Elimination of fastly converging variables, initial slip and fusion hindrance

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Abstract

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1 Introduction

Theoretical description of the fusion of heavy nuclei is a long standing problem in nuclear physics. Fusion hindrance is known to be due to an inner barrier faced by the di-nuclear system at contact towards the compound shape. Few events will reach the compound nucleus state by diffusion. All the others will re-separate before, leading to the so-called quasi-fission.

Large ambiguities remain on the amplitude of the hindrance phenomenon [1, 2] as the size of the inner barrier, the friction strength are not well known. Even the dynamical model varies from one group to another. Assessing the so-called formation probability is necessary to get reliable predictions of fusion-evaporation cross-sections [3].

How to simply describe the diffusion over the inner barrier? One way is to eliminate fast degrees of freedom and only keep the slow variables. In a multi-dimensional system, we are generally not interested in the short time motion but rather in the fate of the system. This is also an old problem in statistical physics. Several seminal articles and textbooks address the subject. See e.g. [4].

Elimination of the fast variables leads to a slip of the initial condition of the slow variables. Such an effect was shown within the context of heavy-ions fusion: elimination of the fast neck degrees of freedom leads to a slip down of the radial one and then to a higher inner barrier. This finally leads to a larger hindrance of the fusion [5]. This was checked numerically [6, 7] within the same physical context.

This is actually a common feature to any non-equilibrium statistical problem. They are many articles devoted to the elimination of fast variables, proposing various methods. It is impossible to list all of them here. Among them, some have a special emphasis on the slip of the initial conditions [8, 9, 10].

Here, we will study the fusion probability with the so-called "fusion by diffusion" model based on a N-dimension Langevin equation. Assuming a Gaussian noise, the probability to pass over a potential barrier, starting from a given initial position is given by an error function [11]

$$P(t; q_{i0}) = \frac{1}{2}\mathrm{erfc}\left[-\frac{\langle q_r(t)\rangle}{\sqrt{2}\sigma_{q_r}}\right], \tag{1}$$

where q_r is the relevant variable used to consider that the system has fused or not. $\langle q_r(t)\rangle$ corresponds to its mean value as a function of time and σ_{q_r} its standard deviation. As shown in Ref. [11], when time goes on a single mode dominates the fusion process (see Eq. (57) in Ref. [11]). As q_r generally corresponds to a slow diffusion, can't we simply reduce the problem to an effective one dimension problem? With high dimensionality, it is not possible to do it analytically. Here we shall try fo find approximate solutions when some degrees of freedom quickly equilibrate.

We will first start with simple cases for which the exact solution is known in order to test the method and then consider more general cases with a N-dimension Langevin equation in order to find an analytical formula to the initial slip of the slow variables.

2 Over-damped approximation as a simple test case

As a first case, we shall study the reduction of the Langevin equation to the overdamped one that corresponds to the Smoluchowski approximation. The velocity is the fast variable.

As the exact solution of the full Langevin equation is known [11, 12], this example is a good test case.

2.1 Starting point

Let us start with a simple Langevin equation with a parabolic barrier:

$$\ddot{q} + \beta\dot{q} - \omega^2 q = r(t). \tag{2}$$

Here β is the reduced friction coefficient, ω, the angular frequency of the potential barrier and $r(t)$ is a Markovian random force which satisfies:

$$\langle r(t)\rangle = 0 \quad \forall t \qquad \text{and} \qquad \langle r(t)r(t')\rangle = \frac{2T\beta}{m}\delta(t-t') \quad \forall t,t'. \tag{3}$$

Introduction the velocity $p = \dot{q}$, this equation can be rewritten as

$$\frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \omega^2 & -\beta \end{bmatrix}\begin{bmatrix} q \\ p \end{bmatrix} + \begin{bmatrix} 0 \\ r(t) \end{bmatrix}. \tag{4}$$

Solutions of these equations were studied in Refs. [11, 12].

2.2 Exact solution of the problem

In this subsection, we will present a quick reminder of the exact solution of the Langevin equation (2) using its Laplace transform:

$$s^2\tilde{q} - sq_0 - p_0 + \beta(s\tilde{q} - q_0) - \omega^2\tilde{q} = \tilde{r}. \tag{5}$$

The mean trajectory is governed by

$$\tilde{q} = q_0\frac{\beta + s}{s^2 + \beta s - \omega^2} + p_0\frac{1}{s^2 + \beta s - \omega^2}. \tag{6}$$

Denominators in the r.h.s. of previous equation has two roots, one positive and one negative,

$$a_\pm = \frac{-\beta \pm \sqrt{\beta^2 + 4\omega^2}}{2}, \tag{7}$$

that can be used to find the mean trajectory:

$$\begin{aligned} \tilde{q} &= q_0\frac{\beta + s}{(s-a_+)(s-a_-)} + \frac{p_0}{(s-a_+)(s-a_-)} && (8) \\ &= \frac{q_0}{a_+ - a_-}\left[\frac{\beta + a_+}{s - a_+} - \frac{\beta + a_-}{s - a_-}\right] + \frac{p_0}{a_+ - a_-}\left[\frac{1}{s - a_+} - \frac{1}{s - a_-}\right]. && (9) \end{aligned}$$

Inverse Laplace transform gives the average trajectory

$$\langle q(t)\rangle = \frac{q_0}{a_+ - a_-}\left[(\beta + a_+)e^{a_+ t} - (\beta + a_-)e^{a_- t}\right] + \frac{p_0}{a_+ - a_-}\left[e^{a_+ t} - e^{a_- t}\right]. \tag{10}$$

When $\beta \gg \omega$, one obviously has $|a_-| \gg |a_+|$. Then, for a time $t > 1/|a_-|$, the mean trajectory becomes

$$\langle q(t)\rangle \simeq \frac{1}{a_+ - a_-}\left[(\beta + a_+)q_0 + p_0\right]e^{a_+ t}. \tag{11}$$

This is the solution of a first-order differential equation ($\dot{q} = a_+ q$) with a shifted initial condition.

Noting that

$$\sqrt{1+x} \simeq 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16}... \qquad \text{when} \qquad x \ll 1, \tag{12}$$

one has

$$a_+ \simeq \frac{\omega^2}{\beta}\left[1 - \frac{\omega^2}{\beta^2} + 2\frac{\omega^4}{\beta^4}...\right] \tag{13}$$

$$a_- \simeq -\beta\left[1 - \frac{\omega^2}{\beta^2} + \frac{\omega^4}{\beta^4} - 2\frac{\omega^6}{\beta^6}...\right]. \tag{14}$$

At the lowest order, one recovers the solution of the overdamped Langevin equation or Smoluchowski equation. Eq. (11) becomes

$$\langle q(t)\rangle \simeq (q_0 + \frac{p_0}{\beta})e^{\frac{\omega^2}{\beta}t}, \tag{15}$$

with a slip of the initial condition.

At higher orders, the solution is not the solution of the same equation. Can we find this equation and the new initial condition without solving the full Langevin equation?

2.3 An intuitive approach

Let us start again from the matrix approach:

$$\frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \omega^2 & -\beta \end{bmatrix}\begin{bmatrix} q \\ p \end{bmatrix} + \begin{bmatrix} 0 \\ r(t) \end{bmatrix}.$$

On the short time scale, from 0 to a short time τ during which the velocity is thermalized, one has for the mean velocity $\dot{p} \simeq -\beta p$ leading to $\langle p(t)\rangle = p_0 e^{-\beta t}$. It vanishes on a time scale $\tau \simeq 1/\beta$. The variance tends to $\sigma_p^2 = \frac{T}{m}$. On this time scale, the first equation $\dot{q} = p$ leads to

$$q(\tau) = \left(q_0 + \frac{p_0}{\beta}\right). \tag{16}$$

Regarding the variance of the initial condition, one gets $\sigma_{q_0}^2 = \frac{T}{m}\sqrt{\tau}$ which is small. We shall neglect it. This is the new initial value of the slow motion during which $\dot{p} \simeq 0$. With such an approximation, one immediately gets

$$\beta\dot{q} - \omega^2 q = r(t) \tag{17}$$

where the inertia term is neglected.

