KIAS Workshop, 5/Sep./2015

Anomalous Driven Motion of Biopolymers

Stretching, Compression & Rotational Dynamics

Takahiro Sakaue

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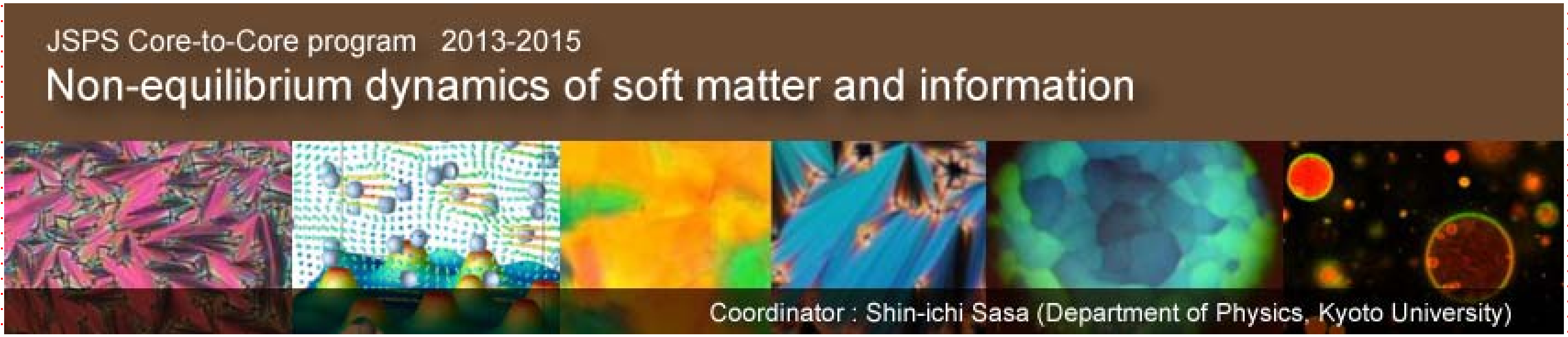
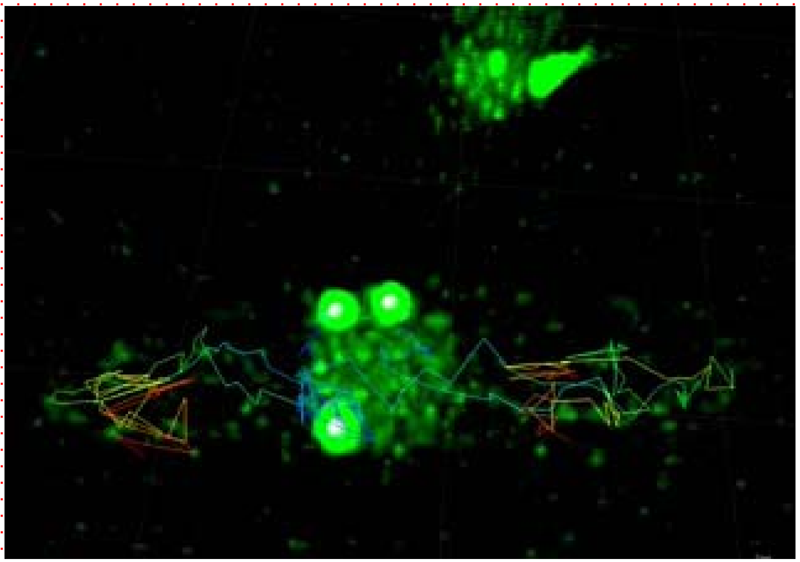
supported by: 科研費 KAKENHI



Chromosome dynamics

M-phase (yeast cell)



Green:
cell nucleus
White:
Spindle pole body (SPB)
Telomere

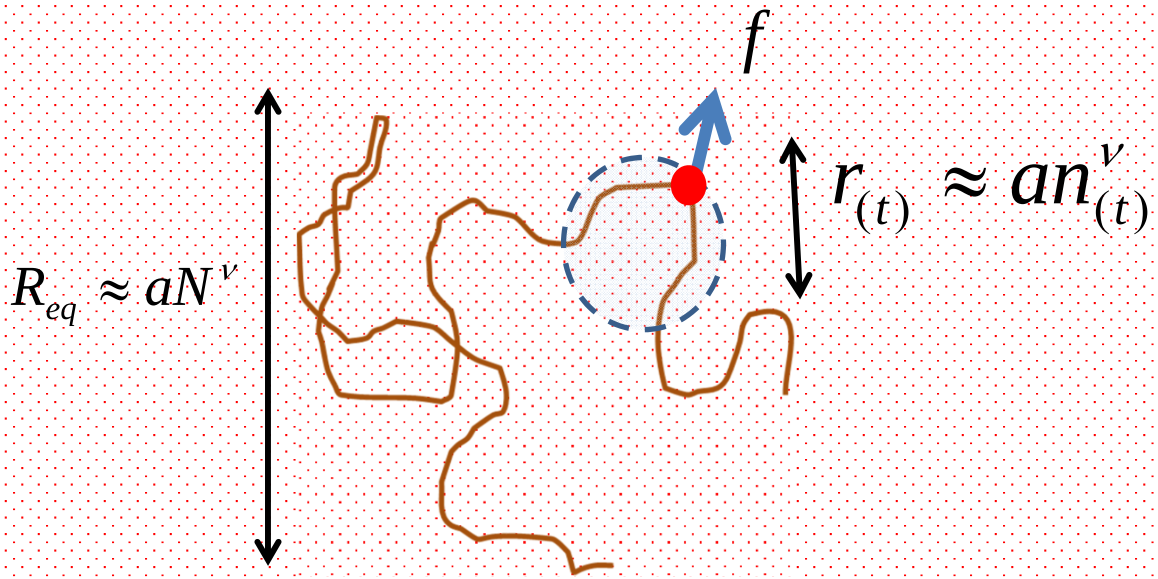
RcMcD
Research Center for the Mathematics
on Chromatin Live Dynamics

Courtesy of T. Sugawara & H. Nishimori (Hiroshima University)

Tagged monomer diffusion: A paradigm of anomalous diffusion

- Time-dependent friction (diffusion coeff.)
- Memory effect
- Visco-elastic response

Tension propagation



<u>Rouse model</u>

$$n(t) \sim t^{1/2}$$

$$\sim \Gamma(t) \sim 1/D(t)$$

sub-diffusion

$$\boxed{r(t) \sim \sqrt{D(t)t} \sim t^{1/4}}$$

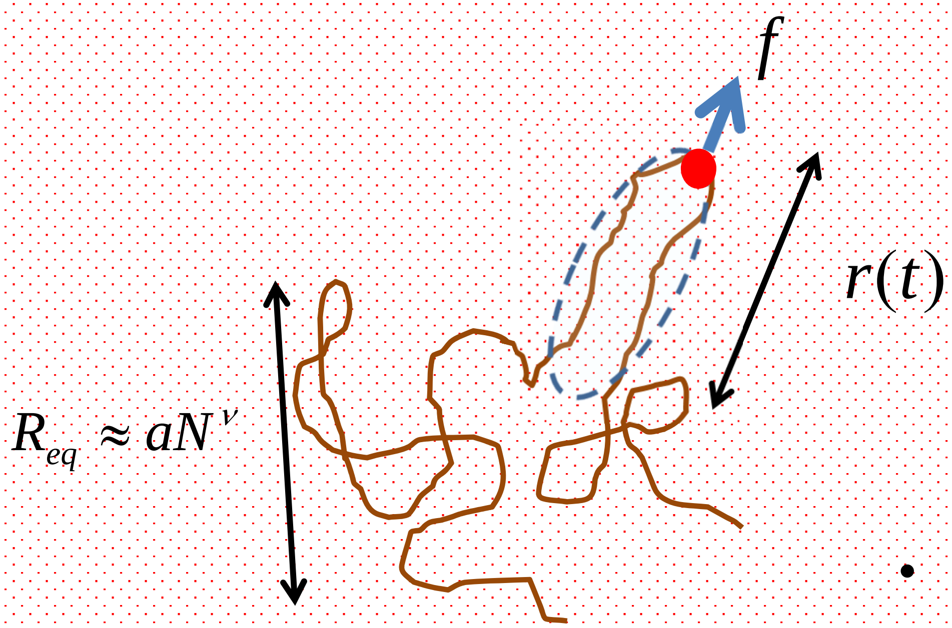
Terminal time

$$n(\tau) \sim N \Leftrightarrow r(\tau) \sim R_{eq}$$

$$\boxed{\tau \sim N^{2}}$$

Strong force (non-equilibrium dynamics)

$$f \gg \frac{k_B T}{R_{eq}}$$



Drift (+ small fluctuation)

