Non-linear Brownian motion: the problem of obtaining the thermal Langevin equation for a non-Gaussian bath

A A Dubkov[1], P Hänggi[2] and I Goychuk[2]

[1] Radiophysics Department, Nizhniy Novgorod State University, Gagarin Avenue 23, 603950 Nizhniy Novgorod, Russia

[2] Institut für Physik, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany

E-mail: dubkov@rf.unn.ru, hanggi@physik.uni-augsburg.de and goychuk@physik.uni-augsburg.de

Abstract. The non-linear dissipation corresponding to a non-Gaussian thermal bath is introduced together with a multiplicative white noise source in the phenomenological Langevin description for the velocity of a particle moving in some potential landscape. Deriving the closed Kolmogorov's equation for the joint probability distribution of the particle displacement and its velocity by use of functional methods and taking into account the well-known Gibbs form of the thermal equilibrium distribution and the condition of 'detailed balance' symmetry, we obtain the exact master equation: given the white noise statistics, this master equation relates the non-linear friction function to the velocity-dependent noise function. In particular, for multiplicative Gaussian white noise this operator equation yields a unique inter-relation between the generally non-linear friction and the (multiplicative) velocity-dependent noise amplitude. This relation allows us to find, for example, the form of velocity-dependent noise function for the case of non-linear Coulomb friction.

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1. Introduction

One hundred years after its original introduction [1, 2] the Langevin approach continues to present a fruitful and powerful tool for investigating the stochastic dynamics of complex macroscopic systems (see e.g. [3]), such as the problem of non-linear Brownian motion [4]. In most cases the presence of the internal thermal fluctuations can be described by introducing a linear dissipation mechanism and, at the same time, an additive Gaussian white noise source; see in this context the recent analysis [5]. Moreover, the intensity of such noise is strongly connected with the linear damping coefficient. This well-known Sutherland–Einstein relation [6] is of the form of the linear fluctuation-dissipation theorem [7], reflecting the fundamental relationship between equilibrium fluctuations and macroscopic irreversibility. When the thermal bath is modeled by Gaussian colored noise, the dissipation remains linear, but non-local, and the stochastic Langevin equation transforms to the generalized Langevin equation with a memory of Kubo–Zwanzig type [8]–[10].

The Gaussian thermal bath constitutes in many cases a good but nevertheless idealized physical situation. Even in the simple case of a Brownian particle interacting with the molecules of solvent, the random collisions can be described in terms of a Poissonian rather than a Gaussian statistics. In the case of frequent and small collision changes (weak collision limit) the central limit theorem then guarantees a Gaussian statistics. On the other hand, infrequent and strong collisions then necessitate a master equation description in terms of a linearized Boltzmann equation with a collision kernel. Two typical such cases refer to the situation of gas in the Rayleigh limit, i.e. a heavy particle colliding with a thermal bath of light particles, yielding a case for the weak collision limit, and the Lorentz limit with a light particle colliding with a thermal bath of heavy particles (strong collision limit); see section V in [10] and the insightful review on the 'linear gas' [11]. Such a situation with non-linear white non-Gaussian noise is omnipresent for chemical reactions scenarios, i.e. the theme of unimolecular rate theory [10].

On the other hand, according to non-linear fluctuation-dissipation theorems and relations [12]–[17], the presence of a non-linear resistor in an electrical circuit intrinsically implies the existence of high-order correlations in equilibrium current fluctuations. A relatively small number of charge carriers in semiconductor thin films can provide a non-Gaussian shot noise; i.e. the central limit theorem is inapplicable for such a situation. Finally, the molecular vibrations in solids are in general anharmonic, and the Gaussian approximation for such a thermal bath is not justified at higher temperatures.

Some first steps towards solving the problem of non-Gaussian thermal fluctuations in non-linear systems by introducing in the Langevin equation, together with non-linear friction, a multiplicative white Gaussian noise were taken in [3], [17]–[20] in the framework of the theory of Markovian stochastic processes. In particular, many authors have tried to construct the Langevin equation for an electrical circuit with a non-linear resistor and condenser [21]–[28] on the basis of the known equilibrium probability distribution and the detailed balance symmetry. They discussed also the possibilities of using the master equation for this purpose and reconstructing the phenomenological voltage–current characteristic for a non-linear diode from the stochastic model. Despite these prior works, the extension of the phenomenological Langevin method to noisy non-linear dynamical systems containing non-Gaussian thermal fluctuations still presents a partially unsolved problem.