The solution leads to probability density function that is Gaussian. The mean value is equal to

$$\langle q(t)\rangle = \left(q_0 + \frac{p_0}{\beta}\right)e^{\frac{\omega^2}{\beta}t}, \tag{18}$$

and a variance to

$$\sigma_q^2(t) = \frac{T}{m\omega^2}\left(e^{2\frac{\omega^2}{\beta}t} - 1\right), \tag{19}$$

with a sharp initial condition. This overdamped approximation is generally valid when $\beta \gg \omega$ and for times $t \gg \beta$.

Regarding the variance, long term expression of the full Langevin solution given in [11, 12] and the overdamped approximation meet.

Finally, we can calculate the probability to cross the potential barrier,

$$\begin{aligned} P(t; q_0, p_0) &= \int_0^{+\infty} W(q, t; q_0, p_0)dq \\ &= \frac{1}{2}\text{erfc}\left(-\frac{\langle q(t)\rangle}{\sqrt{2}\sigma_q(t)}\right). \end{aligned} \tag{20}$$

A comparison of mean exact and approximated trajectories is plotted in Fig.. The same comparison for the probabilities to cross the potential barrier is shown in Fig. *Plots have to be included...*

2.4 Another presentation

Let us denote

$$D = \begin{bmatrix} 0 & 1 \\ \omega^2 & -\beta \end{bmatrix}, \tag{21}$$

the drift matrix. The mean trajectory can be formally written as

$$\begin{bmatrix} \langle q(t) \rangle \\ \langle p(t) \rangle \end{bmatrix} = e^{Dt} \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}. \tag{22}$$

Introducing the intermediate time scale τ, one exactly has

$$\begin{bmatrix} \langle q(t) \rangle \\ \langle p(t) \rangle \end{bmatrix} = e^{D(t-\tau)} e^{D\tau} \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}. \tag{23}$$

The approximation of the previous subsection consists in having different approximate expressions of the drift matrix D on the two time scales:

$$\begin{bmatrix} \langle q(t) \rangle \\ \langle p(t) \rangle \end{bmatrix} \simeq e^{D_2(t-\tau)} e^{D_1\tau} \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}, \tag{24}$$

with

$$D_1 = \begin{bmatrix} 0 & 1 \\ 0 & -\beta \end{bmatrix} \qquad \text{and} \qquad D_2 = \begin{bmatrix} \frac{\omega^2}{\beta} & 0 \\ 0 & -\beta \end{bmatrix}. \tag{25}$$

Actually, what was really done is

$$\begin{bmatrix} \langle q(t) \rangle \\ \langle p(t) \rangle \end{bmatrix} \simeq e^{D_2 t} \lim_{\tau \to \infty} e^{D_1\tau} \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}. \tag{26}$$

I don't know if this helps... I guess not.

2.5 Reduced equation: a systematic expansion

Reduction of the Langevin equation to its Smoluchowski equivalent has already been done, starting either from the Fokker-Plank-Klein-Kramers equation [13] or from the Langevin equation [14]. But none of these works mentions the slip of the initial condition. Inspired by the latter, we will study an expansion to higher orders with a special attention to the initial value.

2.5.1 Formal integration

Let us start again from the matrix approach:

$$\frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \omega^2 & -\beta \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix} + \begin{bmatrix} 0 \\ r(t) \end{bmatrix}.$$

The second row can be seen as a differential equation for p that can be formally integrated using the variation of the constant technique. This leads to

$$\dot{q} = p = p_0 e^{-\beta t} + \omega^2 \int_0^t e^{\beta(t'-t)} q(t') dt' + \int_0^t e^{\beta(t'-t)} r(t'). \tag{27}$$

This is a first order differential equation in q with a memory kernel. This is not a surprise as the reduction of the fast variables always leads to a reduced equation with a memory kernel. Then, one should assume that the fast variables are very fast to recover the Markovian Smoluchowski equation.

The diffusion problem over a parabolic potential barrier with a non-Markovian Langevin equation was solved in Ref. [15]. But this was done introducing an additional variable. Applying this scheme to our problem would mean going back to the original Langevin equation! Here, we shall rather seek an approximative way to solve the non-Markovian Smoluchowski equation, Eq. (27).

2.5.2 First-order expansion when β in large

When β is very large, $e^{\beta(t'-t)} \simeq \delta(t'-t)/\beta$ and the equation become Markovian:

$$\dot{q} = p = p_0 e^{-\beta t} + \frac{\omega^2}{\beta} q(t) + \frac{1}{\beta} r(t). \tag{28}$$

We could have used the Laplace approximation for exponential integrals to find the same result.

On a short time step τ such as $1/\omega \gg \tau \gg 1/\beta$, the mean value of this equation could be integrated:

$$q(\tau) - q_0 = \frac{p_0}{\beta}\left[1 - e^{-\beta\tau}\right] + \frac{\omega^2}{\beta}\int_0^\tau q(t)dt + \frac{1}{\beta}\int_0^\tau r(t)dt. \tag{29}$$

In the first integral term of the r.h.s., we shall assume that $q(t) \simeq q_0$. In addition, τ is such as $e^{-\beta\tau} \simeq 0$. One finally has, at the first order

$$\langle q(\tau)\rangle \simeq q_0 + \frac{p_0}{\beta} \quad \forall \tau. \tag{30}$$

This is the mean value of the new initial conditions of the slow variable that has slipped. The last term of r.h.s. of Eq. (29) gives the standard deviation of theses initial conditions:

$$\sigma_{q(\tau)} = \frac{1}{\beta}\sqrt{\frac{2T\beta}{m}}\sqrt{\tau} = \sqrt{\frac{2T}{m}\frac{\tau}{\beta}}. \tag{31}$$

As $\beta \gg \tau$, we can neglect the dispersion of these initial conditions.

Finally, when $t \gg \tau$, the differential equation satisfied by the slow variable (28) simply becomes:

$$\dot{q} = \frac{\omega^2}{\beta} q(t) + \frac{1}{\beta} r(t), \tag{32}$$

which is nothing else as the overdamped Langevin that is equivalent to the Smoluchowski equation.

2.5.3 Higher order expansion

What if the fast variable is not so fast? Can we perform a higher order expansion? The random force in Eq. (27), $R(t) = \int_0^t e^{\beta(t'-t)} r(t')$, can be easily treated. The mean value is

$$\langle R(t)\rangle = \langle \int_0^t e^{\beta(t'-t)} r(t')\rangle = \int_0^t e^{\beta(t'-t)} \langle r(t')\rangle = 0 \tag{33}$$

and the correlation function

$$\langle R(t_1)R(t_2)\rangle = \int_0^{t_1}\int_0^{t_2} e^{\beta(t_1'-t_1)} e^{\beta(t_2'-t_2)} \langle r(t_1')r(t_2')\rangle dt_1' dt_2' = \frac{2T\beta}{m}\int_0^{t_1}\int_0^{t_2} e^{\beta(t_1'+t_2'-t_1-t_2)} \delta(t_1'-t_2') dt_1' dt_2'. \tag{34}$$

Assuming that $t_2 > t_1$, one has

$$\langle R(t_1)R(t_2)\rangle = \frac{T}{m}\left[e^{-\beta(t_2-t_1)} - e^{-\beta(t_1+t_2)}\right]. \tag{35}$$

More generally, one has

$$\langle R(t_1)R(t_2)\rangle = \frac{T}{m}\left[e^{-\beta|t_2-t_1]} - e^{-\beta(t_1+t_2)}\right] \quad \forall t_1, t_2. \tag{36}$$

Expansion is then easy.

The other integral term in Eq. (27) cannot be calculated as we don't know $q(t)$. Can we expand it? I still have to learn about expansion of exponential integrals from text books. Here is another tentative using successive integrations by part:

$$\omega^2 \int_0^t e^{\beta(t'-t)} q(t') dt' = \frac{\omega^2}{\beta}\left[q(t) - q_0 e^{\beta t}\right] - \frac{\omega^2}{\beta}\int_0^t e^{\beta(t'-t)}\dot{q}(t')dt' \tag{37}$$

$$= \frac{\omega^2}{\beta}\Bigg[q(t) - \frac{\dot{q}(t)}{\beta} + \frac{\ddot{q}(t)}{\beta^2} + \ldots + (-1)^n \frac{q^{(n)}(t)}{\beta^n} + \ldots - \left(q_0 + \frac{\dot{q}_0}{\beta} - \frac{\ddot{q}_0}{\beta^2} + \ldots - (-1)^n \frac{q_0^{(n)}}{\beta^n} + \ldots\right) e^{-\beta t}\Bigg]. \tag{38}$$

We have an expansion in powers of $1/\beta$ but we need many derivatives of the slow variable. This might not be so useful, unfortunately. At least, the first-order is similar to the previous subsection.

