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Non-Markovian diffusion over a saddle with a Generalized Langevin equation

David Boilley* and Yoann Lallouet
GANIL, BP 55076, Caen cedex 5, France

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Abstract

The diffusion over a simple parabolic barrier is exactly solved with a non-Markovian Generalized Langevin Equation. For a short relaxation time, the problem is shown to be similar to a Markovian one, with a smaller effective friction. But for longer relaxation time, the average trajectory starts to oscillate and the system can have a very fast first passage over the barrier. For very long relaxation times, the solution tends to a zero-friction limit.

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1 Introduction

The phenomenological Langevin equation [1], or its Klein-Kramers equivalent [2, 3], has been applied to most fields of physics when thermal fluctuations are to be taken into account. But such an equation is Markovian, which is, in many cases, a very poor approximation. When it is derived from a microscopic model [4, 5, 6, 7, 8, 9, 10], one gets a so-called Generalized Langevin equation (GLE) for which the dissipation and fluctuation parts have a memory. When the relaxation time of the heat bath is very short compared to the brownian particle's characteristic time scale, one recovers the phenomenological Langevin equation.

The diffusion over a potential barrier is a typical case for which the fluctuations play a crucial role. Since the pioneering work of Kramers [3], who derived an analytical expression for the stationary escape rate from a metastable potential well, this problematic has been widely used and studied. For a review, see Ref. [11]. In particular, the influence of the

*boilley@ganil.fr

memory on this rate was already studied in Refs. [12, 13]. The reverse problem of the entrance into the well after passing over a potential barrier has been studied more recently [14, 15] and applied to fusion reactions with heavy ions [16, 17]. Assuming a parabolic potential barrier, the diffusion problem was solved exactly, but with a Markovian approximation. The aim of this paper is to study the influence of the memory kernel on the diffusion over a parabolic barrier with a Generalized Langevin Equation (GLE), generalizing what was done in Refs. [14, 15].

A GLE can be obtained from simple statistical models. It is the case for the motion of a particle coupled to a heat bath as in Refs. [4, 5], assuming a hamiltonian of the form $H = H_0 + H_b + H_{int}$, with the heat bath, $H_b(s_1, \dots, s_n)$, made of an assembly of coupled harmonic oscillators and the brownian particle, $H_0 = m\dot{q}^2/2 + V(q)$, coupled harmonically to the bath and by an arbitrary force to a fixed center,

$$H_{int} = -\sum_i c_i s_i q(t). \quad (1)$$

Here the c_i 's are coupling constants. Assuming, that the degrees of freedom of the heat bath have a smaller inertia than the brownian particle, they can be averaged out, leading to a GLE. The time scale of the memory kernel represents the relaxation time of the heat bath. Such results were extended to non-linear systems in Refs. [6, 7]. For a review of these so-called adiabatic elimination procedures, see Ref. [8].

The Generalized Langevin Equation obtained from these models reads, for small amplitude motion,

$$\ddot{q} + \int_{t_0}^t dt' \Gamma(t-t') \dot{q}(t') + \frac{1}{m} \frac{\partial V}{\partial q} = \rho(t), \quad (2)$$

where the memory kernel reads,

$$\Gamma(t) = \frac{\beta}{\tau} \exp(-\frac{t}{\tau}). \quad (3)$$

In these equations, β is the reduced friction coefficient, m the mass, τ the relaxation time and $\rho(t)$ comes from a Gaussian random force characterized by

$$\langle \rho(t) \rangle = 0 \quad \text{and} \quad \langle \rho(t) \rho(t') \rangle = \frac{T}{m} [\Gamma(|t-t'|) - \Gamma(t+t'-2t_0)], \quad (4)$$

in agreement with the dissipation-fluctuation theorem [18]. In this paper, we set the Boltzmann constant $k_B = 1$ and $\langle \cdot \rangle$ denotes an average over a statistical ensemble. More complicated kernels and especially anomalous diffusion studied in Refs [19, 20], will be ruled out of this paper.

In some problems, it is assumed that the brownian particle has initially thermalized some of its degrees of freedom and the fluctuation-dissipation theorem is simply reduced to

$$\langle \rho(t)\rho(t') \rangle = \frac{T}{m}\Gamma(|t-t'|). \quad (5)$$

In this paper, we will also consider this case. When the arbitrary initial time $t_0 \rightarrow -\infty$, the physics differs from this hypothesis by an additional force that is always acting [18]:

$$m \int_{-\infty}^{t_0} dt' \Gamma(t-t')\dot{q}(t'). \quad (6)$$

When the relaxation time of the heat bath, τ , is small compared to the characteristic time of the macroscopic variable, $q(t)$, which could be mathematically written as $\tau \rightarrow 0$, we can do a two-step approximation:

1. $\int_{t_0}^t dt' \Gamma(t-t')\dot{q}(t') \simeq \dot{q}(t) \int_{t_0}^t dt' \Gamma(t-t')$;
2. $\frac{t-t_0}{\tau} \gg 1$, which is a kind of *Stoßzahlansatz* (molecular chaos assumption) equivalent to $t_0 \rightarrow -\infty$; in this limit $\int_{t_0}^t dt' \Gamma(t-t') \rightarrow \beta$.

Then the Langevin equation becomes Markovian:

$$\ddot{q} + \beta\dot{q} + \frac{1}{m} \frac{\partial V}{\partial q} = r_m(t), \quad (7)$$

where the random force satisfies

$$\langle r_m(t) \rangle = 0 \quad \text{and} \quad \langle r_m(t)r_m(t') \rangle = \frac{2T\beta}{m}\delta(t-t'), \quad (8)$$

in agreement with the dissipation-fluctuation theorem.