- Large deformation
- Non-linear response
- Tension propagation

$$v(t) = \int_{-\infty}^{t} ds\; \underline{\mu(t-s)}\, f(s) + \eta(t)$$

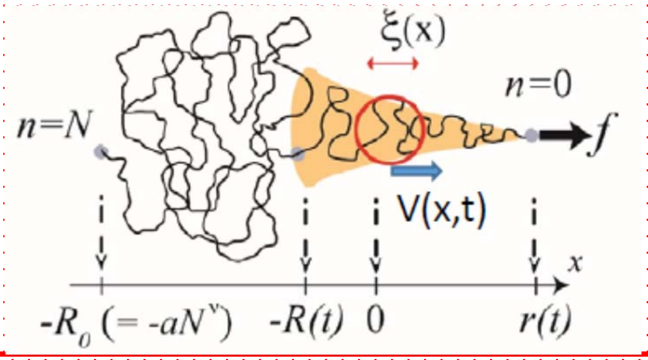
$$\int_{-\infty}^{t} ds\; \underline{\gamma(t-s)}\, v(s) = f(t) + \xi(t)$$

No-linear memory kernel

Driven dynamics of biopolymers

$$f > \frac{k_B T}{R_{eq}}$$

1, Stretching dynamics

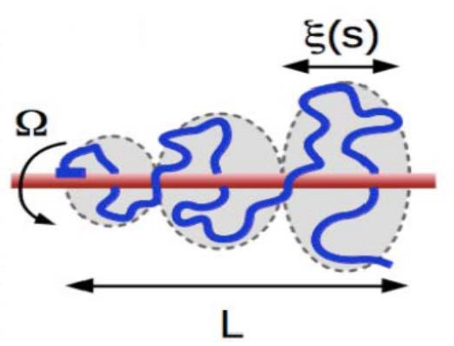


collaboration with T. Saito (Kyoto, Japan)

2, Compression dynamics

collaboration with W. Reisner (McGill, Canada)

3, Rotational dynamics

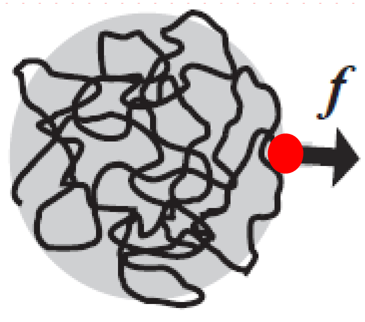


collaboration with E. Carlon (Leuven, Belgium)

Stretching Dynamics (as a paradigm of driven dynamics)

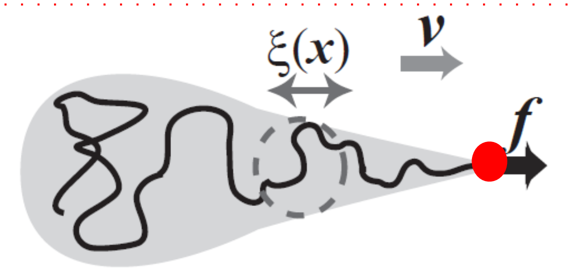
<u>Start pulling at t=0</u>

Equilibrium (at rest) **<u>Steady state</u>** $t > \tau$



?

<u>Transient</u>



$R_{eq} = a\, N^{\nu}$

$R > R_{eq}$

<u>Single molecule experiment, manipulation, chromosome segregation…</u>

How to describe ?

1, Rouse model

Analytical solution

Linear (no EV, no HI)

$$\gamma \frac{\partial x_n}{\partial t} = k \frac{\partial^2 x_n}{\partial n^2} + \eta(t) + f_n(t)$$

viscous elastic

2, Two-phase formalism

Responding and non-responding domains

Steady-state approximation for the responding domain

3, Continuum description (segment line density)

Local force balance (elastic and viscous forces)

Mass conservation

$$\Longrightarrow \quad \frac{\partial \phi(x)}{\partial t} = D_0 \frac{\partial}{\partial x}\left[\phi^{-p}(x)\frac{\partial}{\partial x}\phi(x)\right]$$

4, Non-linear Rouse model

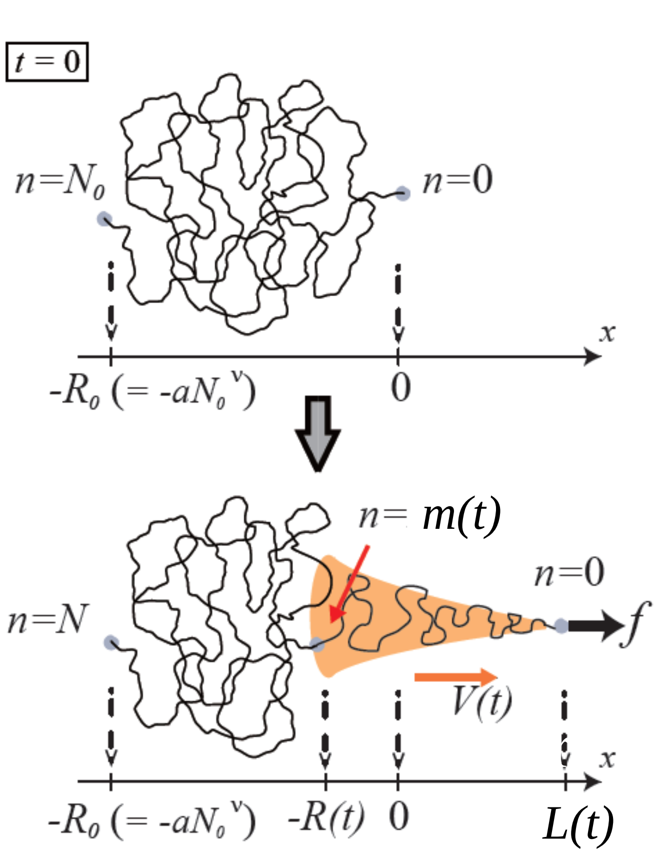
Local force balance (elastic and viscous forces)

$$\frac{\partial x_n}{\partial t} = D_0 \frac{\partial}{\partial n}\left[\left(\frac{\partial x_n}{\partial n}\right)^{p-2}\frac{\partial x_n}{\partial n}\right] + \eta(t)$$

T. Sakaue, T. Saito and H. Wada, Phys. Rev. E **86**, 011804 (2012).
"Dragging a polymer in a viscous fluid: Steady state and transient"
T. Saito and T. Sakaue, Phys. Rev. E **92**, 012601 (2015).
"Driven anomalous diffusion: an example from polymer stretching"

Two-phase picture

Highly non-linear, non-equilibrium process in multi-dimensional space
→ Coarse graining



extension

$$L(t)+R(t) \sim L(t)$$

\# Moving, and quiescent domains

\# Steady-state approximation
for the moving domain

\# Gross variables: size of the moving domain
→ front of the tension propagation

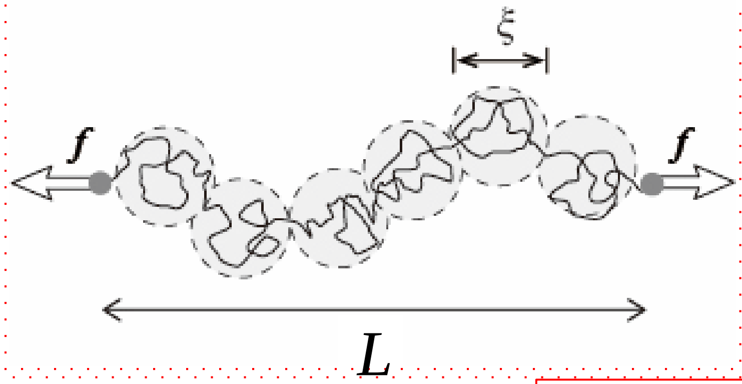
$$\boxed{\Gamma(t)\frac{dL(t)}{dt} \sim f}$$

$$\boxed{\Gamma^{-1}(t) = \frac{\partial V(f,L)}{\partial f}}$$

Steady-state
dynamical Eq. of state

Force-extension (static stretching)

