Brownian motion near a Soft Surface

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1 Framework Introduction

1.1 Theoretical fundamentals

Here are prerequisites 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,

$$m\frac{dv}{dt} = -\xi v + \delta F$$

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 δF representing the effect of the collisions with the molecules of the fluid. The force δF has a Gaussian probability distribution with correlation function $\left\langle \delta F_i(t)\delta F_j(t')\right\rangle = 2\xi k_B T\delta_{ij}\delta(t-t')$

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:

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

which leads to **Itô's chain rule**:

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

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

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

<u>*Derivation from the over-damped Langevin equation*</u>

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 $x \longrightarrow \infty$:

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

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:

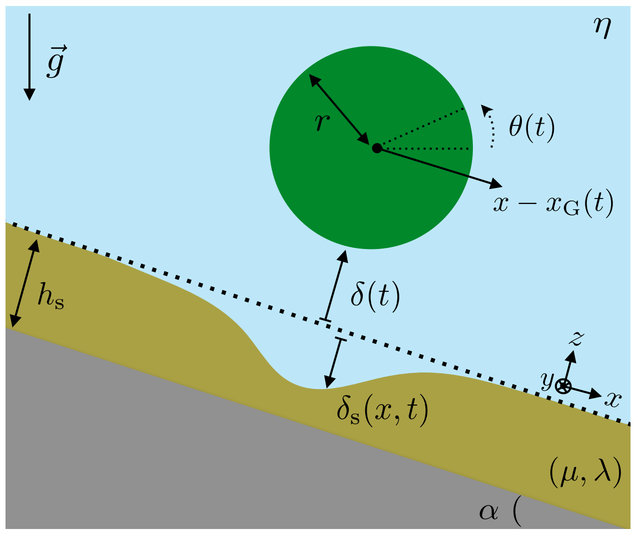

FIG. 1: *Schematic of the system. A negatively buoyant cylinder (green) falls down under the acceleration of gravity $\vec{g}$, inside a viscous fluid (blue), in the vicinity of a thin soft wall (brown). The ensemble lies atop a tilted, infinitely rigid support (grey).*

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

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

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

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

We have for small velocities that

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

and so we find

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

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

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

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

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

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 Brownian Motion in 3D (Δ, X, Θ) near a Soft Surface

Now consider the 3D Brownian motion (perpendicular, vertical, rotation) near a soft surface based on the results shown in the subsection 1.2, with the figure below:

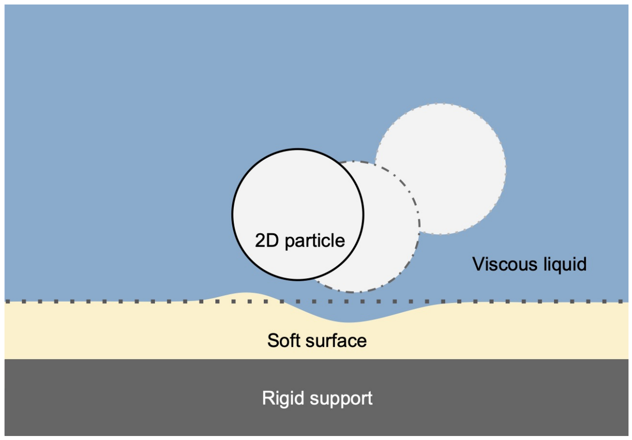

Figure 1: Brownian motion near a soft surface

We exploit Langevin equation to describe the Brownian motion, with the following expression:

$$m\dot{v} = -\xi v + \delta F$$

where the first term refers to systematic put of the environment influence, and the second term δF refers to fluctuation / random put. As the Gaussian white noise, there is no correlation in space and in time so $\langle \delta F(t) \rangle = 0$, and $\langle \delta F(t_1)\delta F(t_2) \rangle = 2B\delta(t_1 - t_2)$. Suppose $\gamma = \xi/m$, we have

$$\dot{v} = -\gamma v + \frac{\delta F}{m}$$

With Laplace transform,

$$\tilde{v}(s) = \frac{v(0)}{s+\gamma} + \frac{\delta\tilde{F}(s)}{m(s+\gamma)}$$

and then the inverse transform

$$v(t) = v(0)e^{-\gamma t} + \int_0^t dt' \frac{\delta F(t')}{m} \exp\left[-\gamma(t-t')\right]$$

At long time limit, $\langle v^2(t) \rangle \to \frac{k_B T}{m}$. According to the expression above, we could calculate

$$\begin{aligned}
\langle v^2(t) \rangle &= \langle v^2(0) \rangle e^{-2\gamma t} + 2e^{-\gamma t} \int_0^t dt' \frac{\langle \delta F(t) v(0) \rangle}{m} e^{-\gamma(t-t')} + \int_0^t dt_1 \int_0^t dt_2 e^{-\gamma(t-t_1)} e^{-\gamma(t-t_2)} \frac{\langle \delta F(t_1)\delta F(t_2) \rangle}{m^2} \\
&= \langle v^2(0) \rangle e^{-2\gamma t} + \int_0^t dt_1 e^{-2\gamma(t-t_1)} \frac{2B}{m^2} = \langle v^2(0) \rangle e^{-2\gamma t} - \frac{1}{2\gamma}(e^{-2\gamma t} - 1) \times \frac{2B}{m^2} \\
&= \langle v^2(0) \rangle e^{-2\gamma t} + \frac{B}{\zeta m}(1 - e^{-2\gamma t})
\end{aligned}$$

thus leading to $B = k_B T \zeta$ or $\langle \delta F(0) \delta F(t) \rangle = 2 k_B T \zeta \delta(t)$. We then write $\delta F(t) = \sqrt{2 k_B T \gamma m} \eta(t)$, following that $\langle \eta(0) \eta(t) \rangle = \delta(t)$.

$$m\dot{v} = -m\gamma v + \sqrt{\frac{2\gamma m}{\beta}}\eta(t)$$

Since $\eta(t)$ is not differentiable, we could define integrals of the process, introducing $W(t)$ as a Wiener process such that $\eta(t) = \mathrm{d}W/\mathrm{d}t$. Consider the external force $f(t)$, we finally writes

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

For our case, 3D Brownian motion should be taken into account. Therefore, additional formula would be needed, including the velocity $\vec{v}$ on each direction, then the mass $\vec{m}$, and γ as a matrix. In this section, we would first consider the second derivatives in Thomas' results, writing the friction matrix; then consider the effective "mass" on different directions, showing $\frac{1}{m}$ as an inverse matrix; finally the amplitude for the noise correlator.

2.1 Friction matrix $\gamma_{\alpha\beta}$ with unit mass

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)

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

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,

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

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

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 $\ddot{\Delta}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\Gamma_{zxz} = \Gamma_{zzx} = \Gamma_{zz\theta} = \Gamma_{z\theta z} = 0 \\
\Gamma_{xzz} = \Gamma_{xxx} = \Gamma_{\theta zz} = \Gamma_{\theta\theta\theta} = 0 \\
\Gamma_{\theta xx} = \Gamma_{x\theta x} = \Gamma_{x\theta\theta} = \Gamma_{\theta x\theta} = 0
\end{aligned} \tag{17}$$

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

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

Note that there would be the spurious drift force, which originates from the derivative of $\gamma_{\alpha\beta}$, equal to $\frac{\partial\gamma_{\alpha\beta}}{\partial v_\beta} = \Gamma_{\alpha\beta\beta}$. We could easily obtain non-zero components:

$$
\begin{aligned}
\frac{\partial\gamma_{zz}}{\partial v_z} &= \Gamma_{zzz} = \frac{42\kappa\xi}{8\Delta^{9/2} - 15\Delta\kappa\xi} \approx \frac{21\kappa\xi}{4\Delta^{9/2}} + \frac{315\kappa^2\xi^2}{32\Delta^8} \\
\frac{\partial\gamma_{zx}}{\partial v_x} &= \Gamma_{zxx} = \frac{2\kappa\xi}{15\kappa\xi - 8\Delta^{7/2}} \approx -\frac{\kappa\xi}{4\Delta^{7/2}} - \frac{15\kappa^2\xi^2}{32\Delta^7} \\
\frac{\partial\gamma_{z\theta}}{\partial v_\theta} &= \Gamma_{z\theta\theta} = \frac{2\kappa\xi}{15\kappa\xi - 8\Delta^{7/2}} \approx -\frac{\kappa\xi}{4\Delta^{7/2}} - \frac{15\kappa^2\xi^2}{32\Delta^7}
\end{aligned}
\tag{20}
$$

