

Brownian motion near a Soft Surface

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Update: March 16, 2023

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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 fluid,

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

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 $\langle \delta F_i(t) \delta F_j(t') \rangle = 2\xi k_B T \delta_{ij} \delta(t - t')$

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:

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

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

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

Derivation from the over-damped Langevin equation

Let $\mathbb{P}(x, t)$ be the probability 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:

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

but using Itô's chain rule:

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

with Langevin's equation

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

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

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

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

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

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:

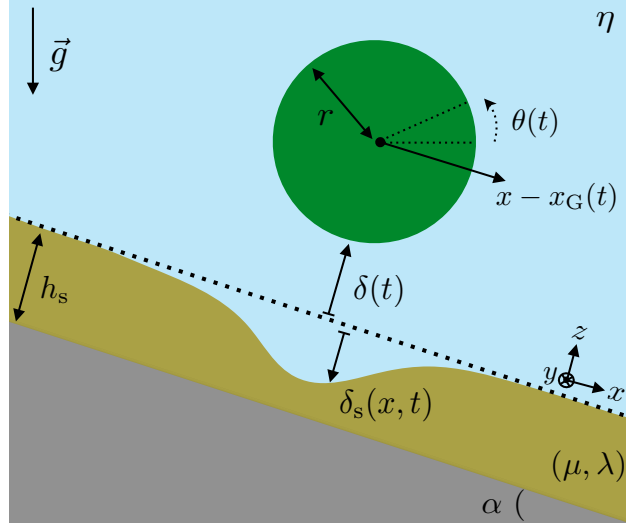


FIG. 1: Schematic of the system. A negatively buoyant cylinder (green) falls down under the acceleration of gravity \vec{g} , inside a viscous fluid (blue), in the vicinity of a thin soft wall (brown). The ensemble lies atop a tilted, infinitely rigid support (grey).

The deformation of the soft wall reads:

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

as well as the dimensionless parameters: $z = Zr\epsilon$, $h = Hr\epsilon$, $\delta = \Delta r\epsilon$, $x = Xr\sqrt{2\epsilon}$, $x_G = X_G r\sqrt{2\epsilon}$, $\theta = \Theta\sqrt{2\epsilon}$, $t = Tr\sqrt{2\epsilon}/c$, $u = Uc$, and $p = P\eta c\sqrt{2}/(r\epsilon^{3/2})$; 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.

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

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

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

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

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

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)

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

and (\mathbf{X}, \mathbf{V}) refer to the position and the velocity, respectively)

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

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

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

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

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

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

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

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

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

The last two terms would vanish since

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

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

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

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

We obtain the GB distribution for the steady state if

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

We have for small velocities that

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

and so we find

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

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

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

and we write

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

and

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

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

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

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

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

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

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

Form this we find that

$$\sum_{\alpha\beta} \Lambda_{z\alpha\beta} V_\alpha V_\beta = \frac{21\kappa\xi}{4} \frac{V_z^2}{Z^{9/2}} - \frac{\kappa\xi}{4} \frac{V_x^2}{Z^{7/2}} \quad (\text{David.14})$$

$$\sum_{\alpha\beta} \Lambda_{x\alpha\beta} V_\alpha V_\beta = \frac{19\kappa\xi\varepsilon}{24} \frac{V_z V_x}{Z^{7/2}}$$

This gives the set of equations

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

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

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

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

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

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

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

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

as well as

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

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

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

which can be written as

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

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

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

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

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

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:

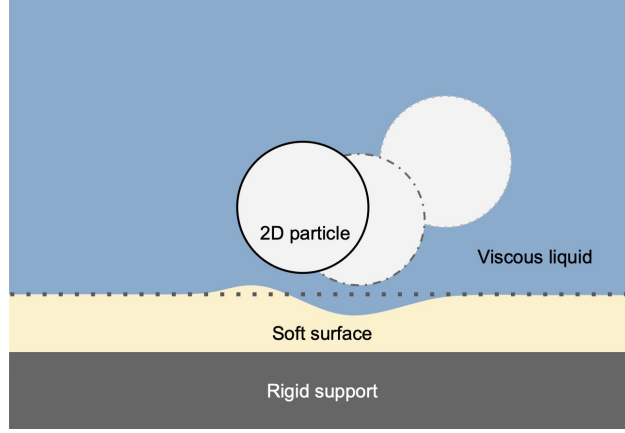


Figure 1: Brownian motion near a soft surface

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

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

At long time limit, $\langle v^2(t) \rangle \rightarrow \frac{k_B T}{m}$. 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 $\langle \delta F(0) \delta F(t) \rangle = 2k_B T \zeta \delta(t)$. We then write $\delta F(t) = \sqrt{2k_B T \gamma m} \eta(t)$, 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 $\eta(t) = dW/dt$. 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)

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

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](#),

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

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

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

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

Similarly, we write the eqs [Salez2015.50](#) and [Salez2015.52](#) as

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

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

with all coefficients we need: $b_1 = \frac{2\xi\xi}{3}$, $b_2 = \frac{19\kappa\xi\xi}{24}$, $b_3 = -\frac{\kappa\xi\xi}{6}$, $b_4 = \frac{\kappa\xi\xi}{12}$, $b_5 = -\frac{\kappa\xi\xi}{12}$, $b_6 = \sin(\alpha = 0) = 0$; and $c_1 = \frac{4\xi\xi}{3}$, $c_2 = \frac{19\kappa\xi\xi}{12}$, $c_3 = -\frac{\kappa\xi\xi}{3}$, $c_4 = \frac{\kappa\xi\xi}{6}$, $c_5 = -\frac{\kappa\xi\xi}{6}$, $c_6 = 0$. 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

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

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

Compare with the eq. [1](#), we finally remove the second derivatives inside each expression

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

See eqs [David.5](#) ~ [David.9](#), we could extract these $\lambda_{\alpha\beta}$ and $\Gamma_{\alpha\beta\beta}$ by

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

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

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

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

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

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

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

$$\lambda_{zx} = \lambda_{xz} = \lambda_{z\theta} = \lambda_{\theta z} = 0 \quad (15)$$

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

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

$$\begin{aligned} \Gamma_{zxz} = \Gamma_{zzx} = \Gamma_{zz\theta} = \Gamma_{z\theta z} &= 0 \\ \Gamma_{xzz} = \Gamma_{xxz} = \Gamma_{\theta zz} = \Gamma_{\theta\theta\theta} &= 0 \end{aligned} \quad (17)$$

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

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

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

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

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

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

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

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

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

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

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

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

Similarly, there are cross terms for X, Θ components

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

$$F_{1hX} = -m_X \left(b_1 \frac{\dot{X}}{\sqrt{\Delta}} + b_2 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + b_3 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + b_6 \right) \quad (30)$$

$$F_{2hXZ} = 0 \quad F_{2hXX} = -\frac{m_X b_5}{\Delta^{5/2}} \quad F_{2hX\Theta} = -\frac{m_X b_4}{\Delta^{5/2}}$$

and

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

$$F_{1h\Theta} = -m_\Theta \left(c_1 \frac{\dot{\Theta}}{\sqrt{\Delta}} + c_2 \frac{\dot{\Delta}\dot{\Theta}}{\Delta^{7/2}} + c_3 \frac{\dot{\Delta}\dot{X}}{\Delta^{7/2}} + c_6 \right) \quad (32)$$

$$F_{2h\Theta Z} = 0 \quad F_{2h\Theta X} = -\frac{m_\Theta c_4}{\Delta^{5/2}} \quad F_{2h\Theta\Theta} = -\frac{m_\Theta c_5}{\Delta^{5/2}}$$

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

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

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

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

and its inverse matrix

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

with the approximation expressed by the series of κ :

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

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

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

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

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

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

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

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

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

where Ψ is zero-order matrix of κ , $\Psi_i = \text{SeriesCoefficients}[\text{Series}[\gamma_{\text{eff},ii}, \{\kappa, 0, 0\}], 0]$; and Φ the first-order one, $\Phi_i = \text{SeriesCoefficients}[\text{Series}[\gamma_{\text{eff},ij}, \{\kappa, 0, 1\}], 1]$. 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

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

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:

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

and non-diagonal elements

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

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

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

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

$$\dot{\mathbf{v}}_{3 \times 1} = -\gamma_{\text{eff}, 3 \times 3} \cdot \mathbf{v}_{3 \times 1} + M_{3 \times 3}^{-1} \cdot \delta F_{3 \times 1} \quad (43)$$

and consider the corresponding Laplace transform

$$\widetilde{\mathbf{v}}_{3 \times 1} = -\widetilde{\gamma_{\text{eff}} \cdot \mathbf{v}} + \widetilde{M^{-1} \cdot \delta F} \quad (44)$$

Note that it contains velocities in γ_{eff} rather than a constant coefficient.

Dissect γ_{eff} as $\gamma_{\text{eff}} = \gamma_0 + \gamma_1(\kappa) + \gamma_{1v}(\kappa, v_i)$,

$$\gamma_0 = \begin{pmatrix} \frac{\xi}{\Delta^{3/2}} & 0 & 0 \\ 0 & \frac{2\xi\epsilon}{3\sqrt{\Delta}} & 0 \\ 0 & 0 & \frac{4\xi\epsilon}{3\sqrt{\Delta}} \end{pmatrix} \quad \gamma_1 = \begin{pmatrix} \frac{15\kappa\xi^2}{8\Delta^4} & 0 & 0 \\ 0 & \frac{\kappa\xi^2\epsilon^2}{18\Delta^3} & -\frac{\kappa\xi^2\epsilon^2}{9\Delta^3} \\ 0 & -\frac{\kappa\xi^2\epsilon^2}{9\Delta^3} & \frac{2\kappa\xi^2\epsilon^2}{9\Delta^3} \end{pmatrix} \quad (45)$$

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

where γ_0 is constant matrix, independent on κ ; γ_1 depends on κ ; and γ_{1v} depends on κ and velocities v_i . Hence we could separate the transform as $\widetilde{\gamma_{\text{eff}} \cdot \mathbf{v}} = \widetilde{\gamma_0 \cdot \mathbf{v}} + \widetilde{\gamma_1 \cdot \mathbf{v}} + \widetilde{\gamma_{1v} \cdot \mathbf{v}}$. 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 i th component turns to

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

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

We are inclined to neglect all $g_{\mu\alpha\beta}(\widetilde{v}^\alpha v^\beta)$ at first, which would be reasonable 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 .

