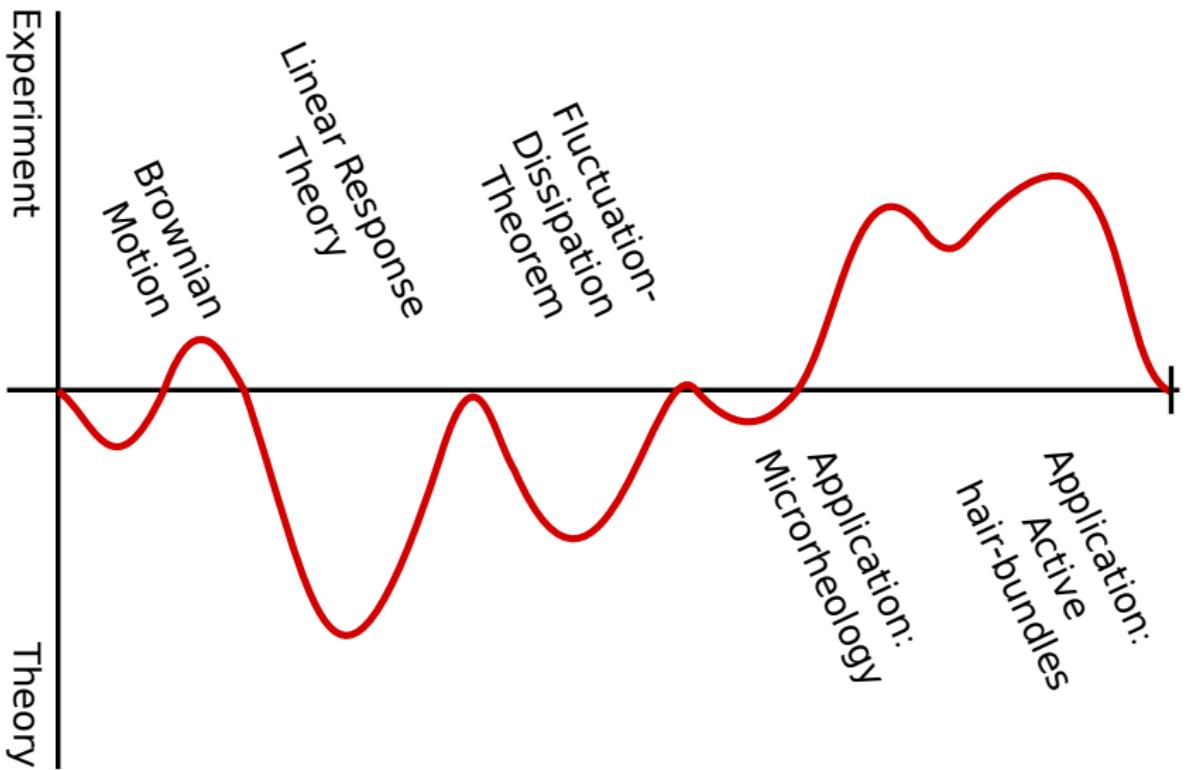


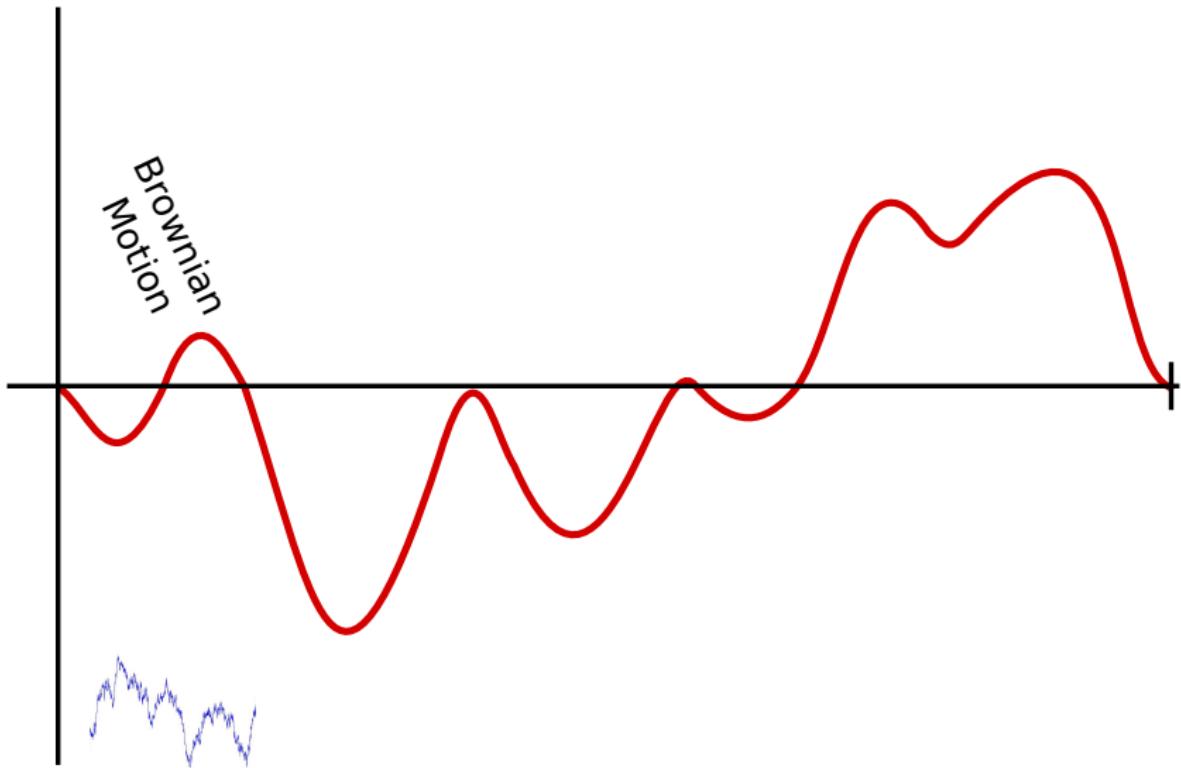
The Fluctuation-Dissipation Theorem

Friedrich Schüßler

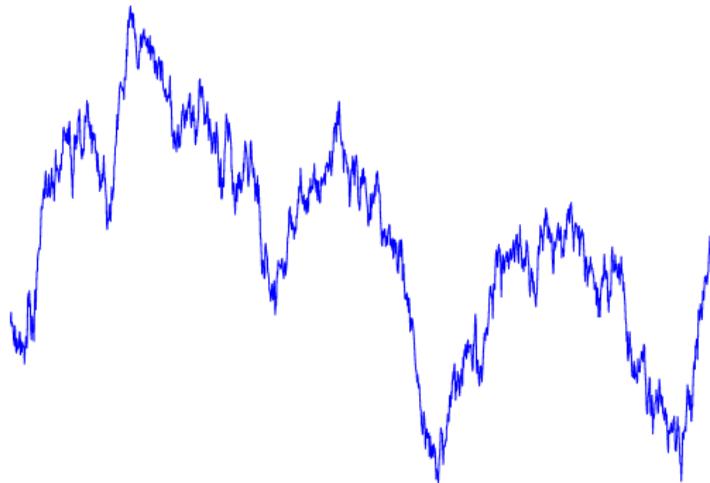
15 January 2016

Supervisor: Prof. Oliver Mülken & Dr. Maxim Dolgushev





Brownian Motion



Brown 1827

Einstein 1905

Smulochowski 1906

Langevin 1908

Perrin 1908

Brownian Motion

Langevin equation:

$$\partial_t u = -\gamma u + L(t)$$

with $\langle L(t) \rangle = 0; \quad \langle L(t)L(t') \rangle = \Gamma \delta(t - t')$

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$$\Rightarrow \boxed{\Gamma = \frac{2\gamma kT}{m}}$$

Perrin's experiment (1908)

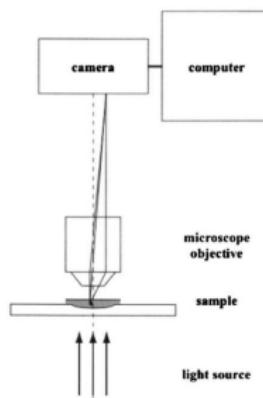
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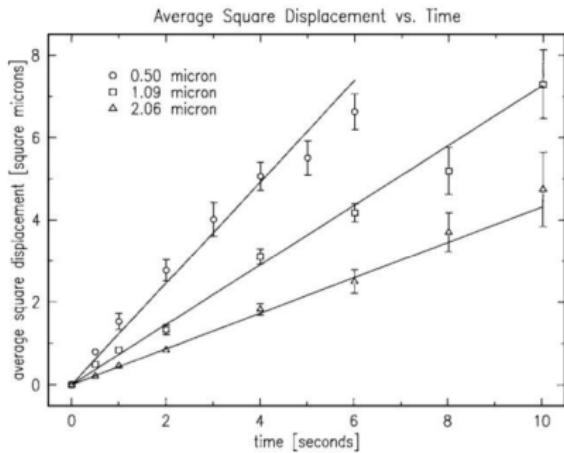
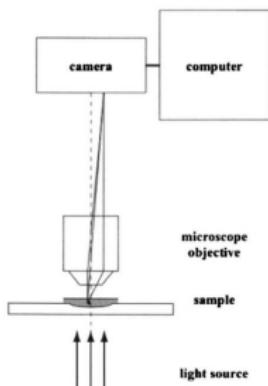
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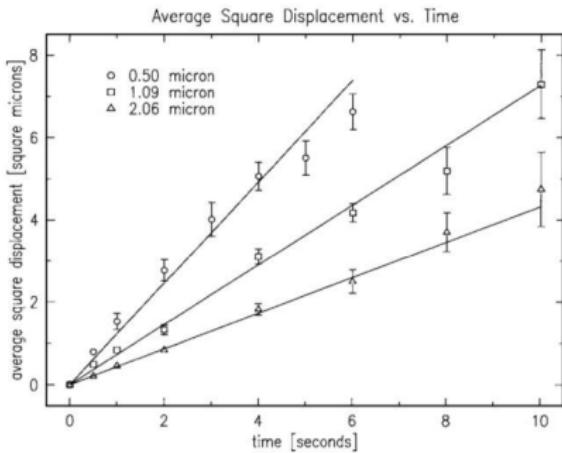
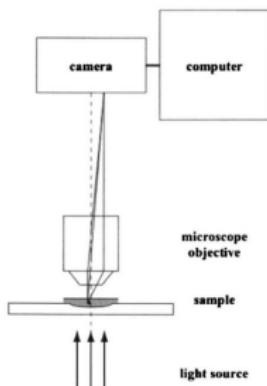
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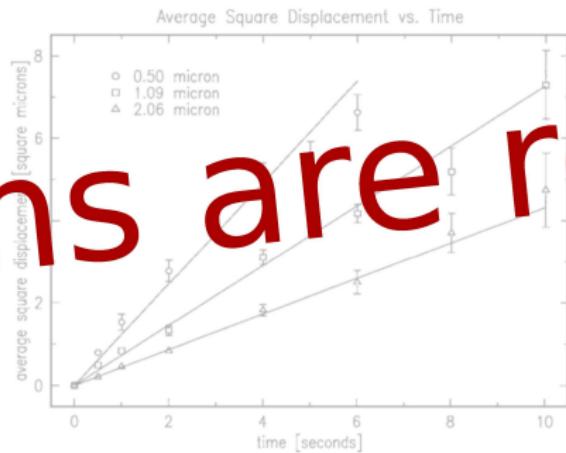
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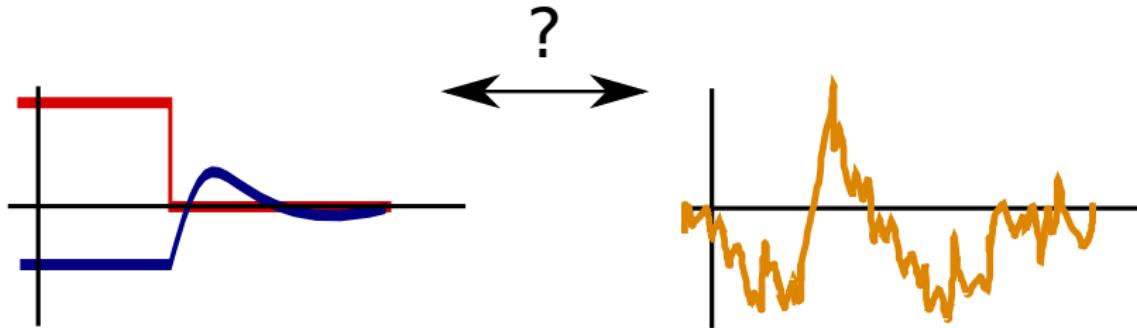
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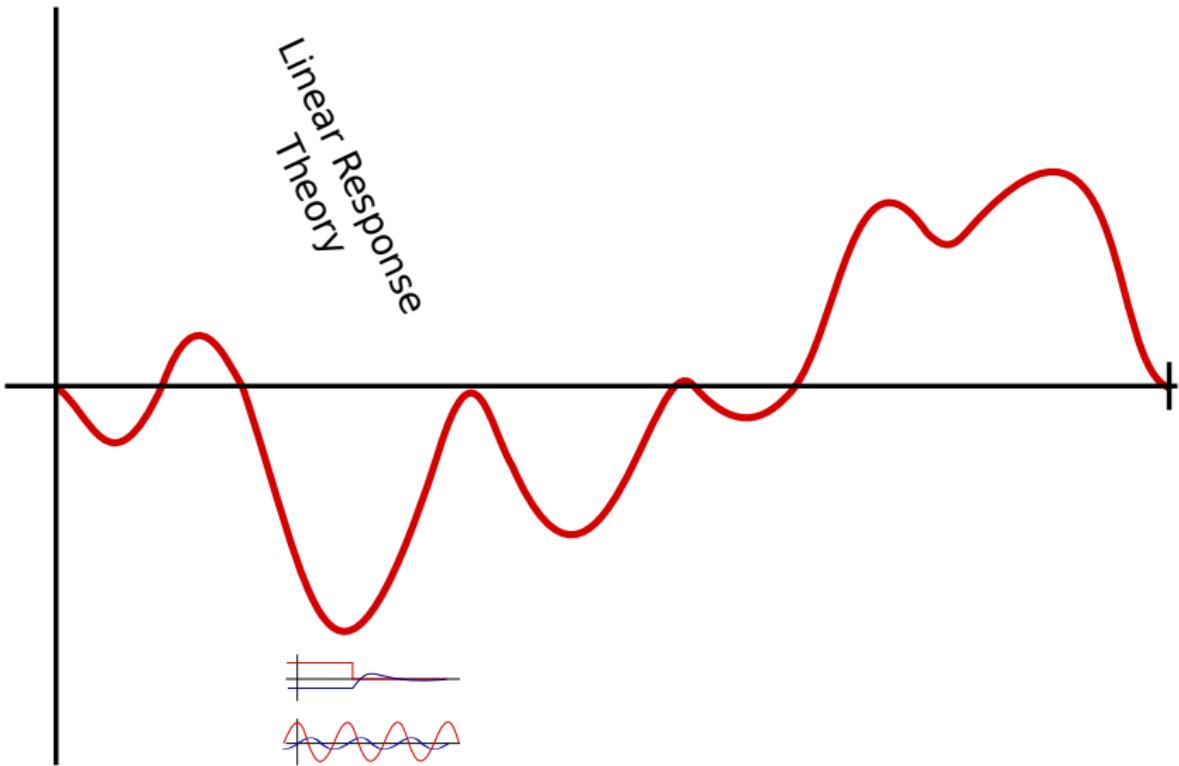