Anyway, the differential equation for the slow variable reads

$$\dot{q} = \frac{\omega^2}{\beta}\left[q(t) - \frac{\dot{q}(t)}{\beta} + \frac{\ddot{q}(t)}{\beta^2} + \ldots + (-1)^n \frac{q^{(n)}(t)}{\beta^n} + \ldots\right] + \left[p_0 - (q_0 - \frac{\dot{q}_0}{\beta} + \cdots + (-1)^n \frac{q_0^{(n)}}{\beta^n} + \ldots)\right] e^{-\beta t} + R(t) \tag{39}$$

In the above equation, the first term of the r.h.s. leads to the reduced differential equation satisfied by the slow variable, the second one corresponds to the initial slip, and, of course, the last one is the random force.

Only keeping the first term of the r.h.s., we can look for a solution $q(t) \propto e^{\alpha t}$. α should then satisfies

$$\alpha = \frac{\omega^2}{\beta}\left[1 - \frac{\alpha}{\beta} + \frac{\alpha^2}{\beta^2} - \frac{\alpha^3}{\beta^3} + \ldots\right] = \frac{\omega^2}{\beta}\frac{1}{1+\frac{\alpha}{\beta}} = \frac{\omega^2}{\beta+\alpha}, \tag{40}$$

if $\alpha < \beta$. Then, α is a root of

$$\alpha^2 + \beta\alpha - \omega^2 = 0. \tag{41}$$

This is the characteristic polynomial of the full Langevin equation. The result is then consistent but we have not reduced the problem.

If the sum is truncated, α is not easy to extract. Assuming that it is truncated as level n, one has

$$\alpha = \frac{\omega^2}{\beta}\frac{1 - (-\frac{\alpha}{\beta})^{n+1}}{1+\frac{\alpha}{\beta}}. \tag{42}$$

Regarding the initial slip, I don't know how to proceed.

3 Simple 2D problem

Let us consider again the neck problem studied in the over-damped approximation

$$\gamma \begin{bmatrix}\dot{\varepsilon}\\ \dot{r}\end{bmatrix} = -\begin{bmatrix}\partial V/\partial\varepsilon\\ \partial V/\partial r\end{bmatrix} + \begin{bmatrix}\rho_1(t)\\ \rho_2(t)\end{bmatrix}, \tag{43}$$

with

$$V(\varepsilon, r) = V_s + \frac{1}{2}g\varepsilon^2 - \frac{1}{2}hr^2. \tag{44}$$

and the random force satisfying the fluctuation-dissipation theorem,

$$\langle \rho_i(t)\rho_j(t')\rangle = 2T\gamma_{ij}\delta(t-t'). \tag{45}$$

Exact and approximate solutions were studied in detail in Ref. [5].

Having to inverse the matrix γ is heavy. Let us consider a simplified case:

$$\frac{d}{dt}\begin{bmatrix}F\\ S\end{bmatrix} = \begin{bmatrix}-g & c_{fs}\\ c_{sf} & w\end{bmatrix}\begin{bmatrix}F\\ S\end{bmatrix} + \begin{bmatrix}r_1(t)\\ r_2(t)\end{bmatrix}, \tag{46}$$

where F and S denote a fast and slow variables respectively. This means that $g \gg |w|$. The new random forces are characterized by

$$\langle r_i(t)\rangle = 0 \qquad \text{and} \qquad \langle r_i(t)r_j(t')\rangle = 2T(\gamma^{-1})_{ij}\delta(t-t') = 2R_{ij}\delta(t-t'). \tag{47}$$

3.1 Initial slip with an intuitive approach

Assuming that the slow variable is frozen, the fast variable's evolution is approximately

$$F(t) \simeq F_0 e^{-gt} + \int_0^t e^{g(t'-t)} r_1(t') dt'. \tag{48}$$

The auto-correlation function can be easily calculated:

$$\begin{aligned}\langle (F(t_1) - \langle F(t_1)\rangle)(F(t_2) - \langle F(t_2)\rangle)\rangle &= \int_0^{t_1}\int_0^{t_2} e^{g(t_1'+t_2'-t_1-t_2)}\langle r_1(t_1')r_1(t_2')\rangle dt_1' dt_2' &(49)\\ &= \frac{R_{11}}{g}\left(e^{-g|t_1-t_2|} - e^{-g(t_1+t_2)}\right). &(50)\end{aligned}$$

The mean value quickly vanishes and the variance converges to $\frac{R_{11}}{g} = \frac{T(\gamma^{-1})_{11}}{g}$.

The fast variable evolution can be written as $F(t) = F_0 e^{-gt} + \delta F(t)$ and injected into the differential equation satisfied by the slow variable S. One has, for the mean value

$$\langle \dot{S}\rangle \simeq c_{sf} F_0 e^{-gt} + w\langle S(t)\rangle, \tag{51}$$

that can be integrated on a small time step τ such as $1/|w| \gg \tau \gg 1/g$ to get, at the first order

$$S(\tau) \simeq S_0 + \frac{c_{sf}}{g} F_0. \tag{52}$$

Note that this is only possible is the fast variable converges to an equilibrium. This would not be correct if it diverges. Then $|g|$ has to be positive. w can be either positive or negative.

As for the variance, one has

$$\begin{aligned}\langle(\delta S(\tau))^2\rangle &= c_{sf}^2 \int_0^\tau dt_1 \int_0^\tau dt_2 \langle \delta F(t_1)\delta F(t_2)\rangle = \frac{c_{sf}^2 R_{11}}{g}\int_0^\tau dt_1 \int_0^\tau dt_2 \left(e^{-g|t_1-t_2|} - e^{-g(t_1+t_2)}\right)\\ &\simeq 2\frac{c_{sf}^2 R_{11}}{g^2}\tau. &(53)\end{aligned}$$

As this result depends on τ, I don't know how to do. Neglect this variance that is small?

3.2 Exact solution of the full equation to test the approximation

To test this result, one can exactly solve the 2D problem. Comparison as still to be done. You can skip this subsection that is not terminated.

Laplace transform of Eq. (46) leads to

$$\begin{aligned}\tilde{F} &= \frac{(s-w)F_0 + c_{fs}S_0 + (s-w)\tilde{r}_1 + c\tilde{r}_2}{(s+g)(s-w) - c_{sf}c_{fs}} &(54)\\ \tilde{S} &= \frac{(s+g)S_0 + c_{sf}F_0 + c\tilde{r}_1 + (s+g)\tilde{r}_2}{(s+g)(s-w) - c_{sf}c_{fs}}. &(55)\end{aligned}$$

Denominator has two roots:

$$a_\pm = \frac{1}{2}\left(-(g-w) \pm \sqrt{(g-w)^2 + 4(c_{sf}c_{fs} + wg)}\right). \tag{56}$$

a_+ is positive and a_- negative. When $g \gg w$ one obviously has $|a_-| \gg |a_+|$. Then, we have

$$\begin{aligned}\tilde{F} &= \frac{F_0 + \tilde{r}_1}{a_+ - a_-}\left[\frac{a_+ - w}{s - a_+} - \frac{a_- - w}{s - a_-}\right] + \frac{c_{fs}(S_0 + \tilde{r}_2)}{a_+ - a_-}\left[\frac{1}{s-a_+} - \frac{1}{s-a_-}\right] &(57)\\ \tilde{S} &= \frac{S_0 + \tilde{r}_2}{a_+ - a_-}\left[\frac{a_+ + g}{s - a_+} - \frac{a_- + g}{s - a_-}\right] + \frac{c_{sf}(F_0 + \tilde{r}_1)}{a_+ - a_-}\left[\frac{1}{s-a_+} - \frac{1}{s-a_-}\right]. &(58)\end{aligned}$$

Inverse Laplace transform finally leads to the following average trajectories

$$\langle F(t)\rangle = \frac{F_0}{a_+ - a_-}\left[(a_+ - w)e^{a_+ t} - (a_- - w)e^{a_- t}\right] + \frac{c_{fs}S_0}{a_+ - a_-}\left[e^{a_+ t} - e^{a_- t}\right] \tag{59}$$

$$\langle S(t)\rangle = \frac{S_0}{a_+ - a_-}\left[(a_+ + g)e^{a_+ t} - (a_- + g)e^{a_- t}\right] + \frac{c_{sf}F_0}{a_+ - a_-}\left[e^{a_+ t} - e^{a_- t}\right]. \tag{60}$$

For times larger than $1/|a_-|$, the mean trajectory of the slow variable becomes

$$\langle S(t)\rangle \simeq \frac{(a_+ + g)S_0 + c_{sf}F_0}{a_+ - a_-}e^{a_+ t}. \tag{61}$$

There is an initial slip as expected.