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

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

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

with the solution as

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

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

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

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:

$$\widetilde{v}_{i0}^2 = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \left[\frac{v_i(0)}{s + \gamma_{0ii0}} + \frac{M_{ii0}^{-1} \widetilde{\delta F}_i(s)}{s + \gamma_{0ii0}} \right] \times \left[\frac{v_i(0)}{p - s + \gamma_{0ii0}} + \frac{M_{ii0}^{-1} \widetilde{\delta F}_i(p - s)}{p - s + \gamma_{0ii0}} \right] ds$$

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

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

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:

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

Note $\mathcal{L}_t \left[\int_0^t f(\tau)g(t-\tau) d\tau \right] (s) = (\mathcal{L}_t[f(t)](s))(\mathcal{L}_t[g(t)](s))$, namely the Laplace transform of convolution is the multiplication of two Laplace transforms.

$$\mathcal{L}_s^{-1} \left[-\frac{\gamma_{0,zz1}}{(\gamma_{0,zz0} + s)^2} \right] (t) = t\gamma_{0,zz1} (-e^{-t\gamma_{0,zz0}}) \quad \mathcal{L}_s^{-1} \left[\frac{1}{\gamma_{0,zz0} + s} \right] (t) = e^{-t\gamma_{0,zz0}}$$

With the inverse Laplace transform above, we get $v_{z1}(t)$

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

We calculate the velocity square average up to 1-order κ :

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

Suppose there exists the correlation between 0-order and 1-order random force, with the relation

$\langle \delta F_{z0}(\tau_1) \delta F_{z1}(\tau_2) \rangle = K_z \cdot \delta(\tau_1 - \tau_2)$. So at long time limit $t \rightarrow \infty$, $\langle v_z^2(t) \rangle$ would converge to

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

Finally, we have the modified noise amplitude of z at 1-order correction.

$$\begin{aligned} \langle \delta F_z(\tau_1) \delta F_z(\tau_2) \rangle &= \langle [\delta F_{z0}(\tau_1) + \delta F_{z1}(\tau_1)] \cdot [\delta F_{z0}(\tau_2) + \delta F_{z1}(\tau_2)] \rangle \\ &= \langle \delta F_{z0}(\tau_1) \delta F_{z0}(\tau_2) \rangle + 2 \langle \delta F_{z0}(\tau_1) \delta F_{z1}(\tau_2) \rangle + \langle \delta F_{z1}(\tau_1) \delta F_{z1}(\tau_2) \rangle \\ &= 2k_B T m_z \gamma_{0,zz0} \delta(\tau_1 - \tau_2) + 2k_B T m_z \left(\gamma_{0,zz1} - 2\gamma_{0,zz0} m_z M_{zz1}^{-1} \right) \delta(\tau_1 - \tau_2) \\ &= 2k_B T m_z \delta(\tau_1 - \tau_2) \cdot \left(\gamma_{0,zz0} + \gamma_{0,zz1} - 2\gamma_{0,zz0} m_z M_{zz1}^{-1} \right) \end{aligned} \quad (50)$$

Note $M_{zz1}^{-1} = \frac{15\kappa\xi}{8\Delta^{5/2}m_z}$, $\gamma_{0,zz} = \frac{\xi}{\Delta^{3/2}} + \frac{15\kappa\xi^2}{8\Delta^4}$, we could calculate

$$\gamma_{0,zz0} + \gamma_{0,zz1} - 2\gamma_{0,zz0} m_z M_{zz1}^{-1} = \frac{\xi}{\Delta^{3/2}} + \frac{15\kappa\xi^2}{8\Delta^4} - 2 \times \frac{15\kappa\xi}{8\Delta^{5/2}} \times \frac{\xi}{\Delta^{3/2}} = \frac{\xi}{\Delta^{3/2}} - \frac{15\kappa\xi^2}{8\Delta^4}$$

and then an amazingly concise result:

$$\langle \delta F_z(\tau_1) \delta F_z(\tau_2) \rangle = 2k_B T m_z \delta(\tau_1 - \tau_2) \cdot (\gamma_{0,zz0} - \gamma_{0,zz1}) \quad (51)$$

which is always valid at 1-order correction, since $\gamma_{0,zz0} = \frac{a_1}{\Delta^{3/2}}$, $\gamma_{0,zz1} = -\frac{a_1 a_5}{\Delta^4}$, $M_{zz1}^{-1} = -\frac{a_5}{\Delta^{5/2} m_z}$.

$$\gamma_{0,zz0} + \gamma_{0,zz1} - 2\gamma_{0,zz0} m_z M_{zz1}^{-1} = \frac{a_1}{\Delta^{3/2}} + \frac{a_5 a_1}{\Delta^4} = \gamma_{0,zz0} - \gamma_{0,zz1}$$

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:

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

with solutions as

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

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

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

with the parameter

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

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

Note that second-order correction of κ has been introduced indirectly owing to γ_s ; to be exact, $\gamma_{0\theta x}\gamma_{0x\theta} = \gamma_{0\theta x1}\gamma_{0x\theta1} \propto \kappa^2$. Therefore, the result after the inverse Laplace transform would be quite complicated, and we could hardly furnish a concise inverse transform including $\widetilde{\delta F_i}$. 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 $\widetilde{v}_\theta = \widetilde{v}_{\theta0} + \widetilde{v}_{\theta1}$. Also, $\delta F_x = \delta F_{x0} + \delta F_{x1}$, and $\delta F_\theta = \delta F_{\theta0} + \delta F_{\theta1}$. Similar for coefficients $\gamma_{0ij} = \gamma_{0ij0} + \gamma_{0ij1}$, $\gamma_{0ij0} = 0$ if $i \neq j$; while $M_{ij}^{-1} = M_{ij0}^{-1} + M_{ij1}^{-1}$, $M_{ij0}^{-1} = 0$ if $i \neq j$. So we expand the Laplace transform to first-order correction of κ as the following expressions:

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

Recall

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

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

$$\begin{aligned} (s + \gamma_{0xx0})\widetilde{v}_{x1} &= -\gamma_{0xx1}\widetilde{v}_{x0} - \gamma_{0x\theta1}\widetilde{v}_{\theta0} + M_{xx1}^{-1}\delta \widetilde{F}_{x0} + M_{x\theta1}^{-1}\delta \widetilde{F}_{\theta0} + M_{xx0}^{-1}\delta \widetilde{F}_{x1} \\ (s + \gamma_{0\theta\theta0})\widetilde{v}_{\theta1} &= -\gamma_{0\theta x1}\widetilde{v}_{x0} - \gamma_{0\theta\theta1}\widetilde{v}_{\theta0} + M_{\theta x1}^{-1}\delta \widetilde{F}_{x0} + M_{\theta\theta1}^{-1}\delta \widetilde{F}_{\theta0} + M_{\theta\theta0}^{-1}\delta \widetilde{F}_{\theta1} \end{aligned} \quad (54)$$

or as the equivalent

$$\begin{aligned}
\widetilde{v_{x1}} &= \frac{1}{s + \gamma_{0xx0}} \times \\
&\quad \left\{ -\frac{\gamma_{0xx1}}{s + \gamma_{0xx0}} \left[v_x(0) + M_{xx0}^{-1} \widetilde{\delta F_{x0}} \right] - \frac{\gamma_{0x\theta1}}{s + \gamma_{0\theta\theta0}} \left[v_\theta(0) + M_{\theta\theta0}^{-1} \widetilde{\delta F_{\theta0}} \right] + M_{xx1}^{-1} \widetilde{\delta F_{x0}} + M_{x\theta1}^{-1} \widetilde{\delta F_{\theta0}} + M_{xx0}^{-1} \widetilde{\delta F_{x1}} \right\} \\
\widetilde{v_{\theta1}} &= \frac{1}{s + \gamma_{0\theta\theta0}} \times \\
&\quad \left\{ -\frac{\gamma_{0\theta x1}}{s + \gamma_{0xx0}} \left[v_x(0) + M_{xx0}^{-1} \widetilde{\delta F_{x0}} \right] - \frac{\gamma_{0\theta\theta1}}{s + \gamma_{0\theta\theta0}} \left[v_\theta(0) + M_{\theta\theta0}^{-1} \widetilde{\delta F_{\theta0}} \right] + M_{\theta x1}^{-1} \widetilde{\delta F_{x0}} + M_{\theta\theta1}^{-1} \widetilde{\delta F_{\theta0}} + M_{\theta\theta0}^{-1} \widetilde{\delta F_{\theta1}} \right\}
\end{aligned} \tag{55}$$

After the inverse Laplace transform, it yields

$$\begin{aligned}
v_{x1}(t) &= -v_x(0)\gamma_{0,xx1}te^{-\gamma_{0,xx0}t} + \frac{v_\theta(0)\gamma_{0,x\theta1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx0}t} - e^{-\gamma_{0,\theta\theta0}t}) \\
&\quad - \gamma_{0,xx1} \int_0^t d\tau (t - \tau) e^{-\gamma_{0,xx0}(t-\tau)} M_{xx0}^{-1} \delta F_{x0}(\tau) \\
&\quad + \frac{\gamma_{0,x\theta1}}{\gamma_{0,\theta\theta0} - \gamma_{0,xx0}} \int_0^t d\tau \left(e^{-\gamma_{0,\theta\theta0}(t-\tau)} - e^{-\gamma_{0,xx0}(t-\tau)} \right) M_{\theta\theta0}^{-1} \delta F_{\theta0}(\tau) \\
&\quad + \int_0^t d\tau e^{-\gamma_{0,xx0}(t-\tau)} \left[M_{xx1}^{-1} \delta F_{x0}(\tau) + M_{x\theta1}^{-1} \delta F_{\theta0}(\tau) + M_{xx0}^{-1} \delta F_{x1}(\tau) \right]
\end{aligned} \tag{56}$$

$$\begin{aligned}
v_{\theta1}(t) &= -v_\theta(0)\gamma_{0,\theta\theta1}te^{-\gamma_{0,\theta\theta0}t} + \frac{v_x(0)\gamma_{0,\theta x1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx0}t} - e^{-\gamma_{0,\theta\theta0}t}) \\
&\quad + \frac{\gamma_{0,\theta x1}}{\gamma_{0,\theta\theta0} - \gamma_{0,xx0}} \int_0^t d\tau \left(e^{-\gamma_{0,\theta\theta0}(t-\tau)} - e^{-\gamma_{0,xx0}(t-\tau)} \right) M_{xx0}^{-1} \delta F_{x0}(\tau) \\
&\quad - \gamma_{0,\theta\theta1} \int_0^t d\tau (t - \tau) e^{-\gamma_{0,\theta\theta0}(t-\tau)} M_{\theta\theta0}^{-1} \delta F_{\theta0}(\tau) \\
&\quad + \int_0^t d\tau e^{-\gamma_{0,\theta\theta0}(t-\tau)} \left[M_{\theta x1}^{-1} \delta F_{x0}(\tau) + M_{\theta\theta1}^{-1} \delta F_{\theta0}(\tau) + M_{\theta\theta0}^{-1} \delta F_{\theta1}(\tau) \right]
\end{aligned} \tag{57}$$