Atoms are real!

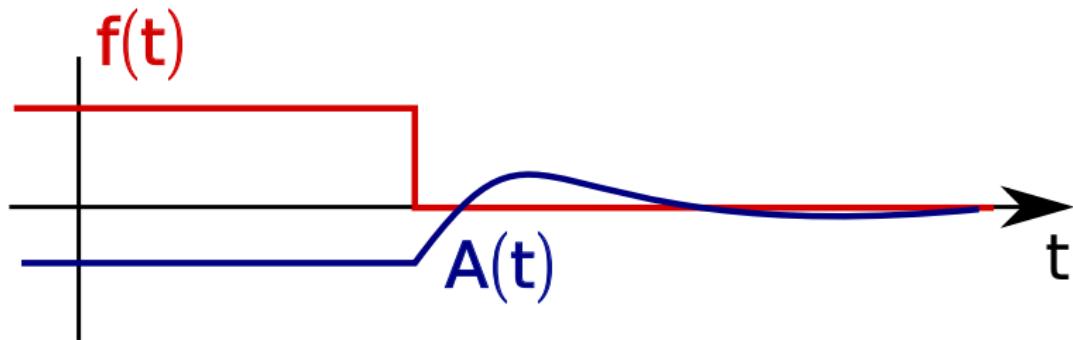
response to
perturbation

equilibrium
fluctuations

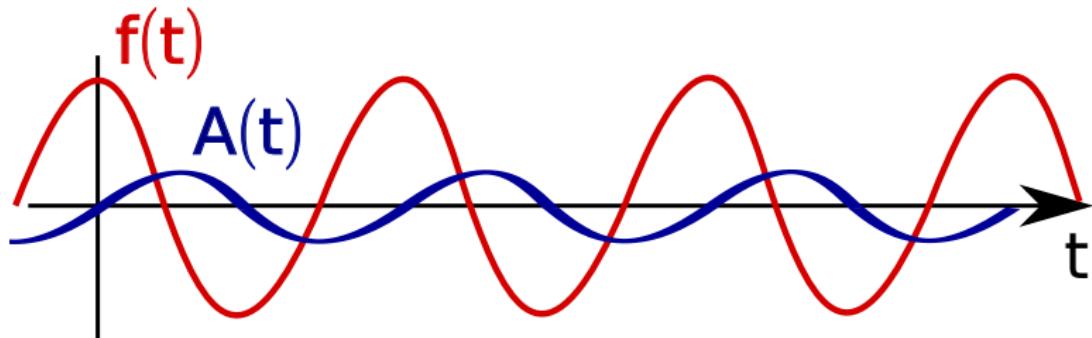
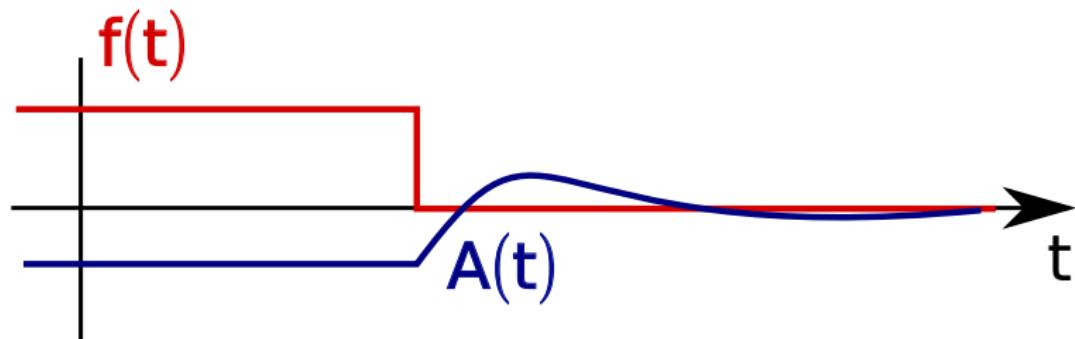