Let us now check calculate the standard deviation of the slow variable as a function of time. As the inverse Laplace transform of a product is the convolution of the inverse functions,

$$\begin{aligned} \delta S(t) &= \frac{1}{a_+ - a_-}\int_0^t \left[(a_+ + g)e^{a_+(t-t')} - (a_- + g)e^{a_-(t-t')}\right] r_2(t')dt' \\ &\quad + \frac{c}{a_+ - a_-}\int_0^t \left[e^{a_+(t-t')} - e^{a_-(t-t')}\right] r_1(t')dt'. \end{aligned} \tag{62}$$

Calculation of the variance is too tedious... I'll do it later.

3.3 Formal reduction of the fast variables

As before, we can first formally integrate the fast variable differential equation

$$\dot{F} = -gF + c_{fs}S + r_1(t) \tag{63}$$

into

$$F(t) = F_0 e^{-gt} + c_{fs}\int_0^t e^{g(t'-t)}S(t')dt' + \int_0^t e^{g(t'-t)}r_1(t')dt'. \tag{64}$$

This can be injected into the slow variable differential equation which becomes

$$\dot{S} = wS + c_{sf}c_{fs}\int_0^t e^{g(t'-t)}S(t')dt' + cF_0e^{-gt} + c_{sf}\int_0^t e^{g(t'-t)}r_1(t')dt' + r_2(t). \tag{65}$$

This equation has memory effect, as usual.

3.3.1 When the fast variable is very fast

When $g \gg |w|$, the integrals in the previous solution, Eq. (65), can be evaluated using Laplace approximation and we get

$$\dot{S} = (w + \frac{c_{sf}c_{fs}}{g})S + c_{sf}F_0e^{-gt} + \frac{c_{sf}}{g}r_1(t) + r_2(t). \tag{66}$$

Introducing again a time scale τ such as $\frac{1}{w} \gg \tau \gg \frac{1}{g}$, one has, as initial condition for the slow motion,

$$S(\tau) \simeq S_0 + \frac{c_{sf}}{g}F_0, \tag{67}$$

at the first order.

3.3.2 Expansion to higher orders

As before, successive integrations by parts give

$$\int_0^t e^{g(t'-t)} S(t')dt' = \frac{1}{g}\left[S(t) - S_0 e^{-gt}\right] - \frac{1}{g^2}\left[\dot{S}(t) - \dot{S}_0 e^{-gt}\right] + \ldots + \frac{(-1)^{n+1}}{g^{n+1}}\left[S^{(n)}(t) - S_0^{(n)} e^{-gt}\right] + \ldots \quad (68)$$

The differential equation (65) satisfied by the slow motion finally becomes

$$\begin{aligned}
\dot{S} \quad = \quad & wS + \frac{c_{sf}c_{fs}}{g}\left[S(t) - \frac{1}{g}\dot{S}(t) + \ldots + \frac{(-1)^n}{g^n} S^{(n)}(t) + \ldots\right] \\
& + \left[c_{sf}F_0 - \frac{c_{sf}c_{fs}}{g}\left(S_0 - \frac{1}{g}\dot{S}_0 + \ldots + \frac{(-1)^n}{g^n} S_0^{(n)} + \ldots\right)\right] e^{-gt} \\
& + c_{sf}\int_0^t e^{g(t'-t)} r_1(t')dt' + r_2(t).
\end{aligned} \quad (69)$$

The structure is as usual: 1st term of the r.h.s. governs the time evolution of the mean value of the slow variable, the 2nd term is responsible of the initial slip and the last two ones are random forces responsible of the diffusion.

4 A general approach to any dimension

In this section, we will generalize what was done in the previous section to a problem with several fast and slow degrees of freedom. We shall assume that there are n_f and n_s fast and slow variables respectively. The model is described by the following differential equation:

$$\frac{d}{dt}\begin{bmatrix} F \\ S \end{bmatrix} = \begin{bmatrix} D_f & C_{fs} \\ C_{sf} & D_s \end{bmatrix}\begin{bmatrix} F \\ S \end{bmatrix} + \begin{bmatrix} R_f(t) \\ R_s(t) \end{bmatrix}, \quad (70)$$

where F is a n_s-dimension vector with the fast variables and S a n_s-dimension vector with the slow degrees of freedom. R_f and R_s are respectively n_f- and n_s-dimension vectors with the random forces. D_f is a $n_f \times n_f$ drift matrix, D_s a $n_s \times n_s$ one, C_{fs} and C_{sf} are $n_f \times n_s$ and $n_s \times n_f$ coupling matrixes.

The random forces auto-correlation functions are defined by two matrixes ρ_f and ρ_s that could be determined with the dissipation-fluctuation theorem

$$\langle R_f(t) \cdot R_f^t(t')\rangle \quad = \quad 2\rho_f \delta(t-t') \quad (71)$$

$$\langle R_s(t) \cdot R_s^t(t')\rangle \quad = \quad 2\rho_s \delta(t-t'). \quad (72)$$

There are also cross-terms, of course.

We will assume that all fast variables quickly converges to a finite value.

4.1 Fast variables

Fast variables satisfy the following set of differential equations

$$\frac{dF}{dt} = D_f \cdot F + C_{fs} \cdot S + R_f(t) \quad (73)$$

This can be formally integrated into

$$F(t) = e^{D_f t} \cdot F_0 + \int_0^t e^{D_f(t-t')} \cdot C_{fs} \cdot S(t')dt' + \int_0^t e^{D_f(t-t')} \cdot R_f(t')dt'. \quad (74)$$

Once again we will assume that the mean value of the fast variables quickly vanishes.

Regarding the random part, the auto-correlation function reads

$$\langle \delta F(t_1) \cdot \delta F^t(t_2)\rangle = 2\int_0^{t_2} e^{D_f(t_1-t)} \cdot \rho_f \cdot e^{D_f^t(t_2-t)}dt, \quad (75)$$

if $t_1 > t_2$. Then, I don't know how to do as I don't think that the matrixes D_f and ρ_f commute.

4.2 Slow variables

Slow variables satisfy the following set of differential equations

$$\frac{dS}{dt} = D_s \cdot S + C_{sf} \cdot F(t) + R_s(t). \tag{76}$$

4.2.1 Approximate initial slip

When the time scale of the fast and slow variables are well separated, one approximately has, at the first order

$$\boxed{S(\tau) \simeq S_0 - C_{sf} \cdot D_f^{-1} \cdot F_0.} \tag{77}$$

This is the mean initial slip.

4.2.2 Effective equation and expansion

Finally, the set of differential equations satisfied by the slow degrees of freedom reads

$$\dot{S} = D_s S + C_{sf} \int_0^t e^{D_f(t-t')} \cdot C_{fs} \cdot S(t')dt' + C_{sf} e^{D_f t} \cdot F_0 + C_{sf} \int_0^t e^{D_f(t-t')} \cdot R_f(t')dt' + R_s(t). \tag{78}$$

In the equation, the first two terms of the r.h.s. correspond to the differential equation with a memory kernel. The third term contributes to the initial slip and the last two ones are the random forces.

When the fast variables are very fast compared to the slow ones, we can use the Laplace approximation for exponential integrals that leads to

$$\boxed{\dot{S} \simeq \left[D_s - C_{sf} \cdot D_f^{-1} \cdot C_{fs}\right] \cdot S + C_{sf} \cdot e^{D_f t} \cdot F_0 - C_{sf} \cdot D_f^{-1} \cdot R_f(t) + R_s(t).} \tag{79}$$

The second term of the r.h.s. represents the initial slip. It can be neglected in the differential equation satisfied by the slow variables that starts after a time step τ.