Eq. of State



Alignment of blobs

$$\boxed{\xi \approx k_B T / f \approx a g^{\nu}}$$

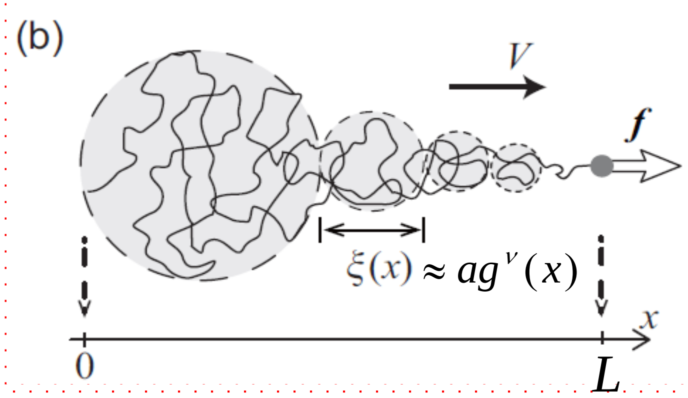
$$\boxed{L \sim \xi\left(\frac{N}{g}\right) \sim N f^{(1-\nu)/\nu}}$$

ν: critical exponent (Flory)

P. Pincus (1976)

Steady State

Dynamical Eq. of State



F. Brochard-Wyart (1993)

Local force balance

$$\boxed{0 = -\eta V + \frac{d}{dx}\frac{k_B T}{\xi(x)}}$$

Boundary condition (f)

$$\boxed{f = \frac{k_B T}{\xi(L)}}$$

$\boxed{L \sim L(N, f)}$: force-extension

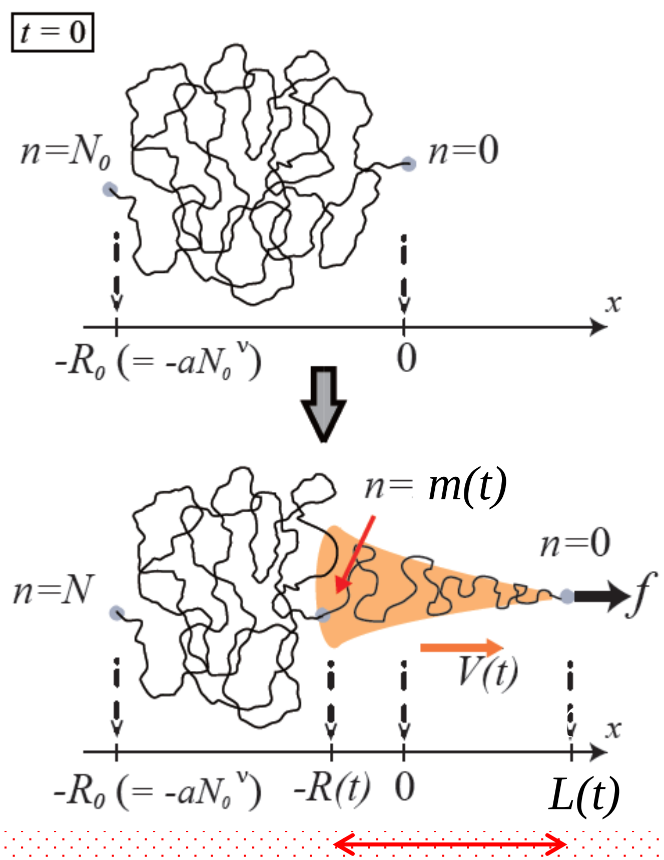
$\boxed{V \sim V(N, f)}$: friction-law

$\boxed{V \sim V(L, f)}$

Two-phase picture

Highly non-linear, non-equilibrium process in multi-dimensional space

→ Coarse graining



extension

$L(t)+R(t)\sim L(t)$

\# Moving, and quiescent domains

\# Steady-state approximation for the moving domain

\# Gross variables: size of the moving domain → front of the tension propagation

$$\boxed{\Gamma(t)\frac{dL(t)}{dt}\sim f} \qquad \boxed{\Gamma^{-1}(t)=\frac{\partial V(L,f)}{\partial f}}$$

$$\left\{\begin{array}{l} L(t)\sim f^{(z/2)-1}t^{1/2} \\ m(t)\sim f^{(z/2)-(1/\nu)}t^{1/2} \\ \tau_f\sim f^{(2/\nu)-z}N^2 \end{array}\right.$$

Anomalous drift !

How to describe ?

1, Rouse model

Analytical solution

Linear (no EV, no HI)

$$\gamma \frac{\partial x_n}{\partial t} = k \frac{\partial^2 x_n}{\partial n^2} + \eta(t) + f_n(t)$$

viscous elastic

2, Two-phase formalism

Responding and non-responding domains

Steady-state approximation for the responding domain

3, Continuum description (segment line density)

Local force balance (elastic and viscous forces)

Mass conservation

$$\Longrightarrow \quad \frac{\partial \phi(x)}{\partial t} = D_0 \frac{\partial}{\partial x}\left[\phi^{-p}(x) \frac{\partial}{\partial x}\phi(x)\right]$$

4, Non-linear Rouse model

Local force balance (elastic and viscous forces) $\frac{\partial x_n}{\partial t} = D_0 \frac{\partial}{\partial n}\left[\left(\frac{\partial x_n}{\partial n}\right)^{p-2} \frac{\partial x_n}{\partial n}\right] + \eta(t)$

T. Sakaue, T. Saito and H. Wada, Phys. Rev. E **86**, 011804 (2012).
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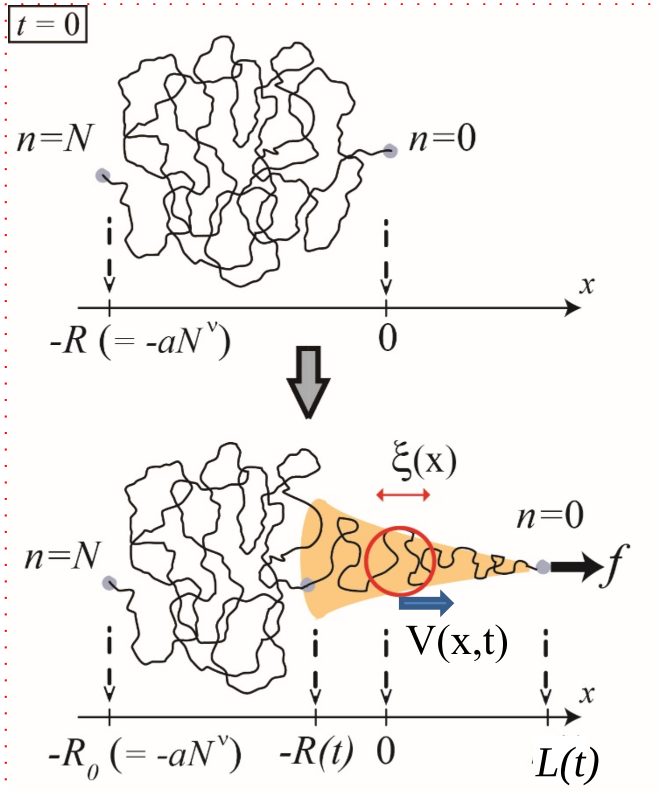
"Driven anomalous diffusion: an example from polymer stretching"

Continuum description : porous medium equation



Local force balance

$$\boxed{\eta\left(\frac{\xi(x,t)}{a}\right)^{z-3} V(x,t) = \frac{d}{dx}\frac{k_B T}{\xi(x,t)}}$$

segment line density

$$\boxed{\phi(x,t) = \frac{g}{\xi} \sim \xi^{(1-\nu)/\nu}}$$

segment flux

$$\boxed{J(x,t) = \phi(x,t) V(x,t)}$$

continuity equation

$$\boxed{\frac{\partial \phi(x,t)}{\partial t} = D_0 \frac{\partial}{\partial x}\left[\phi^{-p}(x,t)\frac{\partial}{\partial x}\phi(x,t)\right]}$$