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

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

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

$$
\begin{aligned}
\gamma_{zx} = \gamma_{xz} &= \frac{2\kappa\xi v_X}{-8\Delta^{7/2} + 15\kappa\xi} + \left(-\frac{25}{18\Delta} - \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{36\Delta^{5/2} - 9\epsilon\kappa\xi}\right) v_\theta \\
&= -\frac{\left(\xi\left(3v_X - 3v_\theta - \epsilon v_\theta\right)\right)\kappa}{12\Delta^{7/2}} + \frac{5\xi^2\left(-27v_X + 27v_\theta + 5\Delta\epsilon^2 v_\theta\right)\kappa^2}{288\Delta^7} + O[\kappa]^3
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
\gamma_{z\theta} = \gamma_{\theta z} &= \left(\frac{25}{18\Delta} + \frac{19\epsilon\kappa\xi}{72\Delta^{7/2}} + \frac{2\kappa\xi}{8\Delta^{7/2} - 15\kappa\xi} + \frac{50\Delta^{3/2}}{9\left(-4\Delta^{5/2} + \epsilon\kappa\xi\right)}\right) v_X + \frac{2\kappa\xi v_\theta}{-8\Delta^{7/2} + 15\kappa\xi} \\
&= -\frac{\left(\xi\left(-3v_X + \epsilon v_X + 3v_\theta\right)\right)\kappa}{12\Delta^{7/2}} - \frac{5\left(\xi^2\left(-27v_X + 5\Delta\epsilon^2 v_X + 27v_\theta\right)\right)\kappa^2}{288\Delta^7} + O[\kappa]^3
\end{aligned}
\tag{23}
$$

$$
\begin{aligned}
\gamma_{xx} &= -\frac{4\epsilon\xi\left(-6\Delta^{5/2} + \epsilon\kappa\xi\right)}{36\Delta^3 - 9\sqrt{\Delta}\epsilon\kappa\xi} + \frac{1}{9}\kappa\xi\left(\frac{18}{8\Delta^{7/2} - 15\kappa\xi} + \frac{\epsilon^2\kappa\xi}{-4\Delta^6 + \Delta^{7/2}\epsilon\kappa\xi}\right) v_z + \frac{19\epsilon\kappa\xi\left(-6\Delta^{5/2} + \epsilon\kappa\xi\right) v_\theta}{-144\Delta^6 + 36\Delta^{7/2}\epsilon\kappa\xi} \\
&= \frac{2\epsilon\xi}{3\sqrt{\Delta}} + \frac{\left(4\sqrt{\Delta}\epsilon^2\xi^2 + 18\xi v_z + 57\epsilon\xi v_\theta\right)\kappa}{72\Delta^{7/2}} + \left(\frac{\epsilon^3\xi^3}{72\Delta^{11/2}} - \frac{\left(-135 + 8\Delta\epsilon^2\right)\xi^2 v_z}{288\Delta^7} + \frac{19\epsilon^2\xi^2 v_\theta}{288\Delta^6}\right)\kappa^2 + O[\kappa]^3
\end{aligned}
\tag{24}
$$

$$\gamma_{\theta\theta} = -\frac{4\epsilon\xi\left(-12\Delta^{5/2}+\epsilon\kappa\xi\right)}{36\Delta^3-9\sqrt{\Delta}\epsilon\kappa\xi} + \frac{19\epsilon^2\kappa^2\xi^2 v_X}{36\left(4\Delta^6-\Delta^{7/2}\epsilon\kappa\xi\right)} + \kappa\xi\left(\frac{23\epsilon}{36\Delta^{7/2}} + \frac{2}{8\Delta^{7/2}-15\kappa\xi} + \frac{34\epsilon}{36\Delta^{7/2}-9\Delta\epsilon\kappa\xi}\right)v_z$$
$$= \frac{4\epsilon\xi}{3\sqrt{\Delta}} + \left(\frac{2\epsilon^2\xi^2}{9\Delta^3} + \frac{(3+19\epsilon)\xi v_z}{12\Delta^{7/2}}\right)\kappa + \left(\frac{\epsilon^3\xi^3}{18\Delta^{11/2}} + \frac{19\epsilon^2\xi^2 v_X}{144\Delta^6} + \frac{\left(135+68\Delta\epsilon^2\right)\xi^2 v_z}{288\Delta^7}\right)\kappa^2 + O[\kappa]^3 \tag{25}$$

$$\gamma_{x\theta} = \gamma_{\theta x} = \frac{4\epsilon^2\kappa\xi^2}{36\Delta^3-9\sqrt{\Delta}\epsilon\kappa\xi} + \left(\frac{2}{15} - \frac{1}{2\Delta} - \frac{3\epsilon\kappa\xi}{8\Delta^{7/2}} + \frac{16}{15\left(-8+\frac{15\kappa\xi}{\Delta^{7/2}}\right)} + \frac{1}{2\Delta-\frac{\epsilon\kappa\xi}{2\Delta^{3/2}}}\right)v_z$$
$$= \left(\frac{\epsilon^2\xi^2}{9\Delta^3} - \frac{(\xi+\epsilon\xi)v_z}{4\Delta^{7/2}}\right)\kappa + \left(\frac{\epsilon^3\xi^3}{36\Delta^{11/2}} + \frac{\left(-15+\Delta\epsilon^2\right)\xi^2 v_z}{32\Delta^7}\right)\kappa^2 + O[\kappa]^3 \tag{26}$$

2.2 Mass vector and effective friction matrix

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)

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

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

$$-\frac{F_{hZ}}{m_Z} = -\dot{v}_z = -\ddot{\Delta} = a_1\frac{\dot{\Delta}}{\Delta^{3/2}} + a_2\frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3\frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3\frac{\dot{X}^2}{\Delta^{7/2}} + a_4\frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_5\frac{\ddot{\Delta}}{\Delta^{7/2}} + a_6 \tag{27}$$

thus

$$F_{1hZ} = -m_Z\left(a_1\frac{\dot{\Delta}}{\Delta^{3/2}} + a_2\frac{\dot{\Delta}^2}{\Delta^{9/2}} + a_3\frac{\dot{\Theta}^2}{\Delta^{7/2}} + a_3\frac{\dot{X}^2}{\Delta^{7/2}} + a_4\frac{\dot{\Theta}\dot{X}}{\Delta^{7/2}} + a_6\right)$$
$$F_{2hZZ} = -\frac{m_Z a_5}{\Delta^{7/2}} \qquad F_{2hZX} = 0 \qquad F_{2hZ\Theta} = 0 \tag{28}$$

Similarly, there are cross terms for X, Θ components

$$-\frac{F_{hX}}{m_X} = -\dot{v}_x = -\ddot{X} = b_1 \frac{\dot{X}}{\sqrt{\Delta}} + b_2 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_4 \frac{\ddot{\Theta}}{\Delta^{5/2}} + b_5 \frac{\ddot{X}}{\Delta^{5/2}} + b_6 \tag{29}$$

$$\begin{aligned} F_{1hX} &= -m_X \left(b_1 \frac{\dot{X}}{\sqrt{\Delta}} + b_2 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_6 \right) \\ F_{2hXZ} &= 0 \qquad F_{2hXX} = -\frac{m_X b_5}{\Delta^{5/2}} \qquad F_{2hX\Theta} = -\frac{m_X b_4}{\Delta^{5/2}} \end{aligned} \tag{30}$$

and

$$-\frac{F_{h\Theta}}{m_\Theta} = -\dot{v}_\theta = -\ddot{\Theta} = c_1 \frac{\dot{\Theta}}{\sqrt{\Delta}} + c_2 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + c_4 \frac{\ddot{X}}{\Delta^{5/2}} + c_5 \frac{\ddot{\Theta}}{\Delta^{5/2}} + c_6 \tag{31}$$

$$\begin{aligned} F_{1h\Theta} &= -m_\Theta \left(c_1 \frac{\dot{\Theta}}{\sqrt{\Delta}} + c_2 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + c_6 \right) \\ F_{2h\Theta Z} &= 0 \qquad F_{2h\Theta X} = -\frac{m_\Theta c_4}{\Delta^{5/2}} \qquad F_{2h\Theta\Theta} = -\frac{m_\Theta c_5}{\Delta^{5/2}} \end{aligned} \tag{32}$$

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

$$\begin{aligned} M_{ZZ} &= m_Z + \frac{m_Z a_5}{\Delta^{5/2}} \\ M_{XX} &= m_X + \frac{m_X b_5}{\Delta^{5/2}} \qquad M_{X\Theta} = \frac{m_X b_4}{\Delta^{5/2}} \\ M_{\Theta X} &= \frac{m_\Theta c_4}{\Delta^{5/2}} \qquad M_{\Theta\Theta} = m_\Theta + \frac{m_\Theta c_5}{\Delta^{5/2}} \end{aligned} \tag{33}$$

