Non-Markovian effects on overdamped systems

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Abstract – We study the consequences of adopting the memory-dependent, non-Markovian, physics with the memory-less overdamped approximation usually employed to investigate Brownian particles. Due to the finite correlation time scale associated with the noise, the stationary behavior of the system is not described by the Boltzmann-Gibbs statistics. However, the presence of a very weak external white noise can be used to regularize the equilibrium properties. Surprisingly, the coupling to another bath effectively restores the dynamical aspects missed by the overdamped treatment.

Introduction. – Brownian motion is an excellent laboratory for probing the microscopic dynamics of fluid systems. For realistic systems, the interaction between the Brownian Particle (BP) and its neighborhood is quite complex since, on top of all the microscopic local interactions of the BP and the bath particles, the BP’s own motion generates (inertial) hydrodynamic fluxes that interact again with it. In consequence, a dissipative memory function arises [1,2], setting the non-Markovian character of the reduced dynamics of the particles. That sort of effect is responsible for the anomalies in velocity-velocity correlation functions first pointed out by Alder and Wainwright [3].

It should be clear from the beginning that non-Markovian properties are not properties of a system itself, but rather of its description by a chosen set of variables [4]. As an example, a BP described only by its position will present a memory-dependent behavior. On the other hand, by describing it by means of position and velocity will recover the Markovian character. For classical systems, the Hamiltonian dynamics, or its equivalent, the Liouville dynamics, is certainly Markovian. In quantum mechanics the von Neumann equation plays an exactly similar role.

The existence of a clear cut time-scale separation, such as that due to the mass difference of a BP and the surrounding thermal bath, allows us to eliminate (most of) the fast variables of the problem via adiabatic elimination treatments [5] or by means of projection operator techniques [6]. This is done by a convenient expansion, of the dynamical equations, in powers of a small parameter, such as the ratio of bath-to-BP masses

$$\varepsilon \equiv \sqrt{\frac{m_{\text{bath}}}{M_{\text{BP}}}}.$$  

A didactically interesting example of that procedure is described by van Kampen [7]. In a more general note, powerful methods have been created that allow us to carefully separate each phenomenon in its correct time-scale, such as the time-extension methods [8,9]. Any remaining slow variables (related to the motion of the BP) are subjected to a dynamics that incorporates the effects of the averaged out variables via a non-Markovian dissipative term and a rapidly fluctuating noise term. That is the physical justification for the Langevin approach. Also, the theory presents a feasible mathematical framework and the stationary properties lead to the well-known equilibrium results.

A BP usually exists in fluid media, at low Reynolds number values (Re), i.e., with a relatively high viscosity, where Stokes’ law applies [10]. Stokes’ force is proportional to the product of the viscosity coefficient \(\eta\) of the fluid, the velocity \(V\) of the BP, and the radius \(R\) of the BP. The dissipative time-scale that arises is proportional to

$$\tau_d = \frac{M_{\text{BP}}}{\gamma} = \frac{\rho_{\text{BP}} R^3}{\eta R} = \frac{\rho_{\text{BP}} R}{\rho} \frac{R V}{\eta} \sim \frac{R}{V} \text{Re.}$$

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A strong approximation is to take the overdamped approximation given by $\Re\to 0$, as $M_{BP}/\gamma \to 0$. In that limit, the BP is too light to be able to make the fluid move by means of its own inertia.

When the presence of induced flows cannot be ignored, they can be taken into account by a memory kernel in the dissipative term of the dynamical equations associated with BP. That kernel is dominated by the time-scale $\tau$ associated with the main contribution from the induced slow hydrodynamic modes. Without an external source of energy, the BP in contact with a thermal bath will tend to an equilibrium state described by the Boltzmann-Gibbs distribution, after a very long transient.

Short-term processes will take the system to an out-of-equilibrium state, unless they are following a very specific quasi-static thermodynamic path. However, even for the non-equilibrium cases, it is possible to find interesting relations between equilibrium and non-equilibrium behaviors [11,12]. Such processes are driven by an external protocol $X(t)$, defined by some time-varying field (such as an external force [13], a magnetic field [14], or the position of the extremity of a spring [15]).

We shall see that using the overdamped approximation, which means assuming a vanishing inertial contribution in the Langevin equation, does not lead to an equilibrium distribution as $t \to \infty$. This can be fixed in two ways: either by taking $\tau \to 0$, i.e., by assuming Markovian behavior of the BP, or by assuming the presence of an arbitrarily weak white-noise source. This is enough to reestablish the equilibrium state, no matter how weak the noise source is.

