Mixing Langevin + ElastoHydroDynamic of cylinder

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1 Framework Introduction

1.1 Theoretical Fundamentals

Here are fundamentals used in the following parts, including Gibbs-Boltzmann distribution, Langevin equation, Fokker-Planck equation.

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

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

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 $\langle \eta_i(t)\eta_j(t')\rangle = 2\lambda k_B T\delta_{ij}\delta(t-t')$

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:

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

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:

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

with Langevin's equation

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

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

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

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

Here we look at Thomas' publication (arxiv: 1412.0162) on 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:

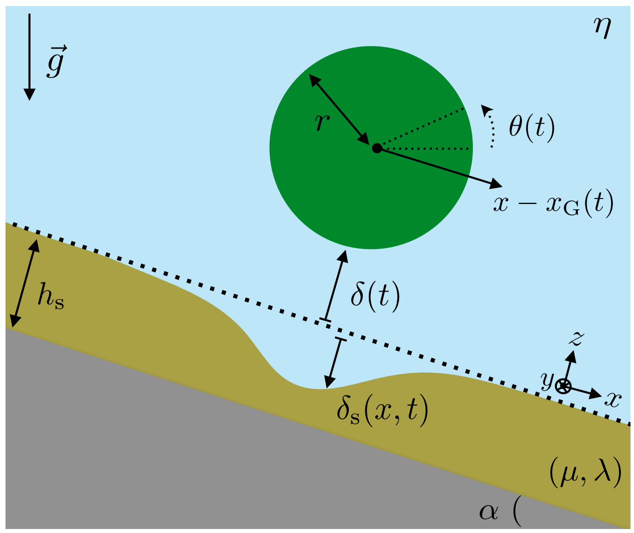

FIG. 1: *Schematic of the system. A negatively buoyant cylinder (green) falls down under the acceleration of gravity $\vec{g}$, inside a viscous fluid (blue), in the vicinity of a thin soft wall (brown). The ensemble lies atop a tilted, infinitely rigid support (grey).*

The deformation of the soft wall reads:

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

as well as the dimensionless parameters: $z = Zr\varepsilon$, $h = Hr\varepsilon$, $\delta = \Delta r\varepsilon$, $x = Xr\sqrt{2\varepsilon}$, $x_G = X_G r\sqrt{2\varepsilon}$, $\theta = \Theta\sqrt{2\varepsilon}$, $t = Tr\sqrt{2\varepsilon}/c$, $u = Uc$, 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

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

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

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

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)*

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

and *($\mathbf{X}, \mathbf{V}$ 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

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

Exploit the Fokker-Planck operator ($\cdots$ refers the similar terms about X_α)

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

Note $\frac{\partial P}{\partial X_\alpha} = P\left(-\beta\frac{\partial\phi}{\partial X_\alpha}\right)$ and $\frac{\partial P}{\partial V_\alpha} = P(-\beta V_\alpha)$. Consider the gravity $\phi(\mathbf{X}) = -mg\Delta$, and then we could derive the eq. David.4, regarding k_B as 1

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

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

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

The last two terms would vanish since

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

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

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

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial V_\alpha}\left[T\gamma_{\alpha\beta}\frac{\partial P}{\partial V_\beta} + U_\alpha P\right] = \frac{\partial}{\partial V_\alpha}\left[\cancel{T}\gamma_{\alpha\beta}P\cdot(-\cancel{\beta}V_\beta) + U_\alpha P\right] = \frac{\partial}{\partial V_\alpha}\left[(U_\alpha - \gamma_{\alpha\beta}V_\beta)\cdot P\right] = 0$$

We obtain the GB distribution for the steady state if

$$U_\alpha = \gamma_{\alpha\beta}V_\beta \qquad \text{(David.5)}$$

We have for small velocities that

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

and so we find

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

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

$$\gamma_{\alpha\beta} = \lambda_{\alpha\beta} + \gamma_{2\alpha\beta} \qquad \text{(David.8)}$$

and we write

$$\gamma_{2\alpha\beta} = \Gamma_{\alpha\beta\gamma}V_\gamma \qquad \text{(David.9)}$$

and

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

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

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

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

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

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

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

$$\begin{aligned}\sum_{\alpha\beta}\Lambda_{z\alpha\beta}V_\alpha V_\beta &= \frac{21\kappa\xi}{4}\frac{V_z^2}{Z^{9/2}} - \frac{\kappa\xi}{4}\frac{V_x^2}{Z^{7/2}}\\ \sum_{\alpha\beta}\Lambda_{x\alpha\beta}V_\alpha V_\beta &= \frac{19\kappa\xi\varepsilon}{24}\frac{V_zV_x}{Z^{7/2}}\end{aligned} \tag{David.14}$$

