Mixing Langevin + ElastoHydroDynamic of cylinder

Yilin YE

Département de Chimie, École Normale Supérieure, 75231 Paris Cedex 05, France Laboratoire Ondes et Matière d'Aquitaine, 33405 Talence Cedex, France

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1 Theoretical Framework

1.1 Fundamentals

Gibbs-Boltzmann distribution The Boltzmann distribution is a probability distribution that gives the probability of a certain state as a function of that state's energy and temperature of the system to which the distribution is applied. It is given as

$$p_i = \frac{\exp(-\beta \varepsilon_i)}{\sum_{i=1}^{M} \exp(-\beta \varepsilon_i)}$$

Langevin equation The original Langevin equation describes Brownian motion, the apparently random movement of a particle in a fluid due to collisions with molecules of the fliud,

$$m\frac{dv}{dt} = -\lambda v + \eta(t)$$

where v is the velocity of the particle, and m is the mass. The force acting on the particle is written as a sum of a viscous force proportional to the particles's velocity, and a noise term $\eta(t)$ representing the effect of the collisions with the molecules of the fluid. The force $\eta(t)$ has a Gaussian probability distribution with correlation function $\langle \eta_i(t)\eta_i(t')\rangle = 2\lambda k_B T \delta_{ij}\delta(t-t')$

There are two common choices of discretization: the Itô and the Stratonovich conventions. Discretization of the Langevin equation:

$$\frac{x_{t+\Delta} - x_t}{\Delta} = -V'(x_t) + \xi_t$$

with an associated discretization of the correlations:

$$\langle f[x(t)] \rangle \to \langle f(x_t) \rangle \quad \langle f[x(t)] \xi(t) \rangle \to \langle f(x_t) \xi_t \rangle \quad \langle f[x(t)] \dot{x}(t) \rangle \to \left\langle f(x_t) \frac{x_{t+\Delta} - x_t}{\Delta} \right\rangle$$

which leads to Itô's chain rule:

$$\frac{d}{dt} \langle f[x(t)] \rangle = \left\langle f'[x(t)] \frac{dx}{dt} \right\rangle + T \langle f''[x(t)] \rangle$$

Fokker-Planck equation In one spatial dimension x, for an Itô process driven by the standard Wiener process W_t and described by the stochastic differential equation (SDE)

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t$$

with drift $\mu(X_t, t)$ and diffusion coefficient $D(X_t, t) = \sigma^2(X_t, t)/2$, the Fokker-Planck equation for the probability density p(x, t) of the random variable X_t is

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\left[\mu(x,t)p(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[D(x,t)p(x,t)\right]$$

Derivation from the over-damped Langevin equation

Let $\mathbb{P}(x,t)$ be the probability density density function to find a particle in [x,x+dx] at time t, and let x satisfy:

$$\dot{x}(t) = -V'(x) + \xi(t)$$

if f is a function, we have:

$$\frac{d}{dt} \left\langle f\left[x(t)\right]\right\rangle = \frac{d}{dt} \int \mathbb{P}(x,t)f(x)dx = \int \frac{\partial \mathbb{P}(x,t)}{\partial t} f(x)dx$$

but using Itô's chain rule:

$$\frac{d}{dt} \langle f[x(t)] \rangle = \left\langle f'[x(t)] \frac{dx}{dt} \right\rangle + T \langle f''[x(t)] \rangle$$

with Langevin's equation

$$\frac{d}{dt} \langle f[x(t)] \rangle = \langle f'[x(t)] \{ -V'[x(t)] + \xi(t) \} \rangle + T \langle f''[x(t)] \rangle$$

since $\langle f'[x(t)]\xi(t)\rangle = 0$, we have

$$\frac{d}{dt} \left\langle f\left[x(t)\right]\right\rangle = \int \left[\frac{df(x)}{dx} \left(-\frac{dV(x)}{dx}\right) + T\frac{d^2f(x)}{dx^2}\right] \mathbb{P}(x,t) dx$$

performing an integration by parts, and using that $\mathbb{P}(x,t)$ is a probability density vanishing at $x \to \infty$:

$$\int \frac{\partial \mathbb{P}(x,t)}{\partial t} f(x) dx = \int \frac{\partial}{\partial x} \left[\frac{dV(x)}{dx} + T \frac{\partial}{\partial x} \right] \mathbb{P}(x,t) f(x) dx$$

this is true for any function f, thus

$$\boxed{\frac{\partial \mathbb{P}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[\frac{dV(x)}{dx} + T \frac{\partial}{\partial x} \right] \mathbb{P}(x,t)}$$

It could be written as $\partial_t \mathbb{P}(x,t) = -H_{FP}\mathbb{P}(x,t)$ with H_{FP} the Fokker-Planck operator shown above.

1.2 Salez2015: Elastohydrodynamics of a sliding, spinning and sedimenting cylinder near a soft wall

arxiv: 1412.0162; Journal of Fluid Mechanics, 779 181 (2015)

This article describes the sedimentation, sliding, and spinning motions of a cylinder near a thin compressible elastic wall by thin-film lubrication dynamics. Below is the illustration.

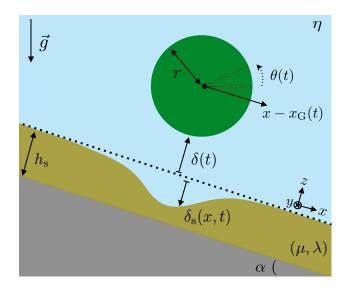


FIG. 1: Schematic of the system. A negatively buoyant cylinder (green) falls down under the acceleration of gravity \vec{g} , inside a viscous fluid (blue), in the vicinity of a thin soft wall (brown). The ensemble lies atop a tilted, infinitely rigid support (grey).