In nuclear physics, specific derivations of the GLE for heavy ion reactions were done, starting from a semi-classical transport equation with a collision term [9, 10, 21]. Then, the relaxation time comes from the linearization of the Boltzmann collision integral and connects the distortion of the Fermi surface with the real space motion. The equation of motion is generally non-linear, but we will restrict our study to small amplitude motions with a linear equation, in order to focus our attention on the effects of the memory kernel. For resonant oscillations of the nuclei, the relaxation time has the same order of magnitude as the inverse of the frequency and thus, the memory kernel must be taken into account to reproduce experimental observations [10, 21]. But for a slow nuclear fission reaction, the Markovian approximation appears to be sufficient [22]. In the case of fusion

reactions, the time scale is short enough to consider that the memory kernel might be relevant. Finally, a recent calculation shows up that the descent time from saddle to scission point is also sensitive to the relaxation time [21]. In this paper, we will consider these two problems as an illustration.

In all these microscopic models, β and τ are correlated, but we will treat them as independent in order to study their influence.

2 Diffusion over a parabolic barrier

The problem of the diffusion over a 1-D parabolic potential barrier, $V(q) = -m\omega^2 q^2/2$, with a sharp given initial condition, $q_0 < 0$ and $p_0 = \dot{q}_0 > 0$, can be solved exactly, following what was done in Ref. [14] or using Laplace transforms, which is faster.

To evaluate the probability of passing over the potential barrier, we only need the reduced distribution obtained when all degrees of freedom but q are integrated out. It is also a Gaussian distribution,

$$w(t, q; q_0, p_0) = \frac{1}{\sqrt{2\pi}\sigma_q(t)} \exp\left(-\frac{(q - \langle q(t) \rangle)^2}{2\sigma_q^2(t)}\right), \quad (9)$$

where $\sigma_q^2(t)$ is the variance and $\langle q(t) \rangle$ the average trajectory. Then, the probability is,

$$P(t; q_0, p_0) = \int_0^{+\infty} w(t, q; q_0, p_0) dq \quad (10)$$

$$= \frac{1}{2} \operatorname{erfc}\left(-\frac{\langle q(t) \rangle}{\sqrt{2}\sigma_q(t)}\right). \quad (11)$$

The problem can be extended to more general cases with a Gaussian distribution of the initial conditions and also be solved exactly, see Ref. [15].

2.1 The Markovian approximation

In this subsection, we will briefly recall the main results of the Markovian diffusion in order to have a better understanding of the influence of the memory kernel. Details can be found in Ref. [14].

The Markovian Langevin equation, written in the following way,

$$\frac{d}{dt} \begin{bmatrix} q \\ p \end{bmatrix} = D \cdot \begin{bmatrix} q \\ p \end{bmatrix} + \begin{bmatrix} 0 \\ r_m(t) \end{bmatrix}, \quad (12)$$

where the drift matrix reads

$$D = \begin{bmatrix} 0 & 1 \\ \omega^2 & -\beta \end{bmatrix}, \quad (13)$$

can be formally integrated into

$$\begin{bmatrix} q \\ p \end{bmatrix} = e^{(t-t_0)D} \cdot \begin{bmatrix} q_0 \\ p_0 \end{bmatrix} + \int_{t_0}^t dt e^{(t-t')D} \cdot \begin{bmatrix} 0 \\ r(t') \end{bmatrix}, \quad (14)$$

where the first term of the r.h.s. corresponds to the average trajectory and the second one to the diffusion.

The eigenvalues of the drift matrix, D , satisfying the following equation,

$$\lambda^2 + \beta\lambda - \omega^2 = (\lambda - a)(\lambda - b) = 0, \quad (15)$$

are

$$\begin{cases} a &= \frac{1}{2}(\sqrt{\beta^2 + 4\omega^2} - \beta) \\ b &= -\frac{1}{2}(\sqrt{\beta^2 + 4\omega^2} + \beta). \end{cases} \quad (16)$$

Note that $a > 0$ and $b < 0$. The average trajectory and the variance can easily be obtained, see Refs. [14, 23, 24, 25], and the probability of passing over the barrier is then known at any time. See Eq. (11).

For large times, $at \gg 1$, the probability to pass over the barrier converges to a finite value,

$$P(t \rightarrow \infty; q_0, p_0) \rightarrow \frac{1}{2} \operatorname{erfc} \left[\frac{\omega}{\sqrt{\beta a}} \left(\sqrt{\frac{B}{T}} - \frac{a}{\omega} \sqrt{\frac{K}{T}} \right) \right], \quad (17)$$

where $K = mp_0^2/2$ denotes the initial kinetic energy and $B = m\omega^2 q_0^2/2$ the barrier height that has to be overcome by the particle. In the case of Kramers' problem, the temperature is solely responsible for the diffusion, because of the initial equilibrium in the metastable well. Here, there is an interplay between dynamics and diffusion: the initial kinetic energy should also be taken into account. In contrast to Kramers' problem, the reverse process is transitive, the flux over the barrier being appreciable only during a given period [15].

To have half of the particles to pass over the barrier, the initial kinetic energy should be,

$$K = \left(\frac{\omega}{a} \right)^2 B = B_{eff}. \quad (18)$$

In the weak friction limit, the previous condition becomes $K \simeq B$, which is a trivial result. Taking usual values of nuclear physics, $\hbar\omega = 1MeV$ and $\beta = 5 \times 10^{21} s^{-1}$, we have $\frac{\beta}{2\omega} = 1.5$ and therefore the effective barrier $B_{eff} \simeq 10B$. This shows the important role played by dissipation.

As it is already discussed in Ref. [15], there are then three regimes, depending on the initial kinetic energy. When $K < B_{eff}$, the average trajectory never reaches the top of the barrier located at $q = 0$. The probability of passing over the barrier is mainly due to the thermal diffusion, which is

a slow process. When $K > B_{eff}$, the average trajectory crosses the barrier and the thermal diffusion does not play an important role anymore. In the critical case where $K = B_{eff}$, the average trajectory converges to the top of the barrier and the probability tends to 1/2, whatever the temperature.