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

$$\begin{aligned}
\langle v_x^2(t) \rangle &= \langle [v_{x0}(t) + v_{x1}(t)]^2 \rangle = \langle v_{x0}^2(t) + 2v_{x0}(t)v_{x1}(t) + v_{x1}^2(t) \rangle = \langle v_{x0}^2(t) \rangle + 2\langle v_{x0}(t)v_{x1}(t) \rangle + \langle v_{x1}^2(t) \rangle \\
&= \langle v_x^2(0) \rangle e^{-2\gamma_{0,xx0}t} + \frac{k_B T}{m_x} \left(1 - e^{-2\gamma_{0,xx0}t} \right) \\
&\quad + 2e^{-\gamma_{0,xx0}t} \left[\langle v_x^2(0) \rangle \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx0}t} - e^{-\gamma_{0,\theta\theta0}t}) - \langle v_x(0)v_\theta(0) \rangle \gamma_{0,\theta\theta1} t e^{-\gamma_{0,\theta\theta0}t} \right] \\
&\quad + 2 \left\langle \int_0^t d\tau_1 \frac{\delta F_{x0}(\tau_1)}{m_x} e^{-\gamma_{0,xx0}(t-\tau_1)} \left[-\gamma_{0,xx1} \int_0^t d\tau_2 (t-\tau_2) e^{-\gamma_{0,xx0}(t-\tau_2)} M_{xx0}^{-1} \delta F_{x0}(\tau_2) \right. \right. \\
&\quad \left. \left. + \int_0^t d\tau_2 e^{-\gamma_{0,xx0}(t-\tau_2)} \left(M_{xx1}^{-1} \delta F_{x0}(\tau_2) + M_{xx0}^{-1} \delta F_{x1}(\tau_2) \right) \right] \right\rangle \\
&= \langle v_x^2(0) \rangle e^{-2\gamma_{0,xx0}t} + \frac{k_B T}{m_x} \left(1 - e^{-2\gamma_{0,xx0}t} \right) \\
&\quad + 2e^{-\gamma_{0,xx0}t} \left[\langle v_x^2(0) \rangle \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx0}t} - e^{-\gamma_{0,\theta\theta0}t}) - \langle v_x(0)v_\theta(0) \rangle \gamma_{0,\theta\theta1} t e^{-\gamma_{0,\theta\theta0}t} \right] \\
&\quad + 2k_B T \left[-\gamma_{0,xx1} M_{xx0}^{-1} \frac{e^{-2\gamma_{0,xx0}t} (-1 + e^{2\gamma_{0,xx0}t} - 2\gamma_{0,xx0}t)}{2\gamma_{0,xx0}} + \left(2\gamma_{0,xx0} M_{xx1}^{-1} + \frac{\beta K_x}{m_x} M_{xx0}^{-1} \right) \frac{1 - e^{-2\gamma_{0,xx0}t}}{2\gamma_{0,xx0}} \right]
\end{aligned}$$

with $\langle \delta F_{x0}(\tau_1)\delta F_{x1}(\tau_2) \rangle = K_x \cdot \delta(\tau_1 - \tau_2)$. So at long time limit $t \rightarrow \infty$, the MSD converge to

$$\begin{aligned}
\langle v_x^2(t) \rangle &= \frac{k_B T}{m_x} + 2k_B T \left(\frac{-\gamma_{0,xx1} M_{xx0}^{-1}}{2\gamma_{0,xx0}} + M_{xx1}^{-1} + \frac{\beta K_x}{m_x} \frac{M_{xx0}^{-1}}{2\gamma_{0,xx0}} \right) = \frac{k_B T}{m_x} \\
K_x &= k_B T m_x \left(\gamma_{0,xx1} - 2m_x M_{xx1}^{-1} \gamma_{0,xx0} \right)
\end{aligned}$$

$$\begin{aligned}
\langle \delta F_x(\tau_1)\delta F_x(\tau_2) \rangle &\approx \langle \delta F_{x0}(\tau_1)\delta F_{x0}(\tau_2) \rangle + 2\langle \delta F_{x0}(\tau_1)\delta F_{x1}(\tau_2) \rangle \\
&= 2k_B T m_x \gamma_{0,xx0} \delta(\tau_1 - \tau_2) + 2K_x \delta(\tau_1 - \tau_2) = 2k_B T m_x \delta(\tau_1 - \tau_2) \left(\gamma_{0,xx0} + \gamma_{0,xx1} - 2m_x M_{xx1}^{-1} \gamma_{0,xx0} \right)
\end{aligned}$$

Note $\gamma_{0,xx} = \frac{2\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi^2\epsilon^2}{18\Delta^3}$, $M_{xx1}^{-1} = \frac{\kappa\xi\epsilon}{12\Delta^{5/2}m_x}$.

$$\gamma_{0,xx0} + \gamma_{0,xx1} - 2m_x M_{xx1}^{-1} \gamma_{0,xx0} = \frac{2\xi\epsilon}{3\sqrt{\Delta}} + \frac{\kappa\xi^2\epsilon^2}{18\Delta^3} - 2 \times \frac{\kappa\xi\epsilon}{12\Delta^{5/2}} \times \frac{2\xi\epsilon}{3\sqrt{\Delta}} = \frac{2\xi\epsilon}{3\sqrt{\Delta}} - \frac{\kappa\xi^2\epsilon^2}{18\Delta^3}$$

Similar to the modified noise correlator on z , we obtain again a concise result:

$$\langle \delta F_x(\tau_1)\delta F_x(\tau_2) \rangle = 2k_B T m_x \delta(\tau_1 - \tau_2) \cdot (\gamma_{0,xx0} - \gamma_{0,xx1}) \quad (58)$$

$$\begin{aligned}
\langle v_\theta^2(t) \rangle &= \langle [v_{\theta 0}(t) + v_{\theta 1}(t)]^2 \rangle = \langle v_{\theta 0}^2(t) + 2v_{\theta 0}(t)v_{\theta 1}(t) + v_{\theta 1}^2(t) \rangle = \langle v_{\theta 0}^2(t) \rangle + 2\langle v_{\theta 0}(t)v_{\theta 1}(t) \rangle + \langle v_{\theta 1}^2(t) \rangle \\
&= \langle v_\theta^2(0) \rangle e^{-2\gamma_{0,\theta\theta 0}t} + \frac{k_B T}{m_\theta} \left(1 - e^{-2\gamma_{0,\theta\theta 0}t} \right) \\
&\quad + 2e^{-2\gamma_{0,\theta\theta 0}t} \left[-\langle v_\theta^2(0) \rangle \gamma_{0,\theta\theta 1} t e^{-\gamma_{0,\theta\theta 0}t} + \frac{\langle v_\theta(0)v_x(0) \rangle \gamma_{0,\theta x 1}}{\gamma_{0,x x 0} - \gamma_{0,\theta\theta 0}} (e^{-\gamma_{0,x x 0}t} - e^{-\gamma_{0,\theta\theta 0}t}) \right] \\
&\quad + \left\langle \int_0^t d\tau_1 \frac{\delta F_{\theta 0}(\tau_1)}{m_\theta} e^{-\gamma_{0,\theta\theta 0}(t-\tau_1)} \cdot \left\{ \int_0^t 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 \\
&\quad + \left\langle \int_0^t d\tau_1 \frac{\delta F_{\theta 0}(\tau_1)}{m_\theta} e^{-\gamma_{0,\theta\theta 0}(t-\tau_1)} \int_0^t d\tau_2 e^{-\gamma_{0,\theta\theta 0}(t-\tau_2)} M_{\theta\theta 0}^{-1} \delta F_{\theta 1}(\tau_2) \right\rangle \\
&= \langle v_\theta^2(0) \rangle e^{-2\gamma_{0,\theta\theta 0}t} + \frac{k_B T}{m_\theta} \left(1 - e^{-2\gamma_{0,\theta\theta 0}t} \right) \\
&\quad + 2e^{-2\gamma_{0,\theta\theta 0}t} \left[-\langle v_\theta^2(0) \rangle \gamma_{0,\theta\theta 1} t e^{-\gamma_{0,\theta\theta 0}t} + \frac{\langle v_\theta(0)v_x(0) \rangle \gamma_{0,\theta x 1}}{\gamma_{0,x x 0} - \gamma_{0,\theta\theta 0}} (e^{-\gamma_{0,x x 0}t} - e^{-\gamma_{0,\theta\theta 0}t}) \right] \\
&\quad + 2k_B T \left[\left(M_{\theta\theta 1}^{-1} + \frac{\beta K_\theta M_{\theta\theta 0}^{-1}}{2m_\theta \gamma_{0,\theta\theta 0}} \right) \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}$$

with $\langle \delta F_{\theta 0}(\tau_1) \delta F_{\theta 1}(\tau_2) \rangle = K_\theta \cdot \delta(\tau_1 - \tau_2)$. So at long time limit $t \rightarrow \infty$, the MSD converge to

$$\begin{aligned}
\langle v_\theta^2(t) \rangle &= \frac{k_B T}{m_\theta} + 2k_B T \left(\frac{-\gamma_{0,\theta\theta 1} M_{\theta\theta 0}^{-1}}{2\gamma_{0,\theta\theta 0}} + M_{\theta\theta 1}^{-1} + \frac{\beta K_\theta}{m_\theta} \frac{M_{\theta\theta 0}^{-1}}{2\gamma_{0,\theta\theta 0}} \right) = \frac{k_B T}{m_\theta} \\
K_\theta &= k_B T m_\theta \left(\gamma_{0,\theta\theta 1} - 2m_\theta M_{\theta\theta 1}^{-1} \gamma_{0,\theta\theta 0} \right)
\end{aligned}$$

$$\begin{aligned}
\langle \delta F_\theta(\tau_1) \delta F_\theta(\tau_2) \rangle &\approx \langle \delta F_{\theta 0}(\tau_1) \delta F_{\theta 0}(\tau_2) \rangle + 2\langle \delta F_{\theta 0}(\tau_1) \delta F_{\theta 1}(\tau_2) \rangle \\
&= 2k_B T m_\theta \gamma_{0,\theta\theta 0} \delta(\tau_1 - \tau_2) + 2K_\theta \delta(\tau_1 - \tau_2) = 2k_B T m_\theta \delta(\tau_1 - \tau_2) \left(\gamma_{0,\theta\theta 0} + \gamma_{0,\theta\theta 1} - 2m_\theta M_{\theta\theta 1}^{-1} \gamma_{0,\theta\theta 0} \right)
\end{aligned}$$

Note $\gamma_{0,\theta\theta} = \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{2\kappa\xi^2\epsilon^2}{9\Delta^3}$, $M_{\theta\theta 1}^{-1} = \frac{\kappa\xi\epsilon}{6\Delta^{5/2}m_\theta}$.