The deformation of the soft wall reads:

$$\delta_s(x,t) = -\frac{h_s p(x,t)}{2\mu + \lambda}$$
 (Salez2015.2)

as well as the dimensionless parameters: $z = Zr\varepsilon$, $h = Hr\varepsilon$, $\delta = \Delta r\varepsilon$, $x = Xr\sqrt{2\varepsilon}$, $x_G = X_Gr\sqrt{2\varepsilon}$, $\theta = \Theta\sqrt{2\varepsilon}$, $t = Tr\sqrt{2\varepsilon}/c$, u = Uc, and $p = P\eta c\sqrt{2}/(r\varepsilon^{3/2})$; a free fall velocity scale $c = \sqrt{2gr\rho^*/\rho}$

and one dimensionless parameter ξ measures the ratio of the free fall time $\sqrt{\rho r \epsilon/(\rho^* g)}$ and the typical lubrication damping time $m\epsilon^{3/2}/\eta$ over which the inertia of the cylinder vanishes.

$$\xi = \frac{3\sqrt{2}\eta}{r^{3/2}\varepsilon\sqrt{\rho\rho^*g}}\kappa = \frac{2h_s\eta\sqrt{g\rho^*}}{r^{3/2}\varepsilon^{5/2}(2\mu + \lambda)\sqrt{\rho}}$$

With perturbation theory in first-order correction of κ , the soft compressible wall gives

$$\ddot{X}_{G} + \frac{2\varepsilon\xi}{3}\frac{\dot{X}_{G}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_{G}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta} - \ddot{X}_{G}}{\Delta^{5/2}}\right] - \sqrt{\frac{\varepsilon}{2}}\sin\alpha = 0$$
 (Salez2015.50)

$$\ddot{\Delta} + \xi \frac{\dot{\Delta}}{\Delta^{3/2}} + \frac{\kappa \xi}{4} \left[21 \frac{\dot{\Delta}^2}{\Delta^{9/2}} - \frac{(\dot{\Theta} - \dot{X}_G)^2}{\Delta^{7/2}} - \frac{15}{2} \frac{\ddot{\Delta}}{\Delta^{7/2}} \right] + \cos \alpha = 0$$
 (Salez2015.51)

$$\ddot{\Theta} + \frac{4\varepsilon\xi}{3}\frac{\dot{\Theta}}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{3}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{X}_G}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{X}_G - \ddot{\Theta}}{\Delta^{5/2}}\right] = 0$$
 (Salez2015.52)

where Δ refers to z and X_G refers to x after the scaling. For the plan case, we set $\alpha = 0$.

1.3 David's note: Determining noise from deterministic forces

Here is the note of David Dean, considering the Brownian motion but only in two dimension (Δ, X) . The rotation had been neglected $(\dot{\Theta} = 0)$, and the second derivatives in the first-order correction of κ as well. To be clear, Fokker-Planck equation would be carefully discussed. Other personal comments are also written in Italic.

Consider the following deterministic equations (α refers to Δ , X these two directions)

$$dX_{\alpha} = V_{\alpha}dt$$
 (David.1)

and (X, V refer to the position and the velocity, respectively)

$$dV_{\alpha} = -U_{\alpha}dt - \nabla\phi(\mathbf{X})dt \tag{David.2}$$

We assume that U_{α} are generated by hydrodynamic interactions which do not however affect the equilibrium Gibbs-Boltzmann distribution which is

$$P_{eq}(\mathbf{X}, \mathbf{V}) = \frac{1}{\bar{Z}} \exp\left(-\frac{\beta \mathbf{V}^2}{2} - \beta \phi(\mathbf{X})\right)$$
 (David.3)

Exploit the Fokker-Planck operator (· · · refers the similar terms about X_{α})

$$\frac{\partial P}{\partial t} = -H_{FP}P = \frac{\partial}{\partial x} \left[\frac{dV}{dx} P + T \frac{\partial}{\partial x} P \right] = \frac{\partial}{\partial V_{\alpha}} \left[(U_{\alpha} + \nabla_{\alpha} \phi) P + T \gamma_{\alpha\beta} \frac{\partial P}{\partial V_{\beta}} \right] + \frac{\partial}{\partial X_{\alpha}} \left[\cdots \right]$$

Note $\frac{\partial P}{\partial X_{\alpha}} = P\left(-\beta \frac{\partial \phi}{\partial X_{\alpha}}\right)$ and $\frac{\partial P}{\partial V_{\alpha}} = P\left(-\beta V_{\alpha}\right)$. Consider the gravity $\phi(\mathbf{X}) = -mg\Delta$, and then we could derive the eq. David.4, regarding k_B as I

$$\begin{split} \frac{\partial}{\partial X_{\alpha}} \left[\frac{dV}{dx} P + T \frac{\partial}{\partial x} P \right] &= \frac{\partial}{\partial X_{\alpha}} \left[\frac{dV}{dX_{\alpha}} P + T \frac{\partial}{\partial X_{\alpha}} P + T \frac{\partial}{\partial V_{\alpha}} P \right] \\ &= \frac{\partial}{\partial X_{\alpha}} \left[(\nabla_{\alpha} \phi) P + \mathcal{T} \cdot P \left(-\beta \frac{\partial \phi}{\partial X_{\alpha}} \right) + T \frac{\partial}{\partial V_{\alpha}} P \right] = \frac{\partial}{\partial X_{\alpha}} \left[T \frac{\partial}{\partial V_{\alpha}} P \right] \\ &= \frac{\partial}{\partial X_{\alpha}} \left[\mathcal{T} \cdot P \left(-\beta V_{\alpha} \right) \right] = -\frac{\partial}{\partial X_{\alpha}} V_{\alpha} P \end{split}$$