This gives the set of equations

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

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

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

$$\Gamma_{xzz} = 0 \tag{David.18}$$

$$\Gamma_{xxx} = 0 \tag{David.19}$$

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

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

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

as well as

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

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

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

which can be written as

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

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

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

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

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

2 Further Analyses

Generally, the Brownian motion would furnish the following equation:

$$dv = \frac{f(t)}{m}dt - \gamma v dt + \sqrt{\frac{2\gamma}{\beta m}}dW(t)$$

where $f(t)$ contains the external forces, γ would be a matrix rather than a constant for v is a velocity vector, the last term shows the random force.

In this section, we would first consider the second derivatives in Thomas' results, updating the γ matrix; then consider the effective "mass" on different directions (Δ, X, Θ), showing $\frac{1}{m}$ as an inverse matrix; finally one numerical procedure to simulate the Langevin equation.

2.1 New $\lambda_{\alpha\beta}, \Gamma_{\alpha\beta\gamma}$ 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)

$$\begin{aligned}
-U_Z &= \dot{v}_\Delta = \ddot{\Delta} = F_\Delta(\Delta, v_\Delta, v_X, v_\Theta, \dot{v}_\Delta) \\
-U_X &= \dot{v}_X = \ddot{X} = F_X(\Delta, v_\Delta, v_X, v_\Theta, \dot{v}_X, \dot{v}_\Theta) \\
-U_\Theta &= \dot{v}_\Theta = \ddot{\Theta} = F_\Theta(\Delta, v_\Delta, v_X, v_\Theta, \dot{v}_X, \dot{v}_\Theta)
\end{aligned} \tag{Yilin.1}$$

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,

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

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

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 $\dot{v}_\Delta$ ($\dot{v}_z$) namely $\ddot{\Delta}$

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

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

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

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

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

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

$$-\dot{v}_\Theta = U_\Theta = \frac{\epsilon\xi\left(\left(16\Delta^3\left(12\Delta^{5/2} - \epsilon\kappa\xi\right) + \kappa\left(228\Delta^{5/2} - 23\epsilon\kappa\xi\right)v_z\right)v_\theta + \kappa v_X\left(\left(-48\Delta^{5/2} + 4\epsilon\kappa\xi\right)v_z + \epsilon\xi\left(16\Delta^3 + 19\kappa v_\theta\right)\right)\right)}{36\left(4\Delta^6 - \Delta^{7/2}\epsilon\kappa\xi\right)} \tag{Yilin.8}$$

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

$$
\begin{aligned}
\dot{v}_\Delta &= F_\Delta(\Delta, v_\Delta, v_X, v_\Theta) \\
\dot{v}_X &= F_X(\Delta, v_\Delta, v_X, v_\Theta) \\
\dot{v}_\Theta &= F_\Theta(\Delta, v_\Delta, v_X, v_\Theta)
\end{aligned}
\tag{Yilin.9}
$$

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

$$
\lambda_{\alpha\beta} = \text{Coefficient}[\mathrm{U}_\alpha, \mathrm{v}_\beta] - \text{Coefficient}[\mathrm{U}_\alpha, \mathrm{v}_\beta \mathrm{v}_\gamma] \times \mathrm{v}_\gamma \tag{Yilin.10}
$$

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

$$
\Gamma_{\alpha\beta\beta} = \text{Coefficient}[\mathrm{U}_\alpha, \mathrm{v}_\beta \mathrm{v}_\beta] \tag{Yilin.11}
$$

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

$$
2\Lambda_{\alpha\beta\gamma} = \text{Coefficient}[\mathrm{U}_\alpha, \mathrm{v}_\beta \mathrm{v}_\gamma] = \Gamma_{\alpha\beta\gamma} + \Gamma_{\alpha\gamma\beta} \tag{Yilin.12}
$$

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

After some calculations verified by *Mathematica*, we list all $\lambda_{\alpha\beta}$

$$
\begin{aligned}
\lambda_{\mathrm{zz}} &= \frac{8\Delta^2 \xi}{8\Delta^{7/2} - 15\kappa\xi} \\
\lambda_{\mathrm{xx}} &= -\frac{4\epsilon\xi\left(-6\Delta^{5/2} + \epsilon\kappa\xi\right)}{36\Delta^3 - 9\sqrt{\Delta}\epsilon\kappa\xi} \\
\lambda_{\theta\theta} &= -\frac{4\epsilon\xi\left(-12\Delta^{5/2} + \epsilon\kappa\xi\right)}{36\Delta^3 - 9\sqrt{\Delta}\epsilon\kappa\xi}
\end{aligned}
\tag{Yilin.13}
$$