In this work the procedure for constructing a consistent Langevin description from a thermodynamical viewpoint for the case of a Brownian particle interacting with a general non-Gaussian thermal bath is proposed. Using the equilibrium Gibbs form of the thermal equilibrium probability and the 'detailed balance' condition [17, 29] we find the general integro-differential operator relationship involving the non-linear friction term and the velocity-dependent noise intensity. The exact results reduce in the commonly used case with linear velocity damping to the known result for an additive white Gaussian noise source.

2. Derivation of basic relations

We consider a Brownian particle moving in the potential $U(x)$ and interacting with a thermal bath at temperature T. The stochastic dynamics is assumed to be governed by the following phenomenological Langevin equation[3]:

$$m\dot{v} = -F(v) - \frac{\mathrm{d}U\,(x)}{\mathrm{d}x} + \Psi(v)\,\xi(t), \tag{1}$$

where $x(t)$ and $v(t) = \dot{x}(t)$ are the displacement and the velocity of the particle respectively. The symbol m denotes the mass of the particle, $F(v)$ is an as yet unknown non-linear dissipation function (the friction force with the minus sign in the case of additive noise, $\Psi(v) = \text{const}$), and $\Psi(v)\,\xi(t)$ denotes a multiplicative random force which can be represented by a non-Gaussian white noise $\xi(t)$ with the velocity-dependent strength $\Psi(v)$. We interpret the white noise $\xi(t)$ as a time derivative of the generalized Wiener process $\eta(t)$ (the Lévy process) [31]–[33] with identically distributed and statistically independent increments at non-overlapping time intervals (see [27]), i.e. $\xi(t) = \dot{\eta}(t)$. According to the

[3] Throughout this work we will interpret this equation in the Stratonovich sense [30].

theory of infinitely divisible distributions, the characteristic function of such increments obeys the Lévy–Khinchin formula (see equation (6) in [31]):

$$\theta_\eta(u) = \langle \mathrm{e}^{\mathrm{i}u[\eta(t)-\eta(0)]} \rangle = \exp\left\{ t \int_{-\infty}^{+\infty} \frac{\mathrm{e}^{\mathrm{i}uz} - 1 - \mathrm{i}uz}{z^2} \rho(z)\,\mathrm{d}z \right\}. \tag{2}$$

Here, the function $\rho(z)$ represents a non-negative kernel function which is proportional to the probability density of jumps and is uniquely determined by the statistics of noise. Specifically, for an ordinary (continuous) Wiener process $\eta(t)$ the kernel function takes the form of a delta function $\rho(z) = 2D\,\delta(z)$, where $2D$ is the intensity of white Gaussian noise $\xi(t)$. Another widespread model in physics is the white Poissonian shot noise [18, 19]

$$\xi(t) = \sum_i a_i\,\delta(t - t_i), \tag{3}$$

where the point process $\{t_i\}, i = 1, 2, \ldots$, represents the Poissonian process of events with the mean rate λ and random amplitudes a_i which are statistically independent and have the identical probability distribution $W_a(z)$. In such a case the kernel function reads $\rho(z) = \lambda z^2 W_a(z)$. For symmetric α-stable Lévy noise $\xi(t)$ which generates anomalous diffusion in the form of Lévy flights [33], one finds $\rho(z) = K|z|^{1-\alpha}$ $(0 < \alpha < 2)$.

According to general fluctuation-dissipation relations [27] one expects definite relationships to hold between the non-linear friction $F(v)$ and the function $\Psi(v)$ for a given statistics of noise $\xi(t)$, similar in spirit to the Sutherland–Einstein relation between the linear damping coefficient and the intensity of additive Gaussian noise. Moreover, we will base our analysis on two main working principles of statistical mechanics: (i) first, we impose the Gibbs form for the resulting equilibrium distribution for the coordinate and velocity of a particle; i.e.,

$$P_{st}(x, v) = Z_0\,\mathrm{e}^{-H_0(x,v)/k_\mathrm{B}T}, \tag{4}$$

where Z_0 is the normalization constant and k_B denotes the Boltzmann constant. Substituting in equation (4) the Hamiltonian $H_0(x, v) = mv^2/2 + U(x)$ of the system (1) we arrive at well-known stationary Maxwell–Boltzmann probability distribution, reading

$$P_{st}(x, v) = Z_0\,\mathrm{e}^{-mv^2/2k_\mathrm{B}T - U(x)/k_\mathrm{B}T}. \tag{5}$$

The second principle (ii) is the 'detailed balance' condition [17], which has its origin in microscopic reversibility. According to this principle and the even parity property $(+1)$ under time reversal transformation of the variable x and odd parity property (-1) of the velocity variable v, the following relation for the joint, two-event equilibrium probability density function with $\tau > 0$ holds (see equation (4.3.6) in [17] and equation (6.85) in [29]):

$$P_{st}(x, v, \tau; x_0, v_0) = P_{st}(x, -v, -\tau; x_0, -v_0) = P_{st}(x_0, -v_0, \tau; x, -v). \tag{6}$$