Response to a perturbation



Response to a perturbation



Perturbed system

Perturbation $f(t)$ coupling to operator A :

$$H(t) = H_0 - A f(t)$$

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Non-equilibrium average:

$$\langle A(t) \rangle_{ne} = \frac{1}{Z} \operatorname{Tr} \rho_0 A(t)$$

where

Z = partition function

ρ_0 = equilibrium density matrix

Average response

$$\delta A(t) := \langle A(t) \rangle_{ne} - \langle A \rangle_{eq}$$

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$A(t)$ evolves due to H_0 :

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Kubo

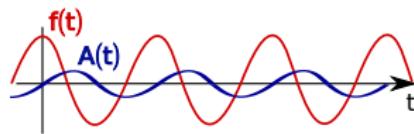
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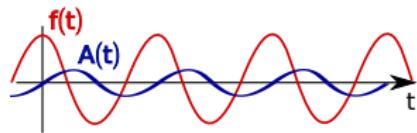
Green

Measure $\chi(\omega)$

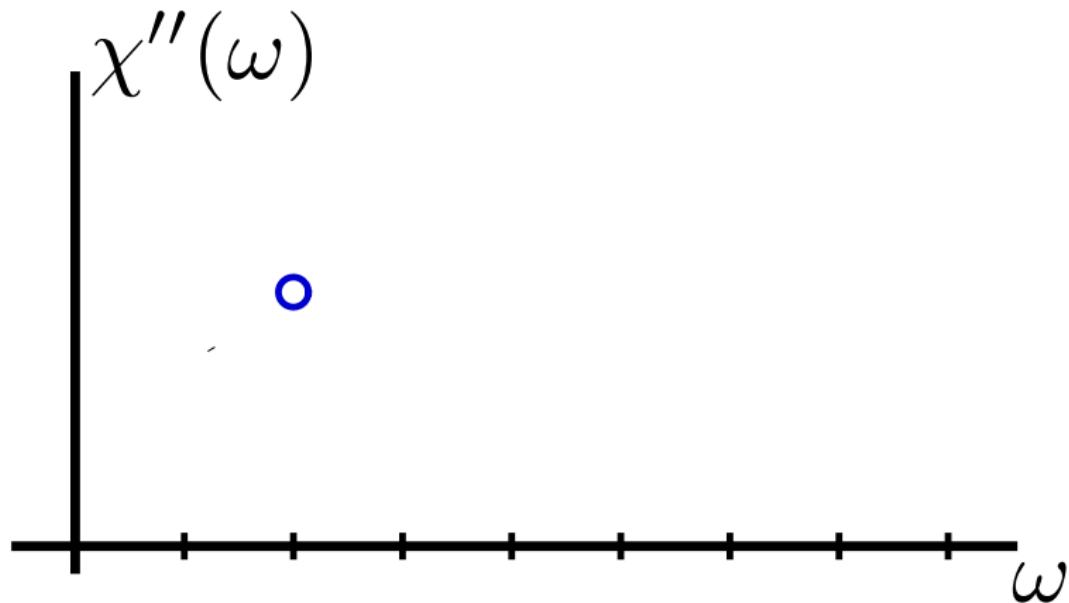


$$\delta A(\omega) = \chi(\omega)f(\omega)$$
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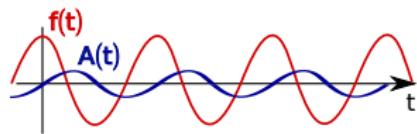
