Brownian motion with inertia

$$\boxed{m\frac{d\underset{\sim}{u}}{dt} = -\gamma \underset{\sim}{u} + \underset{\sim}{A}'(t)}, \quad \frac{d\underset{\sim}{u}}{dt} = -\zeta \underset{\sim}{u} + \underset{\sim}{A}(t) \Rightarrow \underbrace{e^{\zeta t}\left(\frac{d\underset{\sim}{u}}{dt} + \zeta \underset{\sim}{u}\right)}_{\frac{d}{dt}\left(\underset{\sim}{u} e^{\zeta t}\right)} = A e^{\zeta t}$$

$$\underset{\sim}{u}(0) = \underset{\sim}{u}_0$$

so, $\underset{\sim}{u} e^{\zeta t} - \underset{\sim}{u}_0 = \int_0^t dt' e^{\zeta t'} \underset{\sim}{A}(t')$

or $\boxed{\underset{\sim}{U} = \underset{\sim}{u}(t) - \underset{\sim}{u}_0 e^{-\zeta t} = e^{-\zeta t}\int_0^t dt' e^{\zeta t'} \underset{\sim}{A}(t')} \Rightarrow \langle \underset{\sim}{U} \rangle = e^{-\zeta t}\int_0^t dt' e^{\zeta t'} \langle \underset{\sim}{A}(t') \rangle = 0$

higher moments:

$$\langle U^2 \rangle = \langle u^2 \rangle - 2\underbrace{\langle \underset{\sim}{u} \rangle}_{= \underset{\sim}{u}_0 e^{-\zeta t}} \underset{\sim}{u}_0 e^{-\zeta t} + u_0^2 e^{-2\zeta t} = \langle u^2 \rangle - u_0^2 e^{-2\zeta t}$$

$$= e^{-2\zeta t}\int_0^t dt' \int_0^t dt'' e^{\zeta(t'+t'')} \underbrace{\langle \underset{\sim}{A}(t') \cdot \underset{\sim}{A}(t'') \rangle}_{\substack{\phi(|t'-t''|) \\ \text{(hypothesis)}}}$$

let $t'+t'' = x$, $t'-t'' = y$; $t' = \frac{x+y}{2}$, $t'' = \frac{x-y}{2}$

Jacobian $\begin{vmatrix} \partial x/\partial t' & \partial x/\partial t'' \\ \partial y/\partial t' & \partial y/\partial t'' \end{vmatrix} = \left| \begin{vmatrix} 1 & 1 \\ 1 & -1 \end{vmatrix} \right| = 2$

$$= \frac{1}{2} e^{-2\zeta t}\int_0^{2t} e^{\zeta x} dx \underbrace{\overbrace{\int_{-\infty}^{\infty} \phi(y)\, dy}^{\equiv \tau}}_{\substack{\text{extend limits by} \\ \text{virtue of short-range} \\ \text{feature of } \phi}}$$

$$\Rightarrow \langle U^2 \rangle = \frac{1}{2} e^{-2\zeta t} \tau \cdot \frac{1}{\zeta}\left(e^{2\zeta t} - 1\right) = \boxed{\frac{\tau}{2\zeta}\left(1 - e^{-2\zeta t}\right)}$$

as $t \to \infty$, $\langle U^2 \rangle$ satisfies $\frac{1}{2} m \langle U^2 \rangle = \frac{3}{2} k_B T$ (equipartition)

or $\langle U^2 \rangle = 3k_B T/m$

so, $\frac{\tau}{2\zeta} = \frac{3k_B T}{m}$ $\quad \boxed{\langle U^2 \rangle = \frac{3k_B T}{m}\left(1 - e^{-2\zeta t}\right)}$

To evaluate higher moments, we note that since $\langle \underset{\sim}{A} \rangle = 0$, all odd moments $= 0$.
For the even moments we'll have to evaluate expressions of the form

↓

(2)

$$e^{-2n\zeta t}\int dt_1\cdots\int dt_{2n}\, e^{\zeta(t_1+\cdots+t_{2n})}\langle \underset{\sim}{A}(t_1)\underset{\sim}{A}(t_2)\cdots\underset{\sim}{A}(t_{2n})\rangle$$

doing this by pairs will give the same contribution per pair as $\langle U^2\rangle$, yielding $\langle U^2\rangle^n$, with a prefactor given by the number of distinct pairs we can choose from $2n$ labels $t_1,\ldots,t_{2n}$. With $2n$ labels there are n pairs:

the # of ways is $\dfrac{(2n)!}{n!\,2^n} = \dfrac{2n(2n-1)(2n-2)(2n-3)\cdots}{n(n-1)(n-2)\cdots 2^n} = (2n-1)!!$

$n!$ ← permuting pairs; 2^n ← switching within pairs

$$\therefore \boxed{\langle U^{2n}\rangle = (2n-1)!!\langle U^2\rangle^n} = (2n-1)(2n-3)\ldots 5\cdot 3\cdot 1\cdot\langle U^2\rangle^n$$