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

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

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

$$
\begin{aligned}
\Gamma_{\mathrm{zzz}} &= \frac{42\kappa\xi}{8\Delta^{9/2} - 15\Delta\kappa\xi} \\
\Gamma_{\mathrm{xzx}} = \Gamma_{\mathrm{zxx}} &= \frac{2\kappa\xi}{-8\Delta^{7/2} + 15\kappa\xi} \\
\Gamma_{\theta z\theta} = \Gamma_{\mathrm{z}\theta\theta} &= \frac{2\kappa\xi}{-8\Delta^{7/2} + 15\kappa\xi}
\end{aligned}
\tag{Yilin.16}
$$

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

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

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

$$\begin{aligned}
\Gamma_{\mathrm{xxz}} &= \frac{1}{9}\kappa\xi\left(\frac{18}{8\Delta^{7/2}-15\kappa\xi}+\frac{\epsilon^2\kappa\xi}{-4\Delta^6+\Delta^{7/2}\epsilon\kappa\xi}\right)\\
\Gamma_{\mathrm{xx}\theta} &= \frac{19\epsilon\kappa\xi\left(-6\Delta^{5/2}+\epsilon\kappa\xi\right)}{-144\Delta^6+36\Delta^{7/2}\epsilon\kappa\xi}\\
\Gamma_{\theta\theta\mathrm{x}} &= \frac{19\epsilon^2\kappa^2\xi^2}{36\left(4\Delta^6-\Delta^{7/2}\epsilon\kappa\xi\right)}\\
\Gamma_{\theta\theta\mathrm{z}} &= \frac{\epsilon\kappa\xi\left(-228\Delta^{5/2}+23\epsilon\kappa\xi\right)}{-144\Delta^6+36\Delta^{7/2}\epsilon\kappa\xi}
\end{aligned} \tag{Yilin.20}$$

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

2.2 $\gamma_{\alpha\beta}$ and linear approximation of κ

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

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

$$\begin{aligned}
\gamma_{zx} = \gamma_{xz} &= \frac{2\kappa\xi v_X}{-8\Delta^{7/2}+15\kappa\xi}+\left(-\frac{25}{18\Delta}-\frac{19\epsilon\kappa\xi}{72\Delta^{7/2}}+\frac{2\kappa\xi}{8\Delta^{7/2}-15\kappa\xi}+\frac{50\Delta^{3/2}}{36\Delta^{5/2}-9\epsilon\kappa\xi}\right)v_\theta\\
&= -\frac{\left(\xi\left(3v_X-3v_\theta-\epsilon v_\theta\right)\right)\kappa}{12\Delta^{7/2}}+\frac{5\xi^2\left(-27v_X+27v_\theta+5\Delta\epsilon^2 v_\theta\right)\kappa^2}{288\Delta^7}+O[\kappa]^3
\end{aligned} \tag{Yilin.23}$$

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

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

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

$$\gamma_{x\theta} = \gamma_{\theta x} = \frac{4\epsilon^2\kappa\xi^2}{36\Delta^3-9\sqrt{\Delta}\epsilon\kappa\xi} + \left(\frac{2}{15}-\frac{1}{2\Delta}-\frac{3\epsilon\kappa\xi}{8\Delta^{7/2}}+\frac{16}{15\left(-8+\frac{15\kappa\xi}{\Delta^{7/2}}\right)}+\frac{1}{2\Delta-\frac{\epsilon\kappa\xi}{2\Delta^{3/2}}}\right)v_z$$
$$= \left(\frac{\epsilon^2\xi^2}{9\Delta^3}-\frac{(\xi+\epsilon\xi)v_z}{4\Delta^{7/2}}\right)\kappa + \left(\frac{\epsilon^3\xi^3}{36\Delta^{11/2}}+\frac{\left(-15+\Delta\epsilon^2\right)\xi^2 v_z}{32\Delta^7}\right)\kappa^2 + O[\kappa]^3 \tag{Yilin.27}$$

As we could see, $\gamma_{\alpha\beta}$ is a symmetric matrix.