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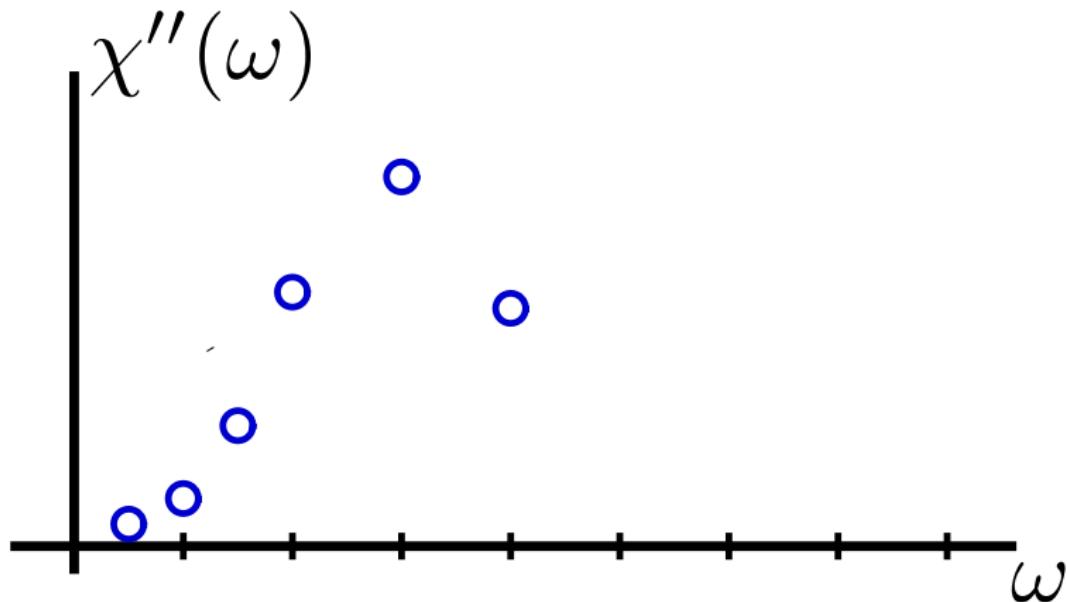
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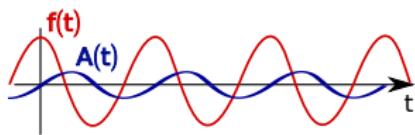
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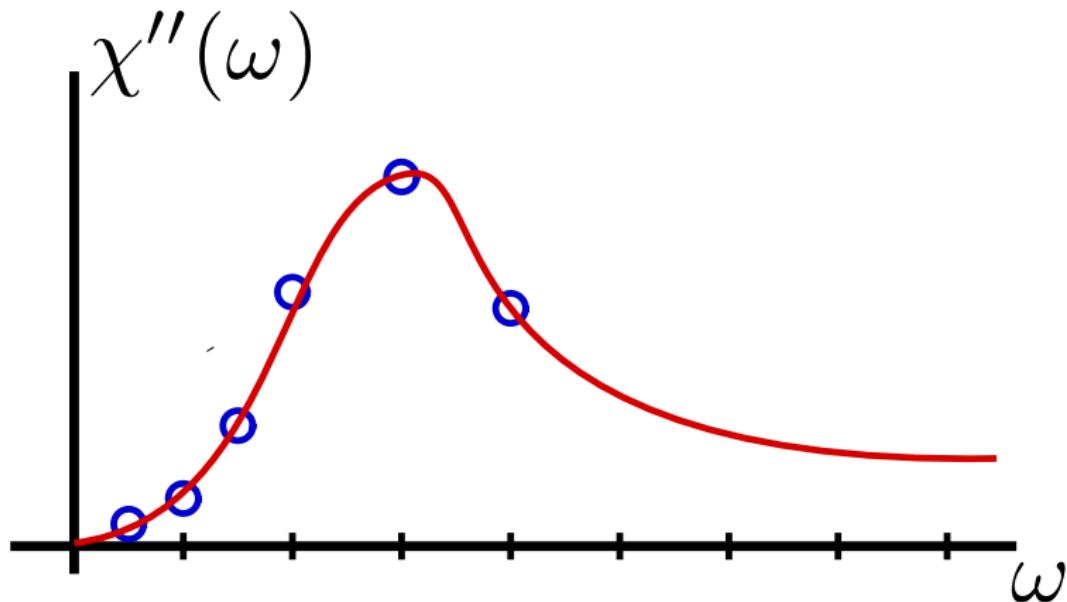
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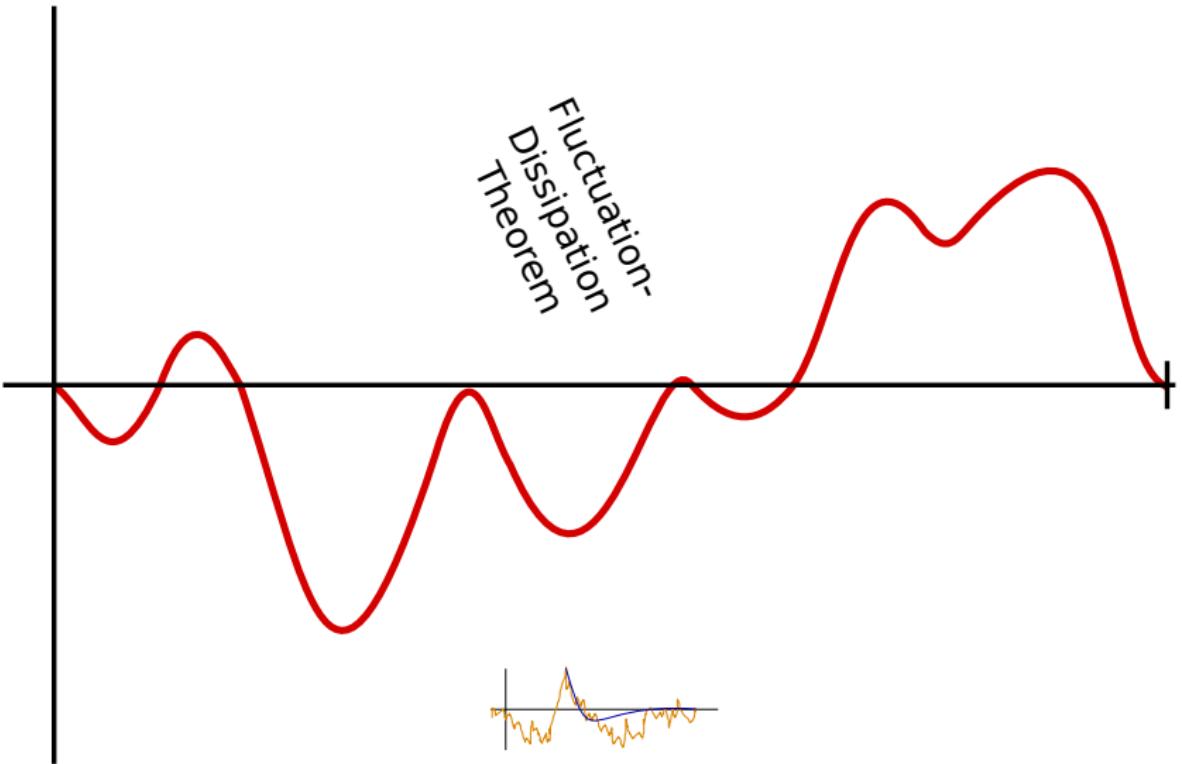


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The fluctuation-dissipation theorem

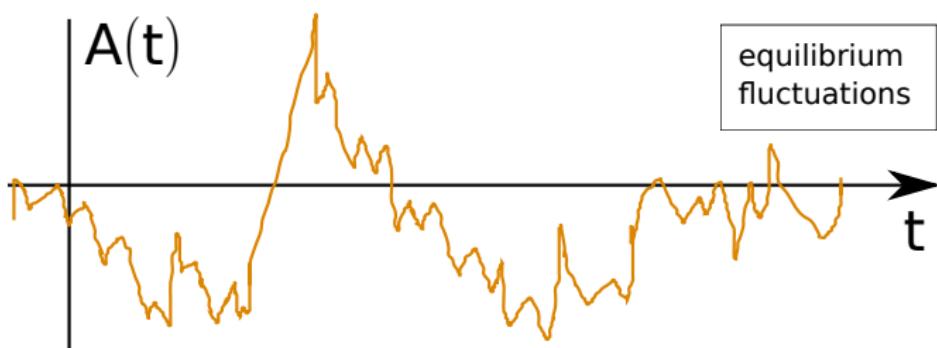
... is based on thermal equilibrium properties!

- ▶ Hamiltonian H_0
- ▶ $\rho = \rho_0$ const.,
- ▶ $A(t) = e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar}$.
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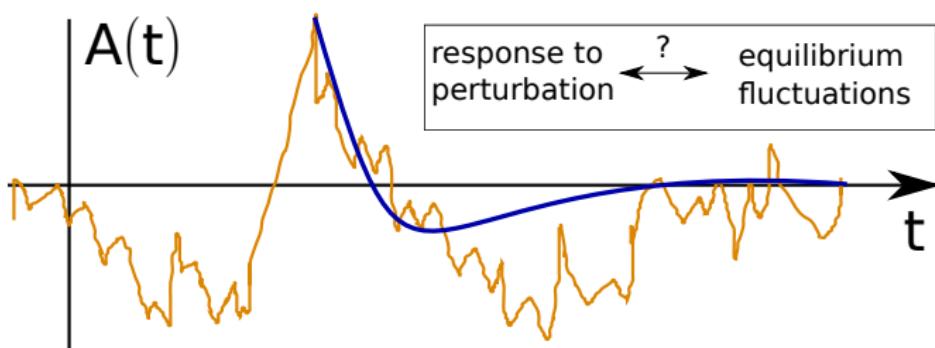
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Symmetries of both functions \implies

$$\boxed{\chi''(\omega) = \frac{1}{\hbar} \tanh \left(\frac{\hbar\omega}{2kT} \right) S(\omega)}$$