For a Gaussian distribution this is exactly the case

$\langle U^2\rangle = 1!\langle U^2\rangle$

$\langle U^4\rangle = 3\langle U^2\rangle^2$

$\langle U^6\rangle = 15\langle U^2\rangle^3$

$$\therefore \boxed{P(\underset{\sim}{u},t;\underset{\sim}{u}_0,0) = \left[\frac{m}{2\pi k_BT(1-e^{-2\zeta t})}\right]^{3/2}\exp\left\{-\frac{m\,|\underset{\sim}{u}-\underset{\sim}{u}_0e^{-\zeta t}|^2}{2k_BT(1-e^{-2\zeta t})}\right\}}$$

since $\underset{\sim}{u}(t) = \underset{\sim}{u}_0e^{-\zeta t} + \int_0^t dt'\,e^{-\zeta(t-t')}\underset{\sim}{A}(t')$; $\underset{\sim}{r}-\underset{\sim}{r}_0 = \int_0^t dt'\,\underset{\sim}{u}(t')$

$$\Rightarrow \underset{\sim}{r}-\underset{\sim}{r}_0 = \int_0^t dt'\left[\underset{\sim}{u}_0e^{-\zeta t'} + \int_0^{t'}dt''\,e^{-\zeta(t'-t'')}\underset{\sim}{A}(t'')\right]$$

$$\boxed{\underset{\sim}{r}-\underset{\sim}{r}_0-\frac{1}{\zeta}(1-e^{-\zeta t})\underset{\sim}{u}_0 = \int_0^t dt'\int_0^{t'}dt''\,e^{-\zeta(t'-t'')}\underset{\sim}{A}(t'')}$$

integrate by parts:

$dv = dt'e^{-\zeta t'}$ $\quad u = \int_0^{t'}dt''e^{\zeta t''}\underset{\sim}{A}(t'')$

$v = -\frac{1}{\zeta}e^{-\zeta t'}$ $\quad du = e^{\zeta t'}\underset{\sim}{A}(t')\,dt'$

$$-\frac{1}{\zeta}e^{-\zeta t'}\int_0^{t'}dt''e^{\zeta t''}\underset{\sim}{A}(t'')\Big|_0^t + \frac{1}{\zeta}\int_0^t dt'\,e^{-\zeta t'}e^{\zeta t'}\underset{\sim}{A}(t')$$

$$= -\frac{1}{\zeta}e^{-\zeta t}\int_0^t dt'e^{\zeta t'}\underset{\sim}{A}(t') + \frac{1}{\zeta}\cdots = \frac{1}{\zeta}\int_0^t dt'\left[1-e^{-\zeta(t-t')}\right]\underset{\sim}{A}(t')$$

change label

$$\Rightarrow \boxed{\langle\underset{\sim}{r}-\underset{\sim}{r}_0\rangle = \frac{\underset{\sim}{u}_0}{\zeta}(1-e^{-\zeta t})}$$

Brownian motion w/inertia

Calculate the variance: $\underset{\sim}{r}-\underset{\sim}{r}_0-\frac{\underset{\sim}{u}_0}{\zeta}(1-e^{-\zeta t}) = \frac{1}{\zeta}\int_0^t dt'\left[1-e^{-\zeta(t-t')}\right]\underset{\sim}{A}(t')$

$$|\underset{\sim}{r}-\underset{\sim}{r}_0|^2-2(\underset{\sim}{r}-\underset{\sim}{r}_0)\cdot\frac{\underset{\sim}{u}_0}{\zeta}(1-e^{-\zeta t})+\frac{\underset{\sim}{u}_0^2}{\zeta^2}(1-e^{-\zeta t})^2$$

$$=\frac{1}{\zeta^2}\int_0^t dt'\int_0^t dt''\left[1-e^{-\zeta(t-t')}\right]\left[1-e^{-\zeta(t-t'')}\right]\underset{\sim}{A}(t')\cdot\underset{\sim}{A}(t'')$$

$$1-e^{-\zeta t+\zeta t'}-e^{-\zeta t+\zeta t''}+e^{-2\zeta t+\zeta(t'+t'')}$$

$\langle\ \rangle \Rightarrow$

$$\langle|\underset{\sim}{r}-\underset{\sim}{r}_0|^2\rangle-\frac{u_0^2}{\zeta^2}(1-e^{-\zeta t})^2=\underbrace{\frac{1}{\zeta^2}\int_0^t dt'\int_0^t dt''\langle\underset{\sim}{A}(t')\cdot\underset{\sim}{A}(t'')\rangle}_{\frac{1}{2}\int_0^{2t}dx\,\tau=t\tau}\underbrace{-e^{-\zeta t}\int_0^t dt'\int_0^t dt''e^{\zeta t'}\langle AA\rangle}_{e^{-\zeta t}\cdot\frac{1}{2}\int_0^{2t}dx\,e^{\zeta x/2}\int dy\,\phi}$$

$$=-\frac{\tau}{\zeta}(1-e^{-\zeta t})$$

$$-e^{-\zeta t}\int_0^t dt'\int_0^t dt''e^{\zeta t''}\langle AA\rangle$$

as previous $=-\frac{\tau}{\zeta}(1-e^{-\zeta t})$

$$+e^{-2\zeta t}\int_0^t dt'\int_0^t dt''e^{\zeta(t'+t'')}\langle AA\rangle$$

$$\frac{\tau}{2\zeta}(1-e^{-2\zeta t})$$

so, $\langle|\underset{\sim}{r}-\underset{\sim}{r}_0|^2\rangle-\frac{u_0^2}{\zeta^2}(1-e^{-\zeta t})^2=\frac{\tau}{\zeta^2}\left[t-\frac{2}{\zeta}(1-e^{-\zeta t})+\frac{1}{2\zeta}(1-e^{-2\zeta t})\right]$

$\tau=\frac{3k_BT}{m}\cdot 2\zeta$

$$=\frac{3k_BT}{m\zeta^2}\left[2\zeta t-4(1-e^{-\zeta t})+1-e^{-2\zeta t}\right]$$

$$=\boxed{\frac{3k_BT}{m\zeta^2}\left(2\zeta t-3+4e^{-\zeta t}-e^{-2\zeta t}\right)}$$

for small t $\cancel{2\zeta t}\cancel{-3}+4\left(\cancel{1-\zeta t+\frac{1}{2}\zeta^2t^2}-\frac{1}{6}\zeta^3t^3+\dots\right)\cancel{-1+2\zeta t-\frac{1}{2}\cdot 4\zeta^2t^2}+\frac{1}{6}\cdot 8\zeta^3t^3+\dots$

$\simeq O(\zeta^3t^3)$

so $\langle|\underset{\sim}{r}-\underset{\sim}{r}_0|^2\rangle\simeq\frac{u_0^2}{\zeta^2}\cdot\zeta^2t^2\simeq u_0^2t^2$ "ballistic"

For small t the initial conditions are remembered.