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

In addition, only three diagonal elements, namely $\gamma_{zz}, \gamma_{xx}, \gamma_{\theta\theta}$ have zero-order term of κ, which describes the compliance. In genenral, this parameter is about $10^{-4} \sim 10^{-3}$. Right now, we could write the equation of motion as:

$$\dot{v}_i = \frac{F_i}{m} - \gamma_{ij}v_j + \eta_i \tag{Yilin.28}$$

where F_i contains the force due to external potentials (gravity and buoyant force), as well as the spurious drift force, which originates from the derivative of $\gamma_{\alpha\beta}$, equal to $\frac{\partial\gamma_{\alpha\beta}}{\partial v_\beta} = \Gamma_{\alpha\beta\beta}$. See eqs

Yilin.16, we could easily obtain non-zero components:

$$\frac{\partial \gamma_{zz}}{\partial v_z} = \Gamma_{zzz} = \frac{42\kappa\xi}{8\Delta^{9/2} - 15\Delta\kappa\xi} \approx \frac{21\kappa\xi}{4\Delta^{9/2}} + \frac{315\kappa^2\xi^2}{32\Delta^8}$$
$$\frac{\partial \gamma_{zx}}{\partial v_x} = \Gamma_{zxx} = \frac{2\kappa\xi}{15\kappa\xi - 8\Delta^{7/2}} \approx -\frac{\kappa\xi}{4\Delta^{7/2}} - \frac{15\kappa^2\xi^2}{32\Delta^7}$$
$$\frac{\partial \gamma_{z\theta}}{\partial v_\theta} = \Gamma_{z\theta\theta} = \frac{2\kappa\xi}{15\kappa\xi - 8\Delta^{7/2}} \approx -\frac{\kappa\xi}{4\Delta^{7/2}} - \frac{15\kappa^2\xi^2}{32\Delta^7}$$

Other $\Gamma_{\alpha\beta\beta}$s are all equal to 0. Thus there is only a spurious force on Δ direction.

To be exact:

$$\begin{pmatrix} \dot{v}_\Delta \\ \dot{v}_X \\ \dot{v}_\Theta \end{pmatrix} = \begin{pmatrix} F_\Delta \\ F_X \\ F_\Theta \end{pmatrix} - \begin{pmatrix} \gamma_{\text{zz}} & \gamma_{\text{zx}} & \gamma_{\text{z}\theta} \\ \gamma_{\text{xz}} & \gamma_{\text{xx}} & \gamma_{\text{x}\theta} \\ \gamma_{\theta\text{z}} & \gamma_{\theta\text{x}} & \gamma_{\theta\theta} \end{pmatrix} \begin{pmatrix} v_\Delta \\ v_X \\ v_\Theta \end{pmatrix} + \begin{pmatrix} \eta_\Delta \\ \eta_X \\ \eta_\Theta \end{pmatrix} \tag{Yilin.29}$$

As for the noise correlator, it 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

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

where Ψ is zero-order matrix of κ, and Φ the first-order one. Also, $\gamma^{1/2}$ 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.

$$\Psi = \begin{pmatrix} \lambda_z & 0 & 0 \\ 0 & \lambda_x & 0 \\ 0 & 0 & \lambda_\theta \end{pmatrix} = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{2\epsilon\xi}{3\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{4\epsilon\xi}{3\sqrt{\Delta}} \end{pmatrix} \tag{Yilin.31}$$

Also, χ is a symmetric matrix, with diagonal components as:

$$\begin{aligned} \chi_{zz} &= \frac{3\xi\left(5\xi + 14\sqrt{\Delta}v_z\right)}{16\Delta^5\sqrt{\frac{\xi}{\Delta^{3/2}}}} \\ \chi_{xx} &= \frac{\xi\left(18v_z + \epsilon\left(4\sqrt{\Delta}\epsilon\xi + 57v_\theta\right)\right)}{48\sqrt{6}\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}} \\ \chi_{\theta\theta} &= \frac{\xi\left(8\sqrt{\Delta}\epsilon^2\xi + (9 + 57\epsilon)v_z\right)}{48\sqrt{3}\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}} \end{aligned} \tag{Yilin.32}$$

and non-diagonal elements

$$
\begin{aligned}
\chi_{zx} = \chi_{xz} &= \frac{\xi\left(-3v_X + (3+\epsilon)v_\theta\right)}{4\Delta^{7/2}\left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + \sqrt{6}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}\right)} \\
\chi_{z\theta} = \chi_{\theta z} &= -\frac{\xi\left(3v_\theta + (\epsilon-3)v_X\right)}{4\Delta^{7/2}\left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + 2\sqrt{3}\sqrt{\frac{\xi\epsilon}{\sqrt{\Delta}}}\right)} \\
\chi_{x\theta} = \chi_{\theta x} &= \frac{\xi\left(4\sqrt{\Delta}\epsilon^2\xi - 9(1+\epsilon)v_z\right)}{12\sqrt{3}\left(2+\sqrt{2}\right)\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}}
\end{aligned}
\tag{Yilin.33}
$$