2.2 Non-Markovian diffusion

2.2.1 Exact solution

In the non-Markovian case we can show that the GLE, Eq. (2), can be transformed into a system of three first-order differential equations,

$$\begin{aligned}\dot{q} &= p \\ \dot{p} &= \omega^2 q + f \\ \dot{f} &= \frac{1}{\tau}[-\beta p - f] + r(t),\end{aligned}\tag{19}$$

where the random term

$$r(t) = \frac{1}{\tau} \sqrt{\frac{2\beta T}{m}} \nu(t),\tag{20}$$

depends on a Gaussian random number, $\nu(t)$, characterized by $\langle \nu(t) \rangle = 0$ and $\langle \nu(t)\nu(t') \rangle = \delta(t - t')$. In Eq. (19), f is a new variable which has the dimension of an acceleration. To get back to the original equation, Eq.(2), one should set its initial value to zero, $f_0 = 0$. Such a choice leads to a correlation function of the noise that depends on the initial time t_0 , see Eq. (4). When f_0 is prepared at its Gaussian equilibrium, $\langle f_0^2 \rangle = \frac{\beta T}{m\tau}$, with a zero mean value [8], it leads to the reduced correlation function of the noise, Eq. (5). In such a case, one should also average the final result on the initial distribution. In order to study both of these cases, we will explicitly keep f_0 in the following derivation.

The eigenvalues of the drift matrix can be obtained by taking the Laplace transform of the GLE and satisfy the characteristic equation

$$\lambda^3 + \frac{1}{\tau}\lambda^2 + \left(\frac{\beta}{\tau} - \omega^2\right)\lambda - \frac{\omega^2}{\tau} = 0,\tag{21}$$

which can be rewritten in the following form,

$$(\lambda - a)(\lambda - b) = \tau\lambda(\omega - \lambda)(\omega + \lambda).\tag{22}$$

Here the l.h.s. corresponds to the Markovian case with the eigenvalues a and b given in Eq. (16), and the r.h.s. to the contribution of the memory kernel. When $\tau \rightarrow 0$, one recovers the Markovian problem. The eigenvalues, λ_1 , λ_2 , and λ_3 , can be explicitly written, but the formulas are somewhat heavy to handle, see Appendix A. Plotting on the same graph

the l.h.s. and the r.h.s. of Eq. (22), it is easy to see that one of the eigenvalues, λ_1 , is always positive. More precisely, $a < \lambda_1 < \omega$. The other two are either negative or complex conjugates. In the latter case, their real part, $(\lambda_2 + \lambda_3)/2 = -(\lambda_1 + \frac{1}{\tau})/2$, is always negative. It can be checked that

$$\lim_{\tau \rightarrow 0} \lambda_1 = a, \quad \lim_{\tau \rightarrow 0} \lambda_2 = b \quad \text{and} \quad \lim_{\tau \rightarrow 0} \lambda_3 = -\infty, \quad (23)$$

which means that we recover the Markovian case when $\tau \rightarrow 0$.

The fact that two eigenvalues become complex when $\tau \in]\tau_1, \tau_2[$, is due to the memory kernel. The critical values of the relaxation time, for which the nature of the eigenvalues changes, are approximatively evaluated in Appendix A:

$$\omega\tau_1 \simeq \frac{1}{8} \frac{2\omega}{\beta} \frac{1 + \left(\frac{\beta}{2\omega}\right)^2}{\frac{5}{4} + \left(\frac{\beta}{2\omega}\right)^2}, \quad (24)$$

$$\omega\tau_2 \simeq \sqrt{3} + 3\frac{\beta}{2\omega}. \quad (25)$$

For example, with $\frac{\beta}{2\omega} = 1.5$, we have $\omega\tau_1 \simeq 0.08$ and $\omega\tau_2 \simeq 6.23$.

Once the eigenvalues are known, the Laplace transform of $q(t)$ can be calculated from Eqs. (19),

$$\tilde{q}(s) = \frac{(s^2\tau + s + \beta)q_0 + (1 + s\tau)p_0 + \tau f_0 + \tau\tilde{r}(s)}{\tau(s - \lambda_1)(s - \lambda_2)(s - \lambda_3)}, \quad (26)$$

where $\tilde{r}(s)$ is the Laplace transform of $r(t)$. Taking the inverse Laplace transform, one gets the average trajectory

$$\langle q(t) \rangle = u(t)q_0 + v(t)p_0 + w(t)f_0, \quad (27)$$

with

$$u(t) = \sum_{i=1}^3 \frac{\lambda_i^2\tau + \lambda_i + \beta}{\tau \prod_{n \neq i} (\lambda_i - \lambda_n)} e^{\lambda_i t}, \quad (28)$$

$$v(t) = \sum_{i=1}^3 \frac{1 + \tau\lambda_i}{\tau \prod_{n \neq i} (\lambda_i - \lambda_n)} e^{\lambda_i t}, \quad (29)$$

$$w(t) = \sum_{i=1}^3 \frac{1}{\prod_{n \neq i} (\lambda_i - \lambda_n)} e^{\lambda_i t}, \quad (30)$$

and the variance

$$\sigma_q^2(t) = \frac{2T\beta}{m\tau^2} \sum_{i=1}^3 \sum_{j=1}^3 \frac{e^{(\lambda_i + \lambda_j)t} - 1}{(\lambda_i + \lambda_j) \prod_{n \neq i} (\lambda_i - \lambda_n) \prod_{m \neq j} (\lambda_j - \lambda_m)}, \quad (31)$$

that enter the Gaussian distribution. Then the probability of passing over the barrier is explicitly known at any time. See Eq. (11).