The Fokker Planck equation at finite temperature which introduces white noise and possibly temperature dependent drifts is $\phi(\mathbf{X})$ is

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial V_{\alpha}} \left[T \gamma_{\alpha\beta} \frac{\partial P}{\partial V_{\beta}} + U_{\alpha} P + \frac{\partial \phi}{\partial X_{\alpha}} P \right] - \frac{\partial}{\partial X_{\alpha}} V_{\alpha} P$$
 (David.4)

The last two terms would vanish since

$$\frac{\partial}{\partial V_{\alpha}} \left(\frac{\partial \phi}{\partial X_{\alpha}} P \right) = \left(\frac{\partial}{\partial V_{\alpha}} \frac{\partial \phi}{\partial X_{\alpha}} \right) \cdot P + \frac{\partial \phi}{\partial X_{\alpha}} \cdot \frac{\partial P}{\partial V_{\alpha}} = \frac{\partial \phi}{\partial X_{\alpha}} \cdot P(-\beta V_{\alpha})$$

$$\frac{\partial}{\partial X_{\alpha}} V_{\alpha} P = \left(\frac{\partial V_{\alpha}}{\partial X_{\alpha}} \right) P + V_{\alpha} \left(\frac{\partial P}{\partial X_{\alpha}} \right) = V_{\alpha} \cdot P \cdot \left(-\beta \frac{\partial \phi}{\partial X_{\alpha}} \right)$$

Therefore, at equilibrium $\frac{\partial P}{\partial t} = 0$

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial V_{\alpha}} \left[T \gamma_{\alpha\beta} \frac{\partial P}{\partial V_{\beta}} + U_{\alpha} P \right] = \frac{\partial}{\partial V_{\alpha}} \left[T \gamma_{\alpha\beta} P \cdot (-\not \beta V_{\beta}) + U_{\alpha} P \right] = \frac{\partial}{\partial V_{\alpha}} \left[(U_{\alpha} - \gamma_{\alpha\beta} V_{\beta}) \cdot P \right] = 0$$

We obtain the GB distribution for the steady state if

$$U_{\alpha} = \gamma_{\alpha\beta} V_{\beta} \tag{David.5}$$

We have for small velocities that

$$U_{\alpha} = \lambda_{\alpha\beta}(\mathbf{X})V_{\beta} + \Lambda_{\alpha\beta\gamma}(\mathbf{X})V_{\beta}V_{\gamma}$$
 (David.6)

and so we find

$$\gamma_{\alpha\beta}V_{\beta} = \lambda_{\alpha\beta}(\mathbf{X})V_{\beta} + \Lambda_{\alpha\beta\gamma}(\mathbf{X})V_{\beta}V_{\gamma}$$
 (David.7)

Written this way the term $\lambda_{\alpha\beta}(\mathbf{X})$ is just the friction tensor in the absence of any elastic effects. We can thus write

$$\gamma_{\alpha\beta} = \lambda_{\alpha\beta} + \gamma_{2\alpha\beta} \tag{David.8}$$

and we write

$$\gamma_{2\alpha\beta} = \Gamma_{\alpha\beta\gamma} V_{\gamma} \tag{David.9}$$

and

$$\Gamma_{\alpha\beta\gamma}(\mathbf{X})V_{\beta}V_{\gamma} = \Lambda_{\alpha\beta\gamma}(\mathbf{X})V_{\beta}V_{\gamma}$$
 (David.10)

where we without loss of generality take $\Lambda_{\alpha\beta\gamma} = \Lambda_{\alpha\gamma\beta}$, which then gives

$$\Gamma_{\alpha\beta\gamma} + \Gamma_{\alpha\gamma\beta} = 2\Lambda_{\alpha\beta\gamma}$$
 (David.11)

We have to solve this system with the constraint that $\Gamma_{\alpha\beta\gamma}V_{\gamma} = \Gamma_{\beta\alpha\gamma}V_{\gamma}$. In Thomas' problem (see subsection 1.2) we have

$$\ddot{\Delta} + \xi \frac{\dot{\Delta}}{\Delta^{3/2}} + \frac{\kappa \xi}{4} \left[21 \frac{\dot{\Delta}^2}{\Delta^{9/2}} - \frac{(\dot{\Theta} - \dot{X}_G)^2}{\Delta^{7/2}} - \frac{15}{2} \frac{\ddot{\Delta}}{\Delta^{7/2}} \right] + \cos \alpha = 0$$

$$\ddot{X}_G + \frac{2\varepsilon\xi}{3}\frac{\dot{X}_G}{\sqrt{\Delta}} + \frac{\kappa\varepsilon\xi}{6}\left[\frac{19}{4}\frac{\dot{\Delta}\dot{X}_G}{\Delta^{7/2}} - \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + \frac{1}{2}\frac{\ddot{\Theta} - \ddot{X}_G}{\Delta^{5/2}}\right] - \sqrt{\frac{\varepsilon}{2}}\sin\alpha = 0$$

where Δ refers to z and X_G refers to x. Note $\dot{\Delta} = -U_z$ and $\dot{X}_G = -U_x$, we write

$$U_z = \xi \frac{V_z}{Z^{3/2}} + \frac{21\kappa\xi}{4} \frac{V_z^2}{Z^{9/2}} - \frac{\kappa\xi}{4} \frac{V_x^2}{Z^{7/2}}$$
 (David.12)

$$U_x = 2\xi\varepsilon \frac{V_x}{3Z^{1/2}} + \frac{19\kappa\xi\varepsilon}{24} \frac{V_z V_x}{Z^{7/2}}$$
 (David.13)

Note $\dot{\Delta} = V_z$ and $\dot{X}_G = V_x$, we could extract the relevant coefficients. But Attention! Here $\dot{\Theta}$ was assumed 0, and the second derivatives in first-order correlation had been ignored.

