Modeling Active Fluctuations in Living Matter

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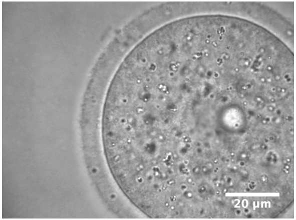

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3. Department of Chemical Physics, Weizmann Institute of Science
4. School of Engineering and Applied Sciences, Harvard University
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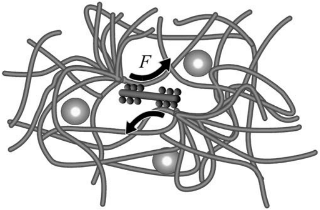
Theory Club

Introduction



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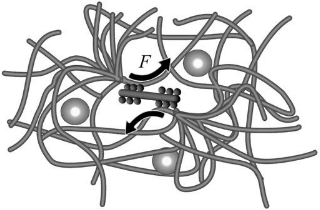
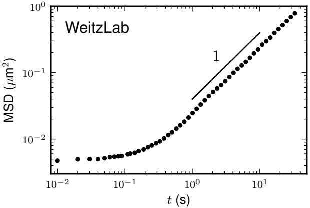
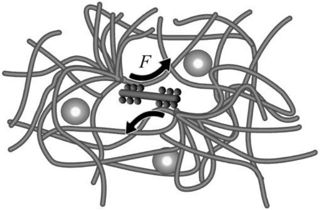


Mean square displacement



Introduction



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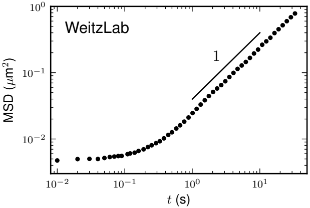
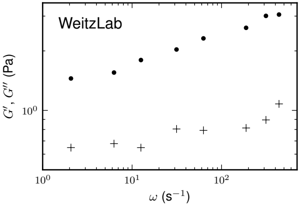


Complex modulus



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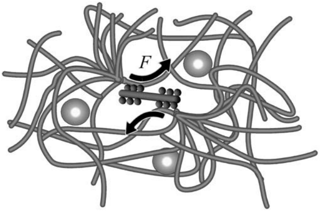
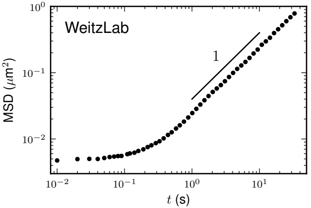
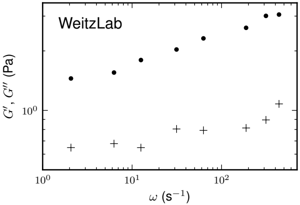


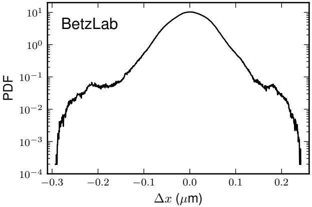
Mean square displacement



Complex modulus



PDF of displacement



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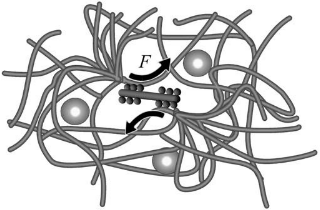
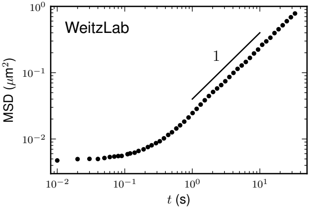
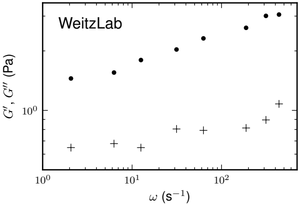


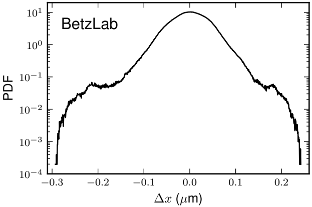
Mean square displacement



Complex modulus



PDF of displacement



Is it possible to extract information about molecular motor activity?

