Computing a non-Maxwellian velocity distribution from first principles

Manuel O. Cáceres*
Centro Atómico Bariloche and Instituto Balseiro, CNEA and Universidad Nacional de Cuyo, 8400 Bariloche, Argentina and Consejo Nacional de Investigaciones Científicas y Técnicas, 8400 Bariloche, Argentina

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We investigate a family of single-particle anomalous velocity distribution by solving a particular class of stochastic Liouville equations. The stationary state is obtained analytically and the Maxwell-Boltzmann distribution is reobtained in a particular limit. We discuss the comparison with other different methods to obtain the stationary state. Extensions when the models cannot be solved in an exact way are also pointed out in connection with the one-ficton approximation.

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I. INTRODUCTION

In recent years there has been an increasing interest in understanding anomalous velocity distributions (non-Maxwellian) that appear—quite ubiquitously—in many different subjects of science; for example, in the study of out of equilibrium (vibrated) granular matter [1], in the analysis of out of equilibrium rodlike thermal molecules rotating freely in a plane [2,3], and in the study of physiological systems [4], etc. In many of these cases the correlation function [of the relevant variable $V(t)$] decays in time with some stretched exponential function; in a similar context, the probability distributions show non-Maxwellian profiles, or they can also show long tails in the configurational velocity space V.

It is well known that the Maxwell (Boltzmann) distribution can be derived by various statistical methods [5]. In particular, the time evolution of the single-particle Maxwell distribution can be analyzed by using the Langevin equation or equivalently by using the Fokker-Planck scheme [6]; in both approaches the important points are that the "dynamics" for the velocity is linear and the fluctuations from the *thermal bath* are Gaussian. Therefore—as expected—the velocity distribution of the Rayleigh particle is Gaussian at all times. A signature of this model is the *singular* character of the random acceleration that the Rayleigh particle feels from the thermal bath; of course this is a necessary condition in order to have a Markovian stochastic process (sp) $V(t)$. In other words, the white-noise nature of the random acceleration leads to a nonvanishing diffusivity

$$D=\lim_{\Delta t\to 0}\frac{\langle \Delta V^2\rangle}{\Delta t}.$$

This is nothing more than a necessary condition to obtain the Fokker-Planck equation.

On the other hand, if we assume a *generalized* Rayleigh particle with a more "realistic" correlation function associated to some external noise, let us say, for example, a color-noise correlation function: $\chi(\tau)=a^2\exp(-2\lambda|\tau|)$, the diffusivity constant D vanishes. It is simple to prove that using a color noise the only way to get nonvanishing diffusivity is in the simultaneous limit: $a^2\to\infty$ and $\lambda\to\infty$, in such a way that $a^2(2\lambda)^{-1}=D$ (but this is just the white-noise case). Note that it is a quite different matter to define a new Markov process $\tilde{V}(t)$ to mimic—in the best way—the non-Markovian one $V(t)$. It is well known that such a Markov sp $\tilde{V}(t)$ exists and fulfills (in the leading order) a Fokker-Planck equation with a *renormalized* diffusivity $D=a^2/(\gamma+2\lambda)$ (see appendix D of van Kampen's paper [8]). Therefore if we want to find a "softer" description for the random accelerations of the *generalized* Rayleigh particle, we should lift the hypothesis of Gaussian noise; this fact will immediately lead to a non-Maxwellian (*anomalous*) velocity profile; for example, a *natural* cutoff for the velocity distribution will appear if the random accelerations are finite.