2.3 Mass vector

We always regarded the mass as 1 in the previous parts, while it should be carefully distinguished later. For z, x components, $m_\alpha = m = \pi r^2\rho$ namely the mass of the column (per unit length). However, $m_\Theta = mr^2/2$ refers to the moment of inertia. Taking that into account, we compare these two versions (Note we re-write U_α as F_α on the left side)

$m_\alpha = 1$	$m_\alpha = (m, m, mr^2/2)$
$dX_\alpha = V_\alpha dt$	$\dot{x}_\alpha = v_\alpha$
$dV_\alpha = -F_\alpha dt - \nabla_\alpha\phi(\mathbf{X})dt$	$m_\alpha \cdot \dot{v}_\alpha = F_{h\alpha}(\mathbf{v}, \dot{\mathbf{v}}, \mathbf{x}) - \nabla_\alpha\phi(\mathbf{x})$
$F_\alpha = \gamma_{\alpha\beta}V_\beta = \lambda_{\alpha\beta}V_\beta + \Gamma_{\alpha\beta\gamma}V_\beta V_\gamma$	$F_{h\alpha}(\mathbf{v}, \dot{\mathbf{v}}, \mathbf{x}) = F_{1h\alpha}(\mathbf{v}, \mathbf{x}) + F_{2h\alpha\beta}(\mathbf{x})\dot{v}_\beta$
	$M_{\alpha\beta} = \delta_{\alpha\beta} \cdot m_\alpha - F_{2h\alpha\beta}(\mathbf{x})$
	$M_{\alpha\beta}\dot{v}_\beta = F_{1h\alpha}(\mathbf{v}, \mathbf{x}) - \nabla_\alpha\phi(\mathbf{x})$

Since $F_{h\alpha}(\mathbf{v}, \dot{\mathbf{v}}, \mathbf{x}) = F_{1h\alpha}(\mathbf{v}, \mathbf{x}) + F_{2h\alpha\beta}(\mathbf{x})\dot{v}_\beta$, we could extract $F_{1h\alpha}(\mathbf{v}, \mathbf{x})$ and $F_{2h\alpha\beta}(\mathbf{x})$ by

$$
-\frac{F_{hZ}}{m_Z} = -\dot{v}_z = -\ddot{\Delta} = a_1\frac{\dot{\Delta}}{\Delta^{3/2}} + a_2\frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3\frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3\frac{\dot{X}^2}{\Delta^{7/2}} + a_4\frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_5\frac{\ddot{\Delta}}{\Delta^{7/2}} + a_6 \tag{Yilin.34}
$$

thus

$$
\begin{aligned}
&F_{1hZ} = -m_Z\left(a_1\frac{\dot{\Delta}}{\Delta^{3/2}} + a_2\frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3\frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3\frac{\dot{X}^2}{\Delta^{7/2}} + a_4\frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_6\right) \\
&F_{2hZZ} = -\frac{m_Z a_5}{\Delta^{7/2}} \qquad F_{2hZX} = 0 \qquad F_{2hZ\Theta} = 0
\end{aligned}
\tag{Yilin.35}
$$

Similarly, there are cross terms for X, Θ components

$$
-\frac{F_{hX}}{m_X} = -\dot{v}_x = -\ddot{X} = b_1\frac{\dot{X}}{\sqrt{\Delta}} + b_2\frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3\frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_4\frac{\ddot{\Theta}}{\Delta^{5/2}} + b_5\frac{\ddot{X}}{\Delta^{5/2}} + b_6 \tag{Yilin.36}
$$

$$
\begin{aligned}
F_{1hX} &= -m_X\left(b_1\frac{\dot X}{\sqrt{\Delta}}+b_2\frac{\dot\Delta\dot X}{\Delta^{7/2}}+b_3\frac{\dot\Delta\dot\Theta}{\Delta^{7/2}}+b_6\right)\\
F_{2hXZ} &= 0 \qquad F_{2hXX} = -\frac{m_X b_5}{\Delta^{5/2}} \qquad F_{2hX\Theta} = -\frac{m_X b_4}{\Delta^{5/2}}
\end{aligned}
\tag{Yilin.37}
$$