For higher orders, the integration by parts can be done as before... but I will skip this problem as the solution for simple examples was not promising. We shall rather apply this scheme to realistic problems.

5 The neck problem revisited

The neck problem was studied in Ref. [5] with the overdamped Langevin equation. We will study it again here, starting from the full Langevin equation for two degrees of freedom, namely the relative distance r and the neck ε. We shall apply the reduction scheme of the previous section.

Assuming that the sole coupling is through the friction tensor β and that potential surface is described by parabolas, the model reads

$$\frac{d}{dt}\begin{bmatrix} p_r \\ p_\varepsilon \\ r \\ \varepsilon \end{bmatrix} = \begin{bmatrix} -\beta_{rr} & -\beta_{r\varepsilon} & \omega_r^2 & 0 \\ -\beta_{\varepsilon r} & -\beta_{\varepsilon\varepsilon} & 0 & -\omega_\varepsilon^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} p_r \\ p_\varepsilon \\ r \\ \varepsilon \end{bmatrix} + \begin{bmatrix} R_r(t) \\ R_\varepsilon(t) \\ 0 \\ 0 \end{bmatrix} \tag{80}$$

Here, $p_r = \dot{r}$, $p_\varepsilon = \dot{\varepsilon}$ and $R_r(t)$ and $R_\varepsilon(t)$ are random forces satisfying the dissipation-fluctuation theorem

$$\left\langle \begin{bmatrix} R_r(t) \\ R_\varepsilon(t) \end{bmatrix} \cdot \begin{bmatrix} R_r(t') & R_\varepsilon(t') \end{bmatrix} \right\rangle = 2T\beta\delta(t-t'). \tag{81}$$

5.1 A step by step approximation

Here we shall first reduce the Langevin equation to its overdamped version and then, as a second step, assume that the neck degree of freedom quickly vanishes.

5.1.1 First step: overdamped approximation

The drift matrix for the fast variables reads

$$D_f = \begin{bmatrix} -\beta_{rr} & -\beta_{r\varepsilon} \\ -\beta_{\varepsilon r} & -\beta_{\varepsilon\varepsilon} \end{bmatrix} = -\beta, \tag{82}$$

and the coupling matrixes

$$C_{sf} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad C_{fs} = \begin{bmatrix} \omega_r^2 & 0 \\ 0 & -\omega_\varepsilon^2 \end{bmatrix}. \tag{83}$$

In this case, the drift matrix for the slow variables is simply $D_s = 0$.

The initial value of the slow variables is slipped as shown in Eq. (77)

$$\begin{bmatrix} r(\tau) \\ \varepsilon(\tau) \end{bmatrix} = \begin{bmatrix} r(0) \\ \varepsilon(0) \end{bmatrix} - C_{sf} \cdot D_f^{-1} \cdot \begin{bmatrix} p_r(0) \\ p_\varepsilon(0) \end{bmatrix}. \tag{84}$$

Consequently,

$$r(\tau) = r(0) + (\beta^{-1})_{rr} p_r(0) + (\beta^{-1})_{r\varepsilon} p_\varepsilon(0) = r(0) + \frac{1}{|\beta|}\left[\beta_{\varepsilon\varepsilon} p_r(0) - \beta_{r\varepsilon} p_\varepsilon(0)\right] \tag{85}$$

$$\varepsilon(\tau) = \varepsilon(0) + (\beta^{-1})_{\varepsilon r} p_r(0) + (\beta^{-1})_{\varepsilon\varepsilon} p_\varepsilon(0) = \varepsilon(0) + \frac{1}{|\beta|}\left[-\beta_{r\varepsilon} p_r(0) + \beta_{rr} p_\varepsilon(0)\right]. \tag{86}$$

The differential equation satisfied by the slow variables is given by Eq. (79)

$$\frac{d}{dt}\begin{bmatrix} r \\ \varepsilon \end{bmatrix} = -C_{sf} \cdot D_f^{-1} \cdot C_{fs} \cdot \begin{bmatrix} r \\ \varepsilon \end{bmatrix} - C_{sf} \cdot D_f^{-1} \cdot \begin{bmatrix} R_r(t) \\ R_\varepsilon(t) \end{bmatrix} \tag{87}$$

$$= \beta^{-1} \cdot \begin{bmatrix} \omega_r^2 & 0 \\ 0 & -\omega_\varepsilon^2 \end{bmatrix} \cdot \begin{bmatrix} r \\ \varepsilon \end{bmatrix} + \begin{bmatrix} \rho_r(t) \\ \rho_\varepsilon(t) \end{bmatrix} \tag{88}$$

$$= \frac{1}{|\beta|}\begin{bmatrix} \omega_r^2 \beta_{\varepsilon\varepsilon} & \omega_\varepsilon^2 \beta_{r\varepsilon} \\ -\omega_r^2 \beta_{r\varepsilon} & -\omega_\varepsilon^2 \beta_{rr} \end{bmatrix} \cdot \begin{bmatrix} r \\ \varepsilon \end{bmatrix} + \begin{bmatrix} \rho_r(t) \\ \rho_\varepsilon(t) \end{bmatrix} \tag{89}$$

where the ρ's are new random forces satisfying

$$\left\langle \begin{bmatrix} \rho_r(t) \\ \rho_\varepsilon(t) \end{bmatrix} \cdot \begin{bmatrix} \rho_r(t') & \rho_\varepsilon(t') \end{bmatrix} \right\rangle = 2T\beta^{-1}\delta(t-t'). \tag{90}$$

5.1.2 Second step: neck elimination

For the second step, we shall directly apply what we did in section 3 to Eq. (89). For the sake of simplicity, we shall define

$$w = \frac{\omega_r^2 \beta_{\varepsilon\varepsilon}}{|\beta|}, \qquad g = \frac{\omega_\varepsilon^2 \beta_{rr}}{|\beta|}, \qquad c_{r\varepsilon} = \frac{\omega_\varepsilon^2 \beta_{r\varepsilon}}{|\beta|} \qquad \text{and} \qquad c_{\varepsilon r} = \frac{-\omega_r^2 \beta_{r\varepsilon}}{|\beta|}. \tag{91}$$

The fast evolution of the neck can be exactly integrated into

$$\varepsilon(t) = \varepsilon(\tau)e^{-gt} + c_{\varepsilon r}\int_0^t e^{g(t'-t)} r(t')\, dt' + \int_0^t e^{g(t'-t)} \rho_\varepsilon(t') dt'. \tag{92}$$

And then, the differential equation satisfied by r reads

$$\dot{r} = wr + c_{r\varepsilon}\left[\varepsilon(\tau)e^{-gt} + c_{\varepsilon r}\int_0^t e^{g(t'-t)} r(t') dt' + \int_0^t e^{g(t'-t)} \rho_\varepsilon(t') dt'\right] + \rho_r(t). \tag{93}$$

If $g \gg w$, Laplace approximation leads to

$$\dot{r} \simeq \left[w + \frac{c_{r\varepsilon} c_{\varepsilon r}}{g}\right] r + c_{r\varepsilon}\varepsilon(\tau)e^{-gt} + \frac{c_{r\varepsilon}}{g}\rho_\varepsilon(t) + \rho_r(t). \tag{94}$$

As we already know, the first term of the r.h.s. leads to the time evolution of the mean value of r, the second one to another slip and the last two ones to the random force.

Consequently, the new initial condition of r is

$$\begin{aligned} r(\tau') &= r(\tau) + \frac{c_{r\varepsilon}}{g}\varepsilon(\tau) \\ &= r(0) + \frac{1}{|\beta|}\left(\beta_{\varepsilon\varepsilon}p_r(0) - \beta_{r\varepsilon}p_\varepsilon(0)\right) + \frac{\beta_{r\varepsilon}}{\beta_{rr}}\left[\varepsilon(0) + \frac{1}{|\beta|}\left(-\beta_{r\varepsilon}p_r(0) + \beta_{rr}p_\varepsilon(0)\right)\right] \\ &= r(0) + \frac{\beta_{r\varepsilon}}{\beta_{rr}}\varepsilon(0) + \frac{1}{\beta_{rr}}p_r(0). \end{aligned} \tag{95}$$

Both initial slips simply add up. Note that the initial velocity of the neck does not affect the initial position of r.