In the context of a *generalized* Rayleigh particle we have studied the time relaxation of its correlation function, and we have proved that if we model the stochastic process $V(t)$ by a generalized Ornstein-Uhlenbeck process, where the fluctuations of the bath are characterized by any arbitrary noise $\xi(t)$ (not necessarily Gaussian), the exact solution of the system is given in terms of the characteristic functional $G_V([z(\bullet)])$; i.e., let the stochastic differential equation (sde) of the process be

$$\frac{dV}{dt}=-\gamma V+\xi(t),\quad \gamma>0, \tag{1}$$

where $\xi(t)$ is an arbitrary noise characterized by its functional

$$G_\xi([k(\bullet)])=\left\langle \exp i\int_0^\infty k(t)\xi(t)\ dt\right\rangle_{P([\xi(\bullet)])};$$

here the notation $G_\xi([k(\bullet)])$ emphasizes that $k(t)$ is a test function. Then the functional of the process $V(t)$ is given by [9,10]

$$G_V([z(\bullet)])=e^{+ik_0V_0}G_\xi\left(\left[\int_t^\infty e^{\gamma(t-s)}z(s)\ ds\right]\right), \tag{2}$$

where V_0 is the initial condition of the sp $V(t)$ and k_0 is a functional of the test function $z(t)$, given by $k_0=\int_0^\infty e^{-\gamma s}z(s)ds$.

*Email address: caceres@cab.cnea.gov.ar

The exact formula (2) solves the problem in a closed way, but of course the difficulty lies in the fact that there are not so many closed expressions for the noise characteristic functional $G_\xi([k(\bullet)])$. Among the many cases that we have been able to work out are: linear sde driven by Lévy noise [11], sde associated with special boundary conditions [12], and also second-order sde driven by arbitrary noises [13], etc. In all of these cases we have been able to calculate correlation functions and higher-order moments and cumulants. In this paper, the problem that we want to tackle is different because we want to know something more about the associated probability distributions, particularly we are interested in the one-time probability density $P(V,t)$ in order to see whether its behavior is anomalous or not. Note that if we had a closed expression for the functional $G_\xi([k(\bullet)])$, the probability density $P(V,t)$ could be obtained by quadrature from Eq. (2), i.e., by Fourier inversion,

$$P(V_1,t_1)=\frac{1}{2\pi}\int_{-\infty}^{\infty}G_V([z(\bullet)=k_1\delta(t-t_1)])\times\exp(-ik_1V_1)dk_1. \tag{3}$$

From this formula, and for any noise $\xi(t)$, we can calculate *in an exact manner* all the one-time cumulants of sp $V(t)$. We emphasize that the probability distribution $P(V_1,t_1)$ depends on the initial condition $V(t_0=0)=V_0$, note however, that due to the intrinsic preparation of the system, this distribution is not the propagator: $P(V_1,t_1|V_0,t_0)$; this is so because in general the system could be non-Markovian. In particular, in Ref. [13] we have found the *exact* stationary nonequilibrium probability distribution $P_{st}(V)$, for the general case when the noise is Gaussian and the correlation is an arbitrary function $\chi(t)$ (not necessarily exponential). Then, for example, it is possible to see that the one-time probability distribution is Gaussian—as expected—but the dispersion, $\langle V(t)^2\rangle$, strongly depends on the character of the correlation function of the bath, in particular this fact leads to the definition of *strongly* or *weakly non-Markovian* dynamics.

II. MODELING THE THERMAL BATH WITH DICHOTOMOUS NOISE: EXACT RESULTS

If the noise $\xi(t)$ is a dichotomous process, characterized by a hopping transition rate λ, all the cumulants of sp $V(t)$ can be calculated. Nevertheless, because the characteristic functional of this noise cannot be expressed in a closed form [it is only possible to write down a series expression for $G_\xi([k(\bullet)])$ [9]], we cannot easily calculate the associated one-time probability distribution using Eq. (3); so here we are going to tackle this problem from a different point of view. Before going ahead with this program we would like to remark that a dichotomous sp is a good candidate to model a thermal bath when the *finite* character of the random accelerations and the nonwhite correlation of the noise are important facts to be considered.

