “physical line”

$$\tau_0 = \tau ; \tau_1 = \xi_d^{-1} \tau ; \tau_2 = \xi_d^{-2} \tau ; \ldots \quad (19)$$

so that

$$P(X,V;\tau) = P^{(0)}(X,V;\tau,\xi_d^{-1} \tau,\xi_d^{-2} \tau,\ldots) + \xi_d^{-1} P^{(1)}(X,V;\tau,\xi_d^{-1} \tau,\xi_d^{-2} \tau,\ldots) + \ldots \quad (20)$$

will be the solution of the Kramers equation (4). Equation (19) indicates that the dependence of the distribution function on $\tau_n$ characterizes the evolution on the time-scale $\tau \sim \xi_d^n \ (n = 0, 1, 2,\ldots)$.

The crucial difference with the standard perturbation method is that outside the physical line (19), the auxiliary distribution function has no physical meaning. Then appropriate boundary conditions can be imposed to require the expansion to be uniform in the small parameter $\xi_d^{-1}$. This freedom will be used to eliminate secular divergences.

The identification of different powers of $\xi_d^{-1}$ in the Kramers equation gives the following
relations

\[ \mathcal{L}_{FP} P^{(0)} = 0 \]
\[ \mathcal{L}_{FP} P^{(1)} = \left[ \frac{\partial}{\partial \tau_0} + V \frac{\partial}{\partial X} + F(X) \frac{\partial}{\partial V} \right] P^{(0)} \]
\[ \mathcal{L}_{FP} P^{(2)} = \left[ \frac{\partial}{\partial \tau_0} + V \frac{\partial}{\partial X} + F(X) \frac{\partial}{\partial V} \right] P^{(1)} + \frac{\partial}{\partial \tau_1} P^{(0)} \]

(21)

The zeroth order equation still imposes a maxwellian velocity distribution

\[ P^{(0)}(X, V; \tau_0, \tau_1, \ldots) = \Phi(X; \tau_0, \tau_1, \ldots) e^{-1/2V^2} \]

where the function \( \Phi \) now depends on all time variables.

The first order term thus obeys to the following equation

\[ \mathcal{L}_{FP} P^{(1)} = \frac{\partial \Phi}{\partial \tau_0} e^{-1/2V^2} + V \left\{ \frac{\partial \Phi}{\partial X} - F \Phi \right\} e^{-1/2V^2} \]

(21b)

The solubility condition then requires the function \( \Phi \) to be independent of the \( \tau_0 \) time-scale

\[ \frac{\partial \Phi}{\partial \tau_0} = 0 \]

(22b)

and the first correction for the distribution function is now given by

\[ P^{(1)}(X, V; \tau_0, \tau_1, \ldots) = -V \left\{ \frac{\partial \Phi(X; \tau_1, \ldots)}{\partial X} - F \Phi(X; \tau_1, \ldots) \right\} e^{-1/2V^2} \]

\[ + \Psi(X; \tau_0, \tau_1, \ldots) e^{-1/2V^2} \]

(23)

The equation for \( P^{(2)} \) becomes

\[ \mathcal{L}_{FP} P^{(2)} = \left\{ \frac{\partial \Psi}{\partial \tau_0} + \frac{\partial \Phi}{\partial \tau_1} - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) \right\} e^{-1/2V^2} + \left\{ \frac{\partial \Psi}{\partial X} - F \Psi \right\} V e^{-1/2V^2} \]

\[ - \left\{ F \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) \right\} (1 - V^2) e^{-1/2V^2} \]

(24)

The solubility condition then requires

\[ \frac{\partial \Psi}{\partial \tau_0} = - \left( \frac{\partial \Phi}{\partial \tau_1} - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) \right) \]

(25)

The r.h.s. of this equation does not depend on \( \tau_0 \) (see eq. (22b)), and one must impose the condition

\[ \frac{\partial \Psi}{\partial \tau_0} = 0 \]

(26)
to eliminate the secular divergence as \( \tau_0 \) grows to infinity. This leads to a closed equation for \( \Phi \)
\[
\frac{\partial \Phi}{\partial \tau_1} - \frac{\partial}{\partial X} \left( \frac{\partial \Phi}{\partial X} - F \Phi \right) = 0
\] (27)

This result has to be compared with eq. (13) of the standard Hilbert procedure, where the
time-dependence of the density was only contained in the first order correction (through
\( \Psi \), see eq. (15)). A correct expansion thus modifies the perturbative scheme and leads to
different couplings between the successive corrections to the probability distribution.