For large t $(\zeta t \gg 1)$,

$$\langle |\underset{\sim}{r} - \underset{\sim}{r}_0|^2 \rangle - \frac{u_0^2}{\zeta^2} \simeq \frac{3k_BT}{m\zeta^2}\left(2\zeta t - 3 \right)$$

↑ dominant term

$$\langle |\underset{\sim}{r} - \underset{\sim}{r}_0|^2 \rangle \simeq \frac{6k_BT}{m\zeta} t$$

but $m\zeta = \gamma$ (original eqn)

$$\frac{6k_BT}{m\zeta} = \frac{6k_BT}{\gamma} = 6D$$

$$\boxed{\langle |\underset{\sim}{r} - \underset{\sim}{r}_0|^2 \rangle \simeq 6Dt}$$

diffusion in three dimensions!

Polymerization

$$j = -D\frac{\partial p}{\partial x} - \frac{F}{\zeta}p \qquad \frac{\partial p}{\partial t} = -\frac{\partial j}{\partial x}$$

$F=0$, steady state $\frac{\partial^2 p}{\partial x^2}=0 \Rightarrow p(x)=A+Bx$ with $\int_0^\ell dx\,p(x)=1$ and $p(\ell)=0$

$$A\ell + \tfrac{1}{2}B\ell^2 = 1 \qquad A+B\ell=0$$

$$A=-B\ell$$

$$-B\ell^2+\tfrac{1}{2}B\ell^2=1=-\tfrac{1}{2}B\ell^2$$

$$B=-\frac{2}{\ell^2}\,;\ A=\frac{2}{\ell}$$

$$j=-D\frac{\partial p}{\partial x}=-D\cdot B=\frac{2D}{\ell^2}$$

$$\boxed{j=\frac{2D}{\ell^2} \Rightarrow \tau_1=\frac{\ell^2}{2D}}$$

"velocity" $=\ell/\tau_1 = 2D/\ell$

$F\neq 0$

$$\boxed{j=-D\frac{dp}{dx} + \frac{F}{\zeta}p}$$

homogeneous solution is just $-D\frac{dp_h}{dx}=\frac{F}{\zeta}p_h$

$p_h = A\exp(-Fx/\zeta D)$ but $D\zeta=k_BT$ (Stokes-Einstein)

$$=\boxed{A\,e^{-\beta Fx}}$$

inhomogeneous (particular) sol'n is $\boxed{p_{in}=-\frac{\zeta j}{F}}$ constant

again, two requirements on the sum $p(x)=Ae^{-\beta Fx}-\frac{\zeta j}{F}$

$$p(\ell)=0\ :\ Ae^{-\beta F\ell}-\frac{\zeta j}{F}=0$$

$$-\frac{\zeta j}{F}=-Ae^{-\beta F\ell}$$

$$\int_0^\ell dx\,p(x)=1=\frac{A}{-\beta F}\left(e^{-\beta F\ell}-1\right)-\frac{\zeta j\ell}{F}$$

$$\frac{A}{\beta F}\left(1-e^{-\beta F\ell}\right)-A\ell e^{-\beta F\ell}=1 \quad \text{or} \quad \frac{A}{\beta F}\left\{1-e^{-\beta F\ell}-\beta F\ell e^{-\beta F\ell}\right\}=1$$

$$A=\frac{\beta F}{1-(1+\beta F\ell)e^{-\beta F\ell}} \qquad j=\frac{FA}{\zeta}e^{-\beta F\ell}=\frac{\beta F^2}{\zeta}\,\frac{e^{-\beta F\ell}}{1-(1+\beta F\ell)e^{-\beta F\ell}}$$

or,
$$j = \frac{\beta F^2}{\zeta} \frac{1}{e^{\beta F\ell} - 1 - \beta F\ell} \qquad \frac{1}{\zeta} = \frac{D}{k_B T} \qquad \frac{\beta F^2}{\zeta} = \frac{1}{(k_B T)^2} F^2 D$$

$$\boxed{j = \frac{DF^2}{(k_B T)^2} \cdot \frac{1}{e^{\beta F\ell} - 1 - \beta F\ell}}$$

as a check, as $F \to 0$
$$e^{\beta F\ell} - 1 - \beta F\ell \simeq \cancel{1} + \cancel{\beta F\ell} + \tfrac{1}{2}(\beta F\ell)^2 - \cancel{1} - \cancel{\beta F\ell} + \dots$$
$$\simeq \tfrac{1}{2}\beta^2 F^2 \ell^2 + \dots$$

and
$$j \to \frac{D\cancel{F^2}}{\cancel{(k_B T)^2}} \cdot \frac{1}{\frac{1}{2}\cancel{\beta^2}\cancel{F^2}\ell^2} \simeq \frac{2D}{\ell^2} \quad \text{as before} \checkmark$$

when $\beta F\ell \gg 1$
$$j \simeq \frac{DF^2 e^{-\beta F\ell}}{(k_B T)^2}$$

$$\tau = \frac{(k_B T)^2}{F^2 D} e^{\beta F\ell}$$

note $k_B T/F$ is a length, call it "δ"

$$\tau \sim \underbrace{\frac{\delta^2}{D}}_{\text{time to diffuse a distance } \delta} \underbrace{e^{\beta F\ell}}_{\text{Boltzmann factor associated with work done on assembling polymer}}$$