$$\gamma_{0,\theta\theta 0} + \gamma_{0,\theta\theta 1} - 2m_\theta M_{\theta\theta 1}^{-1} \gamma_{0,\theta\theta 0} = \frac{4\xi\epsilon}{3\sqrt{\Delta}} + \frac{2\kappa\xi^2\epsilon^2}{9\Delta^3} - 2 \times \frac{\kappa\xi\epsilon}{6\Delta^{5/2}} \times \frac{4\xi\epsilon}{3\sqrt{\Delta}} = \frac{4\xi\epsilon}{3\sqrt{\Delta}} - \frac{2\kappa\xi^2\epsilon^2}{9\Delta^3}$$

Similar again:

$$\langle \delta F_\theta(\tau_1) \delta F_\theta(\tau_2) \rangle = 2k_B T m_\theta \delta(\tau_1 - \tau_2) \cdot (\gamma_{0,\theta\theta 0} - \gamma_{0,\theta\theta 1}) \quad (59)$$

2.4 Mean square displacement

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

$$\begin{aligned}
\langle v_x(0) v_x(t) \rangle &= \langle v_x(0) [v_{x0}(t) + v_{x1}(t)] \rangle = \langle v_x(0) v_{x0}(t) \rangle + \langle v_x(0) v_{x1}(t) \rangle \\
&= \langle v_x^2(0) \rangle e^{-\gamma_{0,xx} t} (1 - \gamma_{0,xx1} t) + \langle v_x(0) v_\theta(0) \rangle \frac{\gamma_{0,x\theta1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx} t} - e^{-\gamma_{0,\theta\theta} t}) \\
&= \frac{k_B T}{m_x} e^{-\gamma_{0,xx} t} (1 - \gamma_{0,xx1} t) + \frac{k_B T}{m_{x\theta}} \frac{\gamma_{0,x\theta1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx} t} - e^{-\gamma_{0,\theta\theta} t}) \\
\langle v_\theta(0) v_\theta(t) \rangle &= \langle v_\theta(0) [v_{\theta0}(t) + v_{\theta1}(t)] \rangle = \langle v_\theta(0) v_{\theta0}(t) \rangle + \langle v_\theta(0) v_{\theta1}(t) \rangle \\
&= \langle v_\theta^2(0) \rangle e^{-\gamma_{0,\theta\theta} t} (1 - \gamma_{0,\theta\theta1} t) + \langle v_\theta(0) v_x(0) \rangle \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx} t} - e^{-\gamma_{0,\theta\theta} t}) \\
&= \frac{k_B T}{m_\theta} e^{-\gamma_{0,\theta\theta} t} (1 - \gamma_{0,\theta\theta1} t) + \frac{k_B T}{m_{x\theta}} \frac{\gamma_{0,\theta x1}}{\gamma_{0,xx0} - \gamma_{0,\theta\theta0}} (e^{-\gamma_{0,xx} t} - e^{-\gamma_{0,\theta\theta} t})
\end{aligned}$$

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

We have the derivatives

$$\begin{aligned}
\frac{d}{dt} \langle \Delta r_x^2(t) \rangle &= 2 \int_0^t d\tau \langle v_x(0) v_x(\tau) \rangle = 2k_B T \times \\
&\left(\frac{1 - e^{-t\gamma_{0,xx}}}{m_x \gamma_{0,xx0}} - \frac{\gamma_{0,xx1} (1 - e^{-t\gamma_{0,xx}} (t\gamma_{0,xx0} + 1))}{m_x \gamma_{0,xx0}^2} + \frac{\gamma_{0,x\theta1}}{m_{x\theta} (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} \left(\frac{1 - e^{-\gamma_{0,xx} t}}{\gamma_{0,xx0}} - \frac{1 - e^{-\gamma_{0,\theta\theta} t}}{\gamma_{0,\theta\theta0}} \right) \right) \\
\frac{d}{dt} \langle \Delta r_\theta^2(t) \rangle &= 2 \int_0^t d\tau \langle v_\theta(0) v_\theta(\tau) \rangle = 2k_B T \times \\
&\left(\frac{1 - e^{-t\gamma_{0,\theta\theta}}}{m_\theta \gamma_{0,\theta\theta0}} - \frac{\gamma_{0,\theta\theta1} (1 - e^{-t\gamma_{0,\theta\theta}} (t\gamma_{0,\theta\theta0} + 1))}{m_x \gamma_{0,\theta\theta0}^2} + \frac{\gamma_{0,\theta x1}}{m_{x\theta} (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} \left(\frac{1 - e^{-\gamma_{0,xx} t}}{\gamma_{0,xx0}} - \frac{1 - e^{-\gamma_{0,\theta\theta} t}}{\gamma_{0,\theta\theta0}} \right) \right)
\end{aligned}$$

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

$$\begin{aligned}
\langle \Delta r_x^2(t) \rangle &= \langle \Delta r_x^2(0) \rangle + \\
&k_B T \left(\frac{\frac{e^{-t\gamma_{0,xx}} - 1}{\gamma_{0,xx0}} + t}{m_x \gamma_{0,xx0}} + \frac{\gamma_{0,x\theta1} \left(\frac{e^{-t\gamma_{0,xx}} - 1}{\gamma_{0,xx0}} + t \right)}{\gamma_{0,xx0} m_{x\theta} (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} - \frac{\gamma_{0,x\theta1} \left(\frac{e^{-t\gamma_{0,\theta\theta}} - 1}{\gamma_{0,\theta\theta0}} + t \right)}{\gamma_{0,\theta\theta0} m_{x\theta} (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} - \frac{\gamma_{0,xx1} \left(t - \frac{2 - e^{-t\gamma_{0,xx}} (t\gamma_{0,xx0} + 2)}{\gamma_{0,xx0}} \right)}{m_x \gamma_{0,xx0}^2} \right) \\
&\approx \frac{t^2 T k_B}{m_x} - \frac{t^3 (T k_B (m_x \gamma_{0,x\theta1} + m_{x\theta} (\gamma_{0,xx0} + \gamma_{0,xx1})))}{3 (m_x m_{x\theta})} + O(t^3)
\end{aligned}$$

$$\begin{aligned}
\langle \Delta r_\theta^2(t) \rangle &= \langle \Delta r_\theta^2(0) \rangle + \\
&k_B T \left(\frac{\frac{e^{-\gamma_{0,\theta\theta 0}} - 1}{\gamma_{0,\theta\theta 0}} + t}{m_\theta \gamma_{0,\theta\theta 0}} + \frac{\gamma_{0,\theta x 1} \left(\frac{e^{-\gamma_{0,xx 0}} - 1}{\gamma_{0,xx 0}} + t \right)}{\gamma_{0,xx 0} m_{x\theta} (\gamma_{0,xx 0} - \gamma_{0,\theta\theta 0})} - \frac{\gamma_{0,\theta x 1} \left(\frac{e^{-\gamma_{0,\theta\theta 0}} - 1}{\gamma_{0,\theta\theta 0}} + t \right)}{\gamma_{0,\theta\theta 0} m_{x\theta} (\gamma_{0,xx 0} - \gamma_{0,\theta\theta 0})} - \frac{\gamma_{0,\theta\theta 1} \left(t - \frac{2 - e^{-\gamma_{0,\theta\theta 0}}(t + \gamma_{0,\theta\theta 0} + 2)}{\gamma_{0,\theta\theta 0}} \right)}{m_\theta \gamma_{0,\theta\theta 0}^2} \right) \\
&\approx \frac{t^2 T k_B}{m_\theta} - \frac{t^3 (T k_B (m_\theta \gamma_{0,\theta x 1} + m_{x\theta} (\gamma_{0,\theta\theta 0} + \gamma_{0,\theta\theta 1})))}{3 (m_\theta m_{x\theta})} + O(t^3)
\end{aligned}$$

In the end, we would like to cross mean "square" displacement between x and θ .

$$\langle \Delta r_x(t) \cdot \Delta r_\theta(t) \rangle = \int_0^t \left[\frac{d}{dt} \langle \Delta r_x(\tau) \cdot \Delta r_\theta(\tau) \rangle \right] d\tau + \langle \Delta r_x(0) \cdot \Delta r_\theta(0) \rangle$$

Since

$$\begin{aligned}
\Delta r_x(t) &= \int_0^t v_x(\tau) d\tau & \Delta r_\theta(t) &= \int_0^t v_\theta(\tau) d\tau \\
\frac{d}{dt} \langle \Delta r_x(t) \cdot \Delta r_\theta(t) \rangle &= \frac{d}{dt} \left\langle \int_0^t v_x(\tau) d\tau \cdot \int_0^t v_\theta(\tau) d\tau \right\rangle = \frac{d}{dt} \left[\int_0^t d\tau_1 \int_0^t d\tau_2 \langle v_x(\tau_1) v_\theta(\tau_2) \rangle \right] \\
&= \int_0^t \langle v_x(t) v_\theta(\tau) \rangle d\tau + \int_0^t \langle v_x(\tau) v_\theta(t) \rangle d\tau
\end{aligned}$$

we focus on cross velocity product average (always to 1-order of κ)

$$\begin{aligned}
\langle v_x(\tau_1) v_\theta(\tau_2) \rangle &= \langle [v_{x0}(\tau_1) + v_{x1}(\tau_1)] \cdot [v_{\theta 0}(\tau_2) + v_{\theta 1}(\tau_2)] \rangle \\
&= \langle v_{x0}(\tau_1) v_{\theta 0}(\tau_2) \rangle + \langle v_{x0}(\tau_1) v_{\theta 1}(\tau_2) \rangle + \langle v_{x1}(\tau_1) v_{\theta 0}(\tau_2) \rangle + \langle v_{x1}(\tau_1) v_{\theta 1}(\tau_2) \rangle
\end{aligned}$$

We still pose that there's no cross correlation, $\langle \delta F_x(\tau_1) \delta F_\theta(\tau_2) \rangle = 0$, $\langle v_i(\tau_1) \delta F_j(\tau_2) \rangle = 0$, we only consider the contribution from $\langle v_x^2(0) \rangle$, $\langle v_\theta^2(0) \rangle$, also $\langle v_x(0) v_\theta(0) \rangle = \frac{k_B T}{m_{x\theta}}$ as we supposed previously.