We next apply known functional methods [18] to the Langevin dynamics equation (1) to obtain the closed equation for the joint probability density function $P(x, v, t)$ [31]. In doing so, we rewrite equation (1) in the form of the following set of equations:

$$\begin{aligned} \dot{x} &= v, \\ \dot{v} &= -\frac{F(v)}{m} - \frac{U'(x)}{m} + \frac{\Psi(v)}{m}\,\xi(t). \end{aligned} \tag{7}$$

Using the expression for $P(x,v,t)$ in the form of a statistical average, i.e.,

$$P(x,v,t) = \langle \delta\left(x - x\left(t\right)\right) \delta\left(v - v(t)\right) \rangle , \tag{8}$$

and taking into account equations (7), we arrive at

$$\begin{aligned} \frac{\partial P}{\partial t} &= -v \frac{\partial P}{\partial x} + \frac{1}{m}\frac{\partial}{\partial v}\left[F\left(v\right)P\right] + \frac{1}{m}U'(x)\frac{\partial P}{\partial v} \\ &\quad - \frac{1}{m}\frac{\partial}{\partial v}\Psi(v)\left\langle \xi(t)\delta\left(x - x(t)\right)\delta\left(v - v(t)\right)\right\rangle . \end{aligned} \tag{9}$$

To split further the average in equation (9) we use the following relation:

$$\langle \xi(t) R_t[\xi] \rangle = \int_{-\infty}^{+\infty} \frac{\rho(z)}{z^2}\, \mathrm{d}z \int_0^z \left[\left\langle \mathrm{e}^{y\delta/\delta\xi(t)} R_t[\xi]\right\rangle - \langle R_t[\xi]\rangle\right] \mathrm{d}y, \tag{10}$$

derived in [31] for the correlation between a non-Gaussian white noise $\xi(t)$ and an arbitrary functional $R_t[\xi]$, with the function $\rho(z)$ defined in equation (2).

Because both $x(t)$ and $v(t)$ are functionals of the random process $\xi(t)$, and moreover, according to equation (7),

$$\frac{\delta x(t)}{\delta \xi(t)} = 0, \qquad \frac{\delta v(t)}{\delta \xi(t)} = \frac{\Psi(v)}{m}, \tag{11}$$

we obtain

$$\frac{\delta}{\delta\xi(t)}\,\delta\left(x - x\left(t\right)\right)\delta\left(v - v(t)\right) = -\frac{1}{m}\frac{\partial}{\partial v}\Psi\left(v\right)\delta\left(x - x(t)\right)\delta\left(v - v(t)\right). \tag{12}$$

Substituting $R_t[\xi] = \delta(x - x(t))\delta(v - v(t))$ in equation (10) and taking into account equations (8) and (12) we find

$$\begin{aligned} \langle \xi(t)\delta\left(x - x(t)\right)\delta(v - v(t))\rangle &= \int_{-\infty}^{+\infty} \frac{\rho(z)}{z^2}\,\mathrm{d}z \\ &\quad \times \int_0^z \left[\exp\left\{-\frac{y}{m}\frac{\partial}{\partial v}\Psi(v)\right\} - 1\right] P\left(x,v,t\right)\,\mathrm{d}y. \end{aligned} \tag{13}$$

Using equation (13) in equation (9) and performing an integration with respect to y we find the following Kolmogorov integro-differential equation for the probability density function $P(x,v,t)$:

$$\begin{aligned} \frac{\partial P}{\partial t} &= -v \frac{\partial P}{\partial x} + \frac{1}{m}\frac{\partial}{\partial v}\left[F\left(v\right)P\right] + \frac{1}{m}U'(x)\frac{\partial P}{\partial v} \\ &\quad + \int_{-\infty}^{+\infty} \frac{\rho(z)}{z^2}\left[\exp\left\{-\frac{z}{m}\frac{\partial}{\partial v}\Psi(v)\right\} - 1 + \frac{z}{m}\frac{\partial}{\partial v}\Psi\left(v\right)\right] P\left(x,v,t\right)\,\mathrm{d}z. \end{aligned} \tag{14}$$