Form this we find that

$$\sum_{\alpha\beta} \Lambda_{z\alpha\beta} V_{\alpha} V_{\beta} = \frac{21\kappa\xi}{4} \frac{V_{z}^{2}}{Z^{9/2}} - \frac{\kappa\xi}{4} \frac{V_{x}^{2}}{Z^{7/2}}$$

$$\sum_{\alpha\beta} \Lambda_{x\alpha\beta} V_{\alpha} V_{\beta} = \frac{19\kappa\xi\varepsilon}{24} \frac{V_{z}V_{x}}{Z^{7/2}}$$
(David.14)

This gives the set of equations

$$\Gamma_{zzz} = \frac{21\kappa\xi}{4Z^{9/2}}$$
 (David.15)

$$\Gamma_{zxx} = -\frac{\kappa \xi}{4Z^{7/2}}$$
 (David.16)

$$\Gamma_{zxz} + \Gamma_{zzx} = 0$$
 (David.17)

$$\Gamma_{xzz} = 0 (David.18)$$

$$\Gamma_{xxx} = 0$$
 (David.19)

$$\Gamma_{xxz} + \Gamma_{xzx} = \frac{19\kappa\xi\varepsilon}{24Z^{7/2}}$$
 (David.20)

The symmetry $\Gamma_{\alpha\beta\gamma} = \Gamma_{\beta\alpha\gamma}$ now gives

$$\Gamma_{xxz} = \frac{19\kappa\xi\varepsilon}{24Z^{7/2}} - \Gamma_{xzx} = \frac{19\kappa\xi\varepsilon}{24Z^{7/2}} - \Gamma_{zxx} = \frac{\kappa\xi}{Z^{7/2}} \left(\frac{19\varepsilon}{24} + \frac{1}{4}\right)$$
 (David.21)

as well as

$$\Gamma_{zxz} = \Gamma_{zzx} = 0$$
(David.22)

The Langevin equation corresponding to this is, using the Itô convention,

$$\frac{dV_{\alpha}}{dt} = -U_{\alpha} - \frac{\partial \phi(\mathbf{X})}{\partial X_{\alpha}} + T \frac{\partial \gamma_{\alpha\beta}}{\partial V_{\beta}} + \eta_{\alpha}(t)$$
 (David.23)

which can be written as

$$\frac{dV_{\alpha}}{dt} = -U_{\alpha} - \frac{\partial \phi(\mathbf{X})}{\partial X_{\alpha}} + T\Gamma_{\alpha\beta\beta} + \eta_{\alpha}(t)$$
 (David.24)

where we use the Einstein summation convention and the noise correlator is given by

$$\langle \eta_{\alpha}(t)\eta_{\beta}(t')\rangle = 2T\gamma_{\alpha\beta}\delta(t-t') = 2T\left[\lambda_{\alpha\beta}(\mathbf{X}) + \Gamma_{\alpha\beta\gamma}(\mathbf{X})V_{\gamma}\right]\delta(t-t')$$
 (David.25)

Putting this together we find (from eq. David.24) with all $\Gamma_{\alpha\beta\beta}$ only depending on Δ, X .

$$\frac{dV_z}{dt} = -V'(Z) - \xi \frac{V_z}{Z^{3/2}} - \frac{21\kappa\xi}{4} \frac{V_z^2}{Z^{9/2}} + \frac{\kappa\xi V_x^2}{4Z^{7/2}} + T \left[\frac{21\kappa\xi}{4Z^{9/2}} - \frac{\kappa\xi}{4Z^{7/2}} \right] + \eta_z(t)
\frac{dV_x}{dt} = -2\xi\varepsilon \frac{V_x}{3Z^{1/2}} - \frac{19\kappa\xi V_z V_x}{24Z^{7/2}} + \eta_x(t)$$
(David.26)

1.4 New Coefficients: $\lambda_{\alpha\beta}$, $\Gamma_{\alpha\beta\gamma}$ in 3D (Δ, X, Θ)

In this part, we would renew coefficients for the motion in 3D (Δ, X, Θ) . Based on the previous subsection, we could repeat the calculation by Fokker-Planck operator, finding the similar results with additional terms about Θ .

For the sake of convenience, we re-write Thomas' differential equations (see subsection 1.2) with \dot{v}_i , (and X refers to X_G)

$$-U_Z = \dot{v}_{\Delta} = \ddot{\Delta} = F_{\Delta}(\Delta, v_{\Delta}, v_{X}, v_{\Theta}, \dot{v}_{\Delta})$$

$$-U_X = \dot{v}_X = \ddot{X} = F_X(\Delta, v_{\Delta}, v_{X}, v_{\Theta}, \dot{v}_{X}, \dot{v}_{\Theta})$$

$$-U_{\Theta} = \dot{v}_{\Theta} = \ddot{\Theta} = F_{\Theta}(\Delta, v_{\Delta}, v_{X}, v_{\Theta}, \dot{v}_{X}, \dot{v}_{\Theta})$$

$$(1)$$

However, we'd like to derive equations for each \dot{v} only depending on Δ and v, without \dot{v} . Therefore, we have to find the proper expression for each \dot{v}_i .