With the expressions, we could easily calculate each term:

$$\begin{aligned}
\langle v_{x0}(\tau_1) v_{\theta 0}(\tau_2) \rangle &= \langle v_x(0) v_\theta(0) \rangle e^{-\gamma_{0,xx 0} \tau_1} e^{-\gamma_{0,\theta\theta 0} \tau_2} \\
\langle v_{x0}(\tau_1) v_{\theta 1}(\tau_2) \rangle &= \langle v_x^2(0) \rangle \frac{e^{-\gamma_{0,xx 0} \tau_1} \gamma_{0,\theta x 1}}{\gamma_{0,xx 0} - \gamma_{0,\theta\theta 0}} (e^{-\gamma_{0,xx 0} \tau_2} - e^{-\gamma_{0,\theta\theta 0} \tau_2}) - \langle v_x(0) v_\theta(0) \rangle \gamma_{0,\theta\theta 1} \tau_2 e^{-\gamma_{0,xx 0} \tau_1} e^{-\gamma_{0,\theta\theta 0} \tau_2} \\
\langle v_{x1}(\tau_1) v_{\theta 0}(\tau_2) \rangle &= \langle v_\theta^2(0) \rangle \frac{e^{-\gamma_{0,\theta\theta 0} \tau_2} \gamma_{0,xx 1}}{\gamma_{0,xx 0} - \gamma_{0,\theta\theta 0}} (e^{-\gamma_{0,xx 0} \tau_1} - e^{-\gamma_{0,\theta\theta 0} \tau_1}) - \langle v_x(0) v_\theta(0) \rangle \gamma_{0,xx 1} \tau_1 e^{-\gamma_{0,xx 0} \tau_1} e^{-\gamma_{0,\theta\theta 0} \tau_2}
\end{aligned}$$

We jump the explicit calculation process, giving the final result directly:

$$\begin{aligned}
\langle \Delta r_x(t) \cdot \Delta r_\theta(t) \rangle &= \langle \Delta r_x(0) \cdot \Delta r_\theta(0) \rangle \\
&+ \frac{\gamma_{0,\theta x1} (e^{t\gamma_{0,xx0}} - 1) e^{-t(\gamma_{0,\theta\theta0} + 2\gamma_{0,xx0})} (\gamma_{0,\theta\theta0} e^{t\gamma_{0,\theta\theta0}} (e^{t\gamma_{0,xx0}} - 1) - \gamma_{0,xx0} (e^{t\gamma_{0,\theta\theta0}} - 1) e^{t\gamma_{0,xx0}})}{\gamma_{0,\theta\theta0} \gamma_{0,xx0}^2 (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} \langle v_x^2(0) \rangle \\
&+ \frac{\gamma_{0,x\theta1} (e^{t\gamma_{0,\theta\theta0}} - 1) e^{-t(2\gamma_{0,\theta\theta0} + \gamma_{0,xx0})} (\gamma_{0,\theta\theta0} e^{t\gamma_{0,\theta\theta0}} (e^{t\gamma_{0,xx0}} - 1) - \gamma_{0,xx0} (e^{t\gamma_{0,\theta\theta0}} - 1) e^{t\gamma_{0,xx0}})}{\gamma_{0,\theta\theta0}^2 \gamma_{0,xx0} (\gamma_{0,xx0} - \gamma_{0,\theta\theta0})} \langle v_\theta^2(0) \rangle \\
&+ \frac{e^{-t(\gamma_{0,\theta\theta0} + \gamma_{0,xx0})}}{\gamma_{0,\theta\theta0}^2 \gamma_{0,xx0}^2} \langle v_x(0) v_\theta(0) \rangle \times \\
&\quad \left[\gamma_{0,xx0} (\gamma_{0,\theta\theta0} ((e^{t\gamma_{0,xx0}} - 1) (e^{t\gamma_{0,\theta\theta0}} + t\gamma_{0,\theta\theta1} - 1) + t\gamma_{0,xx1} (e^{t\gamma_{0,\theta\theta0}} - 1)) \right. \\
&\quad \left. - \gamma_{0,\theta\theta1} (e^{t\gamma_{0,\theta\theta0}} - 1) (e^{t\gamma_{0,xx0}} - 1)) - \gamma_{0,\theta\theta0} \gamma_{0,xx1} (e^{t\gamma_{0,\theta\theta0}} - 1) (e^{t\gamma_{0,xx0}} - 1) \right] \\
&\approx t^2 \langle v_x(0) v_\theta(0) \rangle - \frac{1}{2} t^3 \left[\langle v_x(0) v_\theta(0) \rangle (\gamma_{0,xx0} + \gamma_{0,xx1} + \gamma_{0,\theta\theta0} + \gamma_{0,\theta\theta1}) + \langle v_x^2(0) \rangle \gamma_{0,\theta x1} + \langle v_\theta^2(0) \rangle \gamma_{0,x\theta1} \right]
\end{aligned}$$

We can exploit Kubo's relation toward the diffusion coefficient. Note that D_x, D_θ are both functions of Δ .

$$\begin{aligned}
D_x &= \int_0^\infty \langle v_x(0) v_x(t) \rangle dt = \frac{k_B T}{\gamma_{0,xx0}^2} \left(\frac{\gamma_{0,xx0} - \gamma_{0,xx1}}{m_x} - \frac{\gamma_{0,x\theta1} \gamma_{0,xx0}}{m_{x\theta} \gamma_{0,\theta\theta0}} \right) \\
D_\theta &= \int_0^\infty \langle v_\theta(0) v_\theta(t) \rangle dt = \frac{k_B T}{\gamma_{0,\theta\theta0}^2} \left(\frac{\gamma_{0,\theta\theta0} - \gamma_{0,\theta\theta1}}{m_\theta} - \frac{\gamma_{0,\theta\theta0} \gamma_{0,\theta x1}}{m_{x\theta} \gamma_{0,xx0}} \right)
\end{aligned}$$

We ignored the MSD along z direction, since all γ s depend on the height Δ . Note $\gamma_{0,zz0} = \frac{\xi}{\Delta^{3/2}}$, $\gamma_{0,zz1} = \frac{15\kappa\xi^2}{8\Delta^4}$. In this case, the particle would furnish different diffusion coefficient at different height rather than a constant parameter, even though we could derive the expression of $\langle v_z(0) v_z(t) \rangle$ and the following calculations.

$$\langle v_z(0) v_z(t) \rangle = \langle v_z(0) [v_{z0}(t) + v_{z1}(t)] \rangle = \langle v_z(0) v_{z0}(t) \rangle + \langle v_z(0) v_{z1}(t) \rangle = \langle v_z^2(0) \rangle e^{-\gamma_{0,zz0} t} (1 - \gamma_{0,zz1} t)$$

So we would like to seek a height z_{eq} at equilibrium. Consider the diffusion coefficient D_z as a function of z, t .

$$\begin{aligned}
D_z(\Delta) &= \int_0^\infty \langle v_z(0) v_z(t) \rangle (\Delta) dt = \int_0^\infty \langle v_z^2(0) \rangle \exp\left(-\frac{\xi}{\Delta^{3/2}} t\right) \cdot \left(1 - \frac{15\kappa\xi^2}{8\Delta^4} t\right) dt \\
\langle D_z \rangle &= \frac{1}{z_+ - z_-} \int_{z_-}^{z_+} D_z(\Delta) d\Delta = \frac{1}{z_+ - z_-} \int_{z_-}^{z_+} d\Delta \int_0^\infty dt \langle v_z^2(0) \rangle \exp\left(-\frac{\xi}{\Delta^{3/2}} t\right) \cdot \left(1 - \frac{15\kappa\xi^2}{8\Delta^4} t\right)
\end{aligned}$$

where z_-, z_+ refer to the minimum and maximum height. This average diffusion coefficient would just be corresponding to the value at a given position, namely the typical height z^* .

$$\langle D_z \rangle = D_z(z^*)$$

3 Numerical Simulations

3.1 Discretisation algorithm

Random number generator In the numerical practice, we regard the white noise as a Gaussian random variable at every position and time. We follow the Box-Muller transform to generate normally distributed random variables, which uses two independent random numbers U and V distributed uniformly on $(0, 1)$. Then the two random variables X and Y given by

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

will both have the standard normal distribution, and will be independent with each other. If we take n -dimensional vectors U and V , then $2n$ independent random variables will be furnished.

Euler-Maruyama method In Itô calculus, the Euler–Maruyama method is used for the approximate numerical solution of a stochastic differential equation (SDE). Consider the equation

$$dX_t = a(X_t, t)dt + b(X_t, t)dW_t$$

with initial condition $X_0 = x_0$, where W_t stands for the Wiener process, and suppose that we wish to solve this SDE on some interval of time $[0, T]$. Then the Euler-Maruyama approximation to the true solution X is the Markov chain Y defined as follows:

- partition the interval $[0, T]$ into N equal subintervals of width $\Delta t = T/N > 0$:

$$0 = \tau_0 < \tau_1 < \dots < \tau_N = T$$

- set $Y_0 = x_0$, then recursively define Y_n for $0 \leq n \leq N - 1$ by

$$Y_{n+1} = Y_n + a(Y_n, \tau_n)\Delta t + b(Y_n, \tau_n)\Delta W_n$$

where the random variables ΔW_n are independent and identically distributed normal random variables with expected value zero and variance Δt .

The Euler-Maruyama scheme could be applied in our case as $t_{i+1} = t_i + \Delta t$

$$\mathbf{v}(t_{i+1}) = \mathbf{v}(t_i) + \left[-\gamma_{\text{eff}}(\mathbf{x}, t_i) \cdot \mathbf{v}(t_i) + M^{-1} \cdot \mathbf{F}_{1\alpha}(\mathbf{x}, t_i) \right] \Delta t + \sqrt{\frac{2k_B T (\gamma_0 - \gamma_1)}{m}} \cdot \Delta \mathbf{W}(\Delta t)$$

$$\mathbf{r}(t_{i+1}) = \mathbf{r}(t_i) + \mathbf{v}(t_i)\Delta t$$

where $\mathbf{F}_{1\alpha}(\mathbf{x}, t_i)$ contains the gravity and the spurious force, and even the electrostatic repulsion force added later.

3.2 Dimensional analysis

Three coordinate are included, namely the vertical distance z between the particle and the soft surface; the parallel displacement x ; and the rotation angle θ . Note, dimensionless variables are defined as: $\delta = \Delta \cdot r\epsilon$, $x = X_G \cdot r\sqrt{2\epsilon}$, $\theta = \Theta \cdot \sqrt{2\epsilon}$. r is the particle radius, while $\epsilon \ll 1$ is one dimensionless parameter. Also, we pose that the particle mass $m^* = \pi r^2 \rho$ with the dimension $[MT^{-2}]$ rather than $[LMT^{-2}]$, where ρ the density. Therefore, we would figure out the Langevin formula with 2D mass. To be exact, there should be two steps:

1. Transform the Langevin equation with 3D mass $[M]$ to 2D mass $[ML^{-1}]$, and 3D force $[MLT^{-2}]$ to 2D force $[MT^{-2}]$; $F^* = \frac{F}{\mathcal{L}} \rightarrow [MT^{-2}]$
 2. Transform other parameters to dimensionless ones; $\widehat{F}^* = F^* \cdot \frac{2r}{c^2} = \frac{F}{\mathcal{L}} \cdot \frac{2r}{c^2} \rightarrow [ML^{-1}]$
- namely the tandem nondimensionalization process.