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The protagonists next to Green and Kubo:



Onsager



Nyquist

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δA or S
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Kramers–Kronig relations:

$$\chi = \chi' + i\chi''$$

$$\chi' = P \int \frac{\chi''(\omega')}{\omega' - \omega} \frac{d\omega'}{\pi}$$

$$\chi'' = -P \int \frac{\chi'(\omega')}{\omega' - \omega} \frac{d\omega'}{\pi}$$

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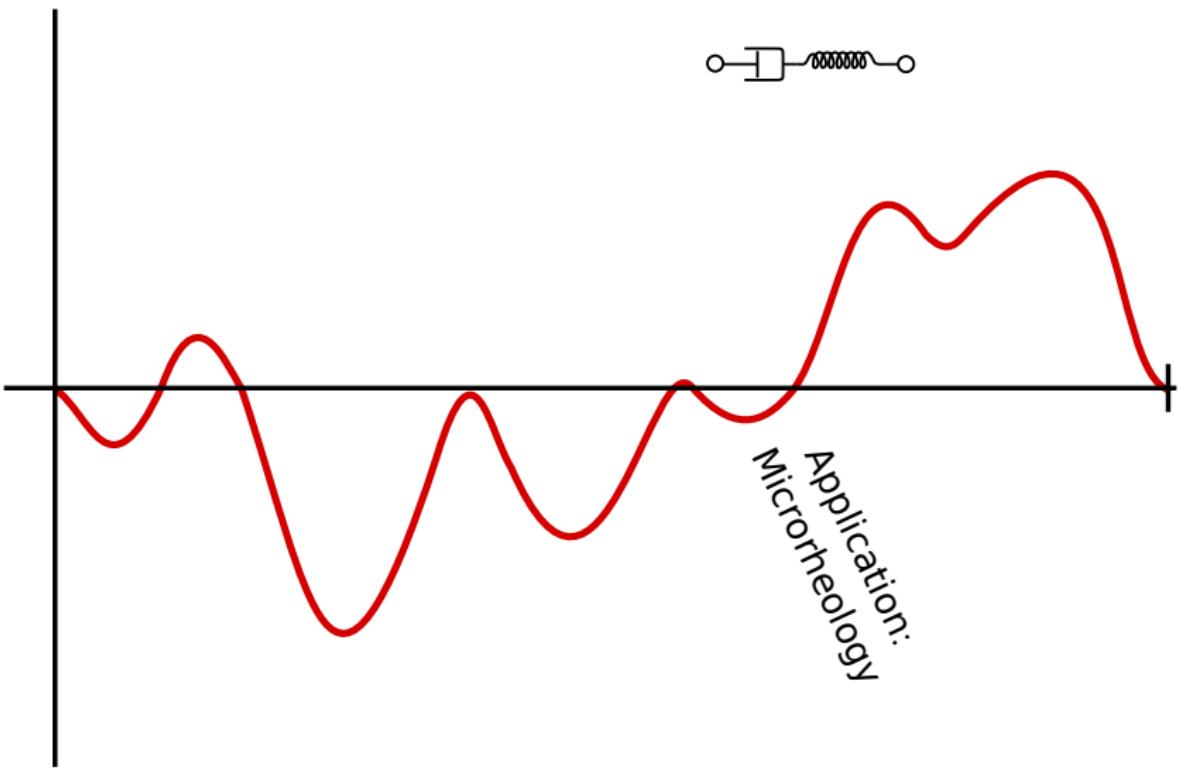
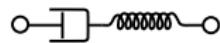
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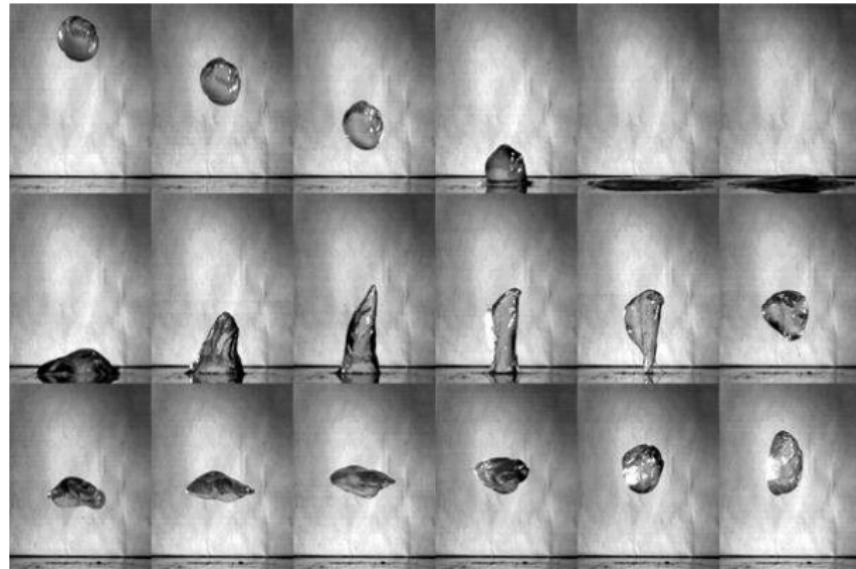
$$\begin{aligned}P &= \frac{1}{T} \int_0^T f(t) \dot{\delta x}(t) dt \\ &= \frac{f_0}{2} \omega \chi''(\omega_0)\end{aligned}$$

In equilibrium:

$$S(\omega) > 0 \implies \chi''(\omega) > 0 \implies P > 0$$



Viscoelastic fluids



R. Zenit,
Instituto de Investigaciones en Materiales,
Universidad Nacional Autonoma de México

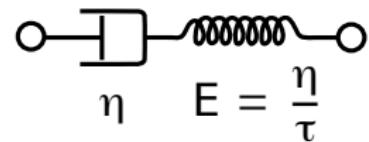
Viscoelastic fluids

Maxwell model:

damper + spring:

$$\sigma = \sigma_D = \sigma_S \quad \text{stress}$$

$$\epsilon = \epsilon_D + \epsilon_S \quad \text{strain}$$



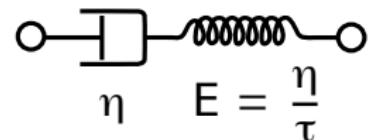
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$$E = \frac{\eta}{\tau}$$