If the noise $\xi(t)$ in Eq. (1) is a symmetric Langevin-like force (producing finite accelerations), it is quite natural to model the *thermal bath* with a dichotomous noise of values $\pm a$; then its stationary correlation function is

$$\langle\xi(t+\tau)\xi(t)\rangle=a^2\exp(-2\lambda|\tau|). \tag{4}$$

Introducing the series expression of $G_\xi([k(\bullet)])$ in Eq. (2), for example, we have shown that the stationary two-point correlation function of the sp $V(t)$ can written in the form [9]

$$\langle\langle V(t+\tau)V(t)\rangle\rangle=\frac{a^2}{\gamma(2\lambda+\gamma)}e^{-\gamma|\tau|}. \tag{5}$$

In general, higher-order cumulants can also be obtained by taking higher-order functional derivatives of $\ln G_V([z(\bullet)])$. Nevertheless, to write the corresponding probability distribution from the information of all these moments is a nontrivial task, thus we are going to bypass this difficulty by introducing an alternative procedure, which in principle is useful—at least—for the one-time probability distribution.

A. Computing the probability distribution

In order to calculate the evolution equation of the one-time probability distribution $P(V,t)$, we start from the stochastic Liouville equation associated to Eq. (1), so defining $\rho(V,t)=\delta(V-V[t,\xi(\bullet)])$ we have

$$\frac{\partial\rho(V,t)}{\partial t}+\frac{\partial}{\partial V}[\dot{V}\rho(V,t)]=0,$$

which is equivalent to

$$\frac{\partial\rho(V,t)}{\partial t}+\frac{\partial}{\partial V}[\{-\gamma V+\xi(t)\}\rho(V,t)]=0. \tag{6}$$

Using van Kampen's lemma [6,7] it follows that the evolution equation for the distribution

$$P(V,t)=\langle\delta(V-V[t,\xi(\bullet)])\rangle$$

is

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=-\left\langle\xi(t)\frac{\partial}{\partial V}\rho(V,t)\right\rangle, \tag{7}$$

where the average is over the ensemble $P([\xi(\bullet)])$. In order to work out this equation we first solve the following Green problem:

$$\left[\frac{\partial}{\partial t}-\gamma-\gamma V\frac{\partial}{\partial V}\right]G(V,V_1;t-t_1)=\delta(V-V_1)\,\delta(t-t_1), \tag{8}$$

where the corresponding Green function is given by

$$G(V,V_1;t-t_1)=e^{\gamma(t-t_1)}\delta[Ve^{\gamma(t-t_1)}-V_1]\Theta(t-t_1), \tag{9}$$

and $\Theta(t)$ is the step function.

The integral solution of Eq. (6) can be written, with the help of the Green function (9), in the form

$$\rho(V,t)=\rho^0(V,t)-\int_{-\infty}^{+\infty}dV_1\int_0^t dt_1 G(V,V_1;t-t_1)\xi(t_1)\frac{\partial}{\partial V_1}\rho(V_1,t_1), \tag{10}$$

where $[\partial/\partial t-\gamma-\gamma V(\partial/\partial V)]\rho^0(V,t)=0$. Now we can introduce Eq. (10) into the right-hand side of Eq. (7),

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=-\left\langle \xi(t)\frac{\partial}{\partial V}\rho^0(V,t)\right\rangle+\left\langle \xi(t)\frac{\partial}{\partial V}\int_{-\infty}^{+\infty}dV_1\int_0^t dt_1 G(V,V_1;t-t_1)\xi(t_1)\frac{\partial\rho(V_1,t_1)}{\partial V_1}\right\rangle. \tag{11}$$

Working out the ensemble average we arrive at

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=\int_{-\infty}^{+\infty}dV_1\int_0^t dt_1 G(V,V_1;t-t_1)e^{\gamma(t-t_1)}\left\langle \xi(t)\xi(t_1)\frac{\partial^2\rho(V_1,t_1)}{\partial V_1^2}\right\rangle, \tag{12}$$

where we have used the fact that in the integral we can replace $\partial/\partial V\to e^{\gamma(t-t_1)}(\partial/\partial V_1)$. Now, because the noise $\xi(t)$ is a dichotomous sp we can use the Bourret-Frisch-Pouquet theorem [14,15] to split the average in two parts; and thus we get the following *exact* equation:

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=\int_{-\infty}^{+\infty}dV_1\int_0^t dt_1 G(V,V_1;t-t_1)e^{\gamma(t-t_1)}\langle\xi(t)\xi(t_1)\rangle\frac{\partial^2 P(V_1,t_1)}{\partial V_1^2}. \tag{13}$$

Integrating over dV_1, changing the variable $\tau=t-t_1$, and using the fact that the correlation function is stationary $\langle\xi(t)\xi(t_1)\rangle\equiv\chi(t-t_1)$, we can write

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=\int_0^t\chi(\tau)\frac{\partial^2}{\partial V^2}P(Ve^{\gamma\tau},t-\tau)d\tau.$$

Now, introducing the operator identity: $P(Ve^{\gamma\tau},t-\tau)=\exp[\gamma\tau V(\partial/\partial V)]P(V,t-\tau)$, and using that

$$\frac{\partial^2}{\partial V^2}\left(V\frac{\partial}{\partial V}\right)^n=\left(V\frac{\partial}{\partial V}+2\right)^n\frac{\partial^2}{\partial V^2},\quad n=0,1,2,\dots,$$

from Eq. (13), after some algebra, we finally obtain

$$\frac{\partial P(V,t)}{\partial t}-\gamma\frac{\partial}{\partial V}[VP(V,t)]=\int_0^t\chi(\tau)\exp\left[\gamma\tau\left(V\frac{\partial}{\partial V}+2\right)\right]\times\frac{\partial^2 P(V,t-\tau)}{\partial V^2}d\tau. \tag{14}$$

This is the exact evolution equation for the one-time probability distribution of the generalized Ornstein-Uhlenbeck process (1), when the thermal bath is modeled by a symmetric dichotomous noise. Now with the help of the Laplace transform, $\int_0^\infty e^{-ut}f(t)dt\equiv\mathcal{L}_u[f(t)]\equiv\hat{f}[u]$, we can rewrite this equation in the form

$$u\hat{P}(V,u)-P(V,0)-\gamma\frac{\partial}{\partial V}[V\hat{P}(V,u)]=\hat{\chi}\left[u-\gamma\left(V\frac{\partial}{\partial V}+2\right)\right]\frac{\partial^2\hat{P}(V,u)}{\partial V^2}. \tag{15}$$

This formula is useful to calculate the stationary distribution of the sp $V(t)$, i.e.,

$$P_{st}(V)\equiv P(V,t\to\infty)=\lim_{u\to 0}u\hat{P}(V,u).$$

Therefore using Eq. (15) and the Laplace transform of the correlation function (4),

$$\hat{\chi}(u)\equiv\mathcal{L}_u[a^2\exp(-2\lambda|t|)]=a^2(u+2\lambda)^{-1},$$

the stationary differential equation for the probability distribution adopts the form

$$\left\{\left[-\gamma\left(V\frac{\partial}{\partial V}+2\right)+2\lambda\right]\left(-\gamma\frac{\partial}{\partial V}V\right)\right\}P_{st}(V)=a^2\frac{\partial^2 P_{st}(V)}{\partial V^2}. \tag{16}$$

To find the solution of this equation we try a normalized function of the form

$$P_{st}(V)=\mathcal{N}(1-BV^2)^A. \tag{17}$$

Note that, in order to have a well defined probability distribution $P_{st}(V)$ some care must be taken in the definition of the domain of the distribution. Inserting Eq. (17) in Eq. (16)

and using that $(1-BV^2)\neq 0$, it is possible to prove, for any $A>-1$, that the constants B and A are given by