**Massive particle and equilibrium properties.** – We initially shall study a 1D Langevin-like model for a massive particle under a harmonic external potential as well a Gaussian colored noise. The system is defined by

$$m \ddot{x} + \int_0^t dt' K(t - t') v(t') + k x = \xi(t),$$

and

$$\dot{x} = v,$$

where $K(t - t')$ is the frictional memory kernel [1,2] and $\xi(t)$ is a stochastic Langevin force. The initial conditions are assumed to be

$$x(0) = 0 \quad \text{and} \quad v(0) = 0.$$

We have chosen a harmonic external potential throughout this paper due to its mathematical convenience, since all calculations herein can be made exact and the role of the kernel’s time-scale can be made explicit.

Nevertheless, it is important to notice that surprising physical effects could arise by assuming a force field that allows metastable states. In fact, there exists a lot of interest in the interplay between nonlinear phenomena and the stochastic character of noisy systems [16–20]. For example, a counterintuitive behavior observed in theoretical models as well experimental investigations is the stabilization enhancement of metastable and unstable states, which is called noise-enhanced stability (NES) [17,20]. This peculiar situation may take place when the intensity of noise fluctuations leads to an increase of the escape time from a locally stable state. Notwithstanding the interest in non-linear relaxation physics, we do believe that it is still worth considering linear systems coupled to distinct baths in order to mimic many different time-scale effects, at least as a first approximation.

The main characteristic of the present method is its exact nature coupled with the fact that averages are taken over an infinite time interval. This last points to more regularized results than the ones obtained by numerical techniques. On the other hand, the obtaining of transition rates becomes a hard problem whenever non-linear potentials are involved.

The Gaussian colored noise is characterized by the cumulants

$$\langle \xi(t) \rangle_c = 0,$$

$$\langle \xi(t) \xi(t') \rangle_c = \frac{\gamma T}{\tau} \exp \left( -\frac{|t - t'|}{\tau} \right),$$

where $T$ is the bath temperature and $\tau$ is the correlation time. Special care should be taken in order to recover the correct limit as $\tau \to 0$. The second cumulant must be

$$2\gamma T \delta(t - t'),$$

which is assured by the expression in (3). All other cumulants are zero, which means that they do not contribute to the dynamics of the system. Also, due to the noise-correlated behavior, the memory kernel should of the type

$$K(t - t') = \frac{\langle \xi(t) \xi(t') \rangle_c}{T},$$

in order to be consistent with the fluctuation dissipation theorem.

The approach we are going to use to solve the problem is a straightforward use of the integral transformation methods [21]. We take the Laplace representation of (1),

$$m \dot{\bar{v}}(s) = -\gamma \frac{\bar{v}(s)}{(s \tau + 1)} - k \bar{v}(s) + \bar{\xi}(s),$$

$$s \bar{x}(s) = \bar{v}(s),$$

and also for the white-noise cumulant [22],

$$\langle \bar{\xi}(z_1) \bar{\xi}(z_2) \rangle = \gamma T \frac{2 + \tau (z_1 + z_2)}{(1 + z_1 \tau)(1 + z_2 \tau)(z_1 + z_2)}.$$
where the roots $\kappa_1, \kappa_2, \kappa_3$ may be obtained exactly in a similar way to that performed by Soares-Pinto and Morgado [22].

The model can be solved exactly by means of time-averaging techniques [15,22]. In fact, the instantaneous probability density associated with (1) can be written as

$$P(x,v,t) = \left( \frac{1}{2\pi} \right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dQ dP e^{iQx + iPv} \times \langle e^{-iQz(t)} - iPv(t) \rangle,$$

where the moment-generating function, as a function of time, is shown explicitly in (11). It is important to bear in mind that $\langle \cdot \rangle$ is the noise average. The equilibrium probability distribution is determined by taking the inverse Fourier transform of

$$G(Q, P) = \lim_{t \to \infty} \langle e^{-iQz(t)} - iPv(t) \rangle,$$

which is the stationary generating function, see eq. (11) on top of the page.