$$\left(p = \frac{\nu(z-2)}{1-\nu}\right)$$

self-similar ansatz

$$\rightarrow \quad L(t) \sim f^{(z/2)-1} t^{1/2}$$

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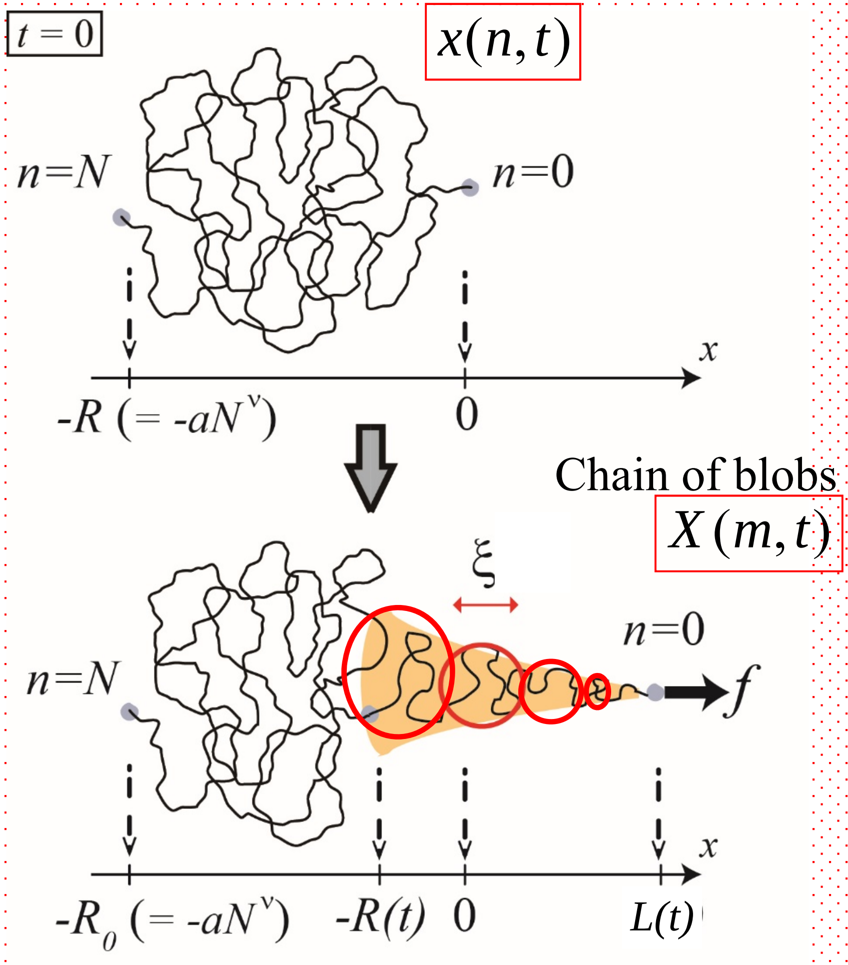
Nonlinear Rouse model: P-Laplacian eq.



\# force balance (coarse-grained)

$$\boxed{\eta a\left(\frac{\xi(m,t)}{a}\right)^{z-2}\frac{\partial X(m,t)}{\partial t}=\frac{\partial}{\partial m}\left(\frac{k_BT}{\xi^2(m,t)}\frac{\partial X(m,t)}{\partial m}\right)}$$

\# X(m,t) → x(n,t) : fine-graining

$$\boxed{\frac{\partial x_n}{\partial t}=D_0\frac{\partial}{\partial n}\left[\left(\frac{\partial x_n}{\partial n}\right)^{p-2}\frac{\partial x_n}{\partial n}\right]+\eta_n(t)+f_n(t)}$$

$$\left(p=\frac{\nu(z-2)}{1-\nu}\right)$$

ν=1/2, z=4
→ Rouse model

self-similar ansatz

$$\Rightarrow\quad L(t)\sim f^{(z/2)-1}t^{1/2}$$

Fluctuations

T. Saito & T. Sakaue, Phys. Rev. E, **92**, 012601 (2015)
Driven Anomalous Diffusion: An example from polymer stretching

\# Anomalous drift, non-linear response

$$\boxed{\langle x(t)\rangle \sim f^{(z/2)-1} t^{1/2}}$$

\# Fluctuation of the driven monomer

$$\boxed{\Delta x(t) \equiv x(t) - \langle x(t)\rangle}$$

$$\boxed{\frac{\partial x_n}{\partial t} = D_0 \frac{\partial}{\partial n}\left[\left(\frac{\partial x_n}{\partial n}\right)^{p-2} \frac{\partial x_n}{\partial n}\right] + \eta(t) + f_n}$$

Gaussian approx.

$$\boxed{\gamma^{(f)} \frac{\partial x_n}{\partial t} = k^{(f)} \frac{\partial^2 x_n}{\partial n^2} + \eta_n^{(f)}(t) + f_n}$$

$$\langle \eta_n^{(f)}(t)\eta_m^{(f)}(s)\rangle = 2\gamma^{(f)} k_B T \delta(n-m)\delta(t-s)$$

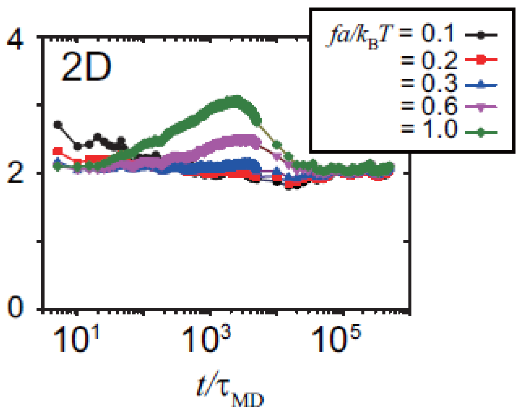
$$k^{(f)} \sim k\ f^{(2\nu-1)/\nu}$$

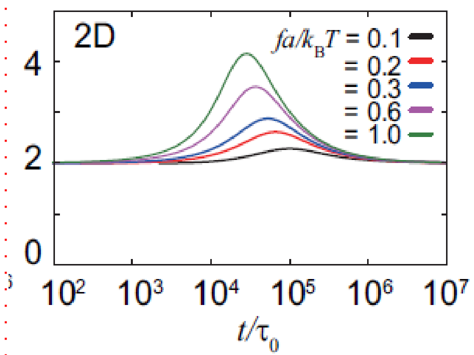
$$\gamma^{(f)} \sim \gamma\ f^{2-z+(1/\nu)}$$

$$\boxed{\langle \Delta x^2(t)\rangle = \frac{2k_B T}{f}\langle x(t)\rangle}$$

?

$$\boxed{f\langle \Delta x^2(t)\rangle / k_B T\langle x(t)\rangle}$$

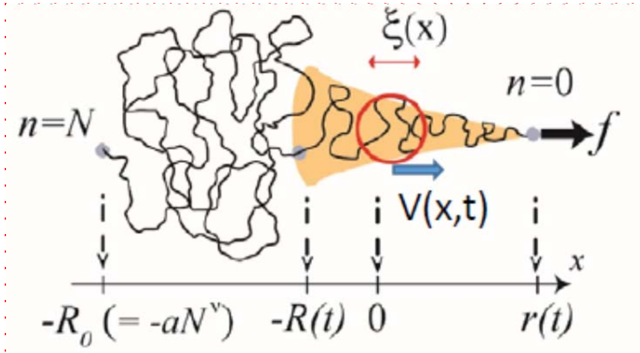




Driven dynamics of biopolymers

$\boxed{f > \frac{k_B T}{R_{eq}}}$

1, Stretching dynamics

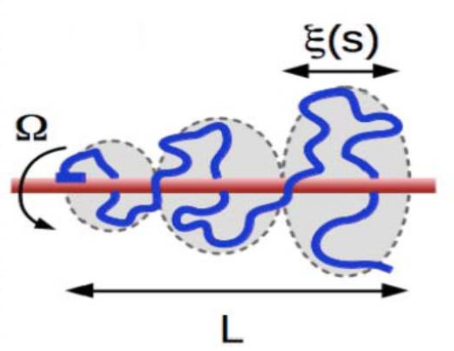


collaboration with T. Saito
(Kyoto, Japan)

2, Compression dynamics

collaboration with W. Reisner
(McGill, Canada)