Propose a model for the tracers' dynamics

Outline

1. Modeling tracer's dynamics

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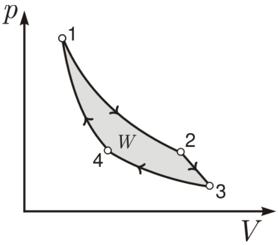
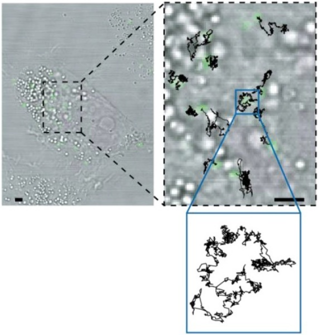
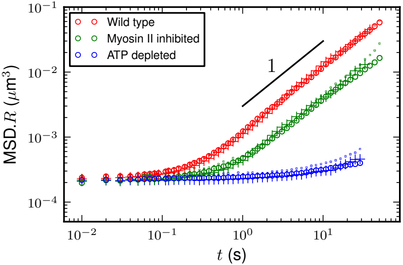
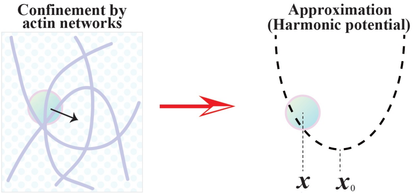
2. New kinds of experiments



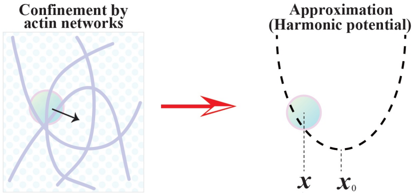



Wild type
Myosin II inhibited
ATP depleted
1
MSD.R (μm^3)
t (s)
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-2}
10^{-1}
10^{0}
10^{1}


Confinement by actin networks
Approximation (Harmonic potential)
x
x_0

Modeling tracer's dynamics

Equation of motion



Tracer's dynamics

$$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = -\boldsymbol{\nabla} U + \mathbf{F}_{\mathrm{S}} + \mathbf{F}_{\mathrm{th}}$$

Harmonic potential: $U = \frac{k}{2}(\mathbf{r} - \mathbf{r_0})^2$

Stokes force: $\mathbf{F}_{\mathrm{S}} = -\gamma\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$

Gaussian white noise: $\mathbf{F}_{\mathrm{th}}$

Tracer's dynamics

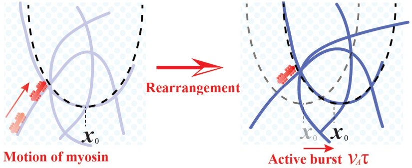
$$\begin{aligned} \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} &= -\frac{1}{\tau_{\mathrm{d}}}(\mathbf{r}-\mathbf{r_0}) + \sqrt{2D_{\mathrm{T}}}\boldsymbol{\xi} \\ \frac{\mathrm{d}\mathbf{r_0}}{\mathrm{d}t} &= -\frac{\varepsilon}{\tau_{\mathrm{d}}}(\mathbf{r_0}-\mathbf{r}) + \sqrt{2\varepsilon D_{\mathrm{T}}}\boldsymbol{\xi_0} \end{aligned}$$

Tracer's dynamics

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\frac{1}{\tau_{\mathrm{d}}}(\mathbf{r}-\mathbf{r_0}) + \sqrt{2D_{\mathrm{T}}}\boldsymbol{\xi}$$

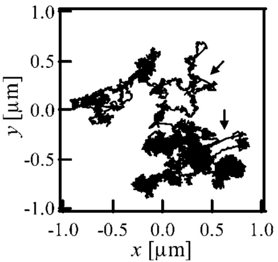
$$\frac{\mathrm{d}\mathbf{r_0}}{\mathrm{d}t} = -\frac{\varepsilon}{\tau_{\mathrm{d}}}(\mathbf{r_0}-\mathbf{r}) + \sqrt{2\varepsilon D_{\mathrm{T}}}\boldsymbol{\xi_0} + \mathbf{v}_{\mathrm{A}}$$