A simple expression for (11) is obtained by using the Gaussian properties of the noise, which allows us to group the averages into products of averages of pairs. The finite time limit will make the corresponding terms of the form

$$\exp [(iq_a + iqb + 2e) t],$$

null, unless one integrates over the thermal pole

$$\frac{1}{iq_a + iqb + 2e},$$

After some straightforward simplifications, the terms $(iq_a + e) \tau + 1$ cancel out and we obtain products of the integrals of the type

$$I_{xx} = \lim_{e \to 0^+} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \left[ \frac{1}{R(iq_1 + e)} \right],$$

$$I_{xv} = \lim_{e \to 0^+} \int_{-\infty}^{\infty} \frac{iq_1 + e}{2\pi} R(iq_1 + e) R(-iq_1 - e) = 0, \quad (14)$$

$$I_{vv} = \lim_{e \to 0^+} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \left[ \frac{(iq_1 + e)^2}{2\pi} R(iq_1 + e) \right] \times \frac{1}{R(-iq_1 - e)} = -\frac{1}{2\gamma m}.$$

Those integrals allow us to find an analytic expression for the distribution function. In fact, since $I_{xx} = 0$, no equilibrium average of the type $\langle \bar{x}\bar{v} \rangle$ may exist. Thus, after some algebraic manipulations, one can find

$$G(Q, P) = \exp \left[ -\frac{T}{2} \left( \frac{Q^2}{k} + \frac{P^2}{m} \right) \right].$$

The stationary distribution can be obtained by means of an inverse Fourier transform, which leads to

$$P_{ss}(x,v) = \frac{\sqrt{k m}}{2\pi T} \exp \left( \frac{-m v^2}{2T} - \frac{k x^2}{2T} \right). (16)$$

As expected, we find the Boltzmann-Gibbs probability for the equilibrium state of BP in contact with a thermal reservoir at temperature $T$. This corresponds to the marginal probability distribution of the complete system, assuming the interaction energy between the thermal bath particles and the BP to be small, where we have averaged out the thermal particles degrees of freedom, which is a good approximation for a system of hard-sphere type.

We should observe, from the result above, that the internal dynamics of a system are of no importance with respect to its equilibrium distribution. For simple ergodic systems in contact with a thermal reservoir at temperature $T$, such as the present one, the final equilibrium state is always given by the Boltzmann-Gibbs statistics, regardless of whether the equilibration process involves memory or not.

**Overdamped case and non-equilibrium distribution.** – We now focus on the fast relaxation dynamics. The idea is to investigate the overdamped limit of (1), which is obtained by taking the limit $m/\gamma \to 0$. Consequently, the Langevin equation is given by

$$kx(t) + \int_0^t dt' K(t - t') \dot{x}(t') = \xi(t). (17)$$

Another equivalent and simpler way to deal with the model is through the cumulant generating function, which is a series expansion of the distribution cumulants. Also, due to the Gaussian noise properties, only the second cumulant is relevant to the problem. Then, we have

$$\ln \langle e^{-iQz(t)} \rangle = \frac{-Q^2}{2} \lim_{e \to 0} \int_{-\infty}^{\infty} \frac{dq_1 e^{(iq_1 + e) t}}{2\pi} \times \frac{dQ e^{iQz(t)}}{2\pi} \times \langle \dot{x}(iq_1 + e) \dot{x}(iq_2 + e) \rangle, \quad (18)$$

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where

$$\ddot{x}(s) = \frac{s \tau + 1}{(\gamma + k \tau)s + k} \ddot{\xi}(s)$$ (19)

is calculated through the Laplace transform of (17). As a result, it is not difficult to show that

$$\ln \left\langle e^{-iQx(t)} \right\rangle = -\frac{Q^2}{2} \frac{\gamma T}{k(kT + \gamma)} \times [1 - (1 - \tau a) e^{-2\tau t}],$$ (20)

where

$$a = \frac{k}{k\tau + \gamma}.$$ (21)

For \(t \to \infty\), the stationary cumulant-generating function is given by

$$\ln G(Q) = -\frac{T \gamma Q^2}{2k(\gamma + k \tau)},$$

which allows us to write the probability distribution

$$P^{xx}(x) = \frac{1}{2\pi} \frac{1}{e^{Qx} \exp \left\{ -\frac{T \gamma Q^2}{2k(\gamma + k \tau)} \right\}}\int_{-\infty}^{\infty} dQ e^{Qx} \exp \left\{ -\frac{k(\gamma + k \tau)}{2\pi T \gamma} x^2 \right\},$$ (22)

Clearly, the stationary state is not described by a Boltzmann-Gibbs distribution.

Note that (22) leads to a renormalization of the temperature felt by the particle,

$$T_{\text{eff}} \equiv \frac{T \gamma}{\gamma + k \tau}.$$ (23)

Clearly, this is unphysical since we have seen that the presence of mass yields the correct physical limit. That result had already been obtained earlier by Cugliandolo and Kurchan [23] and studied in detailed by Soares-Pinto and Morgado [22].