Stress-strain relation

$$\eta \dot{\epsilon}(t) = \sigma(t) + \tau \dot{\sigma}(t)$$

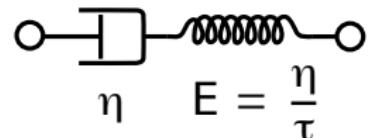
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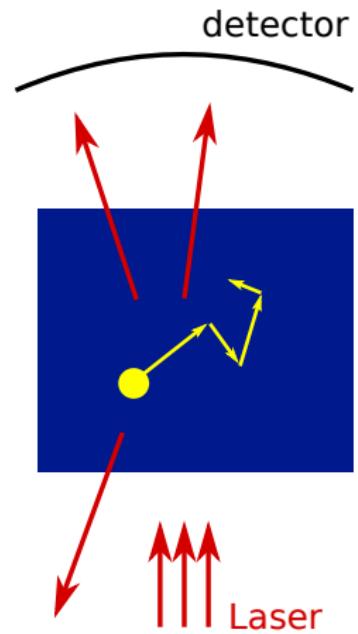
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$$\Rightarrow \tilde{\sigma}(\omega) = -\frac{i\omega\eta}{1 - i\omega\tau} \tilde{\epsilon}(\omega) =: G^*(\omega) \tilde{\epsilon}(\omega)$$

with complex shear modulus $G^*(\omega)$.

Experiment: Bead in viscoelastic fluid



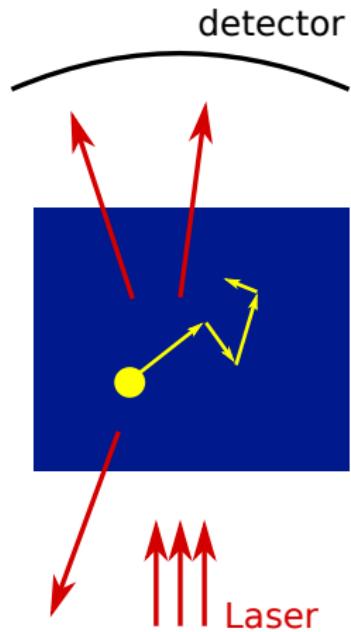
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Generalized Stokes-Einstein equation:

$$\tilde{f}(\omega) = 6\pi a \eta^*(\omega) \tilde{\epsilon}(\omega)$$

with complex viscosity

$$\eta^*(\omega) := \frac{\eta}{1 - i\omega\tau}$$



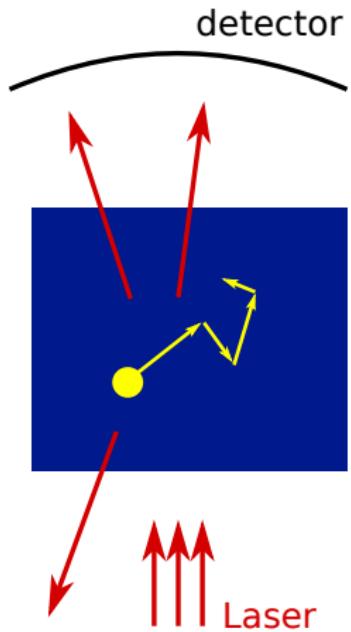
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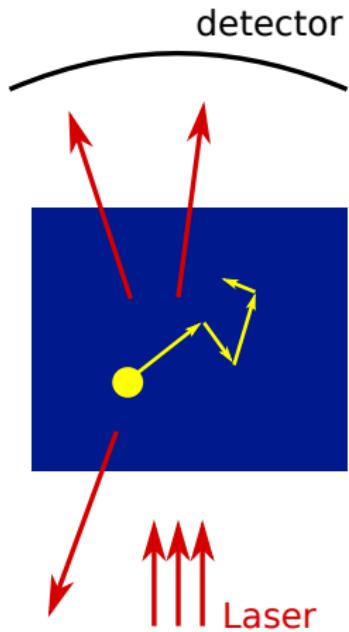
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$$\tilde{\epsilon}(\omega) = \chi(\omega) \tilde{f}(\omega) = \frac{\tilde{f}(\omega)}{6\pi a G^*(\omega)}$$



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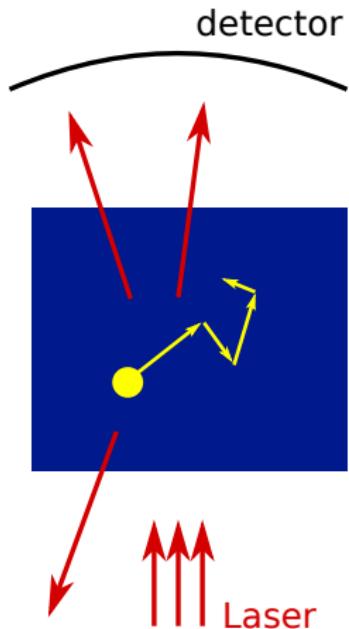
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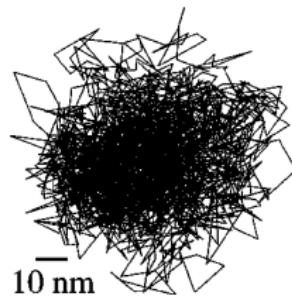
$$\tilde{\epsilon}(\omega) = \chi(\omega) \tilde{f}(\omega) = \frac{\tilde{f}(\omega)}{6\pi a G^*(\omega)}$$

$$\implies G^*(\omega) = \frac{1}{6\pi a \chi(\omega)}$$



Experimental measurement of $G^*(\omega)$

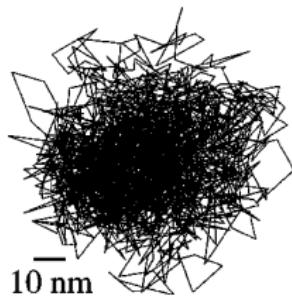
Mason et al., 1997



Trajectory

Experimental measurement of $G^*(\omega)$

Mason et al., 1997

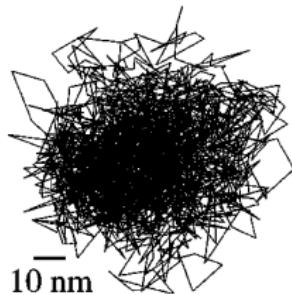


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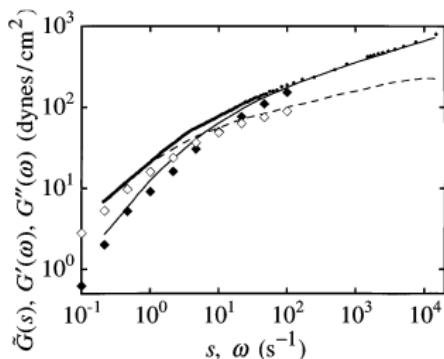
$$r(t) \implies S(\omega) \implies \chi''(\omega) \implies \chi(\omega) \implies G^*(\omega)$$

