Toy Model on Theta

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SITUATION OF THE PROBLEM

To simulate the 3D Brownian motion near the soft surface, we have to solve Langevin equation numerically, depending on the reference «*J. Phys. Chem. B* 2014, 118, 6466».

$$\mathrm{d}v = \frac{f(t)}{m}\mathrm{d}t - \gamma v \mathrm{d}t + \sqrt{\frac{2\gamma}{\beta m}}\mathrm{d}W(t)$$

However, there would be negative variables related to γ shown in square root, leading to undesired results during the calculation.

Therefore, we wish to consider a rather simple case only with one variable θ, namely the rotation angle, for the sake of the possible analytical solution of the noise correlator η. Suppose that we have a differential equation below:

$$m\ddot{\theta} = -\lambda\dot{\theta} - k\theta + \eta^* \tag{1}$$

where $\eta^* = m\eta$ refers to the white noise. If we have $\gamma = \lambda/m$, and $\omega_0^2 = k/m$, then

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} + \gamma\frac{\mathrm{d}\theta}{\mathrm{d}t} + \omega_0^2\theta = \eta \tag{2}$$

INTEGRAL TRANSFORM

Consider the Fourier transform $\hat{\theta}(\omega) = \int_{-\infty}^{+\infty} \theta(t)e^{-i\omega t}\mathrm{d}t$. Since the Fourier transformation of the n-th derivative $f^{(n)}$ is given by $\widehat{f^{(n)}}(\omega) = \mathcal{F}\,\frac{\mathrm{d}^n}{\mathrm{d}t^n}f(t) = (i\omega)^n\hat{f}(\omega)$, we obtain

$$-\omega^2\hat{\theta}(\omega) + i\gamma\omega\hat{\theta}(\omega) + \omega_0^2\hat{\theta}(\omega) = \hat{\eta}(\omega) \tag{3}$$

Thus we solve

$$\hat{\theta}(\omega) = \frac{\hat{\eta}(\omega)}{\omega_0^2 - \omega^2 + i\gamma\omega} \tag{4}$$

After the inverse Fourier transform $\theta(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\hat{\theta}(\omega)e^{i\omega t}\mathrm{d}\omega$, we have the solution as

$$\theta(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{\hat{\eta}(\omega)}{\omega_0^2 - \omega^2 + i\gamma\omega}e^{i\omega t}\mathrm{d}\omega \tag{5}$$

If we know the initial condition, for example, $\theta(0) = \phi, \dot{\theta}(0) = \psi$. We could exploit the Laplace transform $\tilde{\theta}(s) = \int_0^\infty \theta(t)e^{-st}\mathrm{d}t$, with the property $\widetilde{\theta'}(t) = s\tilde{\theta}(s) - \theta(0)$, getting

$$\left[s^2\tilde{\theta}(s) - s\phi - \psi\right] + \gamma\left[s\tilde{\theta}(s) - \phi\right] + \omega_0^2\tilde{\theta}(s) = \tilde{\eta}(s) \tag{6}$$

Thus we solve

$$\begin{aligned}\tilde{\theta}(s) &= \frac{s\phi + (2\gamma^*\phi + \psi) + \tilde{\eta}(s)}{s^2 + 2\gamma^* s + \omega_0^2} \\ &= \frac{\phi(s+\gamma^*)}{(s+\gamma^*)^2 + R} + \frac{\gamma^*\phi + \psi}{(s+\gamma^*)^2 + R} + \frac{\tilde{\eta}(s)}{(s+\gamma^*)^2 + R}\end{aligned} \tag{7}$$

where $\gamma^* = \gamma/2$ and $R = \omega_0^2 - (\gamma^*)^2$. There would be three cases depending on the value of R:

- If $R > 0$, then we pose $R = a^2$ and $a = \sqrt{\omega_0^2 - (\gamma^*)^2}$. After the inverse Laplace transform, we obtain

$$\theta(t) = e^{-\gamma^* t}\left[\phi\cos(at) + \frac{\gamma^*\phi + \psi}{a}\sin(at)\right] + \frac{1}{a}\int_0^t \eta(\tau)e^{-\gamma^*(t-\tau)}\sin\left[a(t-\tau)\right]\mathrm{d}\tau \tag{8}$$