and

$$
-\frac{F_{h\Theta}}{m_\Theta} = -\dot v_\theta = -\ddot\Theta = c_1\frac{\dot\Theta}{\sqrt{\Delta}}+c_2\frac{\dot\Delta\dot\Theta}{\Delta^{7/2}}+c_3\frac{\dot\Delta\dot X}{\Delta^{7/2}}+c_4\frac{\ddot X}{\Delta^{5/2}}+c_5\frac{\ddot\Theta}{\Delta^{5/2}}+c_6 \tag{Yilin.38}
$$

$$
\begin{aligned}
F_{1h\Theta} &= -m_\Theta\left(c_1\frac{\dot\Theta}{\sqrt{\Delta}}+c_2\frac{\dot\Delta\dot\Theta}{\Delta^{7/2}}+c_3\frac{\dot\Delta\dot X}{\Delta^{7/2}}+c_6\right)\\
F_{2h\Theta Z} &= 0 \qquad F_{2h\Theta X} = -\frac{m_\Theta c_4}{\Delta^{5/2}} \qquad F_{2h\Theta\Theta} = -\frac{m_\Theta c_5}{\Delta^{5/2}}
\end{aligned}
\tag{Yilin.39}
$$

We pose that $M_{\alpha\beta} = \delta_{\alpha\beta}m_\alpha - F_{2h\alpha\beta}(\mathbf{x})$, hence $(m_X = m, m_\Theta = mr^2/2)$

$$
\begin{aligned}
M_{ZZ} &= m_Z + \frac{m_Z a_5}{\Delta^{5/2}}\\
M_{XX} &= m_X + \frac{m_X b_5}{\Delta^{5/2}} \qquad M_{X\Theta} = \frac{m_X b_4}{\Delta^{5/2}}\\
M_{\Theta X} &= \frac{m_\Theta c_4}{\Delta^{5/2}} \qquad M_{\Theta\Theta} = m_\Theta + \frac{m_\Theta c_5}{\Delta^{5/2}}
\end{aligned}
\tag{Yilin.40}
$$

We know that $a_5 = -\frac{15\kappa\xi}{8}$, $b_4 = \frac{\kappa\xi\varepsilon}{12}$, $b_5 = -\frac{\kappa\xi\varepsilon}{12}$, $c_4 = \frac{\kappa\xi\varepsilon}{6}$, $c_5 = -\frac{\kappa\xi\varepsilon}{6}$, so

$$
M = \begin{pmatrix}
m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}} & 0 & 0\\
0 & m_X - \frac{\kappa\xi\epsilon m_X}{12\Delta^{5/2}} & \frac{\kappa\xi\epsilon m_X}{12\Delta^{5/2}}\\
0 & \frac{\kappa\xi\epsilon m_\theta}{6\Delta^{5/2}} & m_\theta - \frac{\kappa\xi\epsilon m_\theta}{6\Delta^{5/2}}
\end{pmatrix}
\tag{Yilin.41}
$$

and its inverse matrix

$$
M^{-1} = \begin{pmatrix}
\frac{1}{m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}}} & 0 & 0\\
0 & \frac{12\Delta^{5/2}-2\kappa\xi\epsilon}{12\Delta^{5/2}m_X-3\kappa\xi\epsilon m_X} & \frac{\kappa\xi\epsilon}{3m_\theta\left(\kappa\xi\epsilon-4\Delta^{5/2}\right)}\\
0 & \frac{2\kappa\xi\epsilon}{3m_X\left(\kappa\xi\epsilon-4\Delta^{5/2}\right)} & \frac{12\Delta^{5/2}-\kappa\xi\epsilon}{12\Delta^{5/2}m_\theta-3\kappa\xi\epsilon m_\theta}
\end{pmatrix}
\tag{Yilin.42}
$$

with the approximation expressed by the series of κ:

$$
M_{app}^{-1} \approx \begin{pmatrix}
\frac{1}{m_z}+\frac{15\kappa\xi}{8\Delta^{5/2}m_z}+\frac{225\kappa^2\xi^2}{64\Delta^5 m_z} & 0 & 0\\
0 & \frac{1}{m_X}+\frac{\kappa\xi\epsilon}{12\Delta^{5/2}m_X}+\frac{\kappa^2\xi^2\epsilon^2}{48\Delta^5 m_X} & -\frac{\kappa(\xi\epsilon)}{12\left(\Delta^{5/2}m_\theta\right)}-\frac{\kappa^2\left(\xi^2\epsilon^2\right)}{48\left(\Delta^5 m_\theta\right)}\\
0 & -\frac{\kappa(\xi\epsilon)}{6\left(\Delta^{5/2}m_X\right)}-\frac{\kappa^2\left(\xi^2\epsilon^2\right)}{24\left(\Delta^5 m_X\right)} & \frac{1}{m_\theta}+\frac{\kappa\xi\epsilon}{6\Delta^{5/2}m_\theta}+\frac{\kappa^2\xi^2\epsilon^2}{24\Delta^5 m_\theta}
\end{pmatrix}
\tag{Yilin.43}
$$