The physically relevant equation for \( \rho \) is then obtained by restricting the different
variables \( \tau_i \) to the physical line (19). The time derivative of \( \rho \) can now be written
\[
\frac{\partial}{\partial \tau} \rho(X, \tau) = \sqrt{\frac{2\pi}{\xi_d^2}} \frac{\partial}{\partial \tau_0} \left[ \Phi(X; \tau_1, \ldots) + \xi_d^{-1} \Psi(X; \tau_1, \ldots) + O(\xi_d^{-2}) \right] \bigg|_{\tau_0=\tau, \tau_1=\tau/\xi_d, \ldots} \\
+ \frac{1}{\xi_d} \sqrt{\frac{2\pi}{\xi_d^2}} \frac{\partial}{\partial \tau_1} \left[ \Phi(X; \tau_1, \ldots) + \xi_d^{-1} \Psi(X; \tau_1, \ldots) + O(\xi_d^{-2}) \right] \bigg|_{\tau_0=\tau, \tau_1=\tau/\xi_d, \ldots} \\
- \frac{1}{\xi_d} \sqrt{\frac{2\pi}{\xi_d^2}} \Phi(X; \tau_1, \ldots) \bigg|_{\tau_0=\tau, \tau_1=\tau/\xi_d, \ldots} + O(\xi_d^{-2})
\] (28)

Using (27) and (15), we eventually recover the (dimensionless) Smoluchowski equation
\[
\frac{\partial \rho(X, \tau)}{\partial \tau} = \frac{1}{\xi_d} \frac{\partial}{\partial X} \left( \frac{\partial \rho(X, \tau)}{\partial X} - F(X) \rho(X, \tau) \right) + O(\xi_d^{-2})
\] (29)

IV. DISCUSSION

Let us make a few remarks on the present derivation.

First, as mentioned in the introduction, the Smoluchowski equation governs the spa-
tial evolution of the Brownian particle. This evolution is then expected to occur on a
diffusion time scale \( t_D \sim \ell^2/D \), where \( D = k_BT/M\xi \) is the diffusion coefficient, or in
dimensionless variables, \( \tau_D = \frac{\ell^2}{\xi_d^2} t_D \sim \xi_d \). This feature emerges in a natural way from the
multiple time scale analysis. Indeed, according to equation (27), we have shown that the
spatial density probability evolves on the \( \tau_1 \) time scale, which precisely characterizes the
evolution of the system on time scale \( \tau \sim \xi_d \sim \tau_D \) (see discussion after equation (20)) !

As indicated above, the \( t \gg \xi^{-1} \) limit of \( P^{(0)} \) is just the Maxwellian, which can be
interpreted here as the “local equilibrium approximation” of the Fokker-Planck operator,
\( \mathcal{L}_{FP} \). As shown in eq. (22b), this solution does not evolve on the time-scale \( \tau_0 \), where
this approximated form for \( P^{(0)} \) remains valid. This property confirms the relevance and
the deep physical meaning of the local equilibrium approximation, as a state of the system
which exists over a large time-scale.
Finally, let us remark that the formal analogy between the Kramers equation and the Boltzmann’s equation can serve as an introduction to perturbative expansion methods in Kinetic Theory. It should be noted that the multiple-time scale method is indeed very close in spirit to the Chapman-Enskog procedure. Indeed, the latter introduces an ad-hoc formal expansion of the time derivative in powers of the small parameter $\epsilon$

$$\frac{\partial f}{\partial t} = \sum_{n=0}^{\infty} \epsilon^n \frac{\partial^{(n)} f}{\partial t}$$

(in Kinetic Theory, the Knudsen number is the small parameter). This is a subtle point of the procedure, which stems from the expansion in powers of $\epsilon$ of the functional dependence of the distribution function on the “hydrodynamic” fields Titulaer78, Cercignani. The explicit expressions for the operators $\partial^{(n)}/\partial t$ are computed in the course of the calculation thanks to solubility conditions. Equation (30) is formally equivalent to the multiple time-scale expansion of the time-derivative (18). In this sense, the application of the operator $\partial^{(n)}/\partial t$ of the Chapman-Enskog method characterizes the dynamical evolution of the system on the time-scale $t \sim \epsilon^{-n}$. For the purpose of a pedagogical approach, the multiple time-scale approach seems however more natural to us, since it gives a clear understanding of each term of the expansion. Moreover it explicitly shows the crucial importance of $\epsilon$ dependent corrections in the time derivative (30) to obtain a consistent expansion. Absence of such terms would inevitably lead to inconsistencies identical to those occurring in the naive expansion of the Kramers equation.

To conclude, the study of the Kramers equation in the high friction limit gives a pedagogical and instructive presentation of the multiple time-scale method. Pedagogical, since it can be shown explicitly that the method avoids all the troubles of more naive perturbation expansions; instructive, since it allows a deep insight into the underlying physics. This technique has already been successfully applied to a variety of problems in physics Nayfeh, such as the Lorentz model Jarek, adiabatic systems Anderson or a microscopic (exact) approach to Brownian motion Bocquet to cite some recent work. For such complicated situations, it describes in a systematic way the dynamical evolution of the system on each successive time-scale. This property constitutes the real power of the method.

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