- If $R = 0$, then $a = 0$ and we have

$$\theta(t) = e^{-\gamma^* t}\left[\phi + (\gamma^*\phi + \psi)t\right] + \int_0^t \eta(\tau)(t-\tau)e^{-\gamma^*(t-\tau)}\mathrm{d}\tau \tag{9}$$

- If $R < 0$, then we pose $R = -b^2$ and $b = \sqrt{(\gamma^*)^2 - \omega_0^2}$. Due to the imaginary part, we replace $\sin \to \sinh, \cos \to \cosh, a \to b$

$$\theta(t) = e^{-\gamma^* t}\left[\phi\cosh(bt) + \frac{\gamma^*\phi + \psi}{b}\sinh(bt)\right] + \frac{1}{b}\int_0^t \eta(\tau)e^{-\gamma^*(t-\tau)}\sinh\left[b(t-\tau)\right]\mathrm{d}\tau \tag{10}$$

CORRELATOR AS WHITE NOISE

Without loss of generality, we take $\phi = \psi = 0$. Suppose that $\langle\eta^*(t)\eta^*(t')\rangle = 2B\delta(t-t')$, hence $\langle\eta(t)\eta(t')\rangle = \frac{2B}{m^2}\delta(t-t')$. For the case $R > 0$, we could see

$$\theta(t) = \frac{1}{a}\int_0^t \eta(\tau)e^{-\gamma^*(t-\tau)}\sin\left[a(t-\tau)\right]\mathrm{d}\tau$$

$$\begin{aligned}\left\langle\theta^2(t)\right\rangle &= \frac{1}{a^2}\int_0^t \mathrm{d}\tau_1\int_0^t \mathrm{d}\tau_2 e^{-\gamma^*(t-\tau_1)}\sin\left[a(t-\tau_1)\right]e^{-\gamma^*(t-\tau_2)}\sin\left[a(t-\tau_2)\right]\langle\eta(\tau_1)\eta(\tau_2)\rangle \\ &= \frac{1}{a^2}\int_0^t d\tau_1 e^{-2\gamma^*(t-\tau_1)}\sin^2\left[a(t-\tau_1)\right]\times\frac{2B}{m^2} \\ &= \frac{2B}{m^2a^2}\times\frac{e^{-2\gamma^* t}\left(a^2\left(e^{2\gamma^* t} - 1\right) + \gamma^{*2}\cos(2at) - a\gamma^*\sin(2at) - \gamma^{*2}\right)}{4\gamma^*\left(a^2 + \gamma^{*2}\right)} \\ &\xrightarrow[a>0,\,\gamma^*>0]{t\to\infty} \frac{2B}{m^2a^2}\times\frac{a^2}{4a^2\gamma^* + 4\gamma^{*3}} = \frac{B}{2\gamma^*(\gamma^{*2} + a^2)} = \frac{B}{2m^2\gamma^*\omega_0^2} = \frac{B}{\lambda k} \sim k_BT\end{aligned}$$

thus we have $\boxed{B \sim k_BT\lambda k}$.

For the case $R < 0$, we have the similar result

$$\begin{aligned}
\left\langle \theta^2(t) \right\rangle &= \frac{1}{b^2} \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2 e^{-\gamma^*(t-\tau_1)} \sinh\left[b(t-\tau_1)\right] e^{-\gamma^*(t-\tau_2)} \sinh\left[b(t-\tau_2)\right] \langle \eta(\tau_1)\eta(\tau_2) \rangle \\
&= \frac{1}{b^2} \int_0^t d\tau_1 e^{-2\gamma^*(t-\tau_1)} \sinh^2\left[b(t-\tau_1)\right] \times \frac{2B}{m^2} \\
&= \frac{2B}{m^2 b^2} \times \frac{e^{-2\gamma^* t}\left(b^2\left(e^{2\gamma^* t} - 1\right) - \gamma^*(\gamma^* \cosh(2bt) + b\sinh(2bt)) + \gamma^{*2}\right)}{4\left(\gamma^{*3} - b^2\gamma^*\right)} \\
&\xrightarrow[b>0,\, b<\gamma^*,\, \gamma^*>0]{t\to\infty} \frac{2B}{m^2 b^2} \times \frac{b^2}{4\left(\gamma^{*3} - b^2\gamma^*\right)} = \frac{B}{2m^2\gamma^*(\gamma^{*2} - b^2)} = \frac{B}{2m^2\gamma^*\omega_0^2} = \frac{B}{\lambda k} \sim k_B T
\end{aligned}$$