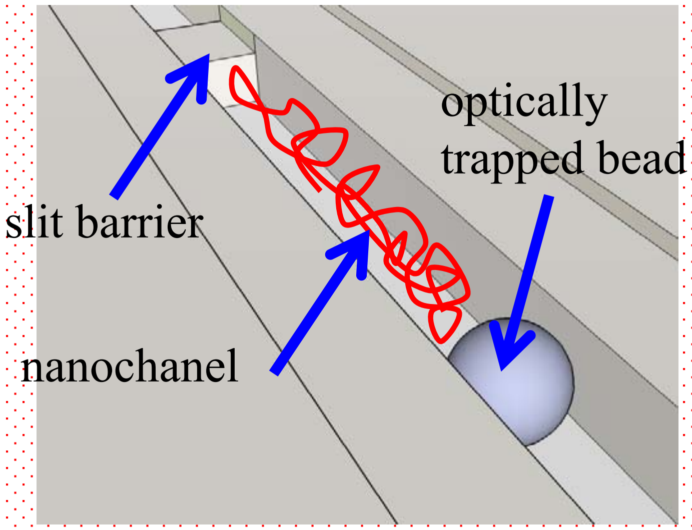
3, Rotational dynamics

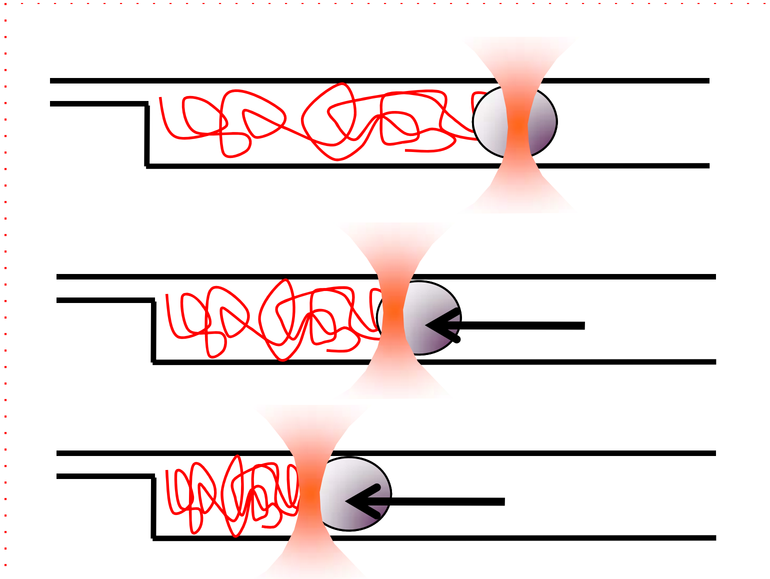


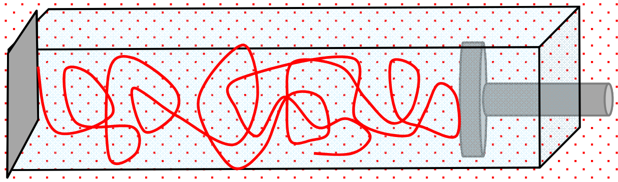
collaboration with E. Carlon
(Leuven, Belgium)

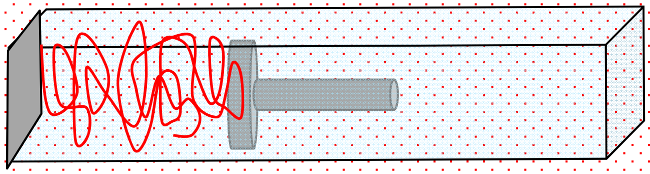
Optical Nonofluidic Piston

- Force-compression relation of confined DNA



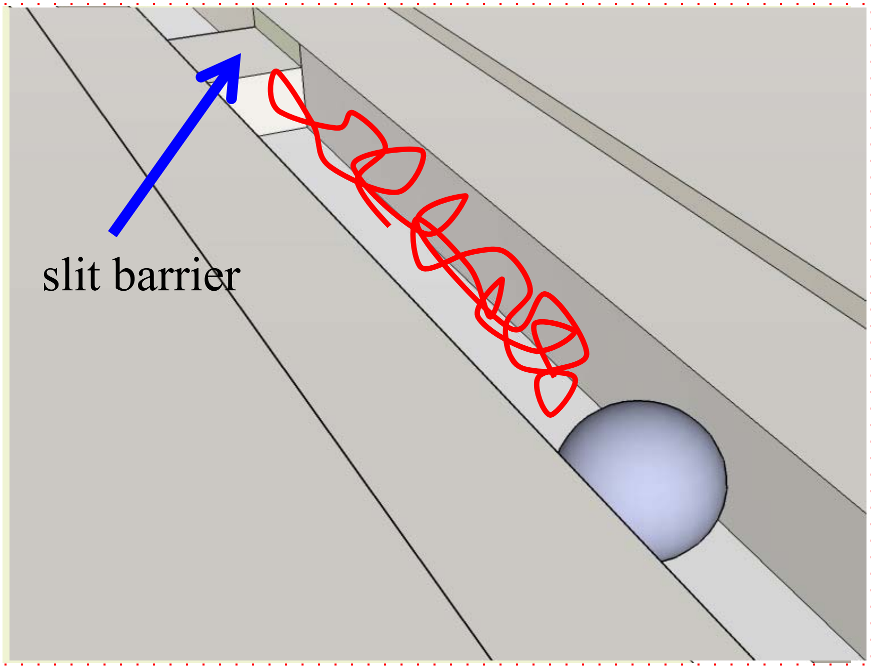






Statics → Dynamics

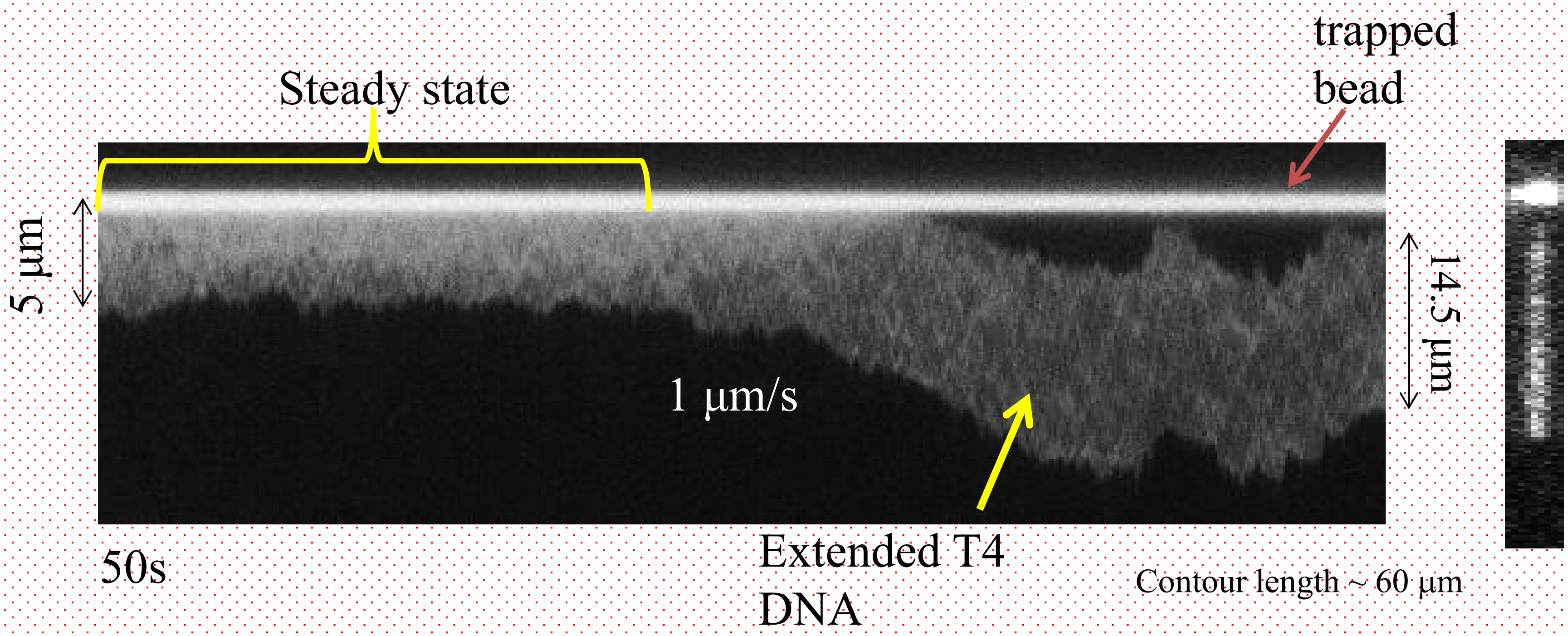
-- *no-wall pushing*



A. Khorshid, P. Zimy, D. Tetreault-La Roche, G. Massaarelli, T. Sakaue & W. Reisner
Phys. Rev. Lett., **113**, 268104 (2014)

Dynamic Compression: Raw time traces

(kymograph)