Wormlike chain

$$\mathcal{E} = \frac{1}{2}A\int_0^L ds\, \kappa^2 - f z$$

(1)

$$z = \int_0^L ds \cos(\theta(s)) \simeq \int_0^L ds\{1 - \frac{1}{2}\theta^2(s) + \dots\} \simeq L - \frac{1}{2}\int_0^L ds\, \underset{\sim}{t}_\perp^2$$

$$|\underset{\sim}{t}_\perp| \sim \theta \qquad \Rightarrow \mathcal{E} \simeq \frac{1}{2}\int_0^L ds\left\{A\left(\frac{\partial \underset{\sim}{t}_\perp}{\partial s}\right)^2 + f\underset{\sim}{t}_\perp^2\right\} + \text{const}$$

define $\underset{\sim}{t}_\perp(s) = \sum_q e^{-iqs}\,\hat{t}_{\perp q}$

then $\mathcal{E} = \frac{1}{2}\int_0^L ds\left\{\sum_q \sum_{q'} e^{-i(q+q')s}\left[-qq'A + f\right]\hat{t}_{\perp q}\hat{t}_{\perp q'}\right\}$ $\qquad \int_0^L ds\, e^{-i(q+q')s} = L\delta_{q,-q'}$

$$= \frac{1}{2}\sum_q L(Aq^2 + f)|\hat{t}_{\perp q}|^2 \quad \Rightarrow \quad \langle|\hat{t}_{\perp q}|^2\rangle = \frac{k_BT}{L(Aq^2+f)}$$

x or y component

$$\text{length change} = \frac{1}{2}\int_0^L ds\, t_\perp^2 = \frac{1}{2}\sum_q \cdot \frac{2Lk_BT}{L(Aq^2+f)} \rightarrow \int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{Lk_BT}{Aq^2+f}$$

$$= \frac{Lk_BT}{2\pi}\cdot\frac{1}{A}\underbrace{\int_{-\infty}^{\infty}\frac{dq}{q^2+f/A}}$$

$$\frac{1}{\sqrt{f/A}}\tan^{-1}\frac{q}{\sqrt{f/A}}\Big|_{-\infty}^{\infty} = \frac{1}{\sqrt{f/A}}\left(\frac{\pi}{2} - (-)\frac{\pi}{2}\right)$$

$$L - Z \simeq \frac{Lk_BT}{2}\cdot\frac{1}{\sqrt{fA}} \quad \text{or} \quad \boxed{1 - \frac{Z}{L} \simeq \frac{k_BT}{\sqrt{4fA}}}$$

$$\boxed{\frac{Z}{L} \simeq 1 - \frac{k_BT}{\sqrt{4fA}}}$$

rewriting this, $\quad \boxed{f = \frac{k_BT}{L_p}\frac{1}{4(1-Z/L)^2}}$

$A = k_BTL_p$

Freely-jointed chain

partition function of one link $$Z_1 = \int_0^{\pi} d\theta \, \sin\theta \, e^{\beta f b \cos\theta}$$

$$= \frac{2\sinh(\beta f b)}{\beta f b}$$

$$\langle \text{displacement} \rangle = \frac{\partial \ln Z_1}{\partial \beta f} = b \left\{ \coth(\beta f b) - \frac{1}{\beta f b} \right\}$$

full $\langle \text{length} \rangle = Nb \left\{ \coth(\beta f b) - \frac{1}{\beta f b} \right\}$ extended length $= Nb$

$$\frac{\Delta\,\text{length}}{Nb} = 1 - z/L = 1 - \coth(\beta f b) + \frac{1}{\beta f b} \underset{\beta f b \gg 1}{\simeq} \frac{k_B T}{f b}$$

$$\Longrightarrow 1 - \frac{z}{L} \simeq \frac{k_B T}{f b} \quad \text{or} \quad \boxed{f \simeq \frac{k_B T}{b} \frac{1}{(1 - z/L)}}$$

Correlation function of WLC $$= \frac{1}{L} \int_0^L dr \left\langle \sum_q e^{-iqr} \hat{t}_\perp(q) \sum_{q'} e^{-iq'(r+s)} \hat{t}_\perp(q') \right\rangle$$

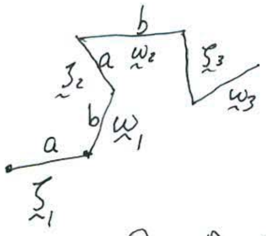
$$= \sum_q e^{iqs} \langle |t_\perp(q)|^2 \rangle = \sum_q \frac{k_B T}{L(A q^2 + f)} e^{iqs} \cdot 2$$

$$= \frac{2 k_B T}{A} \int \frac{dq}{2\pi} \frac{e^{iqs}}{q^2 + f/A} = \frac{k_B T}{\sqrt{fA}} e^{-s\sqrt{f/A}} \quad \boxed{\sim e^{-s/\xi}} \quad \xi = \sqrt{A/f}$$

by contour integration

Polymer chains

a) ab polymer



let $\tilde{\xi}_n$ be bond vector for a type

$\tilde{w}_n$ - - ——— . b ..

$$\tilde{R} \equiv \tilde{r}_{2N} - \tilde{r}_0 = \sum_{m=1}^{N} \tilde{\xi}_m + \sum_{n=1}^{N} \tilde{w}_n \quad \text{with } |\tilde{\xi}_n| = a \equiv l_a \quad |\tilde{w}_n| = b \equiv l_b$$

$$|\tilde{R}^2| = \sum_{m=1}^{N} \tilde{\xi}_m \cdot \sum_{n=1}^{N} \tilde{\xi}_n + 2 \sum_{m=1}^{N} \tilde{\xi}_m \cdot \sum_{n=1}^{N} \tilde{w}_n + \sum_{m=1}^{N} \tilde{w}_m \cdot \sum_{n=1}^{N} \tilde{w}_n$$

taking the average over realisations, we see that all x-terms such as $\langle \tilde{\xi} \cdot \tilde{w} \rangle \to 0$ and all off-diagonal self terms like $\langle \tilde{\xi}_l \cdot \tilde{\xi}_m \rangle \to 0$ for $l \neq m$, leaving only the diagonal terms.