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

$$M = \begin{pmatrix} m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}} & 0 & 0 \\ 0 & m_X - \frac{\kappa\xi\epsilon m_X}{12\Delta^{5/2}} & \frac{\kappa\xi\epsilon m_X}{12\Delta^{5/2}} \\ 0 & \frac{\kappa\xi\epsilon m_\theta}{6\Delta^{5/2}} & m_\theta - \frac{\kappa\xi\epsilon m_\theta}{6\Delta^{5/2}} \end{pmatrix} \tag{34}$$

and its inverse matrix

$$M^{-1} = \begin{pmatrix} \frac{1}{m_z - \frac{15\kappa\xi m_z}{8\Delta^{5/2}}} & 0 & 0 \\ 0 & \frac{12\Delta^{5/2} - 2\kappa\xi\epsilon}{12\Delta^{5/2} m_X - 3\kappa\xi\epsilon m_X} & \frac{\kappa\xi\epsilon}{3m_\theta(\kappa\xi\epsilon - 4\Delta^{5/2})} \\ 0 & \frac{2\kappa\xi\epsilon}{3m_X(\kappa\xi\epsilon - 4\Delta^{5/2})} & \frac{12\Delta^{5/2} - \kappa\xi\epsilon}{12\Delta^{5/2} m_\theta - 3\kappa\xi\epsilon m_\theta} \end{pmatrix} \tag{35}$$

with the approximation expressed by the series of κ:

$$M_{app}^{-1} \approx \begin{pmatrix} \frac{1}{m_z} + \frac{15\kappa\xi}{8\Delta^{5/2} m_z} + \frac{225\kappa^2\xi^2}{64\Delta^5 m_z} & 0 & 0 \\ 0 & \frac{1}{m_X} + \frac{\kappa\xi\epsilon}{12\Delta^{5/2} m_X} + \frac{\kappa^2\xi^2\epsilon^2}{48\Delta^5 m_X} & -\frac{\kappa(\xi\epsilon)}{12(\Delta^{5/2} m_\theta)} - \frac{\kappa^2(\xi^2\epsilon^2)}{48(\Delta^5 m_\theta)} \\ 0 & -\frac{\kappa(\xi\epsilon)}{6(\Delta^{5/2} m_X)} - \frac{\kappa^2(\xi^2\epsilon^2)}{24(\Delta^5 m_X)} & \frac{1}{m_\theta} + \frac{\kappa\xi\epsilon}{6\Delta^{5/2} m_\theta} + \frac{\kappa^2\xi^2\epsilon^2}{24\Delta^5 m_\theta} \end{pmatrix} \tag{36}$$

Only taking the first-order correction, we could verify

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

We have obtained the γ matrix in the subsection 2.1, without mass vector. Here we update the effective matrix γ_{eff} with M^{-1}, starting from

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

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 the original γ as γ^* below. Therefore, we have γ_{eff}, considering $dv = \frac{f(t)}{m} dt - \gamma v dt + \sqrt{\frac{2\gamma}{\beta m}} dW$

$$\gamma_{\text{eff}} = M_{\alpha\beta}^{-1} \cdot \begin{pmatrix} m_Z & 0 & 0 \\ 0 & m_X & 0 \\ 0 & 0 & m_\Theta \end{pmatrix} \cdot \gamma_{\alpha\beta}^* \tag{37}$$

Surprisingly, we recover almost the same $\gamma_{\alpha\beta}$ shown previously except γ_{zz}: (See eq. 21)

$$\begin{aligned} \gamma_{\text{eff},zz} &= \frac{\xi}{\Delta^{3/2}} + \kappa \left(\frac{15\xi^2}{8\Delta^4} + \frac{21\xi v_z}{4\Delta^{9/2}}\right) + O\left(\kappa^2\right) \\ \gamma_{\text{eff},xx} &= \frac{2\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(4\sqrt{\Delta}\xi\epsilon^2 + 18 v_z + 57\epsilon v_\theta\right)}{72\Delta^{7/2}} + O\left(\kappa^2\right) \\ \gamma_{\text{eff},\theta\theta} &= \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi\left(8\sqrt{\Delta}\xi\epsilon^2 + 57\epsilon v_z + 9 v_z\right)}{36\Delta^{7/2}} + O\left(\kappa^2\right) \\ \gamma_{\text{eff},xz} = \gamma_{\text{eff},zx} &= \frac{\kappa\xi\left((\epsilon+3)v_\theta - 3v_X\right)}{12\Delta^{7/2}} + O\left(\kappa^2\right) \\ \gamma_{\text{eff},\theta z} = \gamma_{\text{eff},z\theta} &= -\frac{\kappa\xi\left(3v_\theta + (\epsilon-3)v_X\right)}{12\Delta^{7/2}} + O\left(\kappa^2\right) \\ \gamma_{\text{eff},\theta x} = \gamma_{\text{eff},x\theta} &= -\frac{\kappa\xi\left(16\Delta^3\xi\epsilon^2 + 36\Delta^{5/2}(\epsilon+1)v_z\right)}{144\Delta^6} + O\left(\kappa^2\right) \end{aligned} \tag{38}$$

2.3 Noise correlator amplitude

Up to now, we have derived the effective friction matrix γ_{eff}. Next we consider the amplitude of noise correlator. (See details in beginning of Section 2) So we'd like to find the expression of the square root of γ_{eff}. Suppose that

$$\gamma_{\text{eff}} = \Psi + \kappa\Phi + O[\kappa]^2 \tag{39}$$

where Ψ is zero-order matrix of κ, Ψ_i = SeriesCoefficients[Series[$\gamma_{\text{eff},ii}$, $\{\kappa, 0, 0\}$], 0]; and Φ the first-order one, Φ_i = SeriesCoefficients[Series[$\gamma_{\text{eff},ij}$, $\{\kappa, 0, 1\}$], 1]. We suppose that $\gamma_{\text{eff}}^{1/2}$ shows a similar form such as $\gamma_{\text{eff}}^{1/2} \approx \psi + \kappa\chi$,

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

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, namely

$$\Psi = \begin{pmatrix} \Psi_z & 0 & 0 \\ 0 & \Psi_x & 0 \\ 0 & 0 & \Psi_\theta \end{pmatrix} = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{2\epsilon\xi}{3\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{4\epsilon\xi}{3\sqrt{\Delta}} \end{pmatrix} \tag{40}$$

Then we could verify that χ is a symmetric matrix, $\chi_{ij} = \frac{\Phi_{ij}}{\sqrt{\Psi_i}+\sqrt{\Psi_j}}$, with diagonal components as:

$$\chi_{zz} = \frac{3\xi\left(5\xi + 14\sqrt{\Delta}v_z\right)}{16\Delta^5\sqrt{\frac{\xi}{\Delta^{3/2}}}} \quad \chi_{xx} = \frac{\xi\left(18v_z + \epsilon\left(4\sqrt{\Delta}\epsilon\xi + 57v_\theta\right)\right)}{48\sqrt{6}\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}} \quad \chi_{\theta\theta} = \frac{\xi\left(8\sqrt{\Delta}\epsilon^2\xi + (9 + 57\epsilon)v_z\right)}{48\sqrt{3}\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}} \tag{41}$$

and non-diagonal elements

$$\begin{aligned}
\chi_{zx} = \chi_{xz} &= \frac{\xi\left(-3v_X + (3+\epsilon)v_\theta\right)}{4\Delta^{7/2}\left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + \sqrt{6}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}\right)} \\
\chi_{z\theta} = \chi_{\theta z} &= -\frac{\xi\left(3v_\theta + (\epsilon - 3)v_X\right)}{4\Delta^{7/2}\left(3\sqrt{\frac{\xi}{\Delta^{3/2}}} + 2\sqrt{3}\sqrt{\frac{\xi\epsilon}{\sqrt{\Delta}}}\right)} \\
\chi_{x\theta} = \chi_{\theta x} &= \frac{\xi\left(4\sqrt{\Delta}\epsilon^2\xi - 9(1+\epsilon)v_z\right)}{12\sqrt{3}\left(2+\sqrt{2}\right)\Delta^{7/2}\sqrt{\frac{\epsilon\xi}{\sqrt{\Delta}}}}
\end{aligned} \tag{42}$$

Consider the case without unit mass, we have to calculate the inverse mass matrix as an analogy of $\frac{1}{m}$, hences $\gamma_{\text{eff}}^{1/2} \to \left(\gamma_{\text{eff}} \cdot M^{-1}\right)^{1/2}$ as an asymmetric matrix:

$$\begin{pmatrix} \frac{\xi}{\Delta^{3/2} m_z} + \frac{\kappa(3\xi)\left(\left(5\sqrt{\Delta}\right)\xi + 7v_z(t)\right)}{\left(4\Delta^{9/2}\right)m_z} & -\frac{\kappa\xi(-3v_\theta(t)+3v_X(t)-\epsilon v_\theta(t))}{\left(12\Delta^{7/2}\right)m_X} & -\frac{\kappa\xi(3v_\theta(t)+\epsilon v_X(t)-3v_X(t))}{\left(12\Delta^{7/2}\right)m_\theta} \\ -\frac{\kappa\xi(-3v_\theta(t)+3v_X(t)-\epsilon v_\theta(t))}{\left(12\Delta^{7/2}\right)m_z} & \frac{\xi(2\epsilon)}{\left(3\sqrt{\Delta}\right)m_X} + \frac{\kappa\xi\left(\xi\left(\left(8\sqrt{\Delta}\right)\epsilon^2\right)+18v_z(t)+(57\epsilon)v_\theta(t)\right)}{\left(72\Delta^{7/2}\right)m_X} & \frac{\kappa\xi\left(\xi\left(\left(-288\Delta^{11/2}\right)\epsilon^2\right)-\left(\left(432\Delta^5\right)(\epsilon+1)\right)v_z(t)\right)}{\left(1728\Delta^{17/2}\right)m_\theta} \\ -\frac{\kappa\xi(3v_\theta(t)+\epsilon v_X(t)-3v_X(t))}{\left(12\Delta^{7/2}\right)m_z} & \frac{\kappa\xi\left(\xi\left(\left(-288\Delta^{11/2}\right)\epsilon^2\right)-\left(\left(216\Delta^5\right)(\epsilon+1)\right)v_z(t)\right)}{\left(864\Delta^{17/2}\right)m_X} & \frac{\xi(4\epsilon)}{\left(3\sqrt{\Delta}\right)m_\theta} + \frac{\kappa\xi\left(\xi\left(\left(16\sqrt{\Delta}\right)\epsilon^2\right)+(57\epsilon)v_z(t)+9v_z(t)\right)}{\left(36\Delta^{7/2}\right)m_\theta} \end{pmatrix}$$

Even though we could neglect the non-diagonal elements as the cross-correlated noise since $\kappa \ll 1$, we are still motivated to clarify these terms by proper treatment, such as the diagonalisation. However, we could hardly furnish a simple diagonalized matrix, numerical method would be expected. After extracting noise eigenvalues, we exploit the inverse base transform to furnish the exact contribution on each direction. Further discussion see subsection 3.1.