Only taking the first-order correction, we could verify

$$
M\cdot M_{app}^{-1} = \begin{pmatrix}
1-\frac{225\kappa^2\xi^2}{64\Delta^5} & 0 & 0\\
0 & 1-\frac{\kappa^2\xi^2\epsilon^2}{48\Delta^5} & \frac{\kappa^2\xi^2\epsilon^2 m_X}{48\Delta^5 m_\theta}\\
0 & \frac{\kappa^2\xi^2\epsilon^2 m_\theta}{24\Delta^5 m_X} & 1-\frac{\kappa^2\xi^2\epsilon^2}{24\Delta^5}
\end{pmatrix}
\approx \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}
$$

3 Numerical Practice

3.1 JPCB2014: Discrete-Time Langevin Integration

J. Phys. Chem. B, 2014, 118, 6466-6474, one article about Discrete-Time Langevin Integration. For multiple dimensions, see its Support Information:

https://pubs.acs.org/doi/suppl/10.1021/jp411770f/suppl_file/jp411770f_si_001.pdf

Consider a Langevin equation

$$dv = \frac{f(t)}{m}dt - \gamma v dt + \sqrt{\frac{2\gamma}{\beta m}}dW(t)$$

we have

- Ornstein-Uehlenbeck operator for stochastic thermalization: $\mathscr{L}_o = -\gamma \frac{\partial}{\partial v} v - \frac{\gamma}{\beta m}\frac{\partial^2}{\partial x^2}$
- Deterministic Newtonian evolutions: $\mathscr{L}_v = \frac{f}{m}$, $\mathscr{L}_r = v\frac{\partial}{\partial r}$
- Hamiltonian: $\exp(\mathscr{L}_h \Delta t)\mathscr{H}(n) = \mathscr{H}(n+1)$

where n is the time step index and $t = n\Delta t$.

For this operator splitting, a single update step that advances the simulation clock by Δt is given explicitly by

$$\begin{aligned}
\mathbf{v}\left(n+\frac{1}{4}\right) &= \sqrt{a}\cdot \mathbf{v}(n) + \left[\frac{1}{\beta}(\mathbf{1}-\mathbf{a})\cdot \mathbf{m}^{-1}\right]^{1/2} \cdot \mathbf{N}^{+}(n) \\
\mathbf{v}\left(n+\frac{1}{2}\right) &= \mathbf{v}\left(n+\frac{1}{4}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot \mathbf{m}^{-1}\cdot \mathbf{f}(n) \\
\mathbf{r}\left(n+\frac{1}{2}\right) &= \mathbf{r}(n) + \frac{\Delta t}{2}\mathbf{b}\cdot \mathbf{v}\left(n+\frac{1}{2}\right) \\
\mathscr{H}(n) &\longrightarrow \mathscr{H}(n+1) \\
\mathbf{r}(n+1) &= \mathbf{r}\left(n+\frac{1}{2}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot \mathbf{v}\left(n+\frac{1}{2}\right) \\
v\left(n+\frac{3}{4}\right) &= v\left(n+\frac{1}{2}\right) + \frac{\Delta t}{2}\mathbf{b}\cdot \mathbf{m}^{-1}\cdot \mathbf{f}(n+1) \\
\mathbf{v}(n+1) &= \sqrt{a}\cdot \mathbf{v}\left(n+\frac{3}{4}\right) + \left[\frac{1}{\beta}(\mathbf{1}-\mathbf{a})\cdot \mathbf{m}^{-1}\right]^{1/2} \cdot \mathbf{N}^{-}(n+1)
\end{aligned}$$

where $a_{ij} = \delta_{ij}\exp(-\gamma_i \Delta t)$, $\mathscr{N}^{\pm}$ are independent normally distributed random variables with zero mean and unit variance, $b_{ij} = \delta_{ij}\sqrt{\frac{2}{\gamma_i \Delta t}\tanh\frac{\gamma_i \Delta t}{2}}$