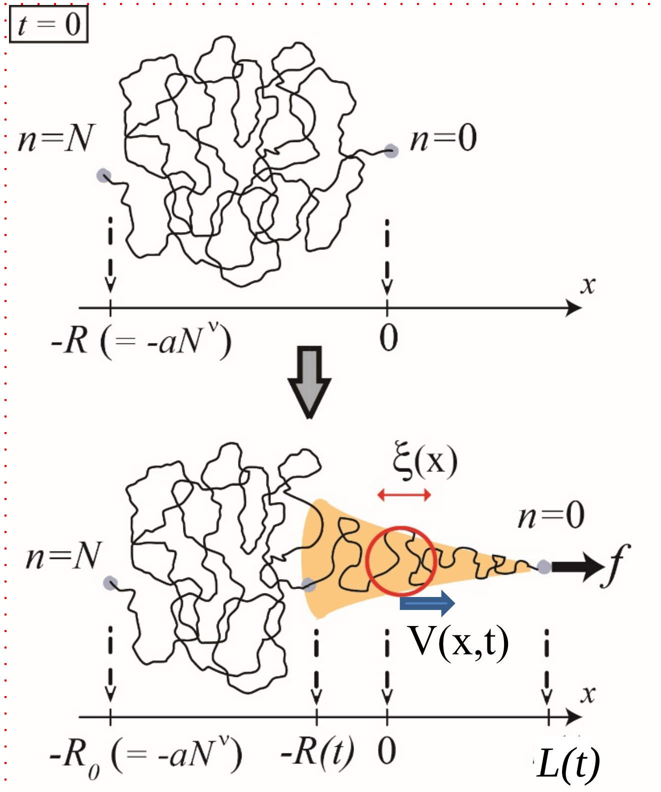
Channel size D= 300 nm

◆Characterization of the steady state

Control parameter: V

recall

Continuum description : porous medium equation



\# Local force balance

$$\eta\left(\frac{\xi(x,t)}{a}\right)^{z-3} V(x,t) = \frac{d}{dx}\frac{k_B T}{\xi(x,t)}$$

\# segment line density

$$\phi(x,t) = \frac{g}{\xi} \sim \xi^{(1-\nu)/\nu}$$

\# segment flux

$$J(x,t) = \phi(x,t) V(x,t)$$

\# continuity equation

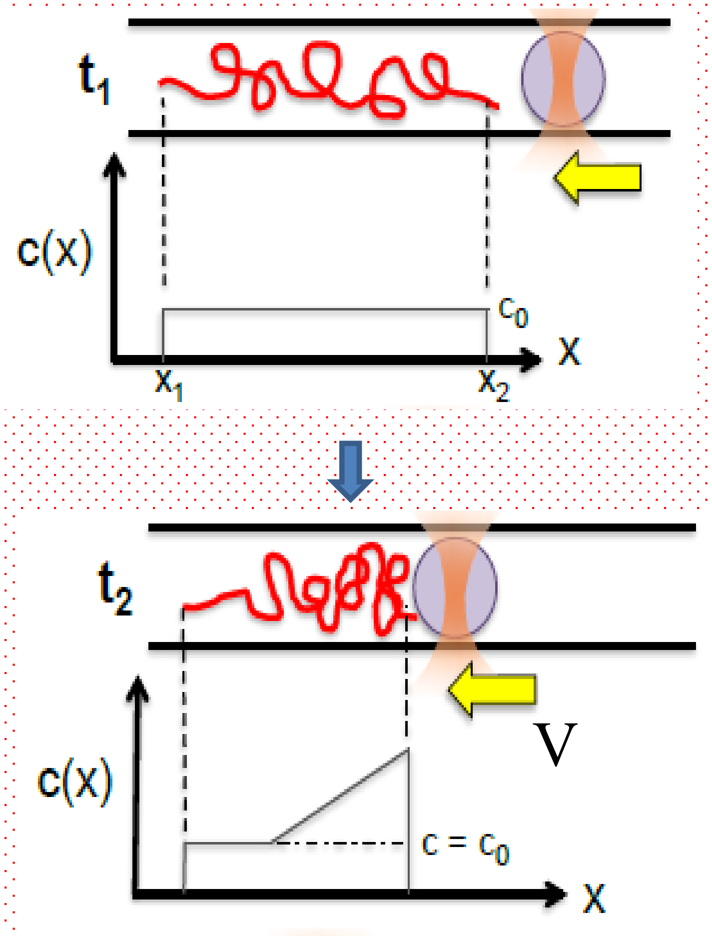
$$\frac{\partial \phi(x,t)}{\partial t} = D_0 \frac{\partial}{\partial x}\left[\phi^{-p}(x,t)\frac{\partial}{\partial x}\phi(x,t)\right]$$

$$\left(p = \frac{\nu(z-2)}{1-\nu}\right)$$

self-similar ansatz

$$\Rightarrow\quad r(t) \sim f^{(z/2)-1} t^{1/2}$$

Continuum description : porous medium equation



Diffusive flux

Convective flux

$$\boxed{\frac{\partial \phi(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\overbrace{D(\phi(x,t))\frac{\partial}{\partial x}\phi(x,t) - \phi(x,t)V}^{-J}\right]}$$

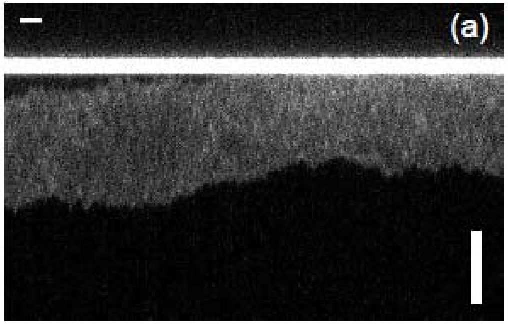
$$D(\phi) = D_0 \phi^{\alpha}$$

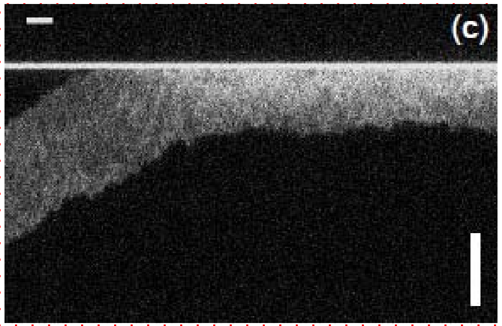
Cooperative diffusion

<u>Steady-state: *j*=0</u>

- Density profile
- Dynamical Eq. of state (f-v-r)