When there is a Gaussian dispersion of the initial conditions,

$$W_0(\bar{q}_0, \sigma_{q_0}; \bar{p}_0, \sigma_{p_0}; \bar{f}_0, \sigma_{f_0}) = \frac{1}{(2\pi)^{3/2} \sigma_{q_0} \sigma_{p_0} \sigma_{f_0}} \\ \times \exp\left[-\frac{(q_0 - \bar{q}_0)^2}{2\sigma_{q_0}^2}\right] \exp\left[-\frac{(p_0 - \bar{p}_0)^2}{2\sigma_{p_0}^2}\right] \exp\left[-\frac{(f_0 - \bar{f}_0)^2}{2\sigma_{f_0}^2}\right], \quad (32)$$

one can easily evaluate the overpassing probability as in Ref. [15],

$$\bar{P}(t; \bar{q}_0, \sigma_{q_0}, \bar{p}_0, \sigma_{p_0}, \bar{f}_0, \sigma_{f_0}) = \int_{-\infty}^{+\infty} dq_0 \int_{-\infty}^{+\infty} dp_0 \int_{-\infty}^{+\infty} df_0 P(t; q_0, p_0, f_0) \\ \times W_0(\bar{q}_0, \sigma_{q_0}; \bar{p}_0, \sigma_{p_0}; \bar{f}_0, \sigma_{f_0}) \\ = \frac{1}{2} \operatorname{erfc}\left(-\frac{\langle \bar{q}(t) \rangle}{\sqrt{2}\sigma'(t)}\right), \quad (33)$$

where $\langle \bar{q}(t) \rangle$ is the same as in Eq. (27) provided that q_0 , p_0 and f_0 are replaced by \bar{q}_0 , \bar{p}_0 and \bar{f}_0 respectively. The variance is larger,

$$\sigma'^2(t) = \sigma^2(t) + u^2(t)\sigma_{q_0}^2 + v^2(t)\sigma_{p_0}^2 + w^2(t)\sigma_{f_0}^2, \quad (34)$$

with $u(t)$, $v(t)$ and $w(t)$ given in Eqs. (28,29,30).

2.2.2 Asymptotic behavior

For long times, only the $e^{\lambda_1 t}$ terms remain and the overpassing probability converges to a finite value. For the first case corresponding to $f_0 = 0$,

$$P(t \rightarrow +\infty; q_0, p_0, f_0 = 0) = \frac{1}{2} \operatorname{erfc}\left[\frac{(1 + \lambda_1 \tau)\omega}{\sqrt{\lambda_1 \beta}} \left(\sqrt{\frac{B}{T}} - \frac{\lambda_1}{\omega} \sqrt{\frac{K}{T}}\right)\right], \quad (35)$$

where K and B are respectively the initial kinetic energy and barrier height previously defined in section 2.1. With an initial distribution in f_0 ,

$$\bar{P}(t \rightarrow +\infty; q_0, p_0, \sigma_{f_0} = \sqrt{\frac{T\beta}{m\tau}}) = \frac{1}{2} \operatorname{erfc}\left[\omega \sqrt{\frac{1 + \lambda_1 \tau}{\beta \lambda_1}} \left(\sqrt{\frac{B}{T}} - \frac{\lambda_1}{\omega} \sqrt{\frac{K}{T}}\right)\right]. \quad (36)$$

These two expressions only differ by the factor $\sqrt{1 + \lambda_1 \tau}$ inside the complementary error function. Therefore, for short relaxation times τ , the probabilities are very close as it can be seen in Fig. 1. For long relaxation times, this is not true anymore.

Figure 1: Asymptotic overpassing probabilities as a function of the initial kinetic energy. The dashed line corresponds to a sharp initial condition $f_0 = 0$ and the solid one to an initial distribution for f_0 (see text). Here, $\frac{\beta}{2\omega} = 1.5$ and $\frac{T}{B} = 0.2$. For the left figure, $\omega\tau = 1$ and for the right one, $\omega\tau = 10$.

In both cases, to have half of the particles to pass over the barrier, the initial kinetic energy should be,

$$K = \left(\frac{\omega}{\lambda_1}\right)^2 B = B_{eff}. \quad (37)$$

This result is very similar to the Markovian case, see Eq. (18). Since $a < \lambda_1 < \omega$, the effective barrier that has to be overcome by the particle is smaller when the relaxation time is larger. The memory kernel tends to decrease the influence of the dissipative process, leading to a reduced effective friction, see Fig. 2 left. For a given relaxation time, such an effect is larger when $\frac{\beta}{2\omega} \simeq 1$, as shown in Fig. 2 right.

Figure 2: Left: $\frac{B_{eff}}{B}$ as a function of $\omega\tau$, for several values of $\frac{\beta}{2\omega}$; $\frac{\beta}{2\omega} = 1$ (long dashed line), $\frac{\beta}{2\omega} = 2$ (short dashed line), $\frac{\beta}{2\omega} = 3$ (solid line). Right: $\frac{B_{eff}}{B_{eff}(\tau=0)}$ is represented as a function of $\frac{\beta}{2\omega}$ for several values of $\omega\tau$ ($\omega\tau = 0.07$: short dashed line, $\omega\tau = 0.4$: long dashed line and $\omega\tau = 1$: solid line).

The average trajectory has to overcome the effective barrier, B_{eff} which takes into account the viscosity and the memory effects. For example, with usual values of nuclear physics, $\hbar\omega = 1MeV$, $\hbar/\tau \simeq 1MeV$ and $\omega\tau \simeq 1$, one gets $B_{eff} \simeq 6.5B$ which is about 40% smaller than in the Markovian case. This shows the important role played by memory effects on the effective barrier.

As we already discussed in the Markovian case, there are still three different regimes, depending on the initial kinetic energy: a thermal diffusion regime when $K < B_{eff}$ and a dynamical crossing when $K > B_{eff}$. In the critical case, $K = B_{eff}$, the average trajectory also converges to the top of the barrier.

Having an initial distribution of f_0 means a larger variance, as shown in Eq. (34), and then a smoother evolution of the probability with the initial kinetic energy. When $K < B_{eff}$, a larger variance means more particles

passing over the barrier. But, when $K > B_{eff}$, a larger variance means more particles staying on the initial side of the barrier and then a smaller probability. Such a behavior is more obvious for large τ , see Fig. 1.

2.2.3 Dynamics

The transient regime to the asymptotic behavior depends on the nature of the eigenvalues. For a small relaxation time, $\tau < \tau_1$, the eigenvalues are real and the situation is very similar to the Markovian case with a slightly reduced friction. When the relaxation time is very large, $\tau > \tau_2$ the eigenvalues are also real and the situation is again similar to the Markovian case with almost no friction.