For the case $R > 0$, also with $\phi = \psi = 0$, we take Leibniz integral rule

$$\begin{aligned}
\dot{\theta}(t) = \frac{\mathrm{d}\theta(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{a}\int_0^t \eta(\tau) e^{-\gamma^*(t-\tau)} \sin\left[a(t-\tau)\right] \mathrm{d}\tau\right\} \\
&= \frac{1}{a}\int_0^t \eta(\tau) e^{\gamma^*(\tau-t)}(a\cos(a(t-\tau)) - \gamma^* \sin(a(t-\tau)))\, d\tau
\end{aligned} \tag{11}$$

Then we consider $\left\langle \dot{\theta}^2(t) \right\rangle$.

$$\begin{aligned}
\left\langle \dot{\theta}^2 \right\rangle &= \frac{1}{a^2}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, e^{\gamma^*(\tau_1 - t)} \left\{a\cos\left[a(t-\tau_1)\right] - \gamma^* \sin\left[a(t-\tau_1)\right]\right\} \\
&\quad \times e^{\gamma^*(\tau_2 - t)} \left\{a\cos\left[a(t-\tau_2)\right] - \gamma^* \sin\left[a(t-\tau_2)\right]\right\} \times \langle \eta(\tau_1)\eta(\tau_2) \rangle \\
&= \frac{1}{a^2}\int_0^t \mathrm{d}\tau_1\, e^{2\gamma^*(\tau_1 - t)} \left\{a\cos\left[a(t-\tau_1)\right] - \gamma^* \sin\left[a(t-\tau_1)\right]\right\}^2 \times \frac{2B}{m^2} \\
&= \frac{2B}{m^2 a^2} \times \frac{a^2 - e^{-2\gamma^* t}\left(a^2 - \gamma^*(\gamma^* \cos(2at) + a\sin(2at)) + \gamma^{*2}\right)}{4\gamma^*} \\
&\xrightarrow[a>0,\, \gamma^*>0]{t\to\infty} \frac{2B}{m^2 a^2} \times \frac{a^2}{4\gamma^*} = \frac{B}{m^2\gamma} \sim k_B T
\end{aligned}$$

If $R < 0$, we have

$$\begin{aligned}
\dot{\theta}(t) = \frac{\mathrm{d}\theta(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{b}\int_0^t \eta(\tau) e^{-\gamma^*(t-\tau)} \sinh\left[b(t-\tau)\right] \mathrm{d}\tau\right\} \\
&= \frac{1}{b}\int_0^t \eta(\tau) e^{\gamma^*(\tau-t)}(b\cosh(b(t-\tau)) - \gamma^* \sinh(b(t-\tau)))\, d\tau
\end{aligned} \tag{12}$$

$$\begin{aligned}
\left\langle \dot{\theta}^2 \right\rangle &= \frac{1}{b^2}\int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_2\, e^{\gamma^*(\tau_1 - t)} \left\{b\cosh\left[b(t-\tau_1)\right] - \gamma^* \sinh\left[b(t-\tau_1)\right]\right\} \\
&\quad \times e^{\gamma^*(\tau_2 - t)} \left\{b\cosh\left[b(t-\tau_2)\right] - \gamma^* \sinh\left[b(t-\tau_2)\right]\right\} \times \langle \eta(\tau_1)\eta(\tau_2) \rangle \\
&= \frac{1}{b^2}\int_0^t \mathrm{d}\tau_1\, e^{2\gamma^*(\tau_1 - t)} \left\{b\cosh\left[b(t-\tau_1)\right] - \gamma^* \sinh\left[b(t-\tau_1)\right]\right\}^2 \times \frac{2B}{m^2} \\
&= \frac{2B}{b^2} \times \frac{e^{-2\gamma^* t}\left(b^2\left(e^{2\gamma^* t} - 1\right) - \gamma^{*2}\cosh(2bt) + b\gamma^* \sinh(2bt) + \gamma^{*2}\right)}{4\gamma^*} \\
&\xrightarrow[b>0,\, b<\gamma^*,\, \gamma^*>0]{t\to\infty} \frac{2B}{m^2 b^2} \times \frac{b^2}{4\gamma^*} = \frac{B}{m^2\gamma} \sim k_B T
\end{aligned}$$

CORRELATOR AS COLORED NOISE

We would like to introduce the Lorentzian for the correlator.