Consider the second derivative in the eq. Salez2015.51,

$$\ddot{\Delta} + a_1 \frac{\dot{\Delta}}{\Delta^{3/2}} + a_2 \frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3 \frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3 \frac{\dot{X}^2}{\Delta^{7/2}} + a_4 \frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_5 \frac{\ddot{\Delta}}{\Delta^{7/2}} + a_6 = 0$$
 (2)

$$\ddot{\Delta} = \left(a_1 \frac{\dot{\Delta}}{\Delta^{3/2}} + a_2 \frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3 \frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3 \frac{\dot{X}^2}{\Delta^{7/2}} + a_4 \frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_6\right) \times \frac{-1}{1 + a_5/\Delta^{7/2}}$$
(3)

We know that $a_1 = \xi$, $a_2 = \frac{21\kappa\xi}{4}$, $a_3 = -\frac{\kappa\xi}{4}$, $a_4 = \frac{\kappa\xi}{2}$, $a_5 = -\frac{15\kappa\xi}{8}$, $a_6 = \cos(\alpha = 0) = 1$. After simple calculation, we could obtain \dot{v}_{Δ} (\dot{v}_z) namely $\ddot{\Delta}$

$$-\dot{v}_{\Delta} = U_z = \frac{8\Delta^{9/2} + 2\xi \left(-\Delta\kappa v_X^2 + 4\Delta^3 v_z + 21\kappa v_z^2 + 2\Delta\kappa v_X v_\theta - \Delta\kappa v_\theta^2\right)}{8\Delta^{9/2} - 15\Delta\kappa\xi} \tag{4}$$

Similarly, we write the eqs Salez2015.50 and Salez2015.52 as

$$\ddot{X} + b_1 \frac{\dot{X}}{\sqrt{\Delta}} + b_2 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_4 \frac{\ddot{\Theta}}{\Delta^{5/2}} + b_5 \frac{\ddot{X}}{\Delta^{5/2}} + b_6 = 0$$
 (5)

$$\ddot{\Theta} + c_1 \frac{\dot{\Theta}}{\sqrt{\Lambda}} + c_2 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + c_4 \frac{\ddot{X}}{\Delta^{5/2}} + c_5 \frac{\ddot{\Theta}}{\Delta^{5/2}} + c_6 = 0 \tag{6}$$

with all coefficients we need: $b_1 = \frac{2\varepsilon\xi}{3}$, $b_2 = \frac{19\kappa\xi\varepsilon}{24}$, $b_3 = -\frac{\kappa\xi\varepsilon}{6}$, $b_4 = \frac{\kappa\xi\varepsilon}{12}$, $b_5 = -\frac{\kappa\xi\varepsilon}{12}$, $b_6 = \sin(\alpha = 0) = 0$; and $c_1 = \frac{4\varepsilon\xi}{3}$, $c_2 = \frac{19\kappa\xi\varepsilon}{12}$, $c_3 = -\frac{\kappa\xi\varepsilon}{3}$, $c_4 = \frac{\kappa\xi\varepsilon}{6}$, $c_5 = -\frac{\kappa\xi\varepsilon}{6}$, $c_6 = 0$. For this system of linear equations, the coefficient matrix has full rank.

$$\begin{pmatrix} 1 + (b_5) & (b_4) \\ (c_4) & 1 + (c_5) \end{pmatrix} \begin{pmatrix} \ddot{X} \\ \ddot{\Theta} \end{pmatrix} = \begin{pmatrix} (b_1 + b_2 + b_3 + b_6) \\ (c_1 + c_2 + c_3 + c_6) \end{pmatrix}$$

Then we could solve $\ddot{X} = \dot{v}_X$ and $\ddot{\Theta} = \dot{v}_{\Theta}$ directly

$$-\dot{v}_X = U_X = \frac{\epsilon \xi \left(\kappa \left(16\Delta^3 \epsilon \xi + \left(-24\Delta^{5/2} + 23\epsilon \kappa \xi\right) v_z\right) v_\theta + v_X \left(-4\epsilon \kappa^2 \xi v_z + \left(6\Delta^{5/2} - \epsilon \kappa \xi\right) \left(16\Delta^3 + 19\kappa v_\theta\right)\right)\right)}{36\left(4\Delta^6 - \Delta^{7/2} \epsilon \kappa \xi\right)}$$

 $-\dot{v}_{\Theta} = U_{\Theta} =$

$$\frac{\epsilon\xi\left(\left(16\Delta^{3}\left(12\Delta^{5/2}-\epsilon\kappa\xi\right)+\kappa\left(228\Delta^{5/2}-23\epsilon\kappa\xi\right)v_{z}\right)v_{\theta}+\kappa v_{X}\left(\left(-48\Delta^{5/2}+4\epsilon\kappa\xi\right)v_{z}+\epsilon\xi\left(16\Delta^{3}+19\kappa v_{\theta}\right)\right)\right)}{36\left(4\Delta^{6}-\Delta^{7/2}\epsilon\kappa\xi\right)}$$
(8)