The results seem plausible and enough with the first-order correction of κ. However, some velocities have been included, which would contribute to Laplace transform. Return to the equation of motion

$$\dot{\mathbf{v}}_{3\times1} = -\gamma_{\text{eff},3\times3} \cdot \mathbf{v}_{3\times1} + M_{3\times3}^{-1} \cdot \delta F_{3\times1} \tag{43}$$

and consider the corresponding Laplace transform

$$\widetilde{\dot{\mathbf{v}}}_{3\times1} = -\widetilde{\gamma_{\text{eff}} \cdot \mathbf{v}} + \widetilde{M^{-1} \cdot \delta F} \tag{44}$$

Note that it contains velocities in γ_{eff} rather than a constant coefficient. We could not extract this friction matrix outside the Laplace transform, while similar for M^{-1}. We try the Laplace transform directly on $-\widetilde{\gamma_{\text{eff}} \cdot \mathbf{v}}$, obtaining

$$\begin{pmatrix} s\widetilde{v_z}(s) - v_z(0) \\ s\widetilde{v_x}(s) - v_x(0) \\ s\widetilde{v_\theta}(s) - v_\theta(0) \end{pmatrix} = \begin{pmatrix} \frac{2\xi}{8\Delta^{9/2}-15\Delta^2\kappa\xi} & 0 & 0 \\ 0 & \frac{\xi\epsilon}{36\left(4\Delta^6-\Delta^{7/2}\kappa\xi\epsilon\right)} & 0 \\ 0 & 0 & \frac{\xi\epsilon}{36\left(4\Delta^6-\Delta^{7/2}\kappa\xi\epsilon\right)} \end{pmatrix}.$$

$$\begin{pmatrix} \left\{\Delta\kappa\left(\widetilde{v_\theta^2} - 2\widetilde{v_\theta v_X}\right) + \Delta\kappa\widetilde{v_X^2} - 4\Delta^3\widetilde{v_z} - 21\kappa\widetilde{v_z^2}\right\} \\ \left\{16\Delta^3(\epsilon\kappa\xi - 6\Delta^{5/2})\widetilde{v_x} + \kappa\left[-4\epsilon\kappa\xi\widetilde{v_x v_z} + 16\Delta^3\epsilon\xi\widetilde{v_\theta} + 19(\epsilon\kappa\xi - 6\Delta^{5/2})\widetilde{v_x v_\theta} + 3(8\Delta^{5/2} + 5\epsilon\kappa\xi)\widetilde{v_z v_\theta}\right]\right\} \\ \left(16\Delta^3\kappa\xi\epsilon - 192\Delta^{11/2}\right)\widetilde{v_\theta} + 16\Delta^3\kappa\xi\epsilon\widetilde{v_X} - 4\kappa\left(\kappa\xi\epsilon - 12\Delta^{5/2}\right)\widetilde{v_X v_z} + 19\kappa^2\xi\epsilon\widetilde{v_\theta v_X} + 3\kappa\left(5\kappa\xi\epsilon - 76\Delta^{5/2}\right)\widetilde{v_\theta v_z} \end{pmatrix}$$

The Laplace transform of multiplication would be quite complex, since

$$\widetilde{f(t)g(t)}(p) = \frac{1}{2\pi i}\lim_{T\to\infty}\int_{c-iT}^{c+iT} \widetilde{f}(s)\widetilde{g}(p-s)ds$$

The integration is done along the vertical line $\mathrm{Re}(s) = c$ that lies entirely within the region of convergence of $\widetilde{f}$. For example, $f(t) = e^t$ does not possess a convergent Laplace integral if $\mathrm{Re}\, p > 1$ or if $\mathrm{Re}\, p < 1$. The strip of convergence has contracted to a line: the integral converges only where $\mathrm{Re}\, p = 1$, and even then not exactly at $p = 1$. We'd like to consider this part after getting the proper formula of v_i. For instance, if $f(t) = e^{-\gamma t}$ with $t > 0$, we have the convergence strip if $\mathrm{Re}\, p > -\gamma$, which could be satisfied in our issue if we have a constant γ.

Dissect γ_{eff} as $\gamma_{\text{eff}} = \gamma_0 + \gamma_1$, where γ_0 is independent on any velocity while γ_1 not:

$$\gamma_0 = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} + \frac{15\kappa\xi^2}{8\Delta^4} & 0 & 0 \\ 0 & \frac{2\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi^2\epsilon^2}{18\Delta^3} & -\frac{\kappa\xi^2\epsilon^2}{9\Delta^3} \\ 0 & -\frac{\kappa\xi^2\epsilon^2}{9\Delta^3} & \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{2\kappa\xi^2\epsilon^2}{9\Delta^3} \end{pmatrix} \tag{45}$$

$$\gamma_1 = \begin{pmatrix} \frac{21\kappa\xi v_z}{4\Delta^{9/2}} & \frac{\kappa\xi((\epsilon+3)v_\theta - 3v_X)}{12\Delta^{7/2}} & -\frac{\kappa\xi(3v_\theta+(\epsilon-3)v_X)}{12\Delta^{7/2}} \\ \frac{\kappa\xi((\epsilon+3)v_\theta - 3v_X)}{12\Delta^{7/2}} & \frac{\kappa\xi(6v_z+19\epsilon v_\theta)}{24\Delta^{7/2}} & -\frac{\kappa\xi(\epsilon+1)v_z}{4\sqrt{\Delta}} \\ -\frac{\kappa\xi(3v_\theta+(\epsilon-3)v_X)}{12\Delta^{7/2}} & -\frac{\kappa\xi(\epsilon+1)v_z}{4\sqrt{\Delta}} & \frac{\kappa\xi(19\epsilon v_z+3v_z)}{12\Delta^{7/2}} \end{pmatrix} \tag{46}$$

hence we could separate the transform as $\widetilde{\gamma_{\text{eff}} \cdot \mathbf{v}} = \widetilde{\gamma_0 \cdot \mathbf{v}} + \widetilde{\gamma_1 \cdot \mathbf{v}}$. Suppose that $\gamma_{1,ij} = g_{ij\alpha} v^\alpha$, where $g_{ij\alpha}$ refers to the coefficient of v_α in $\gamma_{1,ij}$, such as $g_{12x} = -\frac{\kappa\xi v_X}{4\Delta^{7/2}}$. A symmetric γ_{eff} results in symmetric γ_0 and γ_1, so is $g_{ij\alpha}$. In this case, the ith component turns to

$$(\gamma_{\text{eff}} \cdot \mathbf{v})_i = \gamma_{\text{eff},ij} v^j = \left(\gamma_{0,ij} + g_{ij\alpha} v^\alpha\right) v^j$$

$$s\widetilde{v}_\mu - v_\mu(0) = -\gamma_{0,\mu\alpha} \cdot \widetilde{v}^\alpha - g_{\mu\alpha\beta}(\widetilde{v^\alpha v^\beta}) + \widetilde{M^{-1} \cdot \delta F}$$

We are inclined to neglect all $g_{\mu\alpha\beta}(\widetilde{v^\alpha v^\beta})$ at first, which would be raisonnable for the elastic compliance parameter $\kappa \ll 1$ (about $10^{-4} \sim 10^{-3}$). We return to equations of motion in the 0-order correction of κ (see eqs Salez2015.50 - Salez2015.52), obtaining three friction coefficients directly, namely a diagonal friction matrix: $\gamma_{i0} = \gamma_{0,ii0}$, where the first 0 refers to γ_0, ii refers to matrix element index, and the second 0 refers to the terms independent on κ.

$$\gamma_{z0} = \frac{\xi}{\Delta^{3/2}} \qquad \gamma_{x0} = \frac{2\xi\epsilon}{3\sqrt{\Delta}} \qquad \gamma_{\theta 0} = \frac{4\xi\epsilon}{3\sqrt{\Delta}} \tag{47}$$

Also, M^{-1} reduces to the diagonal one as the inverse number of original masses, leading to a simple Langevin equation as $\frac{1}{m_i} = M^{-1}_{ii0}$ with the similar notion as γ_{eff}.

$$\dot{v}_{i0} = -\gamma_i v_{i0} + \frac{\delta F_i}{m_i} \tag{48}$$

with the solution as

$$v_{i0}(t) = v_{i0}(0)e^{-\gamma_{i0}t} + \int_0^t \mathrm{d}\tau \frac{\delta F_i(\tau)}{m_i} \exp\left[-\gamma_{i0}(t-\tau)\right] \tag{49}$$

Follow the same process we have done previously, we get the amplitude of noise correlator:

$$\left\langle \delta F_i(\tau_1)\delta F_j(\tau_2)\right\rangle = 2k_B T m_i \gamma_{i0}\delta_{ij}\delta(\tau_1-\tau_2)$$