$$|\tilde{R}^2| = \sum_{m=1}^{N} \tilde{\xi}_m^2 + \sum_{n=1}^{N} \tilde{w}_n^2 = N \cdot a^2 + N \cdot b^2 = \boxed{N\underbrace{(a^2+b^2)}}$$

effective, average length^2 of compound segment.

stretching

$$\text{total } x = \sum l_n \cos\theta_n = \sum l_n^{(a)} \cos\theta_n^{(a)} + \sum l_n^{(b)} \cos\theta_n^{(b)}$$

$$\langle X \rangle = \boxed{Na \langle \cos\theta^{(a)} \rangle + Nb \langle \cos\theta^{(b)} \rangle}$$

and Energy $E = -fX$

$$\langle \cos\theta_l^{(a)} \rangle = \frac{\int d^2\Omega_1 \cdots \int d^2\Omega_N \cos\theta_l^{(a)} e^{-\beta E}}{\int d^2\Omega_1 \cdots \int d^2\Omega_N e^{-\beta E}}$$

any particular one

reduces to that of a single segment, since E is a linear combination

$$= \frac{\partial \ln Z_1^{(a)}}{\partial \beta f l^{(a)}} = \frac{\partial \ln Z_1^{(a)}}{\partial \beta f a} = \frac{\partial}{\partial \beta f a}\left\{ \text{const.} \frac{\sinh \beta f a}{\beta f a} \right\} = \boxed{\coth \beta f a - \frac{1}{\beta f a}}$$

thus,

$$\boxed{\langle X \rangle = Na\left\{ \coth \beta f a - \frac{1}{\beta f a} \right\} + Nb \left\{ \coth \beta f b - \frac{1}{\beta f b} \right\}}$$

for small argument, $\coth(x) \simeq \frac{1}{x} + \frac{1}{3}x + O(x^3)$

$$\langle X \rangle \simeq Na \cdot \frac{1}{3}\beta f a + Nb \cdot \frac{1}{3}\beta f b \simeq \frac{1}{3}\beta N (a^2+b^2) f$$

$$\Rightarrow \boxed{f \simeq \underbrace{\frac{3k_BT}{N(a^2+b^2)}}_{\kappa\text{, effective spring constant}} \langle X \rangle}$$

b) FJC, a monomers only, restricted $0 \to \frac{\pi}{2}$ only

$$\langle \underset{\sim}{\xi}_m \cdot \underset{\sim}{\xi}_{m+1} \rangle = \langle \cos\theta \rangle = \frac{\cancel{\int_0^{2\pi} d\phi} \int_0^{\pi/2} d\theta \sin\theta \cos\theta}{\cancel{\int_0^{2\pi} d\phi} \int_0^{\pi/2} d\theta \sin\theta}$$

$d\theta \sin\theta = -d\cos\theta$

$$= \frac{\int_0^1 d(\cos\theta)\cos\theta}{\int_0^1 d(\cos\theta)} = \frac{\frac{1}{2}x^2\Big|_0^1 = \frac{1}{2}}{x\Big|_0^1 = 1} = \frac{1}{2}$$

Stretching in electric field

simple: using previous solution of FJC in external field generating a force F,

$$\frac{\langle X \rangle}{L} = \mathcal{L}(\beta F b) \qquad \mathcal{L}(x) = \coth(x) - \frac{1}{x}$$ is Langevin function

$L = Nb$ and $R_0 = \sqrt{N}\,b$ is radius of gyration

$$\boxed{\frac{\langle X \rangle}{R_0} = \sqrt{N}\,\mathcal{L}(f)}$$

in this case, $F = qE = \begin{cases} \text{SI units} & 2\cdot 10^3 \cdot 1.6\times10^{-19} \cdot \underbrace{3\times10^3}_{V/cm} \cdot \underbrace{10^2}_{cm/m} = 9.6\times10^{-11}\ N = 96\ pN \\ \text{cgs} & 2\cdot10^3 \cdot 4.8\times10^{-10} \cdot \cancel{3}\times10^3 \cdot \frac{1}{\cancel{3}00} = 9.6\times10^{-6}\ \text{dyne} \end{cases}$

volts → statvolts   1 dyne $= 10^{-5}$ N ✓

$$\beta F b = \frac{96\ pN \cdot 0.5\ nm}{4\ pN\,nm} \simeq 12 \qquad \mathcal{L}(12) \simeq 0.92,$$ almost fully extended

to obtain 50% extension we need $\mathcal{L}(\beta F_{50} b) = 1/2$

using Matlab:

```
fun = @(x) COTH(x) - 1/x - 1/2 ;
z = fzero(fun, 0.9)
```

↑ guess

$$\Rightarrow \underline{\underline{z = 1.7968}}$$

$$\beta F_{50} b \simeq 1.8$$

$$\frac{F_{50} \cdot 0.5\ nm}{4\ pN\,nm} = 1.8 \Rightarrow \underline{F_{50} \simeq 14.4\ pN}$$

A forced colloidal particle

$$\zeta \dot{x} = F(x - v_T t) \qquad \text{let } \begin{matrix} y = x - v_T t \\ \dot{y} = \dot{x} - v_T \end{matrix} \Big\} \; \dot{x} = \dot{y} + v_T$$

