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# A Remark on the Kramers Problem

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We present new point of view on the old problem, the Kramers problem. The passages from the Fokker–Planck equation to the Smoluchowski equation, including corrections to the Smoluchowski current, is treated through an asymptotic expansion of the solution of the stochastic dynamical equations. The case of an extremely weak force of friction is also discussed.

**KEY WORDS:** Kramers problem; Klyatskin–Novikov theory; stochastic equation; current.

**1.** Evolution of a physical system can be ordered in multi-time-scales. Details of evolution on short-time-scale do not need for description in a closed form of a system evolution on long-time-scale and appears on this scale only in an average form. The prototype of such kind physical systems is dissipative Brownian motion of a particle in an external potential field. In this problem, with the exception of extremely short characteristic time scales of random forces, there are two time scales: (1) time scales of a particle motion in an external field; (2) time scales of relaxation (rate of dissipation) of Brownian particle in a media. It is intuitively absolutely clear that, if the friction force is strong enough (time of free motion is extremely short), then probability distribution of a particle velocity to be rapidly relaxated to the Maxwell distribution and on this background a particle position will be undergoing to slow process of diffusion. In the following we deal with the consideration of approximate reduction of the Fokker–Planck equation for phase-space probability density to the Smoluchowski equation which deals with probability density of a particle position only. In

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the opposite case of extremely weak force of friction we have energy (or action) variable as evident slow one.

**2.** The Kramers problem consist in mathematical description of approximate reductions of the Fokker–Planck equation for dissipative Brownian motion of a particle in an external field to the two limiting cases: (1) to the Smoluchowski equation (extremely strong force of friction) or (2) to equation for probability density of energy (or action) variable (extremely weak force of friction).[1] These reduction procedures are the prototypes of all adiabatic elimination procedures or procedures of separation on slow and fast variables.[2]

The Kramers model,[1] firstly formulated for kinetics of chemical reactions, consists of a partical of mass $m$ moving in an one-dimensional potential field $U(x)$ under influence of a random force $f(t)$ and a linear friction force with a constant dissipation rate $\lambda$. The corresponding set of Langevin equations has the following form

$$\dot{x} = u, \qquad m\dot{u} = -U'(x) - \lambda m u + f(t) \tag{1}$$

where the random force $f(t)$ is generalized Gaussian $\delta$-correlated stochastic processes (white noise) with the following properties (including the fluctuation–dissipation relation)

$$\langle f(t) \rangle = 0, \qquad \langle f(t)\, f(t') \rangle = 2\lambda m k_B T \delta(t - t') \tag{2}$$

$\langle \cdots \rangle$ denotes average over all realizations of random force.

The Langevin (1)–(2) dynamics is stochastically equivalent to the Fokker–Planck equation for the rate of change of probability density $P(u, x; t)$ which has the form (e.g., ref. (2))

$$\partial_t P(u, x; t) = -u\, \partial_x P + \frac{1}{m} U'(x)\, \partial_u P + \frac{\lambda}{m} \partial_u \left[ uP + \frac{k_B T}{m} \partial_u P \right] \tag{3}$$

where $\partial_t = \partial/\partial_t$, $\partial_x = \partial/\partial x$, and $\partial_u = \partial/\partial_u$.

Keeping in mind (1)–(3) we formulate the problem in the following manner: in the case of extremely strong force of friction beginning with (3) or equivalently (1)–(2) to derive the approximate reduction to an equation for the rate of change of probability density $P(x; t)$ in the form of asymptotic expansion by the parameter $\lambda^{-1}$:

$$\partial_t P(x; t) = -\partial_x [\lambda^{-1} J_S + o(\lambda^{-1})] \tag{4}$$

where $J_S$ is the Smoluchowski current,

$$J_S = -[U'(x)\,P(x;t) + k_B T\,\partial_x P(x;t)]/m \tag{5}$$

In other words it is asymptotics of strong force of friction on time scales $\lambda t \gg 1$.

This problem has long history starting since 1940, the date of publication of the Kramers famous work.[1] For relevant references including reviews of the problem, see refs. 2–5. The first treatment of the problem has been down in ref. 6 and the first correct solution has been down in ref. 7 and then in refs. 8–10. The works[10–14] are of importance for the following in respect of treatment of the corrections older then $\lambda^{-3}$ which break the Fokker–Planck structure of (4). Most general treatment of the problem has been down in ref. 15.