The physical reason for the discrepancy is that one of the main roles of a memory kernel is to be the witness to slow modes, such as fluid streamlines, generated in the bath by its interaction with the BP. These flows only appear due to the inertia of the BP that is capable of moving the masses of the particles of the bath out of its way. On the other hand, the overdamped approximation assumes exactly the opposite: the BP inertia is irrelevant! In fact, the relaxation of the BP is supposed to be so fast that it assumes that the BP follows the instantaneous local velocity of the fluid of bath particles. From it we see that by taking \(\tau \to 0\) makes the whole analysis consistent, and (23) becomes \(T_{\text{eff}} = T\), as equilibrium requires.

The discrepancy in (23) is due to artificially mixing the overdamped, memory-less, model with the physics of a non-Markovian model exhibiting a memory function. It is important to bear in mind that our result is consistent with the analysis presented by Soares-Pinto and Morgado [22]. Therein the authors show that, in order to recover the correct equilibrium state, another Gaussian white noise (internal or external) should be included and with the same temperature of the non-Markovian noise. Clearly, the usual equilibrium might also be obtained by taking the limit \(\tau \to 0\) above.

From a mathematical perspective, the presence of mass (independently of its value) implies that \(R(s) = 0\) (see (8)) is a cubic equation with three roots. However, the overdamped limit leads to a simple linear solution, as shown in (19). This suggests that, as \(m \to 0\), two of the cubic roots must move to \(x \to \infty\). The solutions will be quite different.

Let us analyze the problem as \(m/\gamma \to 0\). In this limit, it is straightforward to show that the roots present the asymptotic behavior

$$\kappa_1 \to -\frac{k}{\gamma + k \tau},$$

$$\kappa_2 \to -\frac{\gamma}{2(\gamma + k \tau)} + i \sqrt{\frac{\gamma + k \tau}{m \tau}},$$

$$\kappa_3 \to -\frac{\gamma}{2(\gamma + k \tau)} - i \sqrt{\frac{\gamma + k \tau}{m \tau}},$$ (24)

which can be easily checked out numerically. As a result, the overdamped limit leads to a finite value for \(\kappa_1\), although the other roots tend to \(-c \pm i \infty\). By taking first the limit \(m \to 0\) in (1), which possesses three dynamical poles in Fourier-Laplace representation, we directly obtain (17), which, from (24), presents just a single dynamical pole. It is clear that this is a consequence of taking the mass-less limit, before solving (1), because it makes the other two roots move to infinity, and they no longer participate in the dynamics. Next we see how to regularize that behavior and reach equilibrium once again while still keeping the overdamped non-Markovian character.

The result (23) reminds us of the temperature slip between the interface of a gas and a limiting wall, such as the gas-wall interaction model described in Chapt. 6 of Chapman and Cowling’s book [24]. That slip arises because the particles that are momentarily adsorbed in the wall will be expelled back into the gas, but they will not collide before moving by a typical length of the order of the mean free path, reflecting a decrease in the equilibration efficiency near the wall. Despite the fact that the problem at hand is quite distinct, it is clear that, by neglecting the mass of the particle, the mobility of the BP is clearly reduced and the typical distance it will hover around the origin of the coordinates is reduced by a factor

$$\sqrt{\frac{\gamma}{(\gamma + k \tau)}}.$$ (25)

**Regularizing the equilibration via an additional noise.** – Regularization of the overdamped non-Markovian process can be achieved by replacing the missing kinetic energy of the BP via other means, i.e., an external source such as a thermal bath. That extra noise must be weak enough so that the energy transfer
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from it to the BP is actually negligible compared with that due to the main non-Markovian noise. In fact its role will be to give back the missing particle’s “mobility” due to the extreme rate of damping.