$\downarrow$

$$\frac{dy}{dt} = \frac{F}{\zeta} - v_T \quad \Rightarrow \quad \int_{x_R}^{-x_L} \frac{dy}{F/\zeta - v_T} = \int dt = \Delta t \qquad \text{assume } v_T > \max\left\{\frac{F(y)}{\zeta}\right\}$$

in order of encounter

$$\Delta x = \Delta y + v_T \Delta t = \int_{x_R}^{-x_L} dy \left\{ 1 + \frac{v_T}{F/\zeta - v_T} \right\} = \int_{-x_L}^{x_R} dy \, \frac{F(y)}{\zeta v_T - F(y)}$$

$$\Rightarrow \boxed{\Delta x = \int_{-x_L}^{x_R} dy \, \frac{F(y)}{\zeta v_T - F(y)}} \qquad \text{note, } \frac{F(y)}{\zeta v_T - F(y)} > \frac{F(y)}{\zeta v_T}$$

$$\hookrightarrow > \int_{-x_L}^{x_R} dy \, \frac{F(y)}{\zeta v_T} = \frac{1}{\zeta v_T} \int dy \, F(y) = 0 \quad \text{since } F(y) = -\partial U / \partial y$$

U = trapping potential

$\therefore \underline{\Delta x > 0}$ particle experiences backwards force for a shorter time than forwards force. as long as $v_T - F/\zeta > 0$ Δt is finite

$$\Delta t = \int_{-x_L}^{x_R} \frac{dy}{v_T - F(y)/\zeta}$$

could worry about special case $v_T - F(y)/\zeta \sim y^\alpha$ w/constraint on α

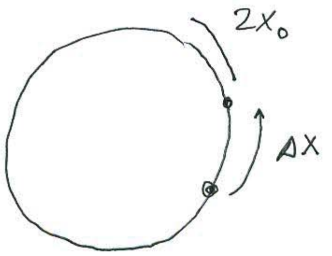
---

for large v_T

$$\Delta x = \int \frac{dy \, F}{\zeta v_T (1 - F/\zeta v_T)} \simeq \int dy \, \frac{(F + F^2/\zeta v_T + \dots)}{\zeta v_T}$$

$$\simeq \int \frac{dy}{(\zeta v_T)^2} F^2(y) \quad \text{manifestly} > 0 .$$

circular orbit :



$\Delta\theta = \frac{\Delta X}{R}$: after 1st kick, particle is caught again w/ extra time $\frac{2\pi R - 2X_0}{v_T}$

$$= \frac{1}{f_T}\left(1 - \frac{X_0}{\pi R}\right) \qquad f_T = \left(\frac{2\pi R}{v_T}\right)^{-1}$$

$\therefore$ angular frequency is

$$\frac{\Delta X}{\Delta t + \frac{1}{f_T}\left(1 - \frac{X_0}{\pi R}\right)} \cdot \frac{1}{2\pi R}$$

for large trap velocity, $\Delta t \simeq \frac{1}{v_T}\int dy = \frac{2X_0}{v_T} = \frac{1}{f_T} \cdot \frac{X_0}{\pi R}$

then $$f_p = \frac{\Delta X}{2\pi R} \; \frac{1}{\frac{1}{f_T}\frac{X_0}{\pi R} + \frac{1}{f_T}\left(1 - \frac{X_0}{\pi R}\right)} \simeq \frac{\Delta X}{2\pi R} f_T$$

---

triangular potential

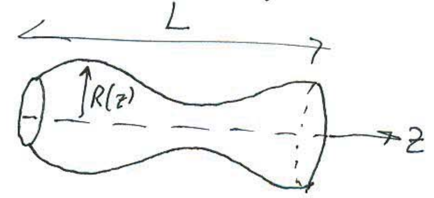
$$\Delta X = \int_{X_0}^{0} dy \, \frac{F}{\zeta v_T - F} + \int dy \, \frac{(-F)}{\zeta v_T + F} = \frac{2X_0 \, v_c^2}{v_T^2 - v_c^2}$$

$$\Delta t = \frac{2X_0 \, v_T}{v_T^2 - v_c^2}$$

then (some algebra)

$$\boxed{\frac{f_p}{f_c} = \left(\frac{X_0}{\pi R}\right) \frac{f_T/f_c}{(f_T/f_c)^2 - 1} \left\{ 1 + \frac{(X_0/\pi R)}{(f_T/f_c)^2 - 1} \right\}^{-1}}$$

Fluctuations of circular objects



volume $V = \int dz\, \pi R^2(z)$

surface area $S = \int dz\, 2\pi R \sqrt{1+R_z^2}$

write $R = \rho_0 + u_q \sin qz$ and adjust ρ_0 to conserve volume up to $O(u_q^2)$ (for consistency with application of equipartition theorem).

$$R^2 = \rho_0^2 + 2\rho_0 u_q \sin qz + u_q^2 \sin^2 qz$$

$$V = \underbrace{\pi R_0^2 L}_{\text{initially}} = \pi\rho_0^2 L + \underset{\substack{\uparrow \\ \int \sin qz = 0}}{0} + \pi u_q^2 \cdot \tfrac{1}{2} L = \pi L \left(\rho_0^2 + \tfrac{1}{2} u_q^2\right)$$

$$\therefore \rho_0 = R_0 \left[1 - u_q^2/2R_0^2\right]^{1/2} \simeq R_0\left(1 - \frac{1}{4}\frac{u_q^2}{R_0^2} + \dots\right)$$

$$\therefore \boxed{\rho_0 \simeq R_0 - \frac{1}{4}\frac{u_q^2}{R_0} + \dots}$$

look at surface area: $R\sqrt{1+R_z^2} = (\rho_0 + \zeta)\left(1 + \frac{1}{2}\zeta_z^2 + \dots\right)$ where $\zeta = u_q \sin qz$