The differential equation satisfied by r is simply

$$\dot{r} = \frac{\omega_r^2}{\beta_{rr}}r + \frac{\beta_{r\varepsilon}}{\beta_{rr}}\rho_\varepsilon(t) + \rho_r(t). \tag{96}$$

The deterministic part is exactly as expected! Regarding the random force, one has

$$\left\langle \left(\frac{\beta_{r\varepsilon}}{\beta_{rr}}\rho_\varepsilon(t) + \rho_r(t)\right)\left(\frac{\beta_{r\varepsilon}}{\beta_{rr}}\rho_\varepsilon(t') + \rho_r(t')\right)\right\rangle = \frac{2T}{\beta_{rr}}\delta(t-t'), \tag{97}$$

as expected!

The intuitive 1D overdamped model is correct as it comes out from the elimination of the fast variables. The only change is the initial condition that is shifted as shown in Eq. (95).

5.2 Direct elimination of all fast variables

Here we will assume that r is the only slow variable and apply the scheme of the previous section to the three other variables that are considered fast, with different time scales.

We shall first reorganize the matrix in order to have r at the last column and raw. The model is the same, but written as

$$\frac{d}{dt}\begin{bmatrix} p_\varepsilon \\ p_r \\ \varepsilon \\ r \end{bmatrix} = \begin{bmatrix} -\beta_{\varepsilon\varepsilon} & -\beta_{r\varepsilon} & -\omega_\varepsilon^2 & 0 \\ -\beta_{\varepsilon r} & -\beta_{rr} & 0 & \omega_r^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} p_\varepsilon \\ p_r \\ \varepsilon \\ r \end{bmatrix} + \begin{bmatrix} R_\varepsilon(t) \\ R_r(t) \\ 0 \\ 0 \end{bmatrix} \tag{98}$$

Then, the drift matrix for the fast variables reads

$$D_f = \begin{bmatrix} -\beta_{\varepsilon\varepsilon} & -\beta_{r\varepsilon} & -\omega_\varepsilon^2 \\ -\beta_{\varepsilon r} & -\beta_{rr} & 0 \\ 1 & 0 & 0 \end{bmatrix}, \tag{99}$$

and the coupling matrixes

$$C_{sf} = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \qquad \text{and} \qquad C_{fs} = \begin{bmatrix} 0 \\ \omega_r^2 \\ 0 \end{bmatrix}. \tag{100}$$

The initial value of the slow variable is slipped as shown in Eq. (77)

$$\begin{aligned} r(\tau) &\simeq r(0) - C_{sf}\cdot D_f^{-1}\cdot \begin{bmatrix} p_\varepsilon(0) \\ p_r(0) \\ \varepsilon(0) \end{bmatrix} \\ &= r(0) + \frac{p_r(0)}{\beta_{rr}} - \frac{\beta_{r\varepsilon}}{\beta_{rr}}\varepsilon(0). \end{aligned} \tag{101}$$

Same result as for the step by step method. Just one sign differs. There must be a mistake somewhere.

The differential equation satisfied by the slow variable is given by Eq. (79) that simply reduces to

$$\dot{r} = \frac{\omega_r^2}{\beta_{rr}} r + \frac{1}{\beta_{rr}} R_r(t), \tag{102}$$

here. This very simple result is the same as the one obtained with the step by step method and corresponds to the intuitive overdamped Langevin equation.

Note that this method if far simpler than all the previous methods I tested like the one of the neck paper [5] or with Laplace transform.

6 With the asymmetry degree of freedom

We shall introduce three variables that are commonly used to study the formation stage, namely the relative distance r, the neck ε and asymmetry α. We shall start from the full Langevin equation and assume that the slow variable is either the relative distance r within the over damped approximation, or both r and α within the same approximation.

Denoting $p_r = \dot{r}$, $p_\varepsilon = \dot{\varepsilon}$ and $p_\alpha = \dot{\alpha}$, the model reads

$$\frac{d}{dt}\begin{bmatrix} p_\varepsilon \\ p_\alpha \\ p_r \\ \varepsilon \\ \alpha \\ r \end{bmatrix} = \begin{bmatrix} -\beta_{\varepsilon\varepsilon} & -\beta_{\varepsilon\alpha} & -\beta_{\varepsilon r} & -\omega_\varepsilon^2 & 0 & 0 \\ -\beta_{\alpha\varepsilon} & -\beta_{\alpha\alpha} & -\beta_{\alpha r} & 0 & -\omega_\alpha^2 & 0 \\ -\beta_{r\varepsilon} & -\beta_{r\alpha} & -\beta_{rr} & 0 & 0 & \omega_r^2 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} p_\varepsilon \\ p_\alpha \\ p_r \\ \varepsilon \\ \alpha \\ r \end{bmatrix} + \begin{bmatrix} R_\varepsilon(t) \\ R_\alpha(t) \\ R_r(t) \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{103}$$

As I don't know if the asymmetry degree of freedom is fast or slow, we shall study two cases:

1. r and α are the only slow variables;
2. r is the only slow variable.

In both cases we shall do the overdamped approximation.

6.1 Two slow variables

If r and α are considered to be the slow variables, the drift matrix of the fast variables reads

$$D_f = \begin{bmatrix} -\beta_{\varepsilon\varepsilon} & -\beta_{\varepsilon\alpha} & -\beta_{\varepsilon r} & -\omega_\varepsilon^2 \\ -\beta_{\alpha\varepsilon} & -\beta_{\alpha\alpha} & -\beta_{\alpha r} & 0 \\ -\beta_{r\varepsilon} & -\beta_{r\alpha} & -\beta_{rr} & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \tag{104}$$

and the coupling matrixes

$$C_{sf} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad C_{fs} = \begin{bmatrix} 0 & 0 \\ -\omega_\alpha^2 & 0 \\ 0 & \omega_r^2 \\ 0 & 0 \end{bmatrix}. \tag{105}$$

The drift matrix of the slow variables $D_s = 0$.

The initial value of the slow variable is slipped as shown in Eq. (77)

$$\begin{aligned}
\begin{bmatrix}\alpha(\tau)\\ r(\tau)\end{bmatrix} &\simeq \begin{bmatrix}\alpha(0)\\ r(0)\end{bmatrix} - C_{sf}\cdot D_f^{-1}\cdot \begin{bmatrix}p_\varepsilon(0)\\ p_\alpha(0)\\ p_r(0)\\ \varepsilon(0)\end{bmatrix}\\
&= \begin{bmatrix}\alpha(0)\\ r(0)\end{bmatrix} - \frac{1}{|\beta|_{r\alpha}}\begin{bmatrix}0 & -\beta_{rr} & -\beta_{r\alpha} & (\beta_{r\alpha}\beta_{r\varepsilon}-\beta_{\alpha\varepsilon}\beta_{rr})\\ 0 & \beta_{r\alpha} & -\beta_{\alpha\alpha} & (\beta_{r\alpha}\beta_{\alpha\varepsilon}-\beta_{\alpha\alpha}\beta_{r\varepsilon})\end{bmatrix}\cdot\begin{bmatrix}p_\varepsilon(0)\\ p_\alpha(0)\\ p_r(0)\\ \varepsilon(0)\end{bmatrix}\\
&= \begin{bmatrix}\alpha(0)\\ r(0)\end{bmatrix} - \frac{1}{|\beta|_{r\alpha}}\begin{bmatrix}-\beta_{rr}p_\alpha(0)-\beta_{r\alpha}p_r(0)+(\beta_{r\alpha}\beta_{r\varepsilon}-\beta_{\alpha\varepsilon}\beta_{rr})\varepsilon(0)\\ \beta_{r\alpha}p_\alpha(0)-\beta_{\alpha\alpha}p_r(0)+(\beta_{r\alpha}\beta_{\alpha\varepsilon}-\beta_{\alpha\alpha}\beta_{r\varepsilon})\varepsilon(0)\end{bmatrix}. \qquad (106)
\end{aligned}$$

Here, $|\beta|_{r\alpha} = \beta_{rr}\beta_{\alpha\alpha} - \beta_{r\alpha}^2$.