- $V_c < V < V^*$
  initial flat profile
  with ϕ_{eq}

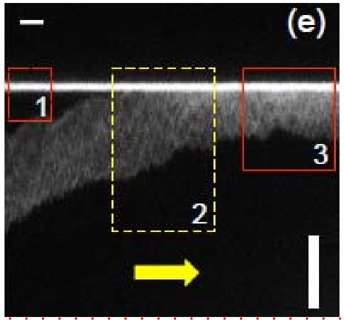




$V^* \approx 1.4\ \mu\text{m/s}$

- V > V*

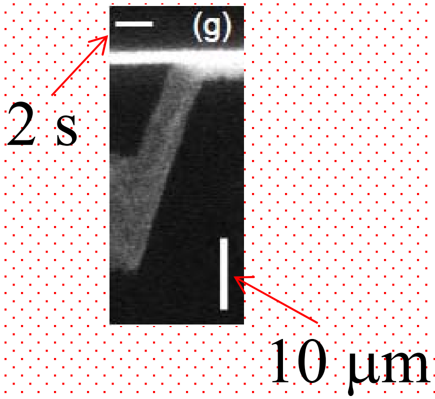
  entire chain deformed

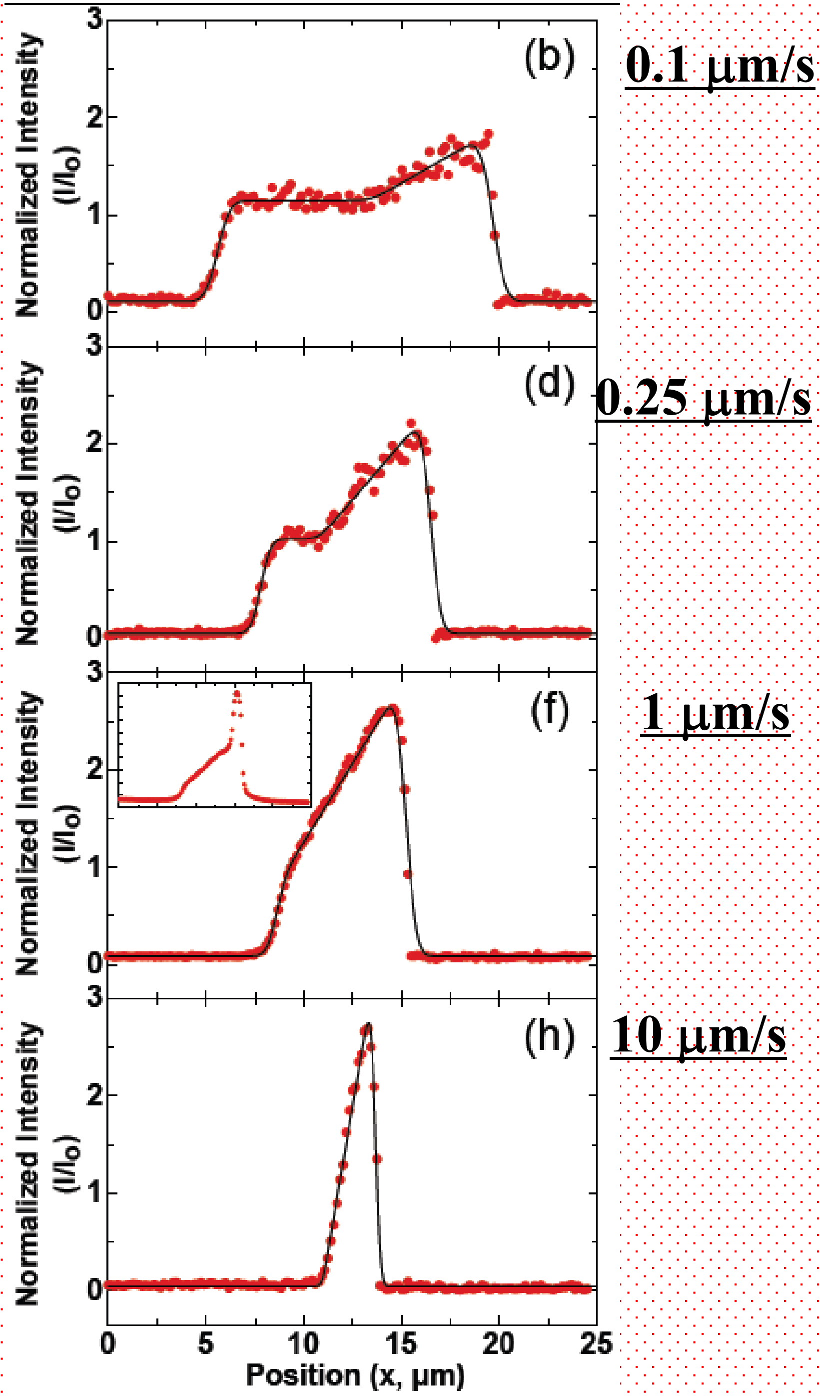


- **Ramp profile**

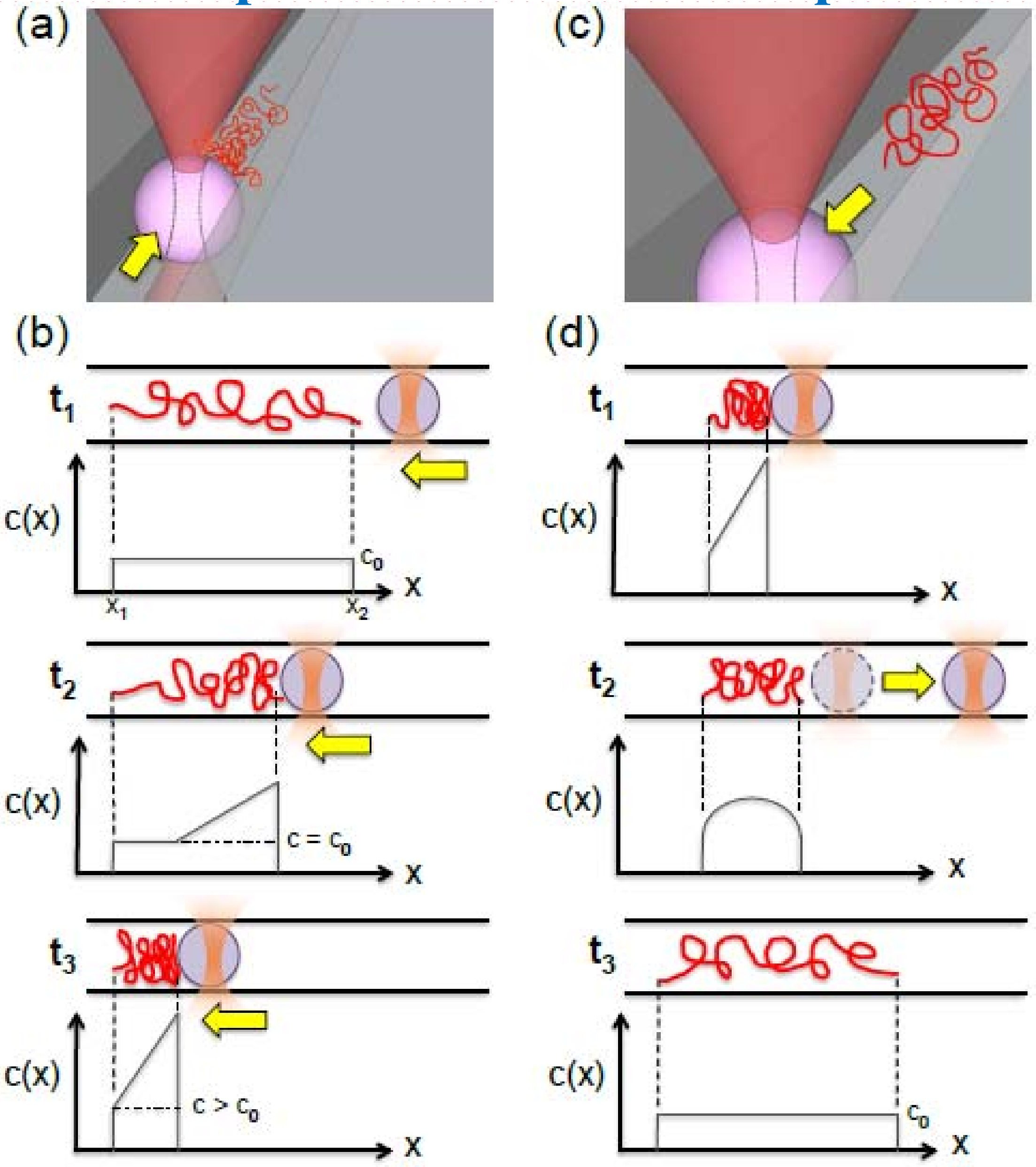
$$\phi_s(x) \sim \left(\mu \frac{x}{D}\right)^{\alpha} \quad (x >> D)$$

$$\alpha = 1$$





Compression Decompression

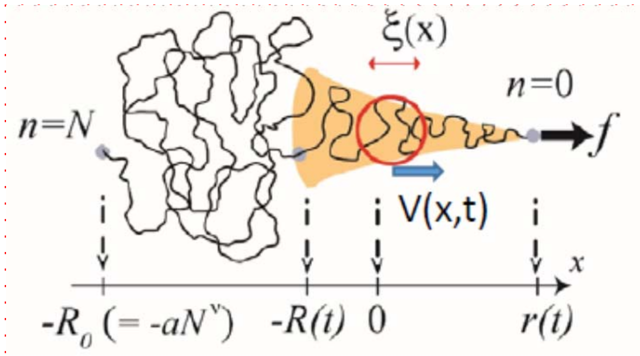


A. Khorshid, S. Amin, Z. Zhang, T. Sakaue & W. Reisner, submitted

Driven dynamics of biopolymers

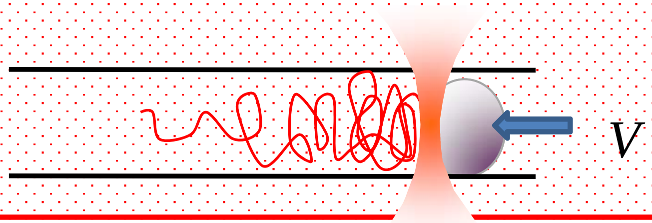
$\boxed{f > \frac{k_B T}{R_{eq}}}$

1, Stretching dynamics



collaboration with T. Saito
(Kyoto, Japan)