We use $*$ to note the 2d variables. For instance, $m^* = m/\mathcal{L}$ with the dimension $[ML^{-1}]$, where \mathcal{L} is the typical length for our particles under the elastohydrodynamic interaction. Since we supposed an infinite long cylindrical particle at first, this \mathcal{L} should be much larger than the particle radius. Besides, $F^* = F/\mathcal{L}$ with the dimension $[MT^{-2}]$. Furthermore, we use $\widehat{}$ to note the dimensionless variables, such as $\Delta = \widehat{\delta} = \delta/(r\epsilon)$.

Consider the Langevin equation with 3d mass with $\gamma = \zeta/m$:

$$m\dot{v} = -\zeta v + \delta F + F_{\text{ext}} \quad \Rightarrow \quad \dot{v} = -\gamma v + \frac{\delta F}{m} + \frac{F_{\text{ext}}}{m}$$

So for the case with 2d mass $[ML^{-1}]$, we pose $\zeta^* = \zeta/\mathcal{L}$, and then $\gamma^* = \zeta^*/m^* = \zeta/m = \gamma$

$$m^*\dot{v} = -\zeta^* v + \delta F^* + F_{\text{ext}}^* \quad \Rightarrow \quad \dot{v} = -\gamma v + \frac{\delta F^*}{m^*} + \frac{F_{\text{ext}}^*}{m^*}$$

Inverse mass matrix We have the matriciel formula with M^* as the 2D mass with the dimension $[ML^{-1}]$:

$$M^* \cdot \dot{\mathbf{v}} = -\zeta^* \cdot \mathbf{v} + \delta \mathbf{F}^* + \mathbf{F}_{\text{ext}}^* \quad \Rightarrow \quad \dot{\mathbf{v}} = -\gamma_{3 \times 3} \cdot \mathbf{v} + (M^*)^{-1} \cdot \delta \mathbf{F}^* + (M^*)^{-1} \cdot \mathbf{F}_{\text{ext}}^*$$

Here, $(M^*)^{-1}$ just corresponds to the inverse mass matrix shown in our previous report, with the dimension as $[LM^{-1}]$: (or m/kg)

$$M^{-1} \simeq \begin{pmatrix} \frac{1}{m_z} + \frac{15\kappa\xi}{8\Delta^{5/2}m_z} & 0 & 0 \\ 0 & \frac{1}{m_x} + \frac{\kappa\xi\epsilon}{12\Delta^{5/2}m_x} & -\frac{\kappa\xi\epsilon}{12\Delta^{5/2}m_\theta} \\ 0 & -\frac{\kappa\xi\epsilon}{6\Delta^{5/2}m_x} & \frac{1}{m_\theta} + \frac{\kappa\xi\epsilon}{6\Delta^{5/2}m_\theta} \end{pmatrix}$$

Effective friction matrix Next, as for the dimensionless variables, we pose $t = T \cdot r \sqrt{2\epsilon}/c$, where for one particle inside the solvent $c = \sqrt{2gr\rho^*}/\rho$ is the maximum dropping speed. To be exact, ρ is the particle density, and $\rho^* = \rho - \rho_{\text{sol}}$ is the density difference for the sake of the buoyancy latter, leading to a dimensionless parameter $\rho^*/\rho = 1 - \rho_{\text{sol}}/\rho$. Thus we have dimensionless speeds and accelerations:

$$\begin{aligned} v_\Delta &= \frac{v_\delta}{c} \sqrt{\frac{2}{\epsilon}} & v_X &= \frac{v_x}{c} & v_\Theta &= v_\theta \cdot \frac{r}{c} \\ \dot{v}_\Delta &= \dot{v}_\delta \cdot \frac{2r}{c^2} & \dot{v}_X &= \dot{v}_x \cdot \frac{\sqrt{2\epsilon}r}{c^2} & \dot{v}_\Theta &= \dot{v}_\theta \cdot \frac{\sqrt{2\epsilon}r^2}{c^2} \end{aligned}$$

leading to dimensionless friction coefficients $\hat{\gamma} = \gamma \cdot \frac{\sqrt{2\epsilon}r}{c}$, since γ has the dimension $[T^{-1}]$. We write dimensionless variables as: $\hat{\gamma}_\delta = \gamma_\Delta$, $\hat{\gamma}_x = \gamma_X$, and $\hat{\gamma}_\theta = \gamma_\Theta$.

$$\gamma_\delta = \gamma_\Delta \cdot \frac{c}{\sqrt{2\epsilon}r} \quad \gamma_x = \gamma_X \cdot \frac{c}{\sqrt{2\epsilon}r} \quad \gamma_\theta = \gamma_\Theta \cdot \frac{c}{\sqrt{2\epsilon}r}$$

Indeed, $\hat{\gamma}$ above without dimension corresponds to the effective friction matrix γ_{eff} derived from equations of motion:

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

By the way, we can solve the dimensionless diffusion coefficient as

$$D_X = \widehat{D}_x = \frac{k_B T}{m_x \gamma_X c^2} \quad D_\Theta = \widehat{D}_\theta = \frac{k_B T r^2}{m_\theta \gamma_\Theta c^2}$$

Random force We give out the modified noise correlator based on the formula shown in the internship report, where a ratio coefficient has been ignored.

$$\langle \delta F(\tau_1) \delta F(\tau_2) \rangle = 2k_B T m \gamma \delta(\tau_1 - \tau_2)$$

Note, we write δF^* with the dimension as $[MT^{-2}]$, and $\widehat{\delta F^*}$ with the dimension as $[ML^{-1}]$, same as the m^* . $\int \delta(t)dt = 1 = \int \widehat{\delta}(T)dT$, so $\widehat{\delta}(T) = \delta(t) \cdot \frac{r\sqrt{2\epsilon}}{c}$. Also, we have $\gamma = \widehat{\gamma} \cdot \frac{c}{\sqrt{2\epsilon}r}$, $\widehat{\delta F^*} = \frac{\delta F}{\mathcal{L}} \cdot \frac{2r}{c^2}$, and therefore:

$$\left\langle \widehat{\delta F_i^*}(\tau_1) \widehat{\delta F_i^*}(\tau_2) \right\rangle = 2k_B T m_i^* \widehat{\delta}(\tau_1 - \tau_2) \cdot (\widehat{\gamma}_{i0} - \widehat{\gamma}_{i1}) \times \frac{2}{\mathcal{L}c^2\epsilon}$$

Since τ_1, τ_2 are dimensionless time variables, $\widehat{\delta}(\tau_1 - \tau_2)$ is also dimensionless. Consider the rest term

$$\frac{k_B T m^*}{\mathcal{L}c^2} \rightarrow \frac{[ML^2T^{-2}] \cdot [ML^{-1}]}{[L] \cdot [LT^{-1}]^2} = [ML^{-1}]^2$$

So in the numerical practice, we consider the random force $\widehat{\delta F_i^*}$ as multiplicative Gaussian white noises,

$$\widehat{\delta F_i^*} = \sqrt{2k_B T m_i^* (\widehat{\gamma}_{i0} - \widehat{\gamma}_{i1}) \times \frac{2}{\mathcal{L}c^2\epsilon}} \cdot \widehat{\Delta\eta_i}$$

where $\widehat{\Delta\eta_i}$ refers to a normal random variable with expected value zero and variance $\widehat{\Delta t}$.

External force There is no external force along the parallel displacement of the rotation. We pose that the external force F_{ext} (3D) probably contains these terms vertically:

$$F_{\text{ext}} = F_{\text{grav}} + F_{\text{buoy}} + F_{\text{spur}} + F_{\text{elec}} + F_{\text{har}}$$

namely the sommation of gravity, buoyancy, the spurious force, given electrostatic repulsion, and supposed harmonic potential. And we suppose that the re-scaling process presents

$$F_{\text{ext}}^* = \frac{F_{\text{ext}}}{\mathcal{L}} \rightarrow [MT^{-2}] \quad \widehat{F_{\text{ext}}^*} = F_{\text{ext}}^* \cdot \frac{2r}{c^2} \rightarrow [ML^{-1}]$$

Below we see each components:

- the gravity $F_{\text{grav}}^* = -m^*g$, where g is the gravity acceleration;
- the buoyancy $F_{\text{buoy}}^* = \rho_{\text{sol}}gV^*$, where ρ_{sol} refers to the fluid density, while $V^* = \pi r^2$ refers to the 2D volume. Consider the gravity and the buoyancy at the same time, we have

$$\widehat{F_{\text{grav}}^*} + \widehat{F_{\text{buoy}}^*} = (-m^*g + \rho_{\text{sol}}gV^*) \cdot \frac{2r}{c^2} = g\pi r^2(-\rho + \rho_{\text{sol}}) \cdot \frac{2r\rho}{2gr(\rho - \rho_{\text{sol}})} = -\pi r^2\rho = -m^*$$

Hence we will always have -1 in the equations of motion, for $(M_{zz}^*)^{-1} \left(\widehat{F_{\text{grav}}^*} + \widehat{F_{\text{buoy}}^*} \right) \simeq -1$.

- the spurious force $F_{\text{spur}} = k_B T \cdot \Gamma_{\alpha\beta\beta}$, where $\Gamma_{\alpha\beta\beta}$ has the dimension as $[M^{-1}]$. For instance, $\Gamma_{\alpha\beta\beta} = \widehat{\Gamma}_{\alpha\beta\beta}/(r\epsilon)$, and $\widehat{\gamma}_{\alpha\beta} = \widehat{\lambda}_{\alpha\beta} + \widehat{\Gamma}_{\alpha\beta\gamma}\widehat{v}_\gamma$ is the effective friction matrix shown previously.
- the electrostatic repulsion $F_{\text{elec}} = k_B T \cdot \frac{B}{\ell_D} \exp\left(-\frac{z}{\ell_D}\right)$, where B is a dimensionless parameter, and ℓ_D is the Debye length, around 50 nm for one particle with radius as 1 μm .

- the ad-hoc harmonic potential $F_{\text{har}} = -k_{\text{har}}(z - z_0)$; we could add this term or not.