Then we consider the term $g_{\mu\alpha\beta}(\widetilde{v^\alpha v^\beta})$ with the 0-order v_i expression of κ and 1-order coefficients $g_{\mu\alpha\beta}$, by the following integration:

$$\widetilde{v_{i0}^2} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\left[\frac{v_i(0)}{s+\gamma_{0ii0}} + \frac{M_{ii0}^{-1}\widetilde{\delta F_i}(s)}{s+\gamma_{0ii0}}\right]\times\left[\frac{v_i(0)}{p-s+\gamma_{0ii0}} + \frac{M_{ii0}^{-1}\widetilde{\delta F_i}(p-s)}{p-s+\gamma_{0ii0}}\right]\mathrm{d}s$$

where $c > -\gamma_{0ii0}$ for instance we taken $c = 0$. Take four terms into account respectively:

$$\int_{-i\infty}^{+i\infty}\frac{v_i(0)v_i(0)}{(\gamma_{0ii0}+s)(\gamma_{0ii0}+p-s)}\,ds = \left.\frac{v_i(0)^2(\log(\gamma_{0ii0}+s)-\log(-\gamma_{0ii0}-p+s))}{2\gamma_{0ii0}+p}\right|_{-\infty}^{+\infty} = 0$$

As a bounded function, $\widetilde{\delta F_i} < \infty$, thus we could repeat the integration above, yielding other three zero integration. So we ignore all $g_{\mu\alpha\beta}(\widetilde{v^\alpha v^\beta})$.

Next, we consider the first-order correction of κ in γ_0. There would be nothing more for γ_{z0} than one additional term: $\gamma_z = \gamma_{z0} \Rightarrow \gamma_z = \gamma_{z0}+\gamma_{z1} = \frac{\xi}{\Delta^3/2}+\frac{15\kappa\xi^2}{8\Delta^4}$. Also, $m_z = m_{z0} \Rightarrow m_z = m_{z0}+m_{z1}$, $v_z(t) = v_{z0}(t)+v_{z1}(t)$, $\delta F_z(t) = \delta F_{z0}(t)+\delta F_{z1}(t)$, where 1 always refers to the first-order correction of κ. Consider Laplace transform again toward κ correction on order 1:

$$\begin{aligned}
s\left(\widetilde{v_{z0}}+\widetilde{v_{z1}}\right) - v_z(0) &= -(\gamma_{0,zz0}+\gamma_{0,zz1})\left(\widetilde{v_{z0}}+\widetilde{v_{z1}}\right) + \left(M_{zz0}^{-1}+M_{zz1}^{-1}\right)\left(\widetilde{\delta F_{z0}}+\widetilde{\delta F_{z1}}\right)\\
s\widetilde{v_{z0}}+s\widetilde{v_{z1}} - v_z(0) &= -\gamma_{0,zz0}\widetilde{v_{z0}} - \gamma_{0,zz0}\widetilde{v_{z1}} - \gamma_{0,zz1}\widetilde{v_{z0}} - \cancel{\gamma_{0,zz1}\widetilde{v_{z1}}}\\
&\quad + M_{zz0}^{-1}\widetilde{\delta F_{z0}} + M_{zz0}^{-1}\widetilde{\delta F_{z1}} + M_{zz1}^{-1}\widetilde{\delta F_{z0}} + \cancel{M_{zz1}^{-1}\widetilde{\delta F_{z1}}}\\
s\widetilde{v_{z0}} - v_z(0) &= -\gamma_{0,zz0}\widetilde{v_{z0}} + M_{zz0}^{-1}\widetilde{\delta F_{z0}}\\
s\widetilde{v_{z1}} &= -\gamma_{0,zz0}\widetilde{v_{z1}} - \gamma_{0,zz1}\widetilde{v_{z0}} + M_{zz0}^{-1}\widetilde{\delta F_{z1}} + M_{zz1}^{-1}\widetilde{\delta F_{z0}}
\end{aligned}$$

$$\widetilde{v_{z1}} = -\frac{\gamma_{0,zz1}}{(s+\gamma_{0,zz0})^2}\left[v_z(0)+M_{zz0}^{-1}\widetilde{\delta F_{z0}}\right) + \frac{1}{s+\gamma_{0,zz0}}\left(M_{zz0}^{-1}\widetilde{\delta F_{z1}} + M_{zz1}^{-1}\widetilde{\delta F_{z0}}\right)$$

After the inverse Laplace transformation, we get $v_{z1}(t)$

$$v_{z1}(t) = -v_z(0)\gamma_{0,zz1}te^{-\gamma_{0,zz0}t} + \int_0^t \mathrm{d}\tau e^{-\gamma_{0,zz0}(t-\tau)}\left\{\left[M_{zz0}^{-1}\delta F_{z1}(\tau)+M_{zz1}^{-1}\delta F_{z0}(\tau)\right] - \gamma_{0,zz1}(t-\tau)M_{zz0}^{-1}\delta F_{z0}(\tau)\right\}$$

$$
\begin{aligned}
\left\langle v_z^2(t)\right\rangle &= \left\langle \left[v_{z0}^2(t)+v_{z1}^2(t)\right]^2\right\rangle = \left\langle v_{z0}^2(t)\right\rangle + 2\left\langle v_{z0}(t)v_{z1}(t)\right\rangle + \cancel{\left\langle v_{z1}^2(t)\right\rangle} \\
&= \left\langle v_{z0}^2(t)\right\rangle e^{-2\gamma_{0,zz0}t} + \frac{k_BT}{m_z}\left(1-e^{-2\gamma_{0,zz0}t}\right) - 2\left\langle v_z^2(0)\right\rangle \gamma_{0,zz1} t e^{-2\gamma_{0,zz0}t} \\
&\quad + 2\left\langle \int_0^t \mathrm{d}\tau_1 \frac{\delta F_{z0}(\tau_1)}{m_z} e^{-\gamma_{0,zz0}(t-\tau_1)} \int_0^t \mathrm{d}\tau_2 e^{-\gamma_{0,zz0}(t-\tau_2)} \left[M_{zz0}^{-1}\delta F_{z1}(\tau_2) + \left(M_{zz1}^{-1} - \gamma_{0,zz1}(t-\tau_2)M_{zz0}^{-1}\right)\delta F_{z0}(\tau_2)\right]\right\rangle \\
&= \left\langle v_{z0}^2(t)\right\rangle e^{-2\gamma_{0,zz0}t} + \frac{k_BT}{m_z}\left(1-e^{-2\gamma_{0,zz0}t}\right) - 2\left\langle v_z^2(0)\right\rangle \gamma_{0,zz1} t e^{-2\gamma_{0,zz0}t} \\
&\quad + 2\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2 \frac{\langle \delta F_{z0}(\tau_1)\delta F_{z1}(\tau_2)\rangle}{m_z} M_{zz0}^{-1} e^{-\gamma_{0,zz0}(t-\tau_1)} e^{-\gamma_{0,zz0}(t-\tau_2)} \\
&\quad + 2k_BT\left[M_{zz1}^{-1}\left(1-e^{-2\gamma_{0,zz0}t}\right) + \frac{\gamma_{0,zz1}M_{zz0}^{-1}}{2\gamma_{0,zz0}} e^{-2\gamma_{0,zz0}t}\left(1-e^{2\gamma_{0,zz0}t}+2\gamma_{0,zz0}t\right)\right]
\end{aligned}
$$

Suppose $\langle \delta F_{z0}(\tau_1)\delta F_{z1}(\tau_2)\rangle = K\cdot\delta(\tau_1-\tau_2)$. At long time limit $t\to\infty$, the expression above would converge to

$$
\begin{aligned}
\left\langle v_z^2(t)\right\rangle &= \frac{k_BT}{m_z}\left(1-e^{-2\gamma_{0,zz0}t}\right) + 2k_BT\left[M_{zz1}^{-1}\left(1-e^{-2\gamma_{0,zz0}t}\right) + \frac{\gamma_{0,zz1}M_{zz0}^{-1}}{2\gamma_{0,zz0}} e^{-2\gamma_{0,zz0}t}\left(1-e^{2\gamma_{0,zz0}t}+2\gamma_{0,zz0}t\right)\right] \\
&\qquad + 2\int_0^t \mathrm{d}\tau \frac{K}{m_z} M_{zz0}^{-1} e^{-2\gamma_{0,zz0}(t-\tau)} \\
&\qquad = k_BT\left[\frac{1}{m_z} + 2\left(M_{zz1}^{-1} - \frac{M_{zz0}^{-1}\gamma_{0,zz1}}{2\gamma_{0,zz0}}\right)\right] + \frac{K}{m_z\gamma_{0,zz0}} M_{zz0}^{-1}\left(1-\cancel{e^{-2\gamma_{0,zz0}t}}\right) = \frac{k_BT}{m_z} \\
&\quad K = k_BTm_z\left(\gamma_{0,zz1} - 2\gamma_{0,zz0}m_zM_{zz1}^{-1}\right)
\end{aligned}
$$