Active motion of local minimum



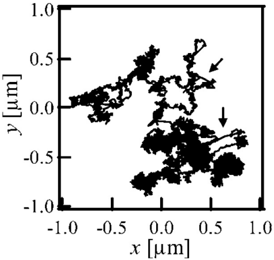
Modeling tracer's dynamics

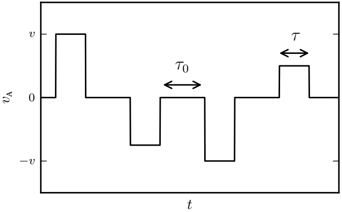
Active burst's statistics

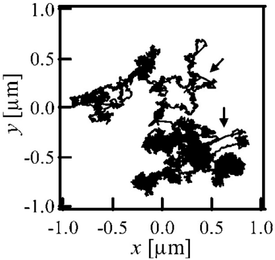


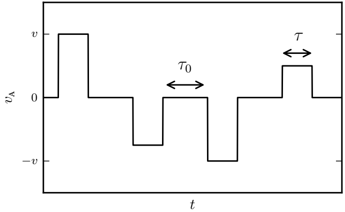
Modeling tracer's dynamics

Active burst's statistics



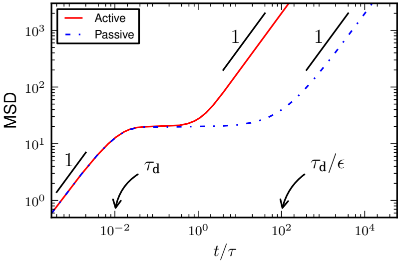






2–time correlation function

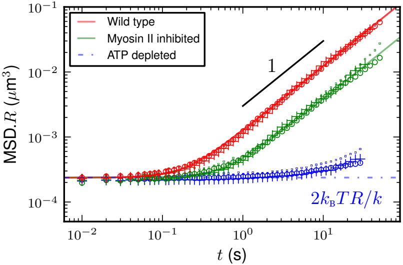
$$\langle v_A(t) v_A(0) \rangle = \frac{D_A}{\tau} e^{-|t|/\tau} \, , \qquad D_A = \frac{(v\tau)^2}{3(\tau + \tau_0)}$$



Active
Passive
MSD
10^0
10^1
10^2
10^3
10^{-2}
10^0
10^2
10^4
t/τ
1
1
1
τ_{d}
$\tau_{\mathrm{d}}/\epsilon$

Short time   Confinement

Large time   Free diffusion
$\text{MSD} \sim 2D_{\mathsf{A}}t$

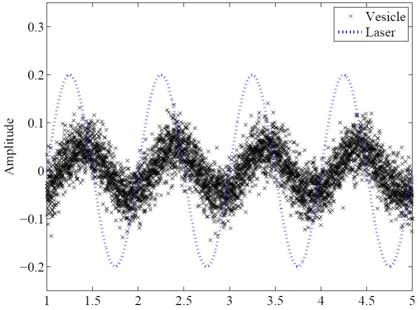


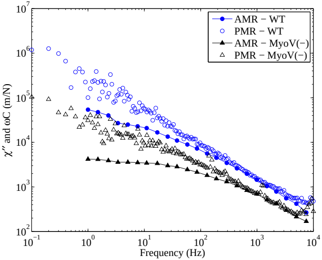
Microscopic features

- Typical time of activity: $\tau_{\mathsf{wt}} \simeq 0.15$ s, $\tau_{\mathsf{b}} \simeq 0.41$ s
- Amplitude of active fluctuations:
  $D_{\mathsf{A,wt}} \simeq 5.2 \cdot 10^{-3} D_{\mathsf{T}},\ D_{\mathsf{A,b}} \simeq 1.6 \cdot 10^{-3} D_{\mathsf{T}}$