**3.** All of the cited works deal with (3) as the input equation for a solution of the problem. The purpose of this paper is to take notice of the fact that (1)–(2) are indeed convenient input equations for an answer to the problem. With respect to solutions of (1)–(2) we use the method of asymptotic expansion by the parameter $\lambda^{-1}$. In the way, the Fokker–Planck type equations (4) to be derived from approximate stochastic dynamical equations in each order of $\lambda^{-1}$. Moreover, Fokker–Planck equation is an approximate equation and in any case must be derived from input dynamical equations. Convenient and powerful method of derivation, in particular, of the Fokker–Planck type equations immediately from stochastic equations has been initiated by Novikov[16] and then it has been sufficiently developed by Klyatskin.[17] In the following we use this method systematically. In this connection it should be pointed out that the Klyatskin–Novikov theory, generally, interprets a stochastic differential equation in the sense of Stratonovich. However, in the case under consideration it does not matter. We refer the reader to refs. 16 and 17 for further information.

The probability density $P(x;t)$ can be written in the form[17]

$$P(x;t) = \langle \delta(x - x(t)) \rangle$$

where $x(t)$ is a stochastic process and $\delta(\cdots)$ is $\delta$-function. Differentiating this definition by time we obtain the equation

$$\partial_t P(x;t) = -\partial_t \langle \dot{x}(t)\,\delta(x - x(t)) \rangle \equiv -\partial_x J(x;t) \tag{6}$$

which has the form of a conservation law and is the proform for an equation of the type (4). If $x(t)$ is defined by (1), our problem is in calculation of asymptotic expansion of $\dot{x}(t)$ by $\lambda^{-1}$ and then the corresponding average in (6). Further insight is gained by making the following construction. Rewrite (1) for $\lambda t \gg 1$ in the form

$$\dot{x}(t) = -\frac{1}{m} \Lambda^{-1} U'(x) + \frac{1}{m} \xi(t) \tag{7}$$

where operator $\Lambda$ has the form $\Lambda = d/dt + \lambda$, and the Ornstein–Uhlenbeck process is introduced:

$$\xi(t) = \Lambda^{-1} f(t) = \exp(-\lambda t) \int_0^t \exp(\lambda t') f(t') \, dt'.$$

Formal expansion of $\Lambda^{-1}$ by $\lambda^{-1}$ has the form

$$\Lambda^{-1} U'(x) = \frac{1}{\lambda} \sum_{n=0}^{N} \frac{(-1)^n}{\lambda^n} \left( \frac{d^n}{dt^n} \right) U'(x) + \cdots$$

Hence, (7) can be written in the form

$$\dot{x}(t) \sim \left[ -\frac{1}{m\lambda} U'(x) + \frac{1}{m} \xi(t) \right] + \frac{1}{m\lambda^2} [U''(x) \dot{x}(t)]$$
$$- \frac{1}{m\lambda^3} [U'''(x)(\dot{x}(t))^2 + U''(x) \ddot{x}(t)] + \cdots$$

The $\dot{x}(t)$, $\ddot{x}(t)$, and so-on, can be excluded from right hand side of last equation repeatedly using iterations of this equation and its time derivatives. Then, and it is important, we are in need of expansion by $\lambda^{-1}$ of the stochastic process $\xi(t)$ or, more precisely, of expansion by $\lambda^{-1}$ of the average in (6) which involves $\xi(t)$. First of all we must remark that the derivatives $\dot{f}(t)$ and so on, have sense only as derivatives of the generalized stochastic process $f(t)$[18] and break the simple Fokker–Planck structure of (6) as of an second order partial differential equation. It is evident in the frame of Klyatskin–Novikov theory.[17] Namely in the process of calculation of the corresponding averages according to ref. 17 we easy detect a complex form of (6) including memory as well as an integral-operator structure. Further, in respect of $\lambda^{-1} f(t)$ it is easy to verify[17] that corresponding averages in (6) have factor $\lambda^{-1}$ because the noise (2) intensity has the order $\lambda$.