Finally, we have the modified noise amplitude of z at 1-order correction. Note $M_{zz1}^{-1} = -M_{zz1} = \frac{15\kappa\xi^2}{8\Delta^4}$

$$
\begin{aligned}
\langle \delta F_z(\tau_1)\delta F_z(\tau_2)\rangle &= \langle [\delta F_{z0}(\tau_1)+\delta F_{z1}(\tau_1)]\cdot[\delta F_{z0}(\tau_2)+\delta F_{z1}(\tau_2)]\rangle \\
&= \langle \delta F_{z0}(\tau_1)\delta F_{z0}(\tau_2)\rangle + 2\langle \delta F_{z0}(\tau_1)\delta F_{z1}(\tau_2)\rangle + \cancel{\langle \delta F_{z1}(\tau_1)\delta F_{z2}(\tau_2)\rangle} \\
&= 2k_BTm_z\gamma_{z0}\delta(\tau_1-\tau_2) + 2k_BTm_z\left(\gamma_{0,zz1} - 2\gamma_{0,zz0}m_zM_{zz1}^{-1}\right)\delta(\tau_1-\tau_2) \\
&= 2k_BTm_z\delta(\tau_1-\tau_2)\cdot\left(\gamma_{0,zz0}+\gamma_{0,zz1}-2\gamma_{0,zz0}m_zM_{zz1}^{-1}\right)
\end{aligned}
\tag{50}
$$

Further treatment would be needed for other components due to non-zero non-diagonal elements $\gamma_{0x\theta} = \gamma_{0\theta x} \neq 0$. Expand $\widetilde{\gamma_0\cdot\mathbf{v}}$ again, we have:

$$
\begin{cases}
s\widetilde{v}_x - v_x(0) = -\gamma_{0xx}\widetilde{v}^x - \gamma_{0x\theta}\widetilde{v}^\theta + M_{xx}^{-1}\widetilde{\delta F_x} + M_{x\theta}^{-1}\widetilde{\delta F_\theta} \\
s\widetilde{v}_\theta - v_\theta(0) = -\gamma_{0\theta x}\widetilde{v}^x - \gamma_{0\theta\theta}\widetilde{v}^\theta + M_{\theta x}^{-1}\widetilde{\delta F_x} + M_{\theta\theta}^{-1}\widetilde{\delta F_\theta}
\end{cases}
\tag{51}
$$

with solutions as

$$
\begin{aligned}
\widetilde{v}_x &= \frac{\gamma_{0x\theta}\left(M^{-1}_{\theta x}\widetilde{\delta F_x} + M^{-1}_{\theta\theta}\widetilde{\delta F_\theta} + v_\theta(0)\right) - (\gamma_{0\theta\theta}+s)\left(M^{-1}_{xx}\widetilde{\delta F_x} + M^{-1}_{x\theta}\widetilde{\delta F_\theta} + v_x(0)\right)}{\gamma_{0\theta x}\gamma_{0x\theta} - (\gamma_{0\theta\theta}+s)(\gamma_{0xx}+s)} \\
\widetilde{v}_\theta &= \frac{\gamma_{0\theta x}\left(M^{-1}_{xx}\widetilde{\delta F_x} + M^{-1}_{x\theta}\widetilde{\delta F_\theta} + v_x(0)\right) - (\gamma_{0xx}+s)\left(M^{-1}_{\theta x}\widetilde{\delta F_x} + M^{-1}_{\theta\theta}\widetilde{\delta F_\theta} + v_\theta(0)\right)}{\gamma_{0\theta x}\gamma_{0x\theta} - (\gamma_{0\theta\theta}+s)(\gamma_{0xx}+s)}
\end{aligned}
\tag{52}
$$

We tried the inverse Laplace transform on terms without $\widetilde{\delta F_i}$ below, getting

$$
\begin{aligned}
v_x &\supset \frac{e^{-(\gamma_{0\theta\theta}+\gamma_{0\mathrm{xx}}-\gamma_s)t/2}}{2\gamma_s}\cdot\left\{2\gamma_{0x\theta}\left(e^{-\gamma_s t}-1\right)v_\theta(0) + \left[e^{-\gamma_s t}(\gamma_s+\gamma_{0xx}-\gamma_{0\theta\theta}) + (\gamma_s+\gamma_{0\theta\theta}-\gamma_{0xx})\right]v_x(0)\right\} \\
v_\theta &\supset \frac{e^{-(\gamma_{0\theta\theta}+\gamma_{0\mathrm{xx}}-\gamma_s)t/2}}{2\gamma_s}\cdot\left\{2\gamma_{0\theta x}\left(e^{-\gamma_s t}-1\right)v_x(0) + \left[e^{-\gamma_s t}(\gamma_s-\gamma_{0xx}+\gamma_{0\theta\theta}) + (\gamma_s-\gamma_{0\theta\theta}+\gamma_{0xx})\right]v_\theta(0)\right\}
\end{aligned}
$$

with the parameter

$$
\gamma_s = \sqrt{4\gamma_{0\theta\mathrm{x}}\gamma_{0\mathrm{x}\theta} + (\gamma_{0\mathrm{xx}}-\gamma_{0\theta\theta})^2} = \frac{1}{18}\sqrt{\frac{9\left(4\Delta^{5/2}\xi\epsilon + \kappa\xi^2\epsilon^2\right)^2 + 16\kappa^2\xi^4\epsilon^4}{\Delta^6}} \approx \frac{\kappa\xi^2\epsilon^2}{6\Delta^3} + \frac{2\xi\epsilon}{3\sqrt{\Delta}} > 0
$$

Two equations converge well since $\gamma_{0\theta\theta}+\gamma_{0\mathrm{xx}}-\gamma_s \approx \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi^2\epsilon^2}{9\Delta^3} > 0$. Take the limit $\kappa \to 0$, $\gamma_s \to \gamma_{0xx} = \gamma_{0\theta\theta}/2$. So v_x, v_θ would return to $v_i(0)e^{-\gamma_i t}$ as $\kappa \to 0$.

Note that second-order correction of κ has been introduced indirectly owing to γ_s. We could hardly solve the inverse transform including $\widetilde{\delta F_i}$. (To be exact, we are able to solve, but the result would be quite complex..) Suppose that $v_x = v_{x0} + v_{x1}$ and $v_\theta = v_{\theta0} + v_{\theta1}$, where the index 1 refers to the term depending on κ; thus $\widetilde{v_x} = \widetilde{v_{x0}} + \widetilde{v_{x1}}$, and $\widetilde{v_\theta} = \widetilde{v_{\theta0}} + \widetilde{v_{\theta1}}$. Similar for coefficients $\gamma_{0ij} = \gamma_{0ij0} + \gamma_{0ij1}$, $\gamma_{0ij0} = 0$ if $i \neq j$; while $M^{-1}_{ij} = M^{-1}_{ij0} + M^{-1}_{ij1}$, $M^{-1}_{ij0} = 0$ if $i \neq j$. So we expand the Laplace transform to first-order correction of κ as the following expressions:

$$
\begin{aligned}
s(\widetilde{v_{x0}} + \widetilde{v_{x1}}) - v_x(0) &= -(\gamma_{0xx0}+\gamma_{0xx1})(\widetilde{v_{x0}} + \widetilde{v_{x1}}) - (\cancel{\gamma_{0x\theta0}} + \gamma_{0x\theta1})(\widetilde{v_{\theta0}} + \cancel{\widetilde{v_{\theta1}}}) \\
&\quad + (M^{-1}_{xx0} + M^{-1}_{xx1})\widetilde{\delta F_x} + (\cancel{M^{-1}_{x\theta0}} + M^{-1}_{x\theta1})\widetilde{\delta F_\theta} \\
s(\widetilde{v_{\theta0}} + \widetilde{v_{\theta1}}) - v_\theta(0) &= -(\cancel{\gamma_{0\theta x0}} + \gamma_{0\theta x1})(\widetilde{v_{x0}} + \cancel{\widetilde{v_{x1}}}) - (\gamma_{0\theta\theta0}+\gamma_{0\theta\theta1})(\widetilde{v_{\theta0}} + \widetilde{v_{\theta1}}) \\
&\quad + (\cancel{M^{-1}_{\theta x0}} + M^{-1}_{\theta x1})\widetilde{\delta F_x} + (M^{-1}_{\theta\theta0} + M^{-1}_{\theta\theta1})\widetilde{\delta F_\theta}
\end{aligned}
\tag{53}
$$

Recall

$$
\begin{aligned}
s\widetilde{v_{x0}} - v_x(0) &= -\gamma_{0xx0}\widetilde{v_{x0}} + M^{-1}_{xx0}\widetilde{\delta F_x} \\
s\widetilde{v_{\theta0}} - v_\theta(0) &= -\gamma_{0\theta\theta0}\widetilde{v_{\theta0}} + M^{-1}_{\theta\theta0}\widetilde{\delta F_x}
\end{aligned}
$$