$$\langle\eta(\tau_1)\eta(\tau_2)\rangle = \delta(\tau_1-\tau_2)\cdot\frac{1}{\pi\Gamma}\frac{\Gamma^2}{(\tau_1-w)^2+\Gamma^2}$$

Hence we should calculate the following integration:

$$\begin{aligned}
&\iint \mathrm{d}\tau_1\mathrm{d}\tau_2\, e^{-\gamma(t-\tau_1)}\cdot\sin\left[a(t-\tau_1)\right]\cdot e^{-\gamma(t-\tau_2)}\cdot\sin\left[a(t-\tau_2)\right]\cdot\frac{\delta(\tau_1-\tau_2)}{\pi\Gamma}\frac{\Gamma^2}{(\tau_1-w)^2+\Gamma^2}\\
&=\int \mathrm{d}\tau\, e^{-2\gamma(t-\tau)}\cdot\sin\left[a(t-\tau)\right]\cdot\frac{1}{\pi\Gamma}\frac{\Gamma^2}{(\tau-w)^2+\Gamma^2}\\
&=-\frac{i}{8\pi}e^{2\gamma(-5i\Gamma-2t+w)}\Big(e^{-2a(\Gamma+i(t+w))+8i\gamma\Gamma+2\gamma t}\Big(e^{4iat}\mathrm{Ei}(2(a+i\gamma)(\Gamma+i(w-\tau)))-e^{4a\Gamma+4iat+4i\gamma\Gamma}\mathrm{Ei}(2i(a+i\gamma)(w+i\Gamma-\tau))\\
&\quad+e^{4a(\Gamma+iw)}\mathrm{Ei}(2(ia+\gamma)(-w+i\Gamma+\tau))-e^{4i(aw+\gamma\Gamma)}\mathrm{Ei}(2(ia+\gamma)(-w-i\Gamma+\tau))\Big)\\
&\quad+2e^{2\gamma(t+6i\Gamma)}\mathrm{Ei}(-2\gamma(w+i\Gamma-\tau))-2e^{2\gamma(t+4i\Gamma)}\mathrm{Ei}(2\gamma(-w+i\Gamma+\tau))\Big)\Big|_0^t\\
&=\frac{i}{8\pi}\exp(-2(a(\Gamma+i(t+w))+\gamma(i\Gamma+t-w)))\Big(-e^{4iat}\left(\mathrm{Ei}(2(-ia+\gamma)(t-w+i\Gamma))-\mathrm{Ei}(2(a+i\gamma)(iw+\Gamma))\right.\\
&\quad\left.+e^{4\Gamma(a+i\gamma)}\mathrm{Ei}(2i(a+i\gamma)(w+i\Gamma))\right)-e^{4a(\Gamma+iw)}\mathrm{Ei}(2(ia+\gamma)(t-w+i\Gamma))\\
&\quad-2e^{2a(\Gamma+i(t+w))}\Big(-\mathrm{Ei}(2\gamma(t-w+i\Gamma))+e^{4i\gamma\Gamma}(\mathrm{Ei}(2\gamma(t-w-i\Gamma))-\mathrm{Ei}(-2\gamma(w+i\Gamma)))+\mathrm{Ei}(2i\gamma\Gamma-2w\gamma)\Big)\\
&\quad+e^{4a\Gamma+4iat+4i\gamma\Gamma}\mathrm{Ei}(2(-ia+\gamma)(t-w-i\Gamma))+e^{4i(aw+\gamma\Gamma)}\mathrm{Ei}(2(ia+\gamma)(t-w-i\Gamma))\\
&\quad-e^{4i(aw+\gamma\Gamma)}\mathrm{Ei}(2(a-i\gamma)(\Gamma-iw))+e^{4a(\Gamma+iw)}\mathrm{Ei}(2(ia+\gamma)(i\Gamma-w))\Big)
\end{aligned}$$

where Ei is the exponential integral. For real non-zero values of x

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty}\frac{e^{-t}}{t}\mathrm{d}t = \int_{-\infty}^{x}\frac{e^{t}}{t}\mathrm{d}t$$

For complex values of the argument, the definition becomes ambiguous due to branch points at 0 and ∞. Instead of Ei, the following notation is used

$$E_1(z) = \int_z^{\infty}\frac{e^{-t}}{t}\mathrm{d}t \qquad |\mathrm{Arg}(z)| < \pi$$

For positive values of x, we have $-E_1(x) = \mathrm{Ei}(-x)$.