2, Compression dynamics



collaboration with W. Reisner
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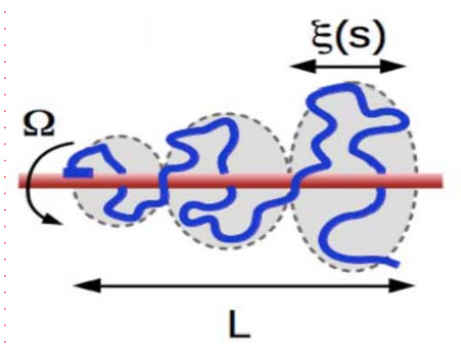
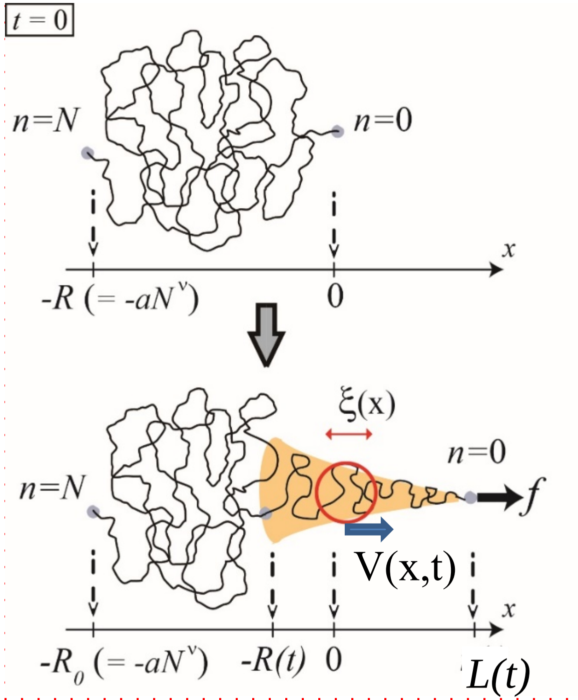
3, Rotational dynamics

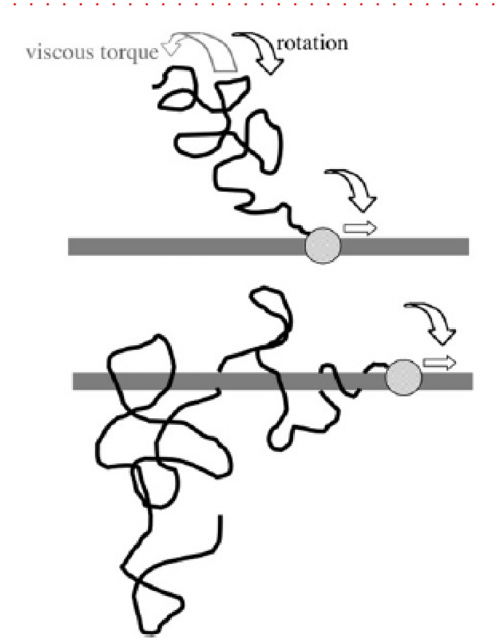


collaboration with E. Carlon
(Leuven, Belgium)

“Torque-induced rotational dynamics in polymers: Torsional blobs and thinning”

M. Laleman, M. Baiesi, B.P. Belotserkovskii, T. Sakaue, J-C. Walter, E. Carlon, *submitted*

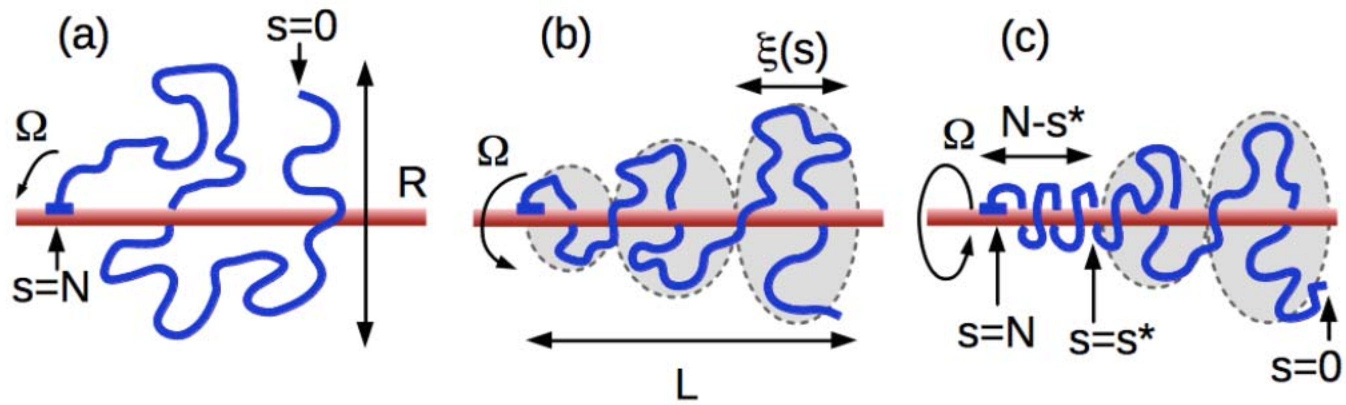




Belotserkovskii, PRE (2014)

- Rotational analogue of the stretching dynamics
- Fundamental polymer dynamics problem
- Relevant to RNA transcription process

Steady state (driven by torque)



Torque- ***torsional blob*** relation

$$\boxed{M(s) \approx \frac{k_B T}{[\ln(\xi(s)/a)]^{\alpha}}}$$

Winding angle distribution

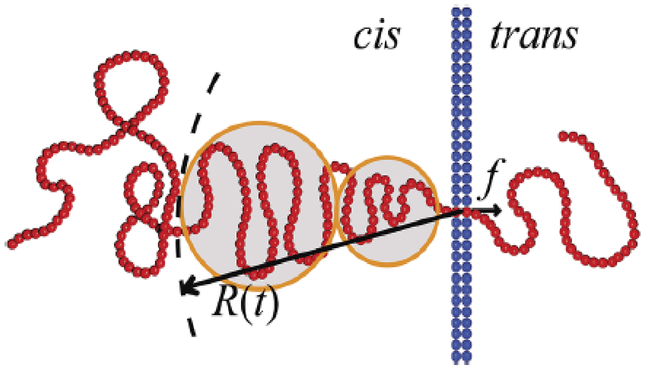
$$P_{\theta}(\theta, N) = f_{\theta}\left(\frac{\theta}{(\ln N)^{\alpha}}\right)$$

cf. force-tensile blob relation $f(s) \approx \dfrac{k_B T}{\xi(s)}$

- ◆ Steady state profile $\xi(s) \sim (\Omega s)^{-1/2}$
- ◆ Torque-angular velocity relation (dynamical eq. of state)
- ◆ Steady elongation

Summary: Driven dynamics of biopolymers

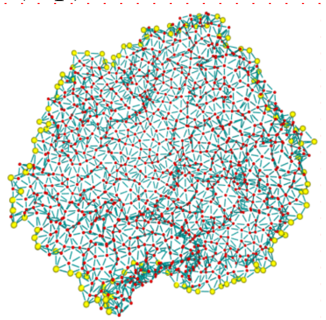
Translocation



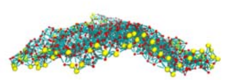
Palyulin et. al, SoftMatter (2014)

Polymerized membrane

(top)

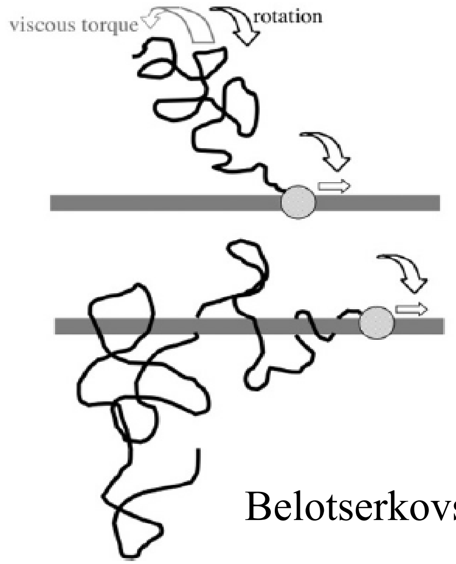


(side)



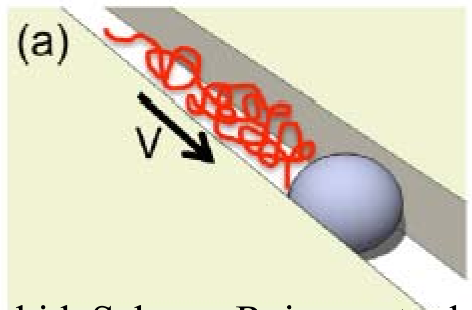
Mizuochi, Nakanishi, Sakaue, EPL (2014)

Transcription



Belotserkovskii, PRE (2014)

Confined DNA (Nanodozer)



Khorshid, Sakaue, Reisner et. al., PRL (2014)

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