$$B=\frac{\gamma^2}{a^2} \quad \text{and} \quad A=\frac{\lambda}{\gamma}-1.$$

This implies a natural cutoff in the domain of the velocity, which is characterized by the value $V_d=\pm a/\gamma$ [this is a clear consequence of the signature of the *finite* random accelerations occurring in the sde (1)]. On the other hand the distribution $P_{st}(V)$ will be a convex or concave function depending on the value of the rate λ/γ; both behaviors can be understood heuristically. The case $\lambda/\gamma \ll 1$ means that the noise correlation $\propto \lambda^{-1}$ is large compared to the dissipation time scale $\propto \gamma^{-1}$, then the noise can be considered strongly persistent (static limit) so we can approximate $\xi(t)$ by a constant in the sde (1); from this fact it follows that asymptotically $|V|\sim a/\gamma$. Therefore, the invariant measure shows a divergence at the points $\pm a/\gamma$. The opposite case, $\lambda/\gamma>1$, applies when the noise is a fluctuating process on the dissipative time scale, and then it is highly improbable to reach the extreme "deterministic" values $V_d=\pm a/\gamma$; that is the reason why, when $\lambda/\gamma>1$, the stationary probability distribution goes suddenly to zero for $V\to V_d$.

It should be emphasized that the time-dependent structure of the corresponding one-time probability distribution $P(V,t)$ is highly complex due to the occurrence of rare events; these events correspond to the stochastic realizations when the dichotomous noise is constant for a long time before jumping—for the first time—to a different value. This fact leads to the occurrence of δ-Dirac contributions (moving away from the initial condition) in the one-time probability distribution $P(V,t)$; this issue has been seen, for example, when solving the simpler sde $\dot{X}=\xi(t)$ driven by a dichotomous noise and in the presence of special boundary conditions [12].

By computing the normalization constant $\mathcal{N}$, in the domain $\mathcal{D}=[-a/\gamma;+a/\gamma]$, the stationary probability distribution (17) can be written in the form

$$P_{st}(V)=\frac{\gamma\Gamma\left(\frac{\lambda}{\gamma}+\frac{1}{2}\right)}{a\sqrt{\pi}\Gamma\left(\frac{\lambda}{\gamma}\right)}\left(1-\frac{\gamma^2}{a^2}V^2\right)^{(\lambda/\gamma-1)}, \quad V\in\mathcal{D}, \tag{18}$$

where $\Gamma(z)$ is the gamma function. From this expression it is quite simple to calculate, for example, the second moment $\langle V^2\rangle$ and see that it is in agreement with Eq. (5). From this expression it is also possible to see that this anomalous velocity distribution goes asymptotically to the Maxwellian distribution $P(V)=\mathcal{N}e^{-\gamma V^2/2D}$ if we take the simultaneous limit: $a\to\infty$ and $\lambda\to\infty$, such that $a^2(2\lambda)^{-1}\to D$ (note that in this case the cutoff disappears restoring the natural Gaussian domain). This limit, of course, corresponds to going from the dichotomous sp to the Gaussian white-noise case. Here we should remark that Eq. (18) fully agrees with the equilibrium density obtained from different methods [16,17].

It is interesting to remark that even when the two-point correlation function (5) does not show any "strange" behavior, the corresponding two-time joint probability distribution should do so. This fact is simple to understand considering the one-time probability distribution; for example, if we calculate the one-time moments $\langle V(t)^n\rangle,\forall n$ we would not see any strange behavior; it is only when we sum all the moments appearing in Eq. (3) that an anomalous behavior is built up in its one-time probability distribution, as shown in the corresponding stationary distribution (18).

An important question is whether it is possible to find another family of anomalous velocity distributions from first principles as we have shown here. Unfortunately, only few stochastic processes can be worked out exactly as we have done with the dichotomous sp, thus if we want to go ahead with this program we should implement some stochastic perturbation theory. This fact has extensively been worked out since the pioneer work of Kraichnan when he studied the problem of turbulence [18], Bourret in the study of wave propagation in random media [19], Kubo when he tackled the problem of linear stochastic differential equations [20], or by using van Kampen's cumulant expansion [21]. A rigorous review showing the "evolution" of the stochastic perturbation theory can be seen in Ref. [22]. In the following section we discuss briefly a possible way of working this program.