Compare with the eq. 1, we finally remove the second derivatives inside each expression

$$\dot{v}_{\Delta} = F_{\Delta}(\Delta, v_{\Delta}, v_{X}, v_{\Theta})$$

$$\dot{v}_{X} = F_{X}(\Delta, v_{\Delta}, v_{X}, v_{\Theta})$$

$$\dot{v}_{\Theta} = F_{\Theta}(\Delta, v_{\Delta}, v_{X}, v_{\Theta})$$
(9)

(7)

See eqs David.5 ~ David.9, we could extract these $\lambda_{\alpha\beta}$ by

$$\lambda_{\alpha\beta} = \text{Coefficient}[U_{\alpha}, v_{\beta}] - \text{Coefficient}[U_{\alpha}, v_{\beta}v_{\gamma}] \times v_{\gamma}$$
(10)

and $\Gamma_{\alpha\beta\beta}$ by

$$\Gamma_{\alpha\beta\beta} = \text{Coefficient}[U_{\alpha}, v_{\beta}v_{\beta}] \tag{11}$$

As for $\Gamma_{\alpha\beta\gamma}$, we should resolve them by

$$2\Lambda_{\alpha\beta\gamma} = \text{Coefficient}[U_{\alpha}, v_{\beta}v_{\gamma}] = \Gamma_{\alpha\beta\gamma} + \Gamma_{\alpha\gamma\beta}$$
 (12)

as well as the constraint $\Gamma_{\alpha\beta\gamma} = \Gamma_{\beta\alpha\gamma}$.

After some calculations with the help of *Mathematica*, we list all $\lambda_{\alpha\beta}$

$$\lambda_{zz} = \frac{8\Delta^2 \xi}{8\Delta^{7/2} - 15\kappa \xi}$$

$$\lambda_{xx} = -\frac{4\epsilon \xi \left(-6\Delta^{5/2} + \epsilon \kappa \xi\right)}{36\Delta^3 - 9\sqrt{\Delta}\epsilon \kappa \xi}$$

$$\lambda_{\theta\theta} = -\frac{4\epsilon \xi \left(-12\Delta^{5/2} + \epsilon \kappa \xi\right)}{36\Delta^3 - 9\sqrt{\Delta}\epsilon \kappa \xi}$$
(13)

$$\lambda_{x\theta} = \lambda_{\theta x} = \frac{4\epsilon^2 \kappa \xi^2}{36\Delta^3 - 9\sqrt{\Delta}\epsilon \kappa \xi} \tag{14}$$

$$\lambda_{zx} = \lambda_{xz} = \lambda_{z\theta} = \lambda_{\theta z} = 0 \tag{15}$$

and then $\Gamma_{\alpha\beta\gamma}$

$$\Gamma_{zzz} = \frac{42\kappa\xi}{8\Delta^{9/2} - 15\Delta\kappa\xi}$$

$$\Gamma_{xzx} = \Gamma_{zxx} = \frac{2\kappa\xi}{-8\Delta^{7/2} + 15\kappa\xi}$$

$$\Gamma_{\theta z\theta} = \Gamma_{z\theta\theta} = \frac{2\kappa\xi}{-8\Delta^{7/2} + 15\kappa\xi}$$
(16)

$$\Gamma_{zxz} = \Gamma_{zzx} = \Gamma_{zz\theta} = \Gamma_{z\theta z} = 0 \tag{17}$$

$$\Gamma_{xzz} = \Gamma_{xxx} = \Gamma_{\theta zz} = \Gamma_{\theta\theta\theta} = 0 \tag{18}$$

$$\Gamma_{\theta xx} = \Gamma_{x\theta x} = \Gamma_{x\theta\theta} = \Gamma_{\theta x\theta} = 0 \tag{19}$$

$$\Gamma_{xxz} = \frac{1}{9} \kappa \xi \left(\frac{18}{8\Delta^{7/2} - 15\kappa \xi} + \frac{\epsilon^2 \kappa \xi}{-4\Delta^6 + \Delta^{7/2} \epsilon \kappa \xi} \right)$$

$$\Gamma_{xx\theta} = \frac{19\epsilon \kappa \xi \left(-6\Delta^{5/2} + \epsilon \kappa \xi \right)}{-144\Delta^6 + 36\Delta^{7/2} \epsilon \kappa \xi}$$

$$\Gamma_{\theta\theta x} = \frac{19\epsilon^2 \kappa^2 \xi^2}{36 \left(4\Delta^6 - \Delta^{7/2} \epsilon \kappa \xi \right)}$$

$$\Gamma_{\theta\theta z} = \frac{\epsilon \kappa \xi \left(-228\Delta^{5/2} + 23\epsilon \kappa \xi \right)}{-144\Delta^6 + 36\Delta^{7/2} \epsilon \kappa \xi}$$
(20)

$$\Gamma_{zx\theta} = \Gamma_{xz\theta} = -\frac{25}{18\Delta} - \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{36\Delta^{5/2} - 9\epsilon\kappa\xi}
\Gamma_{z\theta x} = \Gamma_{\theta zx} = \frac{25}{18\Delta} + \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{9\left(-4\Delta^{5/2} + \epsilon\kappa\xi\right)}
\Gamma_{x\theta z} = \Gamma_{\theta xz} = \frac{2}{15} - \frac{1}{2\Delta} - \frac{3\epsilon\kappa\xi}{8\Delta^{7/2}} + \frac{16}{15\left(-8 + \frac{15\kappa\xi}{\Delta^{7/2}}\right)} + \frac{1}{2\Delta - \frac{\epsilon\kappa\xi}{2\Delta^{3/2}}}$$
(21)