New kinds of experiments

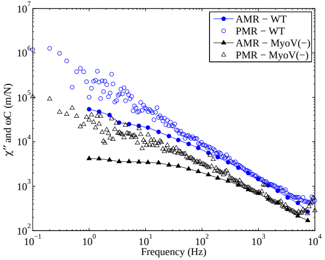
Response function





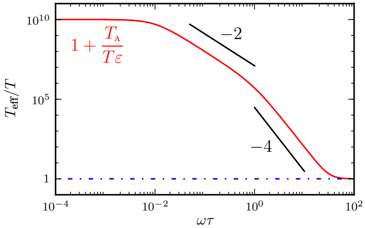
Fluctuation dissipation

$$\chi''(\omega) = \frac{\omega C(\omega)}{2 k_B T}$$



Fluctuation dissipation

$$\chi''(\omega) = \frac{\omega C(\omega)}{2k_\mathrm{B}T}$$

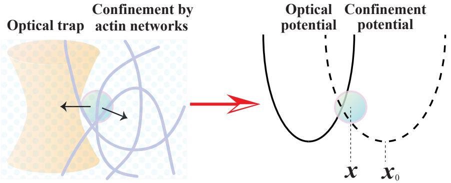


Effective temperature

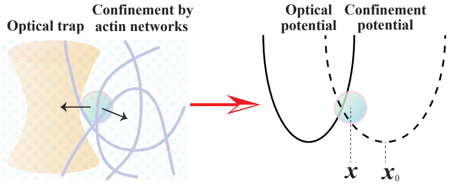
$$k_\mathrm{B}T_\mathrm{eff}(\omega) = \frac{\omega C(\omega)}{2\chi''(\omega)}$$

New kinds of experiments

Applying external quadratic potential



$$U_\mathrm{P} = \frac{k_\mathrm{P}}{2} x^2$$



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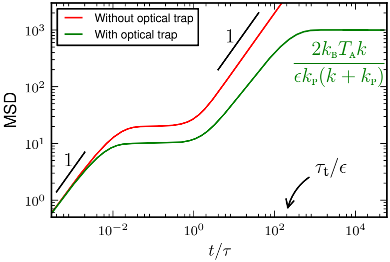

New kinds of experiments

Applying external quadratic potential

$$U_{\mathrm{P}} = U_{\mathrm{P}}(x, \{a_i(t)\}) \quad \rightarrow \quad \mathcal{W} = \sum_i \int \mathrm{d}a_i \frac{\partial U_{\mathrm{P}}}{\partial a_i}$$

New kinds of experiments

Applying external quadratic potential

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Quasistatic protocol

$$U_{\mathrm{P}} = \frac{k_{\mathrm{P}}}{2} x^2, \qquad k_{\mathrm{P}} : k_{\mathrm{i}} \longrightarrow k_{\mathrm{f}}$$

$$W_{\mathrm{H}} = \frac{1}{2} \int_{k_{\mathrm{i}}}^{k_{\mathrm{f}}} \mathrm{d}k_{\mathrm{P}} \left\langle x^2 \right\rangle_{\mathrm{ss}}$$

New kinds of experiments

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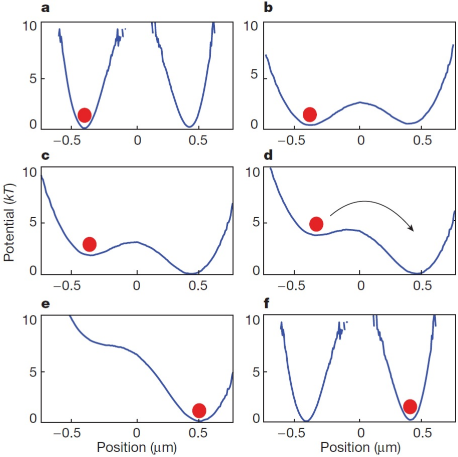
$$W_{\mathrm{H}} = \frac{1}{2} \int_{k_{\mathrm{i}}}^{k_{\mathrm{f}}} \mathrm{d}k_{\mathrm{P}} \left\langle x^2 \right\rangle_{\mathrm{SS}}$$

$$W_{\mathrm{H}} = \frac{T_{\mathrm{A}}}{2\varepsilon} \ln \left[\frac{k_{\mathrm{f}}(k + k_{\mathrm{i}})}{k_{\mathrm{i}}(k + k_{\mathrm{f}})} \right] + \mathcal{O}(\varepsilon^0)$$