Finally, we return to the dimensionless equation

$$\dot{\hat{\mathbf{v}}} = -\widehat{\gamma}(\gamma_{\text{eff}}) \cdot \hat{\mathbf{v}} + (M^*)^{-1} \cdot \widehat{\delta \mathbf{F}^*} + (M^*)^{-1} \cdot \widehat{\mathbf{F}_{\text{ext}}^*}$$

Or the discrete version along the vertical direction with the time gap $\widehat{\Delta t} = \widehat{t}_{i+1} - \widehat{t}_i$

$$\begin{aligned} v_{\Delta}(\widehat{t}_{i+1}) - v_{\Delta}(\widehat{t}_i) = & - \left[\widehat{\gamma}_{z0}(\widehat{t}_i) + \widehat{\gamma}_{z1}(\widehat{t}_i) \right] v_{\Delta}(\widehat{t}_i) \times \widehat{\Delta t} + (M_{zz}^*)^{-1} \cdot \sqrt{2k_B T m_z^* (\widehat{\gamma}_{z0} - \widehat{\gamma}_{z1}) \cdot \frac{2}{\mathcal{L} c^2 \epsilon}} \times \widehat{\Delta \eta_z} \\ & + \left\{ -1 + (M_{zz}^*)^{-1} \cdot \left[k_B T \cdot \frac{\widehat{\Gamma}_{\alpha\beta\beta}}{r\epsilon} + k_B T \cdot \frac{B}{l_D} \exp\left(-\frac{z}{l_D}\right) \right] \cdot \frac{2r}{\mathcal{L} c^2} \right\} \times \widehat{\Delta t} \\ \Delta(\widehat{t}_{i+1}) - \Delta(\widehat{t}_i) = & v(\widehat{t}_i) \times \widehat{\Delta t} \end{aligned}$$

3.3 Parameter estimation

We take these parameters below in the simulations:

$$k_B \sim 10^{-23}(\text{J/K}) \quad T \sim 3 \times 10^2(\text{K}) \quad r \sim 10^{-6}(\text{m}) \quad g \sim 10^1(\text{m/s}^2)$$

$$\rho \sim 10^3(\text{kg/m}^3) \quad \Delta\rho \sim 10^1(\text{kg/m}^3) \quad m^* = \pi r^2 \rho \sim 10^{-9}(\text{kg/m}) \quad c \sim 10^{-3}(\text{m/s})$$

For the sake of simplicity, we rewrite the height at equilibrium in a power version: $\Delta_{\text{eq}} \sim 10^{-d}$. And then we express all external forces with unknown parameters, including B, ℓ_D, κ , etc. **Here**, we know the total effect of gravity and buoyancy is about -1 . Then we estimate other forces below:

↑ **Spurious force**

$$\varepsilon \sim 10^{-1} \quad \xi \sim 10^0 \quad \Delta_{\text{eq}} \sim 10^{-d} \quad \widehat{\Gamma}_{zzz} = \frac{\kappa \xi}{\Delta^{9/2}} \sim 10^{9d/2} \kappa$$

$$\widehat{\Gamma}_{zxx} = \widehat{\Gamma}_{z\theta\theta} = \frac{\kappa \xi}{\Delta^{7/2}} \sim 10^{7d/2} \kappa \quad F_{\text{spur}} = k_B T \cdot \frac{\widehat{\Gamma}_{z\beta\beta}}{r\varepsilon} \sim 10^{9d/2-14} \kappa$$

↑ **Electrostatic repulsion**

$$F_{\text{elec}} = k_B T \cdot \frac{B}{\ell_D} \exp\left(-\frac{\Delta r \varepsilon}{\ell_D}\right) \sim 10^{-14} B \exp\left(-10^{-d}\right)$$

↕ **Noise**

$$\widehat{\delta F_i^*} = \sqrt{2k_B T m_i^* (\widehat{\gamma}_{i0} - \widehat{\gamma}_{i1}) \times \frac{2}{\mathcal{L} c^2 \epsilon}} \cdot \widehat{\Delta \eta_i} \sim \frac{2}{\sqrt{L}} \cdot 10^{\frac{3d}{4} - \frac{23}{2}} \cdot \mathcal{N}(0, dt)$$

We should arrange these forces in proper order, namely with the following assumptions:

1. The height at equilibrium is much smaller than the particle radius; so $\Delta_{\text{eq}} \sim 10^{-d} \ll \varepsilon^{-1}$;

2. The noise / random force is much smaller than the “gravity – buoyancy”; $T \sim 3 \cdot 10^2 (\text{K})$

$$\sqrt{2k_B T m_i^* (\hat{\gamma}_{i0} - \hat{\gamma}_{i1}) \times \frac{2}{\mathcal{L} c^2 \epsilon} \cdot \widehat{\Delta \eta_i}} \ll m^* = \pi r^2 \rho$$

$$\frac{2}{\sqrt{L}} \cdot 10^{\frac{3d}{4} - \frac{23}{2}} \cdot \mathcal{N}(0, dt) \ll 10^{-9} \quad \rightarrow \quad \mathcal{L} \gg \frac{10^{3d/2}}{10^{21} \cdot r^3} (dt)$$

3. Gravity – buoyancy \sim Electrostatic repulsion; $\ell_D \sim 10^{-7} (\text{m})$

$$k_B T \cdot \frac{B}{\ell_D} \exp\left(-\frac{\Delta r \epsilon}{\ell_D}\right) \cdot \frac{2r}{\mathcal{L} c^2} \simeq \pi r^2 \rho \quad \rightarrow \quad B \sim \pi r^2 \mathcal{L} \cdot \frac{10^{23} \ell_D}{\exp(-10^{-d})}$$

3.4 Typical results

Simulation with fixed height (Δ) - Effect of compliance ($\kappa \neq 0$)

We could derive analytical solutions for X, Θ since Δ is completely fixed. Diffusion coefficient depends on vertical positions and soft wall modulus.

$$D(\kappa, \Delta) = D(0, \Delta) \left[1 - \kappa \cdot \frac{\gamma_{i1}(\Delta)}{\gamma_{i0}(\Delta)} \right]$$

In this case, we don't need to consider the external forces, but only the parallel Brownian motion and the corresponding MSD (mean square displacement). Analytical expectations are shown in color bands, while the numerical results in dashed lines could fit that rather well. At short time region, MSD is proportional to ΔT^2 ; while at long time region, it's a linear function of ΔT .

In Fig. 2, we see that the closer to the surface, the less diffusion coefficient we get, which verifies the confined Brownian motion but with soft surface ($\kappa \neq 0$).

In Fig. 3, we see that the softer surface we have, the less diffusion coefficient we get.

Simulation with unfixed height (Δ) & Effect of compliance ($\kappa \neq 0$)

Here we have to consider the external forces with proper selected parameters:

$$r = 10^{-6} (\text{m}) \quad \ell_D = 1.5 \times 10^{-7} (\text{m}) \quad \mathcal{L} = 0.25 (\text{m}) \quad B = 3.0 \times 10^4$$

We started the simulations with 10^5 particles normally distributed around $\Delta \simeq 1.4$ at beginning, focusing on the compliance influence toward PDF (probability distribution function). In Fig. 4, we see no obvious difference for different curves. Then in Fig. 5, we see clearly that PDF peak falls down much quick for the softer case, perhaps due to the asymmetric deformation of the soft surface. Across the equilibrium height, we see that in Fig. 6, the most softer curve (in red) returns back much quicker than others, perhaps due to the larger lift force. Finally, in Fig. 7, we see no difference for all cases, and they would stay around the equilibrium height in the end.

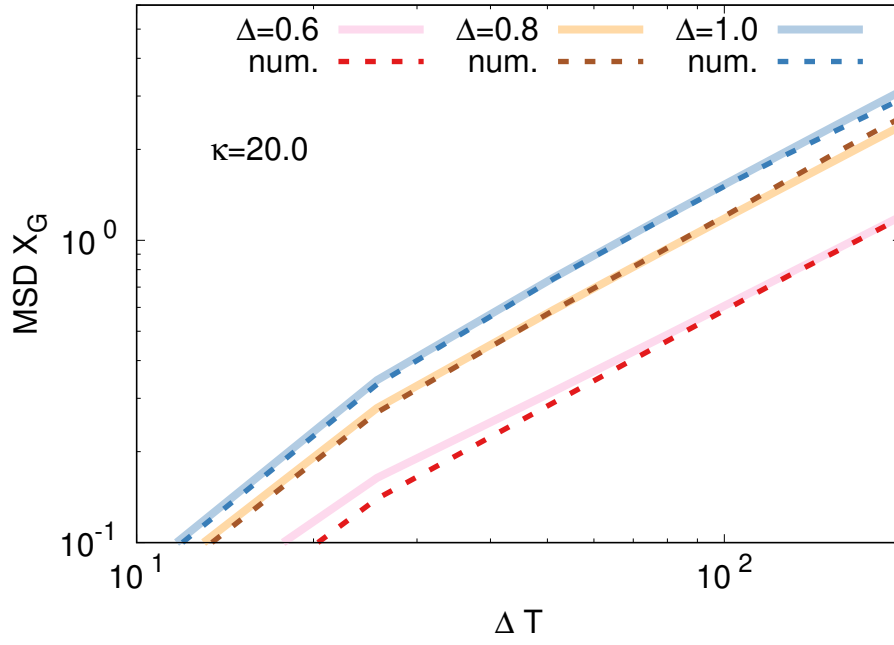


Figure 2: Influence of height with fixed compliance.

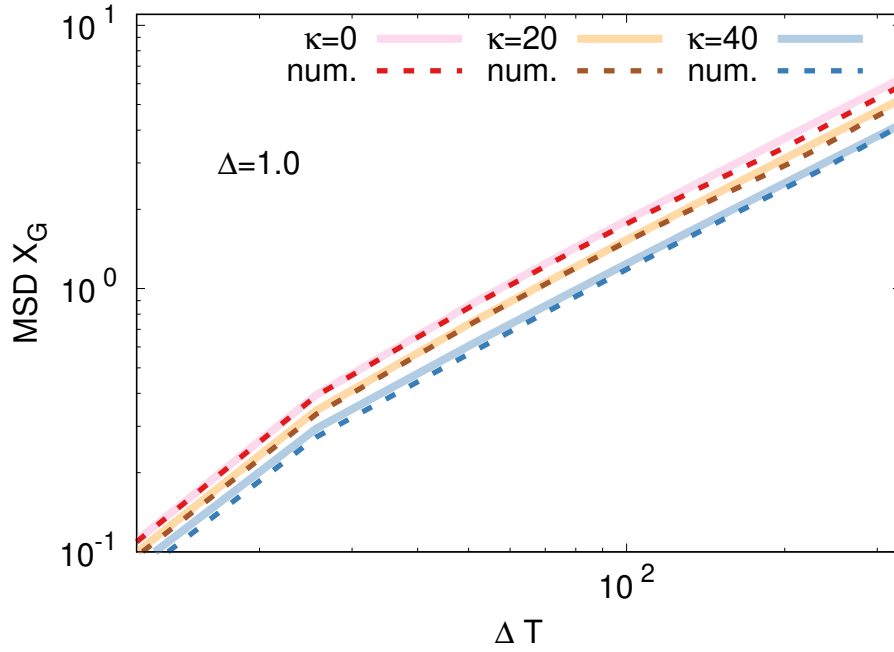


Figure 3: Influence of compliance with fixed height.