B. Discussion

If the noise $\xi(t)$ in Eq. (1) is not a dichotomous process the "partition" of the bracket involved in going from Eq. (12) to Eq. (13) is not exact, therefore Eq. (14) is only an approximation. As a matter of fact, Bourret called this procedure the one-ficton approximation, and later on it was recognized that a rigorous perturbation theory should be done in the Kubo number $\sigma^2 T_{\mathrm{corr}}$. In any case, the one-ficton approximation, or the leading order in the Kubo number, involves in an essential way the two-time correlation function $\chi(\tau)$ of the stochastic coefficients appearing in the Liouville equation. Thus in principle, if $\xi(t)$ is an arbitrary sp the one-ficton approximation can be considered as a first approach to solve this problem, i.e., by adjusting the dispersion, $\sigma^2=\langle\xi^2\rangle$, and the correlation time T_{corr} of the noise to that of a dichotomous process. If we want to go one step further and consider nonexponential correlation functions, a possible way is by generalizing the dichotomous noise using the kangaroo processes (KP) [23]; in fact the KP are Markovian stochastic processes but with arbitrary probability distributions [for the configurational transition rate $\lambda(\xi)$] and correlation function $\chi(\tau)$; however, the amount of algebra involved to tackle this problem could be prohibitive. Thus a qualitative approximation to work out a situation when the correlation function is nonexponential, could be to consider the right-hand side of Eq. (15) even with an arbitrary function $\hat{\chi}(u)$. On the other hand, and thanks to the fact that we can calculate all the cumulants and moments of the sp $V(t)$ [if we know the characteristic functional of the noise, see Eq. (2)], we can always compare these exact one-time moments against the one that we could calculate using the distribution coming from the one-ficton approximation; in this way we can test the goodness or not of Bourret's approximation.

For example, suppose that the correlation function is a power law of the form

$$\chi(\tau)=\frac{\Gamma_2\ T_{\rm corr}^{-1}}{(1+\tau/T_{\rm corr})^{\mu}},\quad 0\leqslant\mu<1;$$

a similar long range correlation function was also used to model anomalous diffusion in a random velocity field [24]. The Laplace transform of $\chi(\tau)$ is given by

$$\hat{\chi}(u)=\Gamma_2(uT_{\rm corr})^{\mu-1}e^{uT_{\rm corr}}\Gamma(1-\mu,uT_{\rm corr}),$$

where

$$\Gamma(v,x)=\int_x^{\infty}t^{\nu-1}e^{-t}dt,\quad x>0,$$

is the incomplete gamma function. Introducing this function $\hat{\chi}(u)$ in Eq. (15) it is simple to work out an approximate differential equation for the stationary distribution $P_{st}(V)$. As a matter of fact, for small $uT_{\rm corr}$, it is possible to see that the dominant contribution leads to a *fractional* differential equation [25], therefore predicting an anomalous velocity distribution. In fact from this ''naive'' approximation it is simple to check that the limit $\mu\to 0$ (the static limit) is in agreement with the exact result (16) in the limit $\lambda\to 0$. Due to the fact that this limit is the worst situation for the one-ficton approximation [26], we expect that from our fractional differential equation we could get some insight in understanding the fascinating issue of the occurence of anomalous velocity distributions. Work along these lines is in progress.

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[27] In the paper Physica A54, 623 (1971), Bourret used implicitly the idea of the stochastic Liouville equation. As a matter of fact, in a somewhat ''obscure'' paper [Can. J. Phys. 44, 2519 (1966)] Bourret also used this idea to get the stationary probability distribution. By the way, in Sec. V of this old paper there is an *avant premiere* concerning the problem of a generalized Rayleigh particle; unfortunately, the derivation is not given and the solution is not well written; but the very interesting point is that this stationary distribution was found almost 15 years before the work of Kitahara, Horsthemke, and R. Lefever [Phys. Lett. 70A, 377 (1979)].