New kinds of experiments
Thermodynamic cycle with quartic potential



Naert *et al.*, Nature 2012

$$U_P = \frac{k_P}{2}x^2 + \frac{b_P}{4}x^4$$

Quasistatic protocol

$$U_{\mathrm{P}} = \frac{k_{\mathrm{P}}}{2}x^2 + \frac{b_{\mathrm{P}}}{4}x^4, \qquad k_{\mathrm{P}} : k_{\mathrm{i}} \longrightarrow k_{\mathrm{f}}$$

$$W_{\mathrm{Q}} = \frac{1}{2}\int_{k_{\mathrm{i}}}^{k_{\mathrm{f}}} \mathrm{d}k_{\mathrm{P}} \left\langle x^2 \right\rangle_{\mathrm{ss}}$$

Quasistatic protocol

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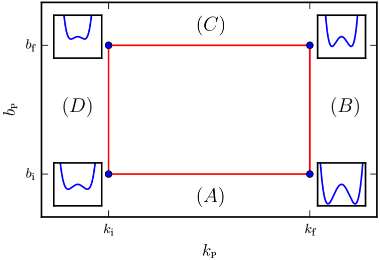
$$W_{\mathrm{Q}} = \frac{1}{2}\int_{k_{\mathrm{i}}}^{k_{\mathrm{f}}} \mathrm{d}k_{\mathrm{P}} \left\langle x^2 \right\rangle_{\mathrm{ss}}$$

$$W_{\mathrm{Q}} = W_{\mathrm{H}} + W_{\mathrm{P}} + \mathcal{O}(b_{\mathrm{P}}^2)$$

$$\frac{W_{\mathrm{P}}}{b_{\mathrm{P}}} = \left(\frac{T_{\mathrm{A}}}{\varepsilon}\right)^2 f(k, k_{\mathrm{i}}, k_{\mathrm{f}}, \tau, \tau_{\mathrm{d}}) + \mathcal{O}(1/\varepsilon)$$

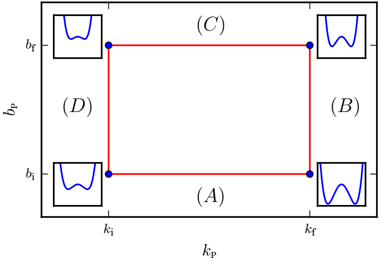
New kinds of experiments

Thermodynamic cycle with quartic potential



New kinds of experiments

Thermodynamic cycle with quartic potential

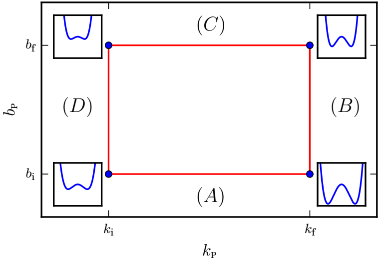


Quasistatic protocol

$$W_\mathcal{C} = \frac{1}{2}\oint_\mathcal{C} \mathrm{d}k_\mathrm{P} \left\langle x^2 \right\rangle_\mathrm{ss} + \frac{1}{4}\oint_\mathcal{C} \mathrm{d}b_\mathrm{P} \left\langle x^4 \right\rangle_\mathrm{ss}$$

New kinds of experiments

Thermodynamic cycle with quartic potential



Quasistatic protocol

$$W_{\mathcal{C}} = \frac{1}{2} \oint_{\mathcal{C}} \mathrm{d}k_{\mathrm{P}} \left\langle x^2 \right\rangle_{\mathrm{ss}} + \frac{1}{4} \oint_{\mathcal{C}} \mathrm{d}b_{\mathrm{P}} \left\langle x^4 \right\rangle_{\mathrm{ss}}$$

$$W_{\mathcal{C}} = \left(\frac{T_{\mathrm{A}}}{\varepsilon} \right)^2 f_{\mathcal{C}}(k, k_{\mathrm{i}}, k_{\mathrm{f}}, b_{\mathrm{i}}, b_{\mathrm{f}}, \tau, \tau_{\mathrm{d}}) + \mathcal{O}(1/\varepsilon)$$