1.5 $\gamma_{\alpha\beta}$ and linear approximation of κ

Since $\gamma_{\alpha\beta} = \lambda_{\alpha\beta} + \Gamma_{\alpha\beta\gamma}V_{\gamma}$, we have

$$\gamma_{zz} = \frac{8\Delta^2 \xi}{8\Delta^{7/2} - 15\kappa \xi} + \frac{42\kappa \xi v_z}{8\Delta^{9/2} - 15\Delta\kappa \xi}
= \frac{\xi}{\Delta^{3/2}} + \left(\frac{15\xi^2}{8\Delta^5} + \frac{21\xi v_z}{4\Delta^{9/2}}\right)\kappa + \left(\frac{225\xi^3}{64\Delta^{17/2}} + \frac{315\xi^2 v_z}{32\Delta^8}\right)\kappa^2 + O[\kappa]^3$$
(22)

$$\gamma_{zx} = \gamma_{xz} = \frac{2\kappa\xi v_X}{-8\Delta^{7/2} + 15\kappa\xi} + \left(-\frac{25}{18\Delta} - \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{36\Delta^{5/2} - 9\epsilon\kappa\xi}\right) v_{\theta}$$

$$= -\frac{(\xi(3v_X - 3v_{\theta} - \epsilon v_{\theta}))\kappa}{12\Delta^{7/2}} + \frac{5\xi^2(-27v_X + 27v_{\theta} + 5\Delta\epsilon^2 v_{\theta})\kappa^2}{288\Delta^7} + O[\kappa]^3$$
(23)

$$\gamma_{z\theta} = \gamma_{\theta z} = \left(\frac{25}{18\Delta} + \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{9\left(-4\Delta^{5/2} + \epsilon\kappa\xi\right)}\right) v_X + \frac{2\kappa\xi v_{\theta}}{-8\Delta^{7/2} + 15\kappa\xi} \\
= -\frac{\left(\xi\left(-3v_X + \epsilon v_X + 3v_{\theta}\right)\right)\kappa}{12\Delta^{7/2}} - \frac{5\left(\xi^2\left(-27v_X + 5\Delta\epsilon^2 v_X + 27v_{\theta}\right)\right)\kappa^2}{288\Delta^7} + O[\kappa]^3$$
(24)

$$\gamma_{xx} = -\frac{4\epsilon\xi \left(-6\Delta^{5/2} + \epsilon\kappa\xi\right)}{36\Delta^{3} - 9\sqrt{\Delta}\epsilon\kappa\xi} + \frac{1}{9}\kappa\xi \left(\frac{18}{8\Delta^{7/2} - 15\kappa\xi} + \frac{\epsilon^{2}\kappa\xi}{-4\Delta^{6} + \Delta^{7/2}\epsilon\kappa\xi}\right)\nu_{z} + \frac{19\epsilon\kappa\xi \left(-6\Delta^{5/2} + \epsilon\kappa\xi\right)\nu_{\theta}}{-144\Delta^{6} + 36\Delta^{7/2}\epsilon\kappa\xi} \\
= \frac{2\epsilon\xi}{3\sqrt{\Delta}} + \frac{\left(4\sqrt{\Delta}\epsilon^{2}\xi^{2} + 18\xi\nu_{z} + 57\epsilon\xi\nu_{\theta}\right)\kappa}{72\Delta^{7/2}} + \left(\frac{\epsilon^{3}\xi^{3}}{72\Delta^{11/2}} - \frac{\left(-135 + 8\Delta\epsilon^{2}\right)\xi^{2}\nu_{z}}{288\Delta^{7}} + \frac{19\epsilon^{2}\xi^{2}\nu_{\theta}}{288\Delta^{6}}\right)\kappa^{2} + O[\kappa]^{3} \tag{25}$$

$$\gamma_{\theta\theta} = -\frac{4\epsilon\xi \left(-12\Delta^{5/2} + \epsilon\kappa\xi\right)}{36\Delta^{3} - 9\sqrt{\Delta}\epsilon\kappa\xi} + \frac{19\epsilon^{2}\kappa^{2}\xi^{2}v_{X}}{36\left(4\Delta^{6} - \Delta^{7/2}\epsilon\kappa\xi\right)} + \kappa\xi \left(\frac{23\epsilon}{36\Delta^{7/2}} + \frac{2}{8\Delta^{7/2} - 15\kappa\xi} + \frac{34\epsilon}{36\Delta^{7/2} - 9\Delta\epsilon\kappa\xi}\right)v_{z} \\
= \frac{4\epsilon\xi}{3\sqrt{\Delta}} + \left(\frac{2\epsilon^{2}\xi^{2}}{9\Delta^{3}} + \frac{(3+19\epsilon)\xi v_{z}}{12\Delta^{7/2}}\right)\kappa + \left(\frac{\epsilon^{3}\xi^{3}}{18\Delta^{11/2}} + \frac{19\epsilon^{2}\xi^{2}v_{X}}{144\Delta^{6}} + \frac{(135+68\Delta\epsilon^{2})\xi^{2}v_{z}}{288\Delta^{7}}\right)\kappa^{2} + O[\kappa]^{3} \tag{26}$$