The transient regime changes drastically when the relaxation time $\tau \in]\tau_1, \tau_2[$. Two eigenvalues are then complex and the average trajectory, the over-passing probability and the current at the top of the barrier, $j = \frac{dP(t)}{dt}$, start to oscillate. See Fig. 3. This would never happen in a Markovian approach.

Figure 3: Average trajectory, over-passing probability and current at the top of the barrier as a function of time for the four regimes, $K = 0$, (first column) $K = B_{eff}/2$ (second column), $K = B_{eff}$ (third column) and $K = 2B_{eff}$ (last column). For each graphic, three different curves are plotted : the Markovian case ($\omega\tau = 0$: solid line), the non-oscillating case ($\omega\tau = 0.07$: short dashed line) and the oscillating case ($\omega\tau = 0.4$: long dashed line). These are non-dimensional plots. Here, $\frac{\beta}{2\omega} = 1.5$, $T = \frac{B}{2}$, $f_0 = 0$ and $\sigma_{f_0} = 0$. Note that each column has a different time scale.

In Fig. 3, the oscillating behavior of the dashed curves is damped because these are average observables. For a single trajectory, the situation is drastically different because the random force excites the oscillations that remain at all times.

In nuclear physics, the oscillations of the average trajectory corresponds to the giant quadrupole resonance [10, 26].

2.2.4 Dispersion of the initial conditions

Up to now, the problem was considered with sharp initial conditions in q and p , and we may wonder whether a dispersion of the initial conditions might affect the results. We will consider the analytically tractable problem of a Gaussian distribution, as in Eq. (32). As previously, one takes $\bar{q}_0 < 0$ and $\bar{p}_0 = \dot{q}_0 > 0$. As for the variances, it is more complicated because the system is not necessarily equilibrated. It depends on the physical

situation. In the case of heavy ion fusion, dissipation already occurs in the approaching phase, generating a dispersion of the initial conditions, q_0 and p_0 [16, 27]. Later, once the nuclei have collided, dissipation is known to be very strong and the internal degrees of freedom are supposed to be quickly equilibrated at temperature T . Not the collective ones, of course. They are coupled to the intrinsic ones through the dissipation-fluctuation terms. As a consequence, in such a situation, a dispersion of the initial conditions should be considered with a different width characterized by T_0 :

$$\sigma_{p_0}^2 = \frac{T_0}{m} \quad \text{and} \quad \sigma_{f_0}^2 = \frac{\beta T_0}{m\tau}. \quad (38)$$

Since there is no potential pocket in this problem, it is not possible to link $\sigma_{q_0}^2$ with the initial temperature. We will therefore drop it in Fig. 4.

The result is given in Eq. (33). It should be noticed that the average trajectory is not affected by the dispersion of the initial conditions and that the oscillations that might occur are not washed out. In Fig. 4, we plot again the over-passing probability as a function of time with various initial widths. Naturally, the diffusion process starts earlier when the initial width is larger. Then, when $K < B_{eff}$, i.e. when the process is dominated by the diffusion, the overpassing probability is also always larger. But when $K \geq B_{eff}$, the transition is smoother and more particles come backward once the average trajectory has passed the saddle. The probability 1/2 corresponds to $\langle q(t) \rangle = 0$ and then does not depend on the variance.

Figure 4: Oscillating over-passing probability ($\omega\tau = 0.4$) as a function of time for three regimes: $\bar{K} = \bar{B}_{eff}/2$ (first column), $\bar{K} = \bar{B}_{eff}$ (second column) and $\bar{K} = 2\bar{B}_{eff}$ (third column). For each graphic three different curves are plotted: $T_0 = T$ (long dashed line), $T_0 = T/2$ (short dashed line) and $T_0 = 0$ (solid line). Here, $\frac{\beta}{2\omega} = 1.5$, $T = \frac{B}{2}$ and $\sigma_{q_0} = 0$.

For large times, ($\lambda_1 t \gg 1$), the probability to pass over the barrier converges to a finite value,

$$\bar{P}(t \rightarrow \infty; \bar{q}_0, \sigma_{q_0}, \bar{p}_0, T_0, \bar{f}_0 = 0, T_0) \rightarrow \frac{1}{2} \operatorname{erfc} \left[\sqrt{\frac{\bar{B}}{T'}} - \frac{\lambda_1}{\omega} \sqrt{\frac{\bar{K}}{T'}} \right], \quad (39)$$

with

$$T' = \frac{\beta\lambda_1 T}{\omega^2(1 + \lambda_1\tau)^2} + m\omega^2\sigma_{q_0}^2 + \left(\frac{\lambda_1}{\omega}\right)^2 \left(1 + \frac{\beta\tau}{(1 + \lambda_1\tau)^2}\right) T_0. \quad (40)$$

Here, $\bar{K} = m\bar{p}_0^2/2$ denotes the average initial kinetic energy, $\bar{B} = m\omega^2\bar{q}_0^2/2$ the average barrier height and T' a generalised dynamical temperature, including memory effects.

The condition to have half of the particles passing over the barrier is not changed

$$\bar{K}_c = \left(\frac{\omega}{\lambda_1}\right)^2 \bar{B} = \bar{B}_{eff}. \quad (41)$$

When $\bar{K} \ll \bar{B}_{eff}$, and moreover if $T' < \bar{B}/10$, the over-passing probability is extremely low and it can be expanded

$$\bar{P}(t \rightarrow +\infty; \bar{q}_0, \sigma_{q_0}, \bar{p}_0, T_0) \simeq \sqrt{\frac{T'}{4\pi\bar{B}}} \exp\left(-\frac{\bar{B}}{T'}\right). \quad (42)$$

The result has an Arrhenius type factor [28] similar to the one obtained in the Markovian case and could be called “*inverse Kramers formula*”, as in Ref. [15].