On the basis of the forward and backward Kolmogorov equation we can rewrite the 'detailed balance' condition (6) in the form of an equivalence between two operators: the kinetic $\hat{L}(x,v)$ and the adjoint $\hat{L}^{+}(x,v)$ yielding the operator relation (see equation (3.7) in [16] or also equation (6.81) in [29])

$$\frac{1}{P_{st}(x,v)}\,\hat{L}(x,v)P_{st}(x,v) = \hat{L}^{+}(x,-v). \tag{15}$$

This relation is meant to operate on an arbitrary function $g(x, v)$. Substituting next in equation (15) the equilibrium Maxwell–Boltzmann distribution from equation (5), using the form of the kinetic operator $\hat{L}(x, v)$ from equation (14) and taking into account the odd parity property of the friction function $F(v)$ and the even parity property of the noise amplitude function $\Psi(v)$, we arrive after some manipulations at

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}v}\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right] + 2F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\frac{\mathrm{d}}{\mathrm{d}v} \\
&\qquad + m\int_{-\infty}^{+\infty}\frac{\rho(z)}{z^2}\left[\exp\left\{-\frac{z}{m}\frac{\mathrm{d}}{\mathrm{d}v}\Psi(v)\right\} + \frac{z}{m}\frac{\mathrm{d}}{\mathrm{d}v}\Psi(v)\right]\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\mathrm{d}z \\
&\qquad = m\int_{-\infty}^{+\infty}\frac{\rho(z)}{z^2}\,\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\left[\exp\left\{-\frac{z}{m}\Psi(v)\frac{\mathrm{d}}{\mathrm{d}v}\right\} + \frac{z}{m}\Psi(v)\frac{\mathrm{d}}{\mathrm{d}v}\right]\mathrm{d}z. \qquad (16)
\end{aligned}$$

Equation (16) assumes the form of an equivalence between two integro-differential operators. If all the relations given by

$$B_n = \int_{-\infty}^{+\infty} z^n \rho(z)\,\mathrm{d}z \qquad (17)$$

are finite, equation (16) can be rewritten in a more compact differential form:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}v}\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right] + 2F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\frac{\mathrm{d}}{\mathrm{d}v} + \sum_{n=2}^{\infty}\frac{(-1)^n B_{n-2}}{m^{n-1}\,n!} \\
&\qquad \times\left\{\left[\frac{\mathrm{d}}{\mathrm{d}v}\Psi(v)\right]^n \mathrm{e}^{-mv^2/2k_\mathrm{B}T} - \mathrm{e}^{-mv^2/2k_\mathrm{B}T}\left[\Psi(v)\frac{\mathrm{d}}{\mathrm{d}v}\right]^n\right\} = 0. \qquad (18)
\end{aligned}$$

These relations constitute the main result of our present work.

3. Applications

First, we analyze equation (18) for multiplicative Gaussian thermal noise. Substituting $\rho(z) = 2D\,\delta(z)$ in equations (17) and (18) we obtain

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}v}\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right] + 2F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\frac{\mathrm{d}}{\mathrm{d}v} \\
&\qquad + \frac{D}{m}\left\{\left[\frac{\mathrm{d}}{\mathrm{d}v}\Psi(v)\right]^2 \mathrm{e}^{-mv^2/2k_\mathrm{B}T} - \mathrm{e}^{-mv^2/2k_\mathrm{B}T}\left[\Psi(v)\frac{\mathrm{d}}{\mathrm{d}v}\right]^2\right\} = 0. \qquad (19)
\end{aligned}$$

After some rearrangements, equation (19) can be written in the form

$$\begin{aligned}
&\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T} + \frac{D}{m}\Psi(v)\left(\Psi(v)\,\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right)'\right]' \\
&\qquad + 2\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T} + \frac{D}{m}\Psi(v)\left(\Psi(v)\,\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right)'\right]\frac{\mathrm{d}}{\mathrm{d}v} = 0. \qquad (20)
\end{aligned}$$

From equation (20) we can now extract a unique fundamental relation between the non-linear friction $F(v)$ and the velocity-dependent noise intensity $\Psi^2(v)$, reading

$$F(v) = \frac{Dv}{k_\mathrm{B}T}\Psi^2(v) - \frac{D}{2m}\left[\Psi^2(v)\right]'. \qquad (21)$$

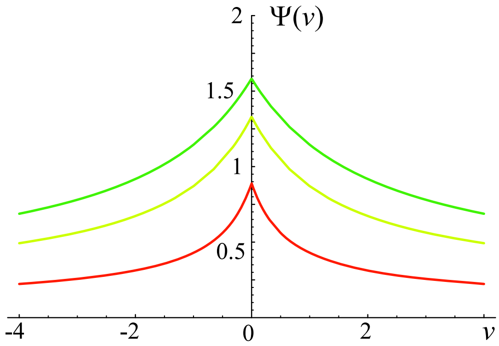

Figure 1. Coulomb friction case: dependence of the thermal multiplicative noise strength $\Psi(v)$ on the particle velocity v for different values of the parameter $\kappa = m/(k_{\mathrm{B}}T)$: $\kappa = 0.5$ (green curve), $\kappa = 1$ (yellow curve), $\kappa = 5$ (red curve). The parameter $\mu\, m/D = 1$.