$$\gamma_{x\theta} = \gamma_{\theta x} = \frac{4\epsilon^{2}\kappa\xi^{2}}{36\Delta^{3} - 9\sqrt{\Delta}\epsilon\kappa\xi} + \left(\frac{2}{15} - \frac{1}{2\Delta} - \frac{3\epsilon\kappa\xi}{8\Delta^{7/2}} + \frac{16}{15\left(-8 + \frac{15\kappa\xi}{\Delta^{7/2}}\right)} + \frac{1}{2\Delta - \frac{\epsilon\kappa\xi}{2\Delta^{3/2}}}\right)v_{z}$$

$$= \left(\frac{\epsilon^{2}\xi^{2}}{9\Delta^{3}} - \frac{(\xi + \epsilon\xi)v_{z}}{4\Delta^{7/2}}\right)\kappa + \left(\frac{\epsilon^{3}\xi^{3}}{36\Delta^{11/2}} + \frac{(-15 + \Delta\epsilon^{2})\xi^{2}v_{z}}{32\Delta^{7}}\right)\kappa^{2} + O[\kappa]^{3}$$
(27)

Finally, we have obtained the all components of $\gamma_{\alpha\beta}$.

$$\gamma = \begin{pmatrix} \gamma_{zz} & \gamma_{zx} & \gamma_{z\theta} \\ \gamma_{xz} & \gamma_{xx} & \gamma_{x\theta} \\ \gamma_{\theta z} & \gamma_{\theta x} & \gamma_{\theta \theta} \end{pmatrix}$$

As we could see, this is a symmetric matrix. In addition, only three diagonal elements, namely γ_{zz} , γ_{xx} , $\gamma_{\theta\theta}$ have zero-order term of κ , which describes the compliance. In general, this parameter is about $10^{-4} \sim 10^{-3}$. Hence we just consider the first-order correction in the following calculations.

Up to now, we have elucidated the drift force. Indeed, there exist the external potential (like gravity) and white noises at the same time.

$$\dot{v}_i = F_i + TF_i^{drift} + \eta_i \tag{28}$$

Since three components are coupled, the equation turns to

$$\begin{pmatrix} \dot{v}_{\Delta} \\ \dot{v}_{X} \\ \dot{v}_{\Theta} \end{pmatrix} = - \begin{pmatrix} \gamma_{zz} & \gamma_{zx} & \gamma_{z\theta} \\ \gamma_{xz} & \gamma_{xx} & \gamma_{x\theta} \\ \gamma_{\theta z} & \gamma_{\theta x} & \gamma_{\theta\theta} \end{pmatrix} \begin{pmatrix} v_{\Delta} \\ v_{X} \\ v_{\Theta} \end{pmatrix} + \begin{pmatrix} \eta_{\Delta} \\ \eta_{X} \\ \eta_{\Theta} \end{pmatrix}$$
(29)

where the noise correlator has been shown in the eq. David.25:

$$\left\langle \eta_{\alpha}(t)\eta_{\beta}(t')\right\rangle = 2T\gamma_{\alpha\beta}\delta(t-t') = 2T\left[\lambda_{\alpha\beta}(\mathbf{X}) + \Gamma_{\alpha\beta\gamma}(\mathbf{X})V_{\gamma}\right]\delta(t-t')$$

So we'd like to find the expression of $\gamma^{1/2}$.

Suppose that

$$\gamma = \Psi + \kappa \Phi + O[\kappa]^2 \tag{30}$$

where Ψ is zero-order matrix of κ , and Φ the first-order one. So $\gamma^{1/2}$ would show a form such as $\gamma^{1/2} \approx \psi + \kappa \chi$,

$$\gamma = \gamma^{1/2} \gamma^{1/2} = (\psi + \kappa \chi)(\psi + \kappa \chi) = \psi \psi + \kappa (\psi \chi + \chi \psi) + O[\kappa]^2$$

we have $\Phi = \chi \psi + \psi \chi$, and $\psi = \sqrt{\Psi}$. Note Ψ is a symmetric matrix and all non-diagonal elements are equal to 0.

$$\Psi = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{2\epsilon\xi}{3\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{4\epsilon\xi}{3\sqrt{\Delta}} \end{pmatrix}$$
(31)

Then we could solve all components of χ

$$\chi_{11} = \frac{3\xi \left(5\xi + 14\sqrt{\Delta}v_z\right)}{16\Delta^5 \sqrt{\frac{\xi}{\Delta^{3/2}}}}$$

$$\chi_{22} = \frac{\xi \left(18v_z + \epsilon \left(4\sqrt{\Delta}\epsilon\xi + 57v_\theta\right)\right)}{48\sqrt{6}\Delta^{7/2} \sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}}$$

$$\chi_{33} = \frac{\xi \left(8\sqrt{\Delta}\epsilon^2\xi + (9 + 57\epsilon)v_z\right)}{48\sqrt{3}\Delta^{7/2} \sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}}$$
(32)

$$\chi_{12} = \chi_{21} = \frac{\xi \left(-3v_X + (3+\epsilon)v_\theta\right)}{4\Delta^{7/2} \left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + \sqrt{6}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}\right)}$$

$$\chi_{13} = \chi_{31} = -\frac{\xi \left(3v_\theta + (\epsilon - 3)v_X\right)}{4\Delta^{7/2} \left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + 2\sqrt{3}\sqrt{\frac{\xi\epsilon}{\sqrt{\Delta}}}\right)}$$

$$\chi_{23} = \chi_{32} = \frac{\xi \left(4\sqrt{\Delta}\epsilon^2\xi - 9(1+\epsilon)v_z\right)}{12\sqrt{3}\left(2+\sqrt{2}\right)\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}}$$
(33)