After eliminate zero-order and second-order terms, we have

$$
\begin{aligned}
(s+\gamma_{0xx0})\widetilde{v_{x1}} &= -\gamma_{0xx1}\widetilde{v_{x0}} - \gamma_{0x\theta1}\widetilde{v_{\theta0}} + M^{-1}_{xx1}\widetilde{\delta F_x} + M^{-1}_{x\theta1}\widetilde{\delta F_\theta} \\
(s+\gamma_{0\theta\theta0})\widetilde{v_{\theta1}} &= -\gamma_{0\theta x1}\widetilde{v_{x0}} - \gamma_{0\theta\theta1}\widetilde{v_{\theta0}} + M^{-1}_{\theta x1}\widetilde{\delta F_x} + M^{-1}_{\theta\theta1}\widetilde{\delta F_\theta}
\end{aligned}
\tag{54}
$$

or as the equivalent

$$
\begin{aligned}
\widetilde{v_{x1}} &= \frac{1}{s+\gamma_{0xx0}}\left\{-\frac{\gamma_{0xx1}}{s+\gamma_{0xx0}}\left[v_x(0)+M^{-1}_{xx0}\widetilde{\delta F_x}\right]-\frac{\gamma_{0x\theta 1}}{s+\gamma_{0\theta\theta 0}}\left[v_\theta(0)+M^{-1}_{\theta\theta 0}\widetilde{\delta F_\theta}\right]+M^{-1}_{xx1}\widetilde{\delta F_x}+M^{-1}_{x\theta 1}\widetilde{\delta F_\theta}\right\}\\
\widetilde{v_{\theta 1}} &= \frac{1}{s+\gamma_{0\theta\theta 0}}\left\{-\frac{\gamma_{0\theta x1}}{s+\gamma_{0xx0}}\left[v_x(0)+M^{-1}_{xx0}\widetilde{\delta F_x}\right]-\frac{\gamma_{0\theta\theta 1}}{s+\gamma_{0\theta\theta 0}}\left[v_\theta(0)+M^{-1}_{\theta\theta 0}\widetilde{\delta F_\theta}\right]+M^{-1}_{\theta x1}\widetilde{\delta F_x}+M^{-1}_{\theta\theta 1}\widetilde{\delta F_\theta}\right\}
\end{aligned}
\tag{55}
$$

After the inverse Laplace transform, it yields

$$
\begin{aligned}
v_{x1}(t) = {} & -v_x(0)\gamma_{0,\mathrm{xx}1}te^{-\gamma_{0,\mathrm{xx}0}t}+\frac{v_\theta(0)\gamma_{0,\mathrm{x}\theta 1}}{\gamma_{0,\mathrm{xx}0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx}0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right)\\
& -\gamma_{0,xx1}\int_0^t \mathrm{d}\tau(t-\tau)e^{-\gamma_{0,xx0}(t-\tau)}M^{-1}_{xx0}\delta F_x(\tau)\\
& +\frac{\gamma_{0,x\theta 1}}{\gamma_{0,\theta\theta 0}-\gamma_{0,xx0}}\int_0^t \mathrm{d}\tau\left(e^{-\gamma_{0,\theta\theta 0}(t-\tau)}-e^{-\gamma_{0,xx0}(t-\tau)}\right)M^{-1}_{\theta\theta 0}\delta F_\theta(\tau)\\
& +\int_0^t \mathrm{d}\tau e^{-\gamma_{0,xx0}(t-\tau)}\left[M^{-1}_{xx1}\delta F_x(\tau)+M^{-1}_{x\theta 1}\delta F_\theta(\tau)\right]
\end{aligned}
\tag{56}
$$

$$
\begin{aligned}
v_{\theta 1}(t) = {} & -v_\theta(0)\gamma_{0,\theta\theta 1}te^{-\gamma_{0,\theta\theta 0}t}+\frac{v_x(0)\gamma_{0,\theta\mathrm{x}1}}{\gamma_{0,\mathrm{xx}0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx}0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right)\\
& +\frac{\gamma_{0,\theta x1}}{\gamma_{0,\theta\theta 0}-\gamma_{0,xx0}}\int_0^t \mathrm{d}\tau\left(e^{-\gamma_{0,\theta\theta 0}(t-\tau)}-e^{-\gamma_{0,xx0}(t-\tau)}\right)M^{-1}_{xx0}\delta F_x(\tau)\\
& -\gamma_{0,\theta\theta 1}\int_0^t \mathrm{d}\tau(t-\tau)e^{-\gamma_{0,\theta\theta 0}(t-\tau)}M^{-1}_{\theta\theta 0}\delta F_\theta(\tau)\\
& +\int_0^t \mathrm{d}\tau e^{-\gamma_{0,\theta\theta 0}(t-\tau)}\left[M^{-1}_{\theta x1}\delta F_x(\tau)+M^{-1}_{\theta\theta 1}\delta F_\theta(\tau)\right]
\end{aligned}
\tag{57}
$$

Finally, we suppose $\left\langle v_i(t_1)\delta F_j(t_2)\right\rangle \equiv 0$ for the calculations toward $\left\langle v_i^2(t)\right\rangle$

$$\begin{aligned}
\left\langle v_x^2(t)\right\rangle &= \left\langle [v_{x0}(t)+v_{x1}(t)]^2\right\rangle = \left\langle v_{x0}^2(t)+2v_{x0}(t)v_{x1}(t)+v_{x1}^2(t)\right\rangle = \left\langle v_{x0}^2(t)\right\rangle + 2\left\langle v_{x0}(t)v_{x1}(t)\right\rangle + \cancel{\left\langle v_{x1}^2(t)\right\rangle}\\
&= \left\langle v_x^2(0)\right\rangle e^{-2\gamma_{0,xx0}t} + \frac{k_BT}{m_x}\left(1-e^{-2\gamma_{0,xx0}t}\right)\\
&\quad + 2e^{-\gamma_{0,xx0}t}\left[\left\langle v_x^2(0)\right\rangle \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,xx0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right) - \left\langle v_x(0)v_\theta(0)\right\rangle \gamma_{0,\theta\theta 1}te^{-\gamma_{0,\theta\theta 0}t}\right]\\
&\quad + \left\langle \int_0^t \mathrm{d}\tau_1 \frac{\delta F_x}{m_x} e^{-\gamma_{0,xx0}(t-\tau_1)}\left[-\gamma_{0,xx1}\int_0^t \mathrm{d}\tau_2 (t-\tau_2)e^{-\gamma_{0,xx0}(t-\tau_2)}M_{xx0}^{-1}\delta F_x(\tau_2)\right.\right.\\
&\qquad \left.\left. + \int_0^t \mathrm{d}\tau_2 e^{-\gamma_{0,xx0}(t-\tau_2)}M_{xx1}^{-1}\delta F_x(\tau_2)\right]\right\rangle\\
&= \left\langle v_x^2(0)\right\rangle e^{-2\gamma_{0,xx0}t} + \frac{k_BT}{m_x}\left(1-e^{-2\gamma_{0,xx0}t}\right)\\
&\quad + 2e^{-\gamma_{0,xx0}t}\left[\left\langle v_x^2(0)\right\rangle \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,xx0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right) - \left\langle v_x(0)v_\theta(0)\right\rangle \gamma_{0,\theta\theta 1}te^{-\gamma_{0,\theta\theta 0}t}\right]\\
&\quad + k_BT\left[M_{xx1}^{-1}\left(1-e^{-2\gamma_{0,xx0}t}\right) - \frac{\gamma_{0,xx1}M_{xx0}^{-1}}{2\gamma_{0,xx0}}e^{-2\gamma_{0,xx0}t}\left(-1+e^{2\gamma_{0,xx0}t}-2t\gamma_{0,xx0}\right)\right]
\end{aligned}$$

$$\begin{aligned}
\left\langle v_\theta^2(t)\right\rangle &= \left\langle [v_{\theta 0}(t)+v_{\theta 1}(t)]^2\right\rangle = \left\langle v_{\theta 0}^2(t)+2v_{\theta 0}(t)v_{\theta 1}(t)+v_{\theta 1}^2(t)\right\rangle = \left\langle v_{\theta 0}^2(t)\right\rangle + 2\left\langle v_{\theta 0}(t)v_{\theta 1}(t)\right\rangle + \cancel{\left\langle v_{\theta 1}^2(t)\right\rangle}\\
&= \left\langle v_\theta^2(0)\right\rangle e^{-2\gamma_{0,\theta\theta 0}t} + \frac{k_BT}{m_\theta}\left(1-e^{-2\gamma_{0,\theta\theta 0}t}\right)\\
&\quad + 2e^{-2\gamma_{0,\theta\theta 0}t}\left[-\left\langle v_\theta^2(0)\right\rangle \gamma_{0,\theta\theta 1}te^{-\gamma_{0,\theta\theta 0}t} + \frac{\left\langle v_\theta(0)v_x(0)\right\rangle \gamma_{0,\theta x1}}{\gamma_{0,xx0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,xx0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right)\right]\\
&\quad + \left\langle \int_0^t \mathrm{d}\tau_1 \frac{\delta F_\theta(\tau_1)}{m_\theta} e^{-\gamma_{0,\theta\theta 0}(t-\tau_1)}\cdot\left\{\int_0^t \mathrm{d}\tau_2 e^{-\gamma_{0,\theta\theta 0}(t-\tau_2)}\delta F_\theta(\tau_2)\left[M_{\theta\theta 1}^{-1}-\gamma_{0,\theta\theta 1}(t-\tau_2)e^{-\gamma_{0,\theta\theta 0}(t-\tau_2)}M_{\theta\theta 0}^{-1}\right]\right\}\right\rangle\\
&= \left\langle v_\theta^2(0)\right\rangle e^{-2\gamma_{0,\theta\theta 0}t} + \frac{k_BT}{m_\theta}\left(1-e^{-2\gamma_{0,\theta\theta 0}t}\right)\\
&\quad + 2e^{-2\gamma_{0,\theta\theta 0}t}\left[-\left\langle v_\theta^2(0)\right\rangle \gamma_{0,\theta\theta 1}te^{-\gamma_{0,\theta\theta 0}t} + \frac{\left\langle v_\theta(0)v_x(0)\right\rangle \gamma_{0,\theta x1}}{\gamma_{0,xx0}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,xx0}t}-e^{-\gamma_{0,\theta\theta 0}t}\right)\right]\\
&\quad + k_BT\left[M_{\theta\theta 1}^{-1}\left(1-e^{-2\gamma_{0,\theta\theta 0}t}\right) - \frac{\gamma_{0,\theta\theta 1}M_{\theta\theta 0}^{-1}}{2\gamma_{0,\theta\theta 0}}e^{-2\gamma_{0,\theta\theta 0}t}\left(-1+e^{2\gamma_{0,\theta\theta 0}t}-2t\gamma_{0,\theta\theta 0}\right)\right]
\end{aligned}$$