Taking into account what has been outlined above the first terms of expansion of $\dot{x}(t)$ by $\lambda^{-1}$ that lead to the current $J(x; t)$ expansion up to order $\lambda^{-3}$ (the maximum-order of saving of the simple Fokker–Planck structure of (6)) can be written in the form

$$\dot{x}(t) \sim \left(1+\frac{1}{m\lambda^2}U''(x)\right)\left[-\frac{1}{m\lambda}U'(x)+\frac{1}{m\lambda}f(t)\right]+\cdots$$

Substituting last expression into the current $J(x;t)$ (6) and performing averaging exactly follow Klyatskin–Novikov theory[17] we obtain

$$\begin{aligned} J(x;t) &= \left\langle \left(1+\frac{1}{m\lambda^2}U''(x)\right)\left[-\frac{1}{m\lambda}U'(x)+\frac{1}{m\lambda}f(t)\right]\delta(x-x(t))\right\rangle + o(\lambda^{-3}) \\ &= \left(1+\frac{1}{m\lambda^2}U''(x)\right) J_S(x;t) + o(\lambda^{-3}) \end{aligned} \tag{8}$$

where $J_S$ is the Smoluchowski current (5). Asymptotic expansions of $\dot{x}(t)$ and $J(x;t)$ (8) together with (2) lead to conventional conclusion: the Smoluchowski equation is valid if: $\lambda t \gg 1$, $l|U'(x)| \ll k_B T$, $l^2|U''(x)| \ll k_B T$,—where a length scale $l=\sqrt{k_B T/m\lambda^2}$ is introduced. (8) contains lowest order correction to the Smoluchowski equation.[8–10] Higher order corrections in $\lambda^{-1}$, involving in averaging time derivatives of the generalized stochastic process $f(t)$, lead to break of simple structure of the Smoluchowski equation as a second order partial differential equation. It was pointed out also in traditional approach.[10–14, 5]

**4.** Consider now the case of extremely weak force of friction. This case more complicated then previous but not so interesting in calculation.

Let $m=1$ in (1). In the case of extremely weak force of friction and on the time-scale $\lambda t \ll 1$ the energy $E=u^2/2+U(x)$ of unperturbed system is evident candidat for slow variable. But previously $E$ must be averaged over period of relatively rapid dynamical oscillations. It is more convenient, however, to consider the action variable $J$ instead of $E$, $J=J(E)$.[1] Let $J$ is action variable averaged over period of rapid dynamical oscillations. Then an equation for the rate of change of probability density $P(J;t)$ can be written in the form (see (6))

$$\partial_t(J;t) = -\partial_J\langle \dot{J}(t)\,\delta(J-J(t))\rangle, \qquad P(J;t)=\langle\delta(J-J(t))\rangle \tag{9}$$

In usual way[1] and taking into account the change of time-scale of the white noise[2, 7] we obtain the equations of motion for slow variables

$$\dot{J}(t) = -\lambda J + \frac{V}{\omega}f(t), \qquad \dot{V} = -\lambda\frac{V}{\omega}J + f(t) \tag{10}$$

where $\omega = \omega(J) = dE/dJ$ is frequency and $V$ is velocity averaged over period of dynamical motion. Substituting (10) in (9) we obtain

$$\partial_t P(J;t) = -\partial_J \left[ -\lambda JP + \frac{1}{\omega(J)} \langle f(t)\, V(t)\, \delta(J - J(t)) \rangle \right] \tag{11}$$

For calculation of the average in right hand side of (11) we can use the Klyatskin–Novikov procedure again. Using (9) and the causality condition[17] we obtain for functional derivatives

$$\frac{\delta V(t)}{\delta f(t)} = 1; \qquad \frac{\delta J(t)}{\delta f(t)} = \frac{V}{\omega}$$

Taking also into account that $V^2/\omega = J$ if $J = \text{const}$, according to ref. 17 we finally obtain

$$\begin{aligned}
\partial_t P(J;t) &= \partial_J \left[ \lambda JP - \frac{\lambda k_B T}{\omega(J)} \left\langle \frac{\delta V(t)}{\delta f(t)}\, \delta(J - J(t)) - V(t)\, \partial_J \delta(J - J(t))\, \frac{\delta J(t)}{\delta f(t)} \right\rangle \right] \\
&= \partial_J \left[ \lambda JP - \frac{\lambda k_B T}{\omega(J)} P + \frac{\lambda k_B T}{\omega(J)} \partial_J (JP) \right] \\
&= \partial_J \left[ \lambda J + \lambda k_B T\, \frac{J}{\omega(J)}\, \partial_J \right] P(J;t)
\end{aligned}$$

It is exactly the Kramers equation. We can derive corrections to this equation but it is slightly more difficult task then in the case of extremely strong force of friction and does not take special interest in the context of this paper.

**5.** In conclusion, we have presented in a simplest framework a unique approach to the kinetic equations for slow variables by taking stochastic dynamical equations as the input instead of the Fokker–Planck equation. We hope that this approach is general enough.

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