In order to see how this works, we replace (17) by

\[ k x(t) + \int_0^t dt' K(t - t') \dot{x}(t') + \Gamma \dot{x}(t) = \eta(t) + \xi(t), \]

where a second Gaussian noise is included,

\[ \langle \eta(t) \eta(t') \rangle = 2 \Gamma T' \delta(t - t'), \]

with zero average and bath temperature \( T' \). Consequently, the transformed Langevin equation can be rewritten as

\[ \ddot{x}(s) = \left( \frac{s \tau + 1}{R_1(s)} \right) \left[ \tilde{\eta}(s) + \tilde{\xi}(s) \right], \]

where\(^1\)

\[ R_1(s) = \gamma T(s - \lambda_+)(s - \lambda_-). \]

The Fourier-Laplace representation of the noise cumulant (27) is given by

\[ \langle \tilde{\eta}(s_1) \tilde{\eta}(s_2) \rangle = \frac{2 \Gamma T'}{s_1 + s_2}. \]

Using the time-averaging treatment, one can find that the system presents a stationary behavior characterized by the cumulant generating function

\[ \ln G(Q) = -Q^2 \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \frac{1}{2\pi} \frac{1}{R(iq_1 + \epsilon)} \times R(-iq_1 - \epsilon) \gamma T + \Gamma T' \times (1 + (iq_1 + \epsilon) \tau) \left( - (iq_1 + \epsilon) \tau + 1 \right) \]

\[ = -\frac{Q^2}{2} T' \tau k + \Gamma T' + \gamma T \]

\[ + \frac{k}{2} \left( k \tau + \gamma + \Gamma \right), \]

which is consistent with the overdamped limit already obtained by Soares-Pinto and Morgado [22].

Now, assuming that the two baths have the same temperature, \( T' = T \), the Gibbsian state is reestablished,

\[ \ln G(Q) = -\frac{Q^2}{2k} T, \]

\[ P_{eq}(x) = \sqrt{\frac{k}{2\pi T}} \exp \left( -\frac{k x^2}{2T} \right), \]

independently of the value of \( \Gamma \). Note that, as long as \( \Gamma \) is small, but not zero, the two dynamical poles \( \lambda_{\pm} \) are still integrated over, and equilibrium is reached. Also, it should be noticed that, for the above, the dissipation and injection of energy due to the additional white noise are negligible. However, the correct equilibration is obtained (almost) cost free as a true regularizing procedure should be. In fact, the rates of energy transfer and dissipation go to zero for vanishing values of \( \Gamma \), although the missing average kinetic energy is restored at equilibrium.

Note that non-harmonic force terms may lead to a more interesting stationary behavior. This is due to the noise-induced effects on non-linear systems [19,20]. In particular, the increase of the characteristic time-scales associated with metastable states. There are many results reporting a non-monotonic behavior of the average escape time as a function of the noise strength [17,18]. These findings suggest that a stationary distribution inconsistent with the Boltzmann-Gibbs statistics could describe complex systems in very rich potential landscapes.

**Conclusions.** – Many physical phenomena are fundamentally influenced by their typical characteristic time-scales. Indeed, the paradigmatic BP model can be viewed basically as a time-scale separation problem: fast degrees of freedom, associated with the fast thermal bath particles, can be averaged out, yielding the much slower dynamics associated with the BP. In that context, the Langevin equation effectively describes the time-scales associated with the mechanical oscillations, the dissipation and the memory or persistence.

The overdamped model assumes that the BP moves in an extremely viscous fluid, where dissipation is very fast. For that to happen it is necessary that \( m/\gamma \to 0 \), which does not unequivocally imply that \( m \to 0 \) since taking \( \gamma \to \infty \) would also do. However, one of the most used forms of the overdamped approximation is to simply take the inertial term \( m \ddot{x} \) to zero on the Langevin equation. Such a choice leads to a much rougher trajectory for the BP when compared with the massive case [25].

We have seen that another consequence of the simple choice for the overdamped approximation, in the context of non-Markovian dynamics, is that the stationary state will not correspond to the Boltzmann-Gibbs form of the equilibrium distribution. This happens because taking \( m \to 0 \) in the dynamics means to make two dynamical poles move to infinity where they will not contribute to shaping the equilibrium state. In fact, any non-zero value for the mass, no matter how small, would lead to the correct equilibrium distribution at long times.

It is still possible to regularize the overdamped non-Markovian behavior through an additional (white) Gaussian noise with a dissipative factor arbitrarily small. The inclusion of an extra thermal bath guarantees that the final equilibrium state will arise despite the presence of an extremely weak uncorrelated noise.

We focus our analysis on a quadratic external potential, which allows to deal with all the calculations in a feasible way. However, it is possible that an even more complex behavior may take place due to the non-linear forces and noise properties, as discussed by Spagnolo.
and collaborators [17,18,20]. Then, it is interesting as further investigation to study the dynamical aspects of non-linear systems with many different stochastic forces, in particular, the effects of noise fluctuations on the characteristic time-scales associated with locally stable states.

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