$$= \rho_0 + u_q \sin qz + \frac{1}{2}\rho_0 q^2 u_q^2 \cos^2 qz + \dots$$

$$\therefore S = 2\pi\rho_0 L + 2\pi \cdot \frac{1}{2}\rho_0 q^2 u_q^2 \cdot \frac{1}{2} L = 2\pi L \rho_0 \left(1 + \frac{1}{4} q^2 u_q^2 + \dots\right)$$

$$= 2\pi L R_0 \left(1 - \frac{1}{4}\frac{u_q^2}{R_0^2} + \dots\right)\left(1 + \frac{1}{4} q^2 u_q^2 + \dots\right)$$

hence, the energy is

$$\sigma S = 2\pi L R_0 \sigma \left\{1 + \frac{1}{4R_0^2}\left(q^2 R_0^2 - 1\right) u_q^2 + \dots\right\}$$

$$= \text{const} + \underbrace{\frac{\pi}{2}\frac{L}{R_0}\sigma\left[(qR_0)^2 - 1\right] u_q^2}_{= \frac{1}{2} k_B T \text{ when averaged}} + \dots$$

equipartition $\Rightarrow$ $\boxed{\langle u_q^2 \rangle = \dfrac{k_B T R_0}{\pi L \sigma\left[(qR_0)^2 - 1\right]}}$

clearly, for $qR_0 < 1$ there is a problem – the Rayleigh instability!

Circular domain

write $\underset{\sim}{r}(\theta) = (\rho_0 + \zeta)\,\hat{e}_r$ $\qquad \underset{\sim}{r}_\theta = \zeta_\theta \hat{e}_r + (\rho_0 + \zeta)\,\hat{e}_\theta$

area $A = \int d\theta \, \frac{1}{2} \underset{\sim}{r} \times \underset{\sim}{r}_\theta = \int d\theta \, \frac{1}{2} (\rho_0 + \zeta)^2$

initial area $= \pi R_0^2 = \pi \rho_0^2 + 0 + \frac{1}{2} \int d\theta \, u_q^2 \sin^2 q\theta$

$= \pi \rho_0^2 + \frac{1}{2} u_q^2 \cdot \frac{1}{\cancel{2}} \cdot \cancel{2}\pi = \pi \rho_0^2 + \frac{\pi}{2} u_q^2$

$$\Rightarrow \underline{\rho_0 = R_0 \left(1 - u_q^2 / 2R_0^2\right)^{1/2}} \quad \text{as above}$$

length of fluctuating domain:

$$L = \int d\theta \sqrt{g} = \int d\theta \left[(\rho_0 + \zeta)^2 + \zeta_\theta^2\right]^{1/2} = \rho_0 \left[\left(1 + \frac{\zeta}{\rho_0}\right)^2 + \frac{\zeta_\theta^2}{\rho_0^2}\right]^{1/2}$$

$g = \underset{\sim}{r}_\theta \cdot \underset{\sim}{r}_\theta$

$$\left[1 + \frac{2\zeta}{\rho_0} + \frac{\zeta^2}{\rho_0^2} + \frac{\zeta_\theta^2}{\rho_0^2}\right]^{1/2} \simeq 1 + \frac{\zeta}{\rho_0} + \frac{1}{2}\left(\cancel{\frac{\zeta^2}{\rho_0^2}} + \frac{\zeta_\theta^2}{\rho_0^2}\right) - \frac{1}{8} \cdot \cancel{\frac{4\zeta^2}{\rho_0^2}} + \cdots$$

so, $L = \int d\theta \, \rho_0 \left\{1 + \frac{\zeta}{\rho_0} + \frac{1}{2} \frac{\zeta_\theta^2}{\rho_0^2} + \cdots\right\} \simeq 2\pi \rho_0 + 0 + \frac{1}{2\rho_0} \cdot \cancel{2\pi} \cdot \frac{1}{\cancel{2}} \cdot q^2 \cdot u_q^2$

energy:

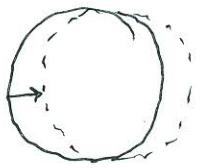
$$\gamma L = 2\pi \rho_0 \gamma + \frac{\gamma}{2\rho_0} \pi q^2 u_q^2 = 2\pi \gamma R_0 \left(1 - \frac{1}{4} \frac{u_q^2}{R_0^2} + \cdots\right) + \frac{\pi}{2} \gamma q^2 \frac{u_q^2}{R_0} \quad \text{to leading order}$$

$$= \boxed{2\pi \gamma R_0 + \frac{\pi \gamma}{2R_0}\left((qR_0)^2 - 1\right) u_q^2}$$

equipartition

$$\frac{\pi \gamma}{2R_0}\left[(qR_0)^2 - 1\right] \langle u_q^2 \rangle = \frac{1}{2} k_B T \qquad \boxed{\langle u_q^2 \rangle = \frac{k_B T R_0}{\pi \gamma \left[(qR_0)^2 - 1\right]}}$$

note: $qR_0 = 1$ mode is a translation; no energy cost



Elastic filament fluctuations

a) $\mathcal{E} = \frac{1}{2}A\int_0^L dx\, h_{xx}^2$ Euler-Lagrange operator is ∂_{4x}, and for it to be self-adjoint we need:

$$\int_0^L h_{4x}\, g\, dx = \int h\, g_{4x}\, dx$$

integrate by parts

$$\to h_{3x}g\Big|_0^L - \int_0^L h_{3x}g_x\, dx$$

$$- h_{xx}g_x\Big|_0^L + \int_0^L h_{xx}\, g_{xx}\, dx$$

$$h_x g_{xx}\Big|_0^L - \int_0^L h_x g_{3x}\, dx$$

$$- h g_{3x}\Big|_0^L + \int_0^L h g_{4x}\, dx$$

surface terms are

$$\boxed{h_{3x}g\Big|_0^L - h_{xx}g_x\Big|_0^L + h_x g_{xx}\Big|_0^L - hg_{3x}\Big|_0^L}$$

self-adjointness requires these to vanish, and if b.c.s are symmetric (same at both ends), we need only consider, say, the 1st 2 terms. In each case, we choose 1 out of 2 factors in $h_{3x}g$ and 1 out of 2 in $h_{xx}g_x$ $\Rightarrow$ $\boxed{\text{4 possibilities}}$