This result can be compared to the result obtained using Laplace transform to solve the full overdamped Langevin equation and expand the eigenvalues to get approximate values [16]:

$$r(t) = r_{2D}\left(\alpha_0 \to \alpha_0 - \frac{\gamma_{\epsilon r}\gamma_{\alpha r}-\gamma_{rr}\gamma_{\alpha\epsilon}}{|\gamma|_{\alpha r}}\epsilon_0, r_0 \to r_0 - \frac{\gamma_{\alpha\epsilon}\gamma_{\alpha r}-\gamma_{\alpha\alpha}\gamma_{\epsilon r}}{|\gamma|_{\alpha r}}\epsilon_0, t\right) + \frac{\gamma_{\alpha\epsilon}\gamma_{\alpha r}-\gamma_{\alpha\alpha}\gamma_{\epsilon r}}{|\gamma|_{\alpha r}}\epsilon_0 e^{a_- t} \qquad (107)$$

The present method with the matrix formalism is far simpler and also includes the initial velocity.

The differential equation satisfied by the slow variables is given by Eq. (79) that simply reduces to

$$\begin{aligned}
\frac{d}{dt}\begin{bmatrix}\alpha\\ r\end{bmatrix} &= \frac{1}{|\beta|_{r\alpha}}\begin{bmatrix}\beta_{rr}\omega_\alpha^2 & \beta_{r\alpha}\omega_r^2\\ -\beta_{r\alpha}\omega_\alpha^2 & -\beta_{\alpha\alpha}\omega_r^2\end{bmatrix}\cdot\begin{bmatrix}\alpha\\ r\end{bmatrix} + \frac{1}{|\beta|_{r\alpha}}\begin{bmatrix}\beta_{rr}R_\alpha(t)-\beta_{r\alpha}R_r(t)\\ -\beta_{r\alpha}R_\alpha(t)+\beta_{\alpha\alpha}R_r(t)\end{bmatrix}\\
&= [\beta]_{r\alpha}^{-1}\cdot\left(\begin{bmatrix}-\omega_\alpha^2 & 0\\ 0 & \omega_r^2\end{bmatrix}\cdot\begin{bmatrix}\alpha\\ r\end{bmatrix} + \begin{bmatrix}R_\alpha(t)\\ R_r(t)\end{bmatrix}\right). \qquad (108)
\end{aligned}$$

Here $[\beta]_{r\alpha} = \begin{bmatrix}\beta_{\alpha\alpha} & \beta_{r\alpha}\\ \beta_{r\alpha} & \beta_{rr}\end{bmatrix}$. This is nothing else as the 2D overdamped Langevin equation. The only change is once again the initial shift given in Eq. (106).

6.2 A unique slow variable r

If r is the only slow variable, the drift matrix for fast variables reads

$$D_f = \begin{bmatrix}-\beta_{\varepsilon\varepsilon} & -\beta_{\varepsilon\alpha} & -\beta_{\varepsilon r} & -\omega_\varepsilon^2 & 0\\ -\beta_{\alpha\varepsilon} & -\beta_{\alpha\alpha} & -\beta_{\alpha r} & 0 & -\omega_\alpha^2\\ -\beta_{r\varepsilon} & -\beta_{r\alpha} & -\beta_{rr} & 0 & 0\\ 1 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0\end{bmatrix}, \qquad (109)$$

and the coupling matrixes

$$C_{sf} = \begin{bmatrix}0 & 0 & 1 & 0 & 0\end{bmatrix} \qquad C_{fs} = \begin{bmatrix}0\\ 0\\ \omega_r^2\\ 0\\ 0\end{bmatrix}. \qquad (110)$$

The drift matrix of the slow variables $D_s = 0$.

The initial value of the slow variable is slipped as shown in Eq. (77)

$$r(\tau) \simeq r(0) + \frac{p_r(0)}{\beta_{rr}} + \frac{\beta_{r\varepsilon}}{\beta_{rr}}\varepsilon(0) + \frac{\beta_{r\alpha}}{\beta_{rr}}\alpha(0). \qquad (111)$$

The differential equation satisfied by the slow variable is given by Eq. (79) that simply reduces to

$$\dot{r} = \frac{\omega_r^2}{\beta_{rr}}r + \frac{1}{\beta_{rr}}R_r(t), \qquad (112)$$

As expected.

7 Conclusions

This method appears to be very powerful. There are only two formulas written in Eqs. (77) and (79) that can be easily applied. It is more powerful than what we did in the neck paper [5] as it includes the initial slip coming from the initial velocities.

What remains to be done are:

1. check the formulas as there might be many trivial mistakes in these notes;
2. compare the approximate solution obtained here with the exact solution coming from a numerical simulation of the exact Langevin equation;
3. study higher orders when fast variables are not so fast as the present work turned out to be useless;
4. apply these formulas to realistic problems...

I put in the appendix calculations that turned out to be useless but that I don't want to erase... There are put here for memory.

A Simple 3D problems

As a next step, we shall now consider a system with either two slow and one fast variables or with one slow and two fast variables. As the next section presents a N-dimension case, you can skip this section.

A.1 Two slow and one fast variables

Let us consider the following case:

$$\frac{d}{dt}\begin{bmatrix} F \\ S_1 \\ S_2 \end{bmatrix} = \begin{bmatrix} -g & c_1 & c_2 \\ c_1 & w_1 & c_s \\ c_2 & c_s & w_2 \end{bmatrix} \begin{bmatrix} F \\ S_1 \\ S_2 \end{bmatrix} + \begin{bmatrix} r_f(t) \\ r_1(t) \\ r_2(t) \end{bmatrix}, \tag{113}$$

where F and S_i denote fast and slow variables respectively. This means that $g \gg |w_1|$ and $g \gg |w_2|$. In addition, $g > 0$ to have a converging fast variable.

A.1.1 Exact solution?

Finding the exact solution means finding the roots of the third-order polynomial that is quite heavy. We can fin approximate solutions to the problem using the Laplace transform as we already did.

A.1.2 Intuitive approach

As in the 2D case, the evolution of the mean value of the fast variable can be approximately described by

$$F(t) \simeq F_0 e^{-gt}. \tag{114}$$

Injecting it into the differential equations satisfied by slow variables, one gets

$$\dot{S}_1 \simeq c_1 F_0 e^{-gt} + w_1 S_1 + c_s S_2 + r_1(t) \tag{115}$$

$$\dot{S}_2 \simeq c_2 F_0 e^{-gt} + c_s S_1 + w_2 S_2 + r_2(t). \tag{116}$$

This can be integrated on a small time-step τ to get, at the first order

$$S_1(\tau) \simeq S_{10} + F_0 \frac{c_1}{g} \tag{117}$$

$$S_2(\tau) \simeq S_{20} + F_0 \frac{c_2}{g} \tag{118}$$

only keeping the deterministic part.

A.2 Differential equations for the slow motion

As before, the can first formally integrate the fast motion differential equation to get

$$F(t) = F_0 e^{-gt} + \int_0^t e^{g(t'-t)} \left[c_1 S_1(t') + c_2 S_2(t')\right] dt' + \int_0^t e^{g(t'-t)} r_f(t') dt'. \tag{119}$$

This solution can be injected into the equations satisfied by the slow variables

$$\dot{S}_1 = w_1 S_1 + c_s S_2 + c_1 F_0 e^{-gt} + c_1 \int_0^t e^{g(t'-t)} \left[c_1 S_1(t') + c_2 S_2(t')\right] dt' + c_1 \int_0^t e^{g(t'-t)} r_f(t') dt' + r_1(t) \tag{120}$$

$$\dot{S}_2 = w_2 S_2 + c_s S_1 + c_2 F_0 e^{-gt} + c_2 \int_0^t e^{g(t'-t)} \left[c_1 S_1(t') + c_2 S_2(t')\right] dt' + c_2 \int_0^t e^{g(t'-t)} r_f(t') dt' + r_2(t) \tag{121}$$

These are coupled differential equations with a memory kernel.