3.2 Update γ_{eff}

We have obtained the γ matrix in the subsection 2.2, without mass vector. Here we update the effective matrix γ_{eff} with M^{-1}, starting from

$$\begin{aligned}
m_\alpha \cdot \dot{v}_\alpha &= F_\alpha(t) - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta = \left[F_{1\alpha}(\mathbf{x}) + F_{2\alpha\beta}(\mathbf{x})\dot{v}_\beta\right] - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta \\
m_\alpha \cdot \dot{v}_\alpha - F_{2\alpha\beta}(\mathbf{x})\dot{v}_\beta &= \left(m_\alpha \cdot \delta_{\alpha\beta} - F_{2\alpha\beta}(\mathbf{x})\right)\dot{v}_\beta = F_{1\alpha}(\mathbf{x}) - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta \\
\dot{v}_\beta &= \left(m_\alpha \cdot \delta_{\alpha\beta} - F_{2\alpha\beta}(\mathbf{x})\right)^{-1}\left(F_{1\alpha}(\mathbf{x}) - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta\right) = M^{-1}_{\alpha\beta}\left(F_{1\alpha}(\mathbf{x}) - m_\alpha \cdot \gamma_{\alpha\beta} v_\beta\right)
\end{aligned}$$

Note that the γ matrix above only contains terms about first derivatives

$$\begin{aligned}
\gamma_{Z\beta} v_\beta &= a_1 \frac{\dot{\Delta}}{\Delta^{3/2}} + a_2 \frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3 \frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3 \frac{\dot{X}^2}{\Delta^{7/2}} + a_4 \frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} \\
\gamma_{X\beta} v_\beta &= b_1 \frac{\dot{X}}{\sqrt{\Delta}} + b_2 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} \\
\gamma_{\Theta\beta} v_\beta &= c_1 \frac{\dot{\Theta}}{\sqrt{\Delta}} + c_2 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}}
\end{aligned}$$

To avoid the possible confusion, we write γ^* below. Consider $dv = \frac{f(t)}{m}dt - \gamma v dt + \sqrt{\frac{2\gamma}{\beta m}}dW$, we have γ_{eff} :

$$\gamma_{\text{eff}} = M^{-1}_{\alpha\beta} \cdot \begin{pmatrix} m_Z & 0 & 0 \\ 0 & m_X & 0 \\ 0 & 0 & m_\Theta \end{pmatrix} \cdot \gamma^*_{\alpha\beta} \tag{Yilin.44}$$

Surprisingly, we recover almost the same $\gamma_{\alpha\beta}$ shown previously

$$\begin{aligned}
\gamma_{\text{eff},zz} &= \frac{\xi}{\Delta^{3/2}} + \kappa\left(\frac{15\xi^2}{8\Delta^4} + \frac{21\xi v_z}{4\Delta^{9/2}}\right) + O\left(\kappa^2\right) \\
\gamma_{\text{eff},xx} &= \frac{2\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(4\sqrt{\Delta}\xi\epsilon^2 + 18v_z + 57\epsilon v_\theta\right)}{72\Delta^{7/2}} + O\left(\kappa^2\right) \\
\gamma_{\text{eff},\theta\theta} &= \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(8\sqrt{\Delta}\xi\epsilon^2 + 57\epsilon v_z + 9v_z\right)}{36\Delta^{7/2}} + O\left(\kappa^2\right) \\
\gamma_{\text{eff},zx} &= \frac{\kappa\xi\left((\epsilon+3)v_\theta - 3v_X\right)}{12\Delta^{7/2}} + O\left(\kappa^2\right) \\
\gamma_{\text{eff},z\theta} &= -\frac{\kappa\left(\xi\left(3v_\theta + (\epsilon-3)v_X\right)\right)}{12\Delta^{7/2}} + O\left(\kappa^2\right) \\
\gamma_{\text{eff},x\theta} &= -\frac{\kappa\left(\xi\left(16\Delta^3\xi\epsilon^2 + 36\Delta^{5/2}(\epsilon+1)v_z\right)\right)}{144\Delta^6} + O\left(\kappa^2\right)
\end{aligned}$$

3.3 Possible modification

Here we consider the following approaches for the sake of better numerical practices

- Solve Langevin equation numerically or solve Fokker-Planck equation directly;
- Add second derivatives or not; ($b_4 = b_5 = c_4 = c_5 = 0$)
- Ignore rotation and fix $\Theta = 0$
- Modify Gaussian random force with "Heaviside" function or not; to avoid sudden collapse $z < 0$
- How to determine the initial z value near the equilibrium position;
- Add Coulomb interaction or not; ($\frac{Q^2}{4\pi\varepsilon z}\exp(-\lambda_D/z)$)
- Diagonalize M matrix or not? physical meaning?
- Consider κ correction to which order?