3 Application to heavy ion reactions

Reaction dynamics of heavy ion collisions is often studied in terms of a few relevant variables which evolve according to a Langevin equation or its Klein-Kramers equivalent [29]. Most of the studies are based on phenomenological equations, which are Markovian, although microscopic derivations lead to memory dependent equations that have seldomly been used in this domain.

3.1 Fusion probability

For the synthesis of super-heavy elements by the means of heavy-ion fusion at near-barrier energies, the formation probabilities are so low that some simple toy-models are also developed to appreciate the results based on huge numerical statistics. In the fusion problem, one has to consider the potential pocket that is beyond the barrier. If we call P_{CN} the probability to have a compound nucleus, i.e. that the particle is inside the pocket limited by the saddle, one has,

$$\frac{dP_{CN}}{dt} = -\Gamma_K P_{CN} + j(t), \quad (43)$$

where Γ_K is Kramers' escape rate and j the entrance current over the barrier evaluated with the parabolic approximation. Assuming that $P_{CN}(0) = 0$, this equation can be easily integrated into,

$$P_{CN}(t) = \int_0^t e^{-\Gamma_K(t-t')} j(t') dt' \simeq e^{-\Gamma_K t} \int_0^t j(t') dt' = e^{-\Gamma_K t} P(t), \quad (44)$$

because $1/\Gamma_K$ is very large compared to the time range where the fusion current $j(t)$ is not vanishing. See Fig. 3. Then, the passing probability over a simple parabolic barrier $P(t)$ is a useful tool to study the entrance behavior into a potential pocket and has been widely used [14, 15, 16, 17, 19, 30, 31, 32, 33].

As we already mentioned, in the nuclear context, the memory effects are linked to the relaxation of the Fermi sphere and τ comes from the linearization of the collision integral of the Boltzmann equation. Using the result of Ref. [34] for a quadrupolar distortion and usual values of nuclear physics, one gets that $\hbar/\tau \simeq 1MeV$, which is similar to $\hbar\omega \simeq 1MeV$. Memory effects should then play a crucial role in the fusion probability.

In Ref. [19], the passage over the parabolic barrier is studied with non-Ohmic noise. The dynamics also exhibit some oscillations that are not explained. From this study, it appears that they are rather linked to the non-Markovian character of the noise.

When we consider the case of the quantum diffusion over the barrier [30, 31, 32, 33], the noise is always non-Markovian, but the memory kernel is more complicated than the one that is used here. The comparison can only be qualitative. The correlation time evaluated in [33] is about $\hbar/\tau \simeq 10MeV$, the other parameters being unchanged. This is beyond the oscillation interval. The average trajectory should then have a Markovian behavior with a vanishing friction. Noticing that

$$\lim_{\tau \rightarrow \infty} \lambda_1 = \omega, \quad \lim_{\tau \rightarrow \infty} \lambda_2 = 0 \quad \text{and} \quad \lim_{\tau \rightarrow \infty} \lambda_3 = -\omega, \quad (45)$$

it appears that the diffusion tends to a zero-friction limit, as in the quantum cases for low temperatures [31].

3.2 Saddle to scission time

The reverse process, starting from the top of the barrier down to a so-called scission point is also of interest in nuclear physics. In Ref. [21], the authors claim that, due to the memory effects, the saddle-to-scission time grows by a factor of about 3. Such a result could appear in contradiction with the fact that the memory kernel tends to decrease the friction coefficient.

For a metastable state in a thermal environment, the saddle-to-scission time is defined as the average time to reach the scission point beyond the barrier minus the average time to reach the saddle point [35]. Therefore, we cannot calculate directly this time with our model, but we can guess how it is affected by the memory effects.

For another set of initial conditions $q_0 = 0$ and $p_0 > 0$, we plot in Fig.

5 the average trajectory as a function of time,

$$\frac{\langle q(t) \rangle}{q_s} = v(t)\omega\sqrt{\frac{K}{B_s}}. \quad (46)$$

Here $B_s = m\omega^2 q_s^2/2$ is the barrier from the top of the saddle ($q = 0$) to q_s , the scission point, and $v(t)$ is given in Eq. (29). As expected, for a given friction parameter the non-Markovian dynamics leads to a weaker viscosity and then to a shorter saddle-to-scission time.

But, when the friction parameter is derived from a microscopic model [9, 10, 21], it depends then on the relaxation time chosen for the memory kernel. In Refs. [9, 10], β is proportional to this relaxation time. Then, a larger relaxation time means a larger viscosity with a net effect of a longer saddle-to-scission time as shown in Fig. 5.

Figure 5: $\frac{\langle q(t) \rangle}{q_s}$ is represented as a function of $\omega\tau$ with $K = B/10$. Three regimes are plotted: $\frac{\beta}{2\omega} = 1.5$, $\omega\tau = 0$ (solid line), $\frac{\beta}{2\omega} = 1.5$, $\omega\tau = 1$ (short dashed line) and $\frac{\beta}{2\omega} = 3$, $\omega\tau = 2$ (long dashed line).

4 Conclusion

In this paper, we have studied the role played by the memory kernel on the diffusion over a parabolic barrier. It leads to a reduction of the dissipation. The larger the relaxation time the larger the effect. For a specific range of relaxation times, some oscillations appear that change drastically the fate of the average trajectory and the time dependent over-passing probability. In the context of heavy ion reactions, these oscillations are at the frequency of the giant quadrupole resonance and are rarely taken into account in the dynamics.

These properties also interest the quantum diffusion over a parabolic barrier which has some applications in matter sciences [36, 37]. These models, together with the models developed in the nuclear context [30, 31, 32, 33] have a non-Markovian noise. Some features observed in the quantum approaches could be explained classically by the non-Markovian properties of the noise.