When the fast variable is very fast

When the fast variable is very fast compared to the slow ones, one can use the usual Laplace approximation for exponential integrals and get

$$\dot{S}_1 \simeq \left[w_1 + \frac{c_1^2}{g}\right] S_1(t) + \left[c_s + \frac{c_1 c_2}{g}\right] S_2(t) + c_1 F_0 e^{-gt} + \frac{c_1}{g} r_f(t) + r_1(t) \tag{122}$$

$$\dot{S}_2 \simeq \left[w_2 + \frac{c_2^2}{g}\right] S_2(t) + \left[c_s + \frac{c_1 c_2}{g}\right] S_1(t) + c_2 F_0 e^{-gt} + \frac{c_2}{g} r_f(t) + r_2(t) \tag{123}$$

In these Eqs., the first two terms of the r.h.s. correspond to the time evolution of the mean value of the slow variables, the third term to the initial slip and the last ones to the random forces.

The initial slip for each of the slow variables is the same as the one found with the intuitive approach.

Expansion to higher orders

As we already did several times, successive integrations by part leads to

$$\begin{aligned}
\int_0^t e^{g(t'-t)} \left[c_1 S_1(t') + c_2 S_2(t')\right] dt' &= \frac{1}{g}\left([c_1 S_1(t) + c_2 S_2(t)] - [c_1 S_{10} + c_2 S_{20}] e^{-gt}\right) \\
&\quad - \frac{1}{g} \int_0^t e^{g(t'-t)} \left[c_1 \dot{S}_1(t') + c_2 \dot{S}_2(t')\right] dt' \qquad (124) \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{g^{n+1}} [c_1 S_1^{(n)}(t) + c_2 S_2^{(n)}(t)] \\
&\quad - \left(\sum_{n=0}^{\infty} \frac{(-1)^n}{g^{n+1}} [c_1 S_1^{(n)}(0) + c_2 S_2^{(n)}(0)]\right) e^{-gt}. \qquad (125)
\end{aligned}$$

Then, it is as before: how to do with such a result that is exact? Truncation leads to a high order differential equation. What have we won? I'm afraid that it is useless.

A.3 Two fast and one slow variables

Let us consider the following case:

$$\frac{d}{dt}\begin{bmatrix} F_1 \\ F_2 \\ S \end{bmatrix} = \begin{bmatrix} -g_1 & c_f & c_1 \\ c_f & -g_2 & c_2 \\ c_1 & c_2 & w \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ S \end{bmatrix} + \begin{bmatrix} r_1(t) \\ r_2(t) \\ r_s(t) \end{bmatrix}, \tag{126}$$

where F_i and S denote fast and slow variables respectively. This means that $g_1 \gg |w|$ and $g_2 \gg |w|$. In addition, $g_1 > 0$ and $g_2 > 0$ to have a converging fast variables.

A.3.1 Intuitive approach

Let us first integrate the two coupled differential equations related to the fast motion,

$$\begin{aligned} \dot{F}_1 &= -g_1F_1 + c_fF_2 + c_1S + r_1(t) \simeq -g_1F_1 + c_fF_2 + r_1(t) && (127) \\ \dot{F}_2 &= -g_2F_2 + c_fF_2 + c_2S + r_2(t) \simeq -g_2F_2 + c_fF_2 + r_2(t), && (128) \end{aligned}$$

by using their Laplace transform

$$\begin{aligned} s\tilde{F}_1 - F_{10} &\simeq -g_1\tilde{F}_1 + c_F\tilde{F}_2 + \tilde{r}_1 && (129) \\ s\tilde{F}_2 - F_{20} &\simeq -g_2\tilde{F}_2 + c_F\tilde{F}_1 + \tilde{r}_2. && (130) \end{aligned}$$

Few lines of calculation lead to

$$\begin{aligned} \tilde{F}_1 &\simeq \frac{1}{a_1 - a_2}\left(\frac{(a_1+g_2)F_{10} + c_fF_{20}}{s-a_1} - \frac{(a_2+g_2)F_{10} + c_fF_{20}}{s-a_2}\right. \\ &\quad \left. + \tilde{r}_1\left[\frac{a_1+g_2}{s-a_1} - \frac{a_2+g_2}{s-a_2}\right] + c_f\tilde{r}_2\left[\frac{1}{s-a_1} - \frac{1}{s-a_2}\right]\right) && (131) \\ \tilde{F}_2 &\simeq \frac{1}{a_1 - a_2}\left(\frac{(a_1+g_1)F_{20} + c_fF_{10}}{s-a_1} - \frac{(a_2+g_1)F_{20} + c_fF_{10}}{s-a_2}\right. \\ &\quad \left. + \tilde{r}_2\left[\frac{a_1+g_1}{s-a_1} - \frac{a_2+g_1}{s-a_2}\right] + c_f\tilde{r}_1\left[\frac{1}{s-a_1} - \frac{1}{s-a_2}\right]\right) && (132) \end{aligned}$$

with a_1 and a_2 being the two negative roots of $s^2 + (g_1+g_2)s + g_1g_2 - c_f^2$, namely

$$a_1 = \frac{1}{2}\left[-(g_1+g_2) + \sqrt{(g_1-g_2)^2 + c_f^2}\right] \qquad \text{and} \qquad a_2 = \frac{1}{2}\left[-(g_1+g_2) - \sqrt{(g_1-g_2)^2 + c_f^2}\right]. \tag{133}$$

Then, the time evolution of the mean values of the fast variables reads

$$\begin{aligned} \langle F_1(t)\rangle &\simeq \frac{1}{a_1-a_2}\left([(a_1+g_2)F_{10} + c_fF_{20}]e^{a_1t} - [(a_2+g_2)F_{10} + c_fF_{20}]e^{a_2t}\right) && (134) \\ \langle F_2(t)\rangle &\simeq \frac{1}{a_1-a_2}\left([(a_1+g_1)F_{20} + c_fF_{10}]e^{a_1t} - [(a_2+g_1)F_{20} + c_fF_{10}]e^{a_2t}\right). && (135) \end{aligned}$$

The differential equation satisfied by the mean value of the slow variable

$$\langle\dot{S}\rangle \simeq w\langle S\rangle + c_1\langle F_1(t)\rangle + c_2\langle F_2(t)\rangle, \tag{136}$$

can be integrated over a time step τ to find the initial slip

$$\begin{aligned} \langle S(\tau)\rangle &\simeq S_0 + \frac{F_{10}}{a_1-a_2}\left[\frac{c_1(a_2+g_2) + c_2c_f}{a_2} - \frac{c_1(a_1+g_2) + c_2c_f}{a_2}\right] \\ &\quad + \frac{F_{20}}{a_1-a_2}\left[\frac{c_2(a_2+g_1) + c_1c_f}{a_2} - \frac{c_2(a_1+g_1) + c_1c_f}{a_2}\right]. && (137) \end{aligned}$$

This expression is quite heavy. We shall redo the same thing using matrix formalism that is more elegant.

A.3.2 Using matrix formalism

The differential equation satisfied by the fast variables reads

$$\frac{d}{dt}\begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = D_f\begin{bmatrix} F_1 \\ F_2 \end{bmatrix} + \begin{bmatrix} c_1S \\ c_2S \end{bmatrix} + \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix}, \tag{138}$$

with

$$D_f = \begin{bmatrix} -g_1 & c_f \\ c_f & -g_2 \end{bmatrix}. \tag{139}$$

The differential equation satisfied by the slow variable reads

$$\dot{S} = wS + \begin{bmatrix} c_1 & c_2 \end{bmatrix} \cdot \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} + r_s(t). \tag{140}$$

The initial slip can be written as

$$S(\tau) \simeq S_0 - \begin{bmatrix} c_1 & c_2 \end{bmatrix} \cdot D_f^{-1} \cdot \begin{bmatrix} F_{10} \\ F_{20} \end{bmatrix}. \tag{141}$$

A formal integration of the fast variables leads to

$$\begin{bmatrix} F_1(t) \\ F_2(t) \end{bmatrix} = e^{D_f t} \cdot \begin{bmatrix} F_{10} \\ F_{20} \end{bmatrix} + \int_0^t e^{D_f(t-t')} \cdot \begin{bmatrix} c_1 S(t') \\ c_2 S(t') \end{bmatrix} dt' + \int_0^t e^{D_f(t-t')} \cdot \begin{bmatrix} r_1(t') \\ r_2(t') \end{bmatrix} dt'. \tag{142}$$

This expression can be injected into Eq. (140). Then, as before, we can use Laplace approximation to exponential integrals to get an approximate differential equation satisfied by the slow variable.

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