2.4 Mean square displacement

Since there is no correlation between $v_i(t)$ and $\delta F_j(t)$, $\left\langle v_i(t_1)\delta F_j(t_2)\right\rangle = 0$. Note $m_x \left\langle v_x^2(0)\right\rangle/2 = k_B T/2$, $m_\theta \left\langle v_\theta^2(0)\right\rangle/2 = k_B T/2$, we suppose $\langle v_x(0)v_\theta(0)\rangle = \langle v_\theta(0)v_x(0)\rangle = k_B T/m_{x\theta}$.

$$\begin{aligned}
\langle v_x(0)v_x(t)\rangle &= \langle v_x(0)\left[v_{x0}(t)+v_{x1}(t)\right]\rangle = \langle v_x(0)v_{x0}(t)\rangle + \langle v_x(0)v_{x1}(t)\rangle \\
&= \left\langle v_x^2(0)\right\rangle e^{-\gamma_{0,xx0}t}\left(1-\gamma_{0,xx1}t\right) + \langle v_x(0)v_\theta(0)\rangle \frac{\gamma_{0,\mathrm{x}\theta 1}}{\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx0}}t}-e^{-\gamma_{0,\theta\theta 0}t}\right) \\
&= \frac{k_B T}{m_x} e^{-\gamma_{0,xx0}t}\left(1-\gamma_{0,xx1}t\right) + \frac{k_B T}{m_{x\theta}}\frac{\gamma_{0,\mathrm{x}\theta 1}}{\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx0}}t}-e^{-\gamma_{0,\theta\theta 0}t}\right) \\
\langle v_\theta(0)v_\theta(t)\rangle &= \langle v_\theta(0)\left[v_{\theta 0}(t)+v_{\theta 1}(t)\right]\rangle = \langle v_\theta(0)v_{\theta 0}(t)\rangle + \langle v_\theta(0)v_{\theta 1}(t)\rangle \\
&= \left\langle v_\theta^2(0)\right\rangle e^{-\gamma_{0,\theta\theta 0}t}\left(1-\gamma_{0,\theta\theta 1}t\right) + \langle v_\theta(0)v_x(0)\rangle \frac{\gamma_{0,\theta\mathrm{x}1}}{\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx0}}t}-e^{-\gamma_{0,\theta\theta 0}t}\right) \\
&= \frac{k_B T}{m_\theta} e^{-\gamma_{0,\theta\theta 0}t}\left(1-\gamma_{0,\theta\theta 1}t\right) + \frac{k_B T}{m_{x\theta}}\frac{\gamma_{0,\theta\mathrm{x}1}}{\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}}\left(e^{-\gamma_{0,\mathrm{xx0}}t}-e^{-\gamma_{0,\theta\theta 0}t}\right)
\end{aligned}$$

$$\left\langle \Delta r_x^2(t)\right\rangle = \left\langle \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2 v_x(\tau_1)v_x(\tau_2)\right\rangle \qquad \left\langle \Delta r_\theta^2(t)\right\rangle = \left\langle \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2 v_\theta(\tau_1)v_\theta(\tau_2)\right\rangle$$

We have the derivatives

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Delta r_x^2(t)\right\rangle = 2\int_0^t \mathrm{d}\tau \,\langle v_x(0)v_x(\tau)\rangle = 2k_B T\times$$
$$\left(\frac{1-e^{-t\gamma_{0,\mathrm{xx0}}}}{m_x\gamma_{0,\mathrm{xx0}}} - \frac{\gamma_{0,\mathrm{xx1}}\left(1-e^{-t\gamma_{0,\mathrm{xx0}}}\left(t\gamma_{0,\mathrm{xx0}}+1\right)\right)}{m_x\gamma_{0,\mathrm{xx0}}^2} + \frac{\gamma_{0,x\theta 1}}{m_{x\theta}(\gamma_{0,xx0}-\gamma_{0,\theta\theta 0})}\left(\frac{1-e^{-\gamma_{0,xx0}t}}{\gamma_{0,xx0}} - \frac{1-e^{-\gamma_{0,\theta\theta 0}t}}{\gamma_{0,\theta\theta 0}}\right)\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Delta r_\theta^2(t)\right\rangle = 2\int_0^t \mathrm{d}\tau \,\langle v_\theta(0)v_\theta(\tau)\rangle = 2k_B T\times$$
$$\left(\frac{1-e^{-t\gamma_{0,\theta\theta 0}}}{m_\theta\gamma_{0,\theta\theta 0}} - \frac{\gamma_{0,\theta\theta 1}\left(1-e^{-t\gamma_{0,\theta\theta 0}}\left(t\gamma_{0,\theta\theta 0}+1\right)\right)}{m_x\gamma_{0,\theta\theta 0}^2} + \frac{\gamma_{0,\theta x 1}}{m_{x\theta}(\gamma_{0,xx0}-\gamma_{0,\theta\theta 0})}\left(\frac{1-e^{-\gamma_{0,xx0}t}}{\gamma_{0,xx0}} - \frac{1-e^{-\gamma_{0,\theta\theta 0}t}}{\gamma_{0,\theta\theta 0}}\right)\right)$$

Then the second integration for $\left\langle \Delta r_i^2(t)\right\rangle$

$$\left\langle \Delta r_x^2(t)\right\rangle = \left\langle \Delta r_x^2(0)\right\rangle +$$
$$k_B T\left(\frac{\frac{e^{-t\gamma_{0,\mathrm{xx0}}}-1}{\gamma_{0,\mathrm{xx0}}}+t}{m_x\gamma_{0,\mathrm{xx0}}} + \frac{\gamma_{0,\mathrm{x}\theta 1}\left(\frac{e^{-t\gamma_{0,\mathrm{xx0}}}-1}{\gamma_{0,\mathrm{xx0}}}+t\right)}{\gamma_{0,\mathrm{xx0}}m_{x\theta}\left(\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}\right)} - \frac{\gamma_{0,\mathrm{x}\theta 1}\left(\frac{e^{-t\gamma_{0,\theta\theta 0}}-1}{\gamma_{0,\theta\theta 0}}+t\right)}{\gamma_{0,\theta\theta 0}m_{x\theta}\left(\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}\right)} - \frac{\gamma_{0,\mathrm{xx1}}\left(t-\frac{2-e^{-t\gamma_{0,\mathrm{xx0}}}\left(t\gamma_{0,\mathrm{xx0}}+2\right)}{\gamma_{0,\mathrm{xx0}}}\right)}{m_x\gamma_{0,\mathrm{xx0}}^2}\right)$$

$$\left\langle \Delta r_\theta^2(t)\right\rangle = \left\langle \Delta r_x^2(0)\right\rangle +$$
$$k_B T\left(\frac{\frac{e^{-t\gamma_{0,\theta\theta 0}}-1}{\gamma_{0,\theta\theta 0}}+t}{m_\theta\gamma_{0,\theta\theta 0}} + \frac{\gamma_{0,\theta\mathrm{x}1}\left(\frac{e^{-t\gamma_{0,\mathrm{xx0}}}-1}{\gamma_{0,\mathrm{xx0}}}+t\right)}{\gamma_{0,\mathrm{xx0}}m_{x\theta}\left(\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}\right)} - \frac{\gamma_{0,\theta\mathrm{x}1}\left(\frac{e^{-t\gamma_{0,\theta\theta 0}}-1}{\gamma_{0,\theta\theta 0}}+t\right)}{\gamma_{0,\theta\theta 0}m_{x\theta}\left(\gamma_{0,\mathrm{xx0}}-\gamma_{0,\theta\theta 0}\right)} - \frac{\gamma_{0,\theta\theta 1}\left(t-\frac{2-e^{-t\gamma_{0,\theta\theta 0}}(t+\gamma_{0,\theta\theta 0}+2)}{\gamma_{0,\theta\theta 0}}\right)}{m_\theta\gamma_{0,\theta\theta 0}^2}\right)$$

3 Numerical Practice

3.1 Discretisation algorithm

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

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

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, $b_{ij} = \delta_{ij}\sqrt{\frac{2}{\gamma_i\Delta t}\tanh\frac{\gamma_i\Delta t}{2}}$

We follow the Box–Muller transform to generate normally distributed random variables. This method uses two independent random numbers U and V distributed uniformly on $(0,1)$. Then the two random variables X and Y

$$X = \sqrt{-2\ln U}\cos(2\pi V) \qquad Y = \sqrt{-2\ln U}\sin(2\pi V)$$

will both have the standard normal distribution, and will be independent.

3.2 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?