3.1. Linear friction

For an additive noise source ($\Psi(v) = 1$) we obtain from equation (21) the well-known linear friction result

$$F(v) = \gamma v, \tag{22}$$

with the damping strength γ satisfying the Sutherland–Einstein relation

$$\gamma = \frac{D}{k_{\mathrm{B}}T}. \tag{23}$$

3.2. Coulomb friction

More generally, we can readily solve the first-order linear differential equation (21) to find for a given non-linear friction $F(v)$ for the multiplicative function $\Psi(v)$ in equation (1) the result

$$\Psi^2(v) = \frac{2m}{D}\,\mathrm{e}^{mv^2/k_{\mathrm{B}}T}\int_v^{+\infty} F\,(u)\,\mathrm{e}^{-mu^2/k_{\mathrm{B}}T}\,\mathrm{d}u. \tag{24}$$

For example, for a Coulomb friction, reading $F(v) = \mu\,\mathrm{sgn}(v)$ [34], we obtain from equation (24)

$$\Psi^2(v) = \frac{\mu\, m}{D}\sqrt{\frac{\pi}{\kappa}}\,\mathrm{e}^{\kappa v^2}\mathrm{erfc}\left(\sqrt{\kappa}|v|\right), \tag{25}$$

where $\kappa = m/(k_{\mathrm{B}}T)$ and $\mathrm{erfc}(z)$ is the complementary error function. The velocity-dependent noise amplitude $\Psi(v)$ from equation (25) is depicted in figure 1 for different values of dimensionless parameter κ. According to equation (25), for large values of the particle velocity v the multiplicative noise strength $\Psi(v) \sim 1/\sqrt{|v|}$.

3.3. Non-Gaussian thermal shot noise

For a non-Gaussian thermal noise, such as white shot noise (3), equation (18) yields

$$\frac{\mathrm{d}}{\mathrm{d}v}\left[F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\right]+2F(v)\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\frac{\mathrm{d}}{\mathrm{d}v}+\nu\sum_{n=2}^{\infty}\frac{(-1)^n\left\langle a^n\right\rangle}{m^{n-1}\,n!}$$
$$\times\left\{\left[\frac{\mathrm{d}}{\mathrm{d}v}\Psi(v)\right]^n\mathrm{e}^{-mv^2/2k_\mathrm{B}T}-\mathrm{e}^{-mv^2/2k_\mathrm{B}T}\left[\Psi\left(v\right)\frac{\mathrm{d}}{\mathrm{d}v}\right]^n\right\}=0. \qquad (26)$$

This operator relation (26) evidently presents a complicated structure. Clearly, this relation in our case seems not readily solvable. The same situation arises already for additive, i.e. $\Psi(v) = 1$, non-Gaussian white noise. Thus, the problem of obtaining the correct multiplicative noise structure remains open.

4. Conclusions

We have proposed a procedure for constructing a Langevin-type equation for a particle moving in some potential and interacting with a non-Gaussian thermal bath. The approach developed is based on two main principles of statistical mechanics: we use the Gibbs form of the equilibrium distribution and detailed balance symmetry. We obtain an exact operator expression relating the non-linear friction $F(v)$ to the statistics of non-Gaussian thermal noise in terms of its corresponding velocity-dependent noise strength $\Psi(v)$. For multiplicative white Gaussian noise this operator relation reduces to a single equation which explicitly connects the non-linear dissipation function and the velocity-dependent noise intensity. As an example, we evaluated this multiplicative velocity noise function for the case of Coulomb friction. Unfortunately, however, for a non-Gaussian white noise source this operator relation seemingly is difficult to solve; it may not even possess a solution which is consistent with the ansatz given with equation (1). More generally, one may be forced to generalize the ansatz in the Langevin equation (1) by including a non-factorizing, velocity-dependent white noise source or even a sum of multiplicative white noise sources, possessing quite different statistics. Alternatively, one may start out directly from the physical master equation and then derive from it the corresponding Langevin equation with generalized white noise sources [18]–[20]. Nevertheless, the stochastic Langevin equation so constructed can serve as a starting point for future investigations of non-linear, non-Gaussian diffusion in different contexts. In this sense, this Langevin approach provides a new playground for investigating thermal non-linear Brownian motion.

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