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A Eigenvalues

The eigenvalues of the non-Markovian problem can be calculated from Eq. (21), see e.g. [38], and one gets

$$\begin{aligned}
\lambda_1 &= -\frac{1}{3\tau} \\
&- \frac{1}{3\tau} \frac{-1 + 3\beta\tau - 3(\omega\tau)^2}{\left[-1 + \frac{9}{2}\beta\tau + 9(\omega\tau)^2 + \left[(-1 + \frac{9}{2}\beta\tau + 9(\omega\tau)^2)^2 + (-1 + 3\beta\tau - 3(\omega\tau)^2)^3\right]^{1/2}\right]^{1/3}} \\
&+ \frac{1}{3\tau} \left[-1 + \frac{9}{2}\beta\tau + 9(\omega\tau)^2 + \left[(-1 + \frac{9}{2}\beta\tau + 9(\omega\tau)^2)^2 + (-1 + 3\beta\tau - 3(\omega\tau)^2)^3\right]^{1/2}\right]^{1/3}, \\
\lambda_2 &= -\frac{1}{2}\left(\frac{1}{\tau} + \lambda_1\right) + iv, \\
\lambda_3 &= -\frac{1}{2}\left(\frac{1}{\tau} + \lambda_1\right) - iv,
\end{aligned} \tag{47}$$

with $i^2 = -1$ and $v^2 = \frac{1}{\tau^2}\left(-\frac{1}{4}(1 + \lambda_1\tau)^2 + \frac{\omega^2}{\lambda_1}\tau\right)$.

If λ_2 and λ_3 are real, $v^2 < 0$ therefore $v = -\frac{i}{\tau}\sqrt{\frac{1}{4}(1 + \lambda_1\tau)^2 - \frac{\omega^2}{\lambda_1}\tau}$. On the contrary, if λ_2 and λ_3 are complex conjugate, $v^2 > 0$ and $v = \frac{1}{\tau}\sqrt{-\frac{1}{4}(1 + \lambda_1\tau)^2 + \frac{\omega^2}{\lambda_1}\tau}$.

The first eigenvalue λ_1 is always real and positive. The nature of λ_2 and λ_3 can be determined with the help of the generalized discriminant Δ given by

$$\Delta\tau^4 = \frac{1}{\tau^2} \left[4 \left(-\frac{1}{3} + \beta\tau - (\omega\tau)^2 \right)^3 + 3 \left(\frac{2}{9} - \beta\tau - 2(\omega\tau)^2 \right)^2 \right]. \tag{48}$$

If $\Delta > 0$ λ_2 and λ_3 are complex conjugate. If $\Delta < 0$ they are real.

For very small τ , $\Delta < 0$, up to τ_1 that can be approximately be estimated by expanding $\Delta\tau^4$ to the first order in $\omega\tau$. The result is given in Eq. (24).

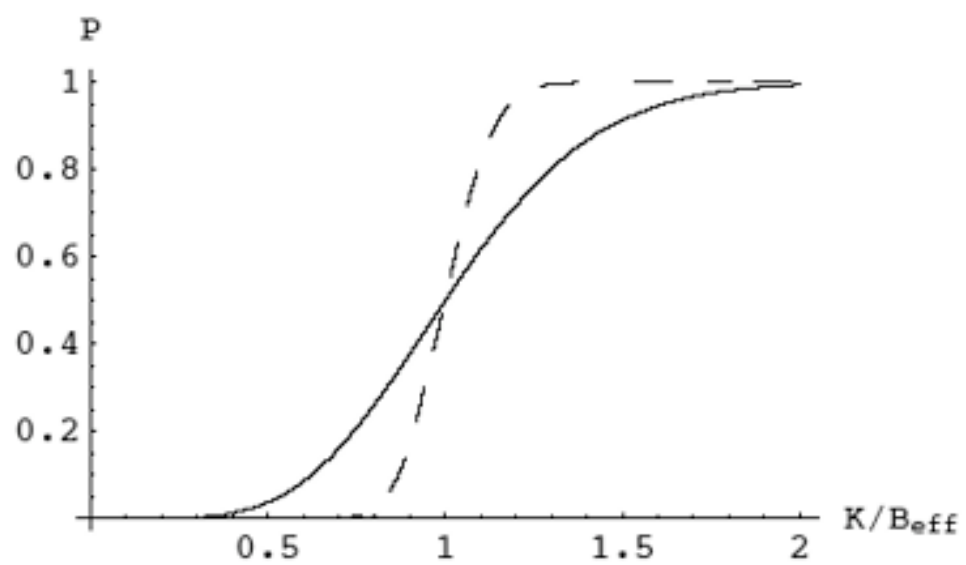
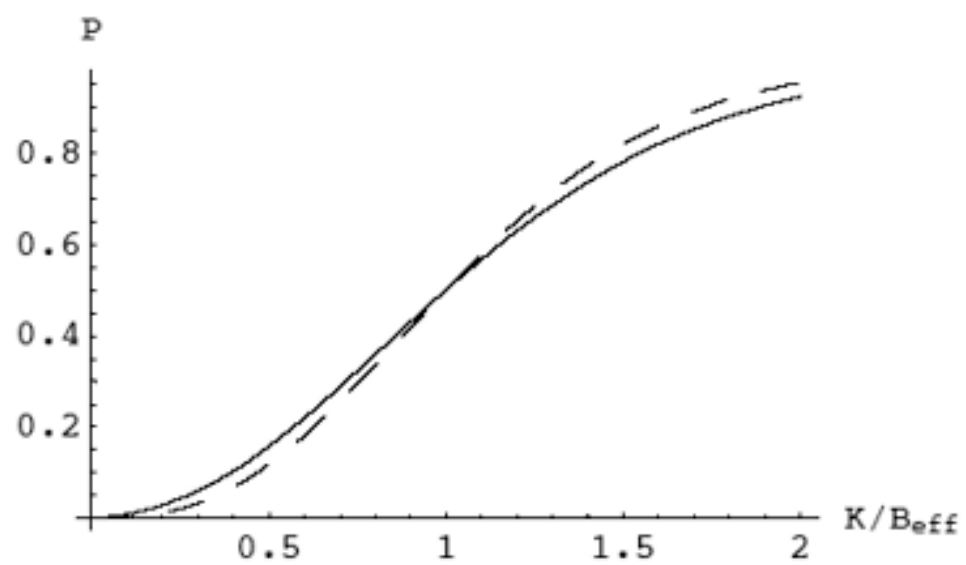
The determination of τ_2 , when λ_2 and λ_3 become again real, is more tricky. Graphically, it could be seen that it approximately corresponds to the negative minimum of the r.h.s. of Eq. (22) being tangent to the l.h.s.. This is how we got $\omega\tau_2$ in Eq. (25).