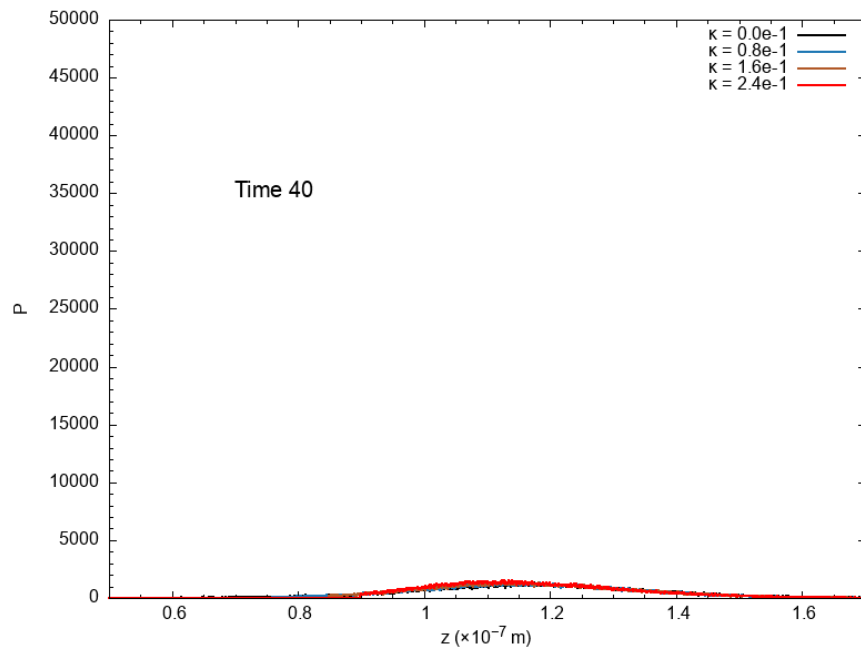


Figure 4

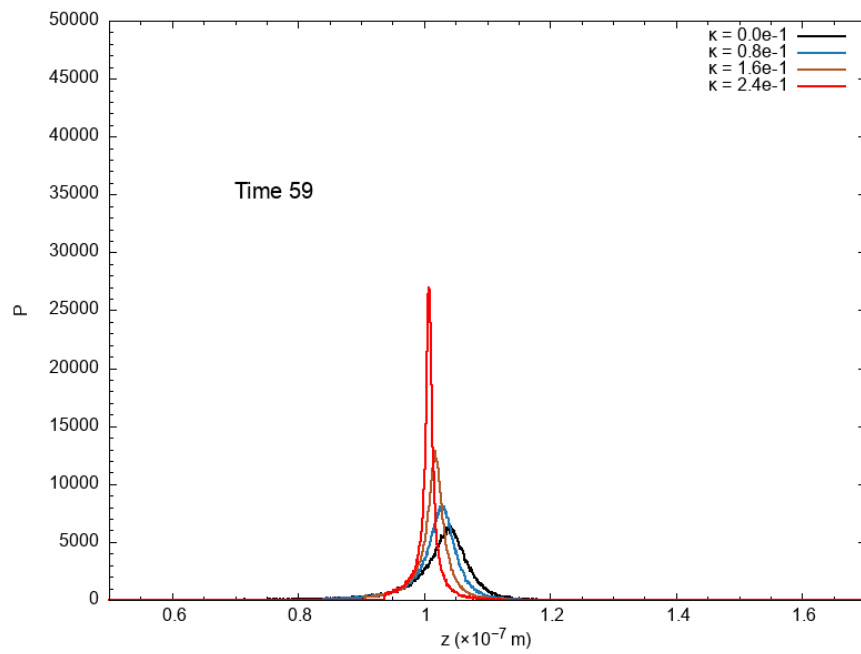


Figure 5

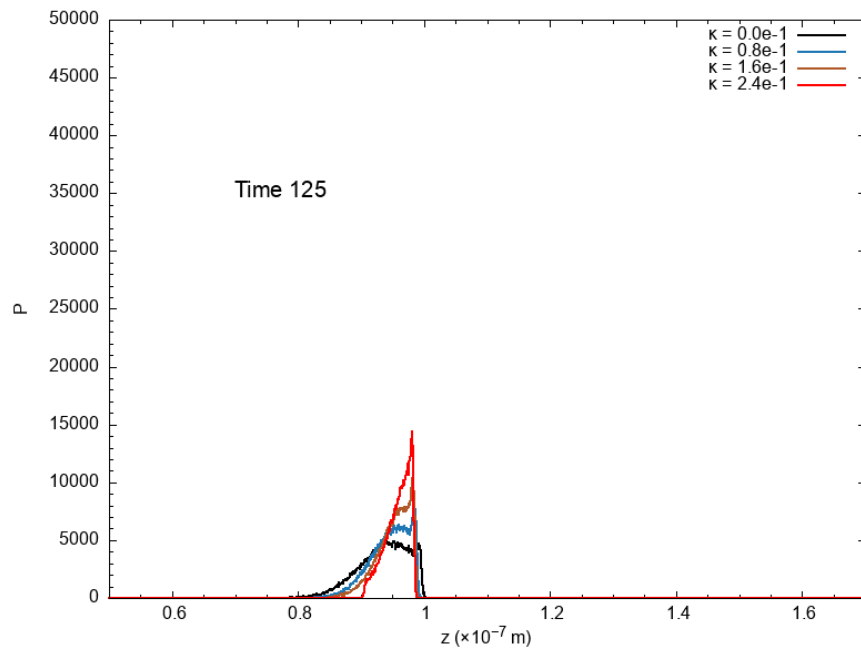


Figure 6

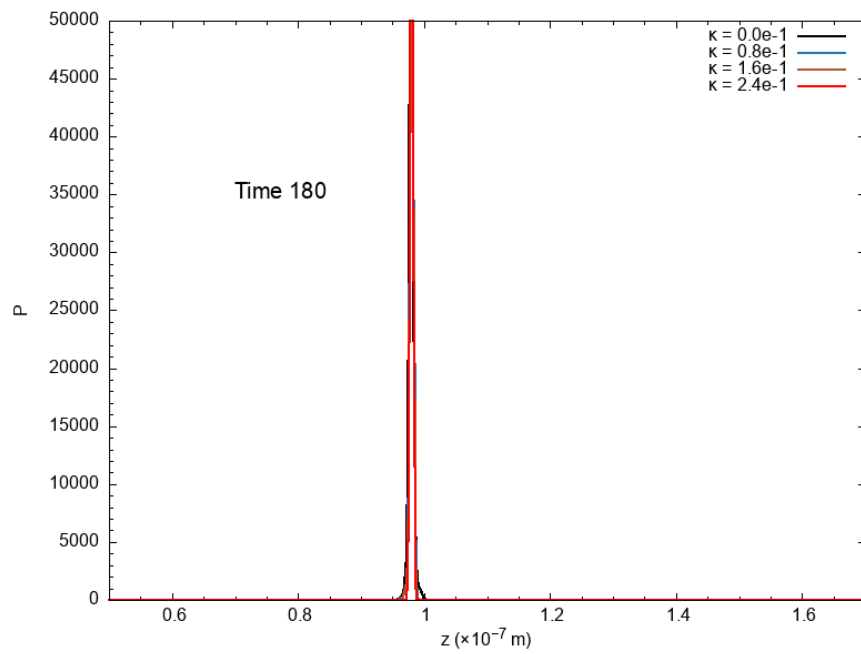


Figure 7

Réfléchir

	Figure 2	Figure 3	Figure 4	Note
1	$\mathbb{P}(x, \kappa, t), \mathbb{P}(v, \kappa, t)$	MSD w/(o) fixed Δ	$\langle D \rangle (\kappa)$ w/(o) fixed Δ	MSD w/ fixed Δ in SI
2	$\mathbb{P}(z/x, t, \kappa), \mathbb{P}(v_{z/x}, t, \kappa)$	MSD(t, κ) w/o fixed Δ	$D(\kappa)$	2+3+4, $\mathbb{P}(X/V_{x/\theta})$
3.A	$\mathbb{P}(\Delta) \times (2\kappa, 4t)$	MSD($\bar{\Delta}$) $\times (3\kappa)$, th.+num.	$\langle D \rangle (\kappa)$ fixed Δ	2d figures: time $\times\kappa$
3.B	$\mathbb{P}(v_\Delta) \times (2\kappa, 4t)$	MSD(Δ) $\times (3\kappa)$	$\langle D \rangle (\kappa)$ unfixed	

Discussion 20230302

$$\begin{aligned}
 M\dot{v} &= -\gamma(v, x)v + \Delta M\dot{v} & M^*v &= -\gamma(v, x)v + F + Tu + \eta \\
 \frac{\partial P}{\partial t} &= \nabla_v [Tp\Gamma\nabla_v P + \frac{1}{M^*}\gamma v P - \frac{1}{M^*}(\nabla\phi)P] - \nabla_x [vP] + \beta\nabla_x\phi v P \\
 P(v, x) &= \exp\left(-\frac{1}{2}\beta m v^2 - \beta\phi\right) & H(v, \delta) &= \frac{1}{2}Mv^2 + \int P\delta + \int \frac{\delta^2}{2\kappa} \\
 \exp(-\beta H_{\text{eff}}) &= \int \exp[-\beta H(v, \delta)] d\delta = \exp\left(-\frac{1}{2}\beta M v^2\right) + \frac{1}{2}\beta \int \kappa P \\
 &\rightarrow \exp\left(-\frac{1}{2}\beta M^2\right) + \frac{1}{2}\beta v^2 \int \kappa f^2(x) dx \rightarrow \exp\left(-\frac{1}{2}\beta M^* v^2\right)
 \end{aligned}$$

on pose que $P \simeq v f(x)$ lineaire.

1. $M \rightarrow M^*$ check fluc-diss? $D = D_0$ independent of κ
2. + harmonic potential,

Energy check

$$\begin{aligned}
 [1 + \delta M_1(\kappa, \Delta)] \ddot{\Delta} &= F_1 [X_G, \Delta, \dot{X}_G, \dot{\Delta}, \kappa] \\
 [1 + \delta M_2(\kappa, \Delta)] \ddot{X}_G &= F_2 [X_G, \Delta, \dot{X}_G, \dot{\Delta}, \kappa] \\
 H &= \frac{\dot{\Delta}^2}{2} + \frac{\dot{X}_G^2}{2} + \int dX P \Delta_s + \int dX \frac{\Delta_s^2}{2\kappa} = \frac{1}{2} \{ [1 + \delta M_1(\kappa, \Delta)] \dot{\Delta}^2 + [1 + \delta M_2(\kappa, \Delta)] \dot{X}_G^2 \} \\
 \frac{dv}{dt} &= f + \eta, \quad \rightarrow \quad v_{i+1} = v_i + \sqrt{2D(z)} \times w_i + f_i \\
 \frac{dx}{dt} &= v \quad \rightarrow \quad x_{i+1} = x_i + v_{i+1} \times \Delta t
 \end{aligned}$$