$h_{3x}=0$	$h_{xx}=0$	$h=0$	$h_{xx}=0$
$h_{3x}=0$	$h_x=0$	$h=0$	$h_x=0$

h = position

h_x = slope (if 0, "clamped")

h_{xx} = curvature

(Ah_{xx} is a torque)

h_{3x} = curvature density

(Ah_{3x} is a force)

clamped: $h = h_x = 0$ @ $x = 0, L$

hinged: $h = h_{xx} = 0$ @ $x = 0, L$ no torque

torqued: $h_x = h_{3x} = 0$ @ $x = 0, L$ no force

free: $h_{xx} = h_{3x} = 0$ @ $x = 0, L$ force free, torque free

b) for C-C conditions $W(x) = A\cos kx + B\sin kx + D\cosh kx + E\sinh kx$

$W(0) = \boxed{0 = A + D}$ $\quad W(L) = \boxed{A\cos kL + B\sin kL + D\cosh kL + E\sinh kL = 0}$

$$W_x = k\left[-A\sin kx + B\cos kx + D\sinh kx + E\cosh kx\right]$$

$\therefore W_x(0) = \boxed{k(B+E)=0}$ $\quad \boxed{W_x(L) = k[-A\sin kL + B\cos kL + D\sinh kL + E\cosh kL] = 0}$

4 eqns for 4 unknowns (A, B, D, E)

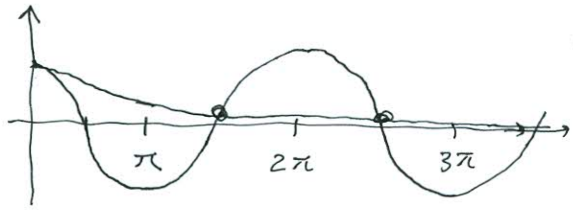
$\Rightarrow D = -A$, $E = -B$ and the remaining 2 eqns reduce to:

$$A\{\cos kL - \cosh kL\} + B\{\sin kL - \sinh kL\} \Rightarrow B = \frac{\cos kL - \cosh kL}{\sinh kL - \sin kL} A$$

and $A\{\sin kL + \sinh kL\} = B\{\cos kL - \cosh kL\} = \dfrac{[\cos kL - \cosh kL]^2}{\sinh kL - \sin kL} A$

$$\Rightarrow (\cos kL - \cosh kL)^2 = \sinh^2 kL - \sin^2 kL$$

or $\boxed{\cos kL \cosh kL = 1}$ $\Rightarrow$ $\boxed{\cos kL = \frac{1}{\cosh kL}}$



one root @ $k=0$

$kL \gg 1 \quad (n+\frac{1}{2})\pi = (2n+1)\frac{\pi}{2} \quad n = 1, 2 \ldots$

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c) $\mathcal{E} = \frac{1}{2}A\int_0^L dx\, h_{xx}^2 = \frac{1}{2}A\left\{\cancel{h_x h_{xx}}\Big|_0^L - \int_0^L dx\, h_x h_{3x}\right.$ $\left. - \cancel{h h_{3x}}\Big|_0^L + \int_0^L dx\, h h_{4x}\right\}$ $= \frac{1}{2}A\int_0^L dx\, h h_{4x}$

but if $h = \sum_n a_n W^{(n)}(x)$, $h_{4x} = \sum_n a_n W_{4x}^{(n)}$ and $W_{4x}^{(n)} = k^{(n)4} W^{(n)}$

$$\Rightarrow \boxed{\mathcal{E} = \frac{1}{2}A\int_0^L dx \sum_m a_m W^{(m)} \sum_n a_n k^{(n)4} W^{(n)}}$$

if we assume the Ws are orthonormal $\quad \mathcal{E} = \frac{1}{2}A\sum_m k^{(m)4} a_m^2$

so, by equipartition $\boxed{\langle a_m^2\rangle = \frac{k_BT}{Ak^{(m)4}}}$

and $\langle h^2(x)\rangle = \left\langle \sum_m \sum_n a_m a_n W^{(m)}_{(x)} W^{(n)}_{(x)}\right\rangle$ $\quad$ and $\langle a_m a_n\rangle = \underline{\quad}\, \delta_{m,n}$ since modes are independent and Gaussian

$$= \boxed{\sum_n \frac{k_BT}{Ak^{(n)4}} W^{(n)}(x)^2}$$

d) if $\mathcal{E} = \frac{1}{2}\int_0^L dx \left\{ A h_{xx}^2 + \sigma(x) h_x^2 \right\}$ $\quad \sigma(0) = \sigma(L) = 0$

$\downarrow$ integrate by parts $\Rightarrow \cancel{\sigma h_x h\Big|_0^L} - \int_0^L dx\, (\sigma h_x)_x\, h$

hence, E-L eqn is $\boxed{A h_{4x} - [\sigma(x) h_x]_x = 0}$

if $A W_{4x}^{(n)} - [\sigma(x) W_x^{(n)}]_x = \lambda^{(n)} W^{(n)}$ (not solving explicitly)

$$\mathcal{E} = \frac{1}{2}\int dx \left\{ A h_{4x} - [\sigma(x) h_x]_x \right\} h \Rightarrow \frac{1}{2}\int_0^L dx \sum_m \lambda^{(m)} a_m W^{(m)}(x) \sum_n a_n W^{(n)}$$

$$= \frac{1}{2}\sum_m \lambda^{(m)} a_m^2$$

and equipartition can be applied in the usual way.