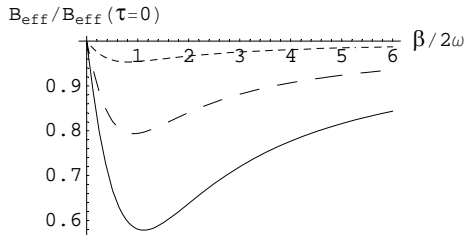
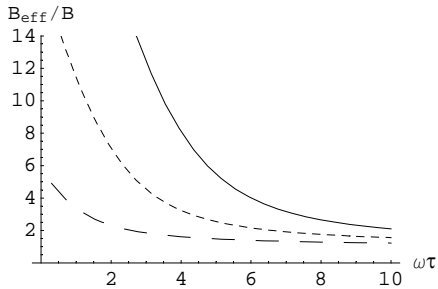
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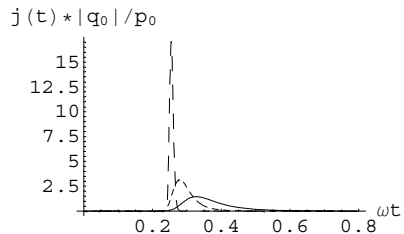
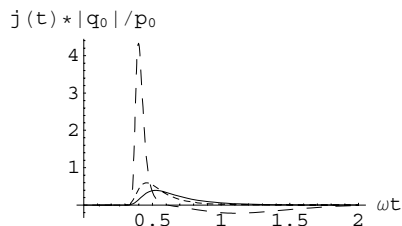
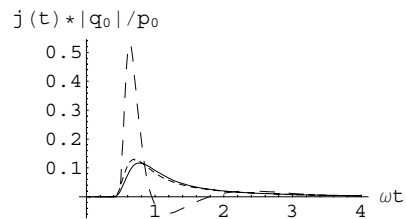
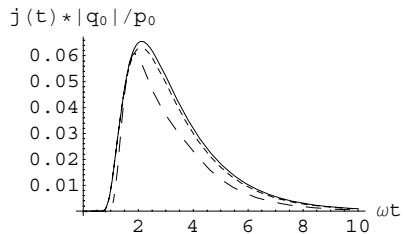
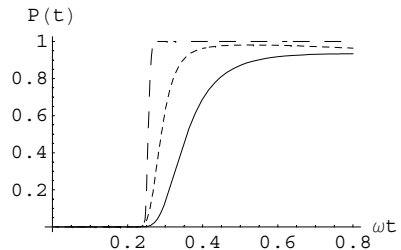
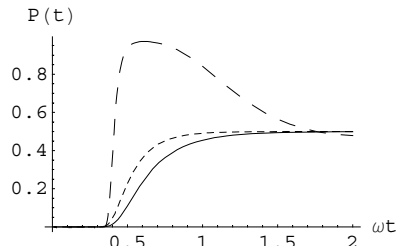
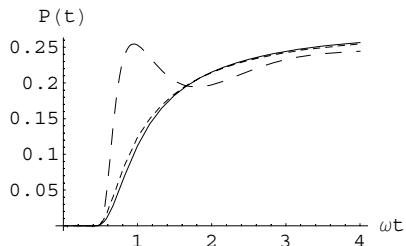
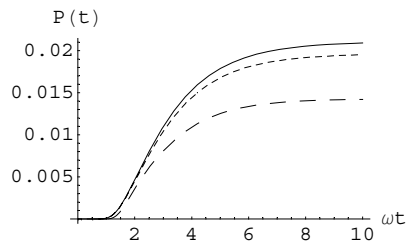
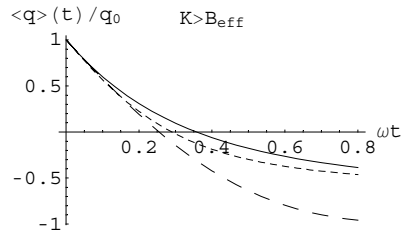
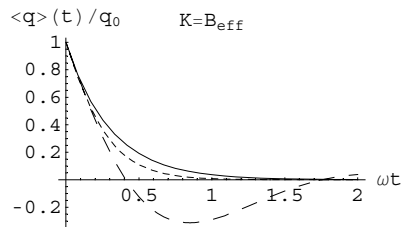
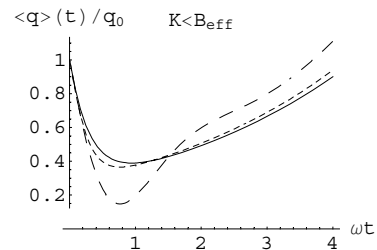
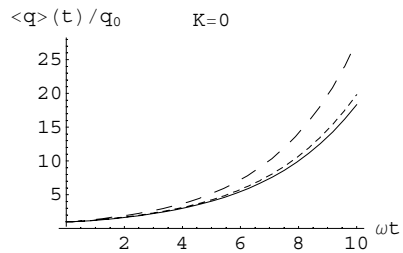
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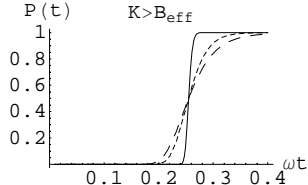
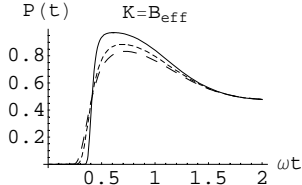
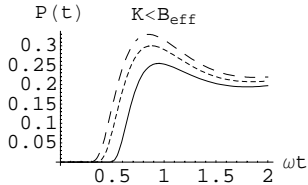
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$\langle q \rangle (t) / q_s$