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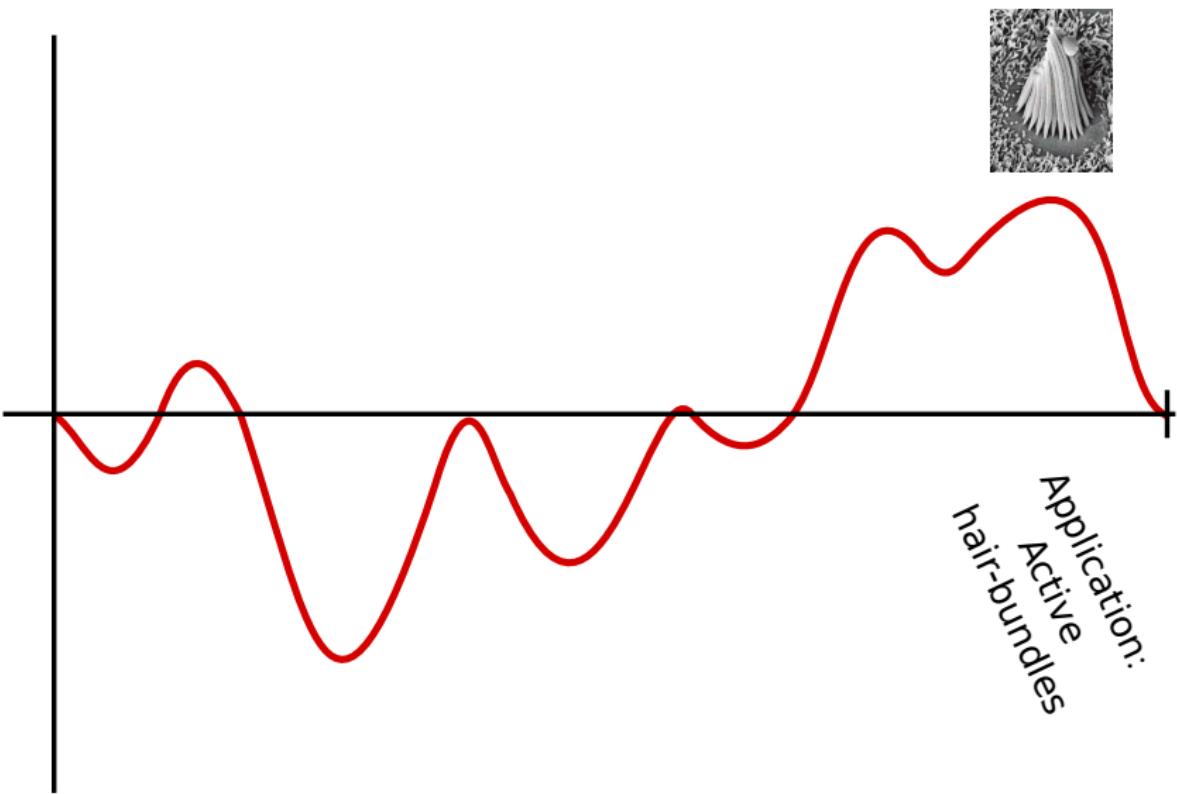


Trajectory



Shear modulus

$$r(t) \implies S(\omega) \implies \chi''(\omega) \implies \chi(\omega) \implies G^*(\omega)$$



Is our system in equilibrium?

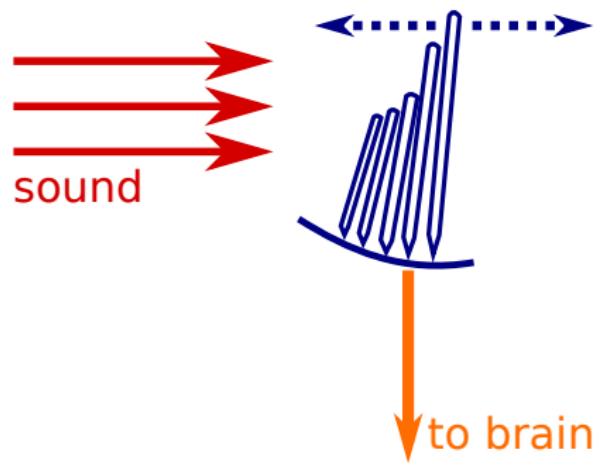
Fluctuation-dissipation theorem:

$$\chi''(\omega) = \frac{\omega}{2kT} S(\omega)$$

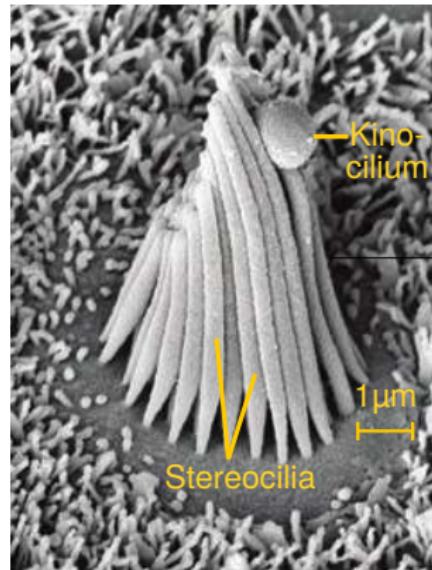
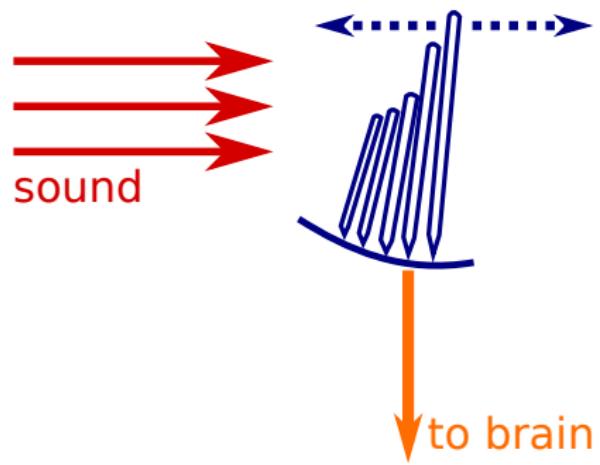
Effective temperature:

$$T_{\text{eff}}(\omega) := \frac{\omega}{2k} \frac{S(\omega)}{\chi''(\omega)}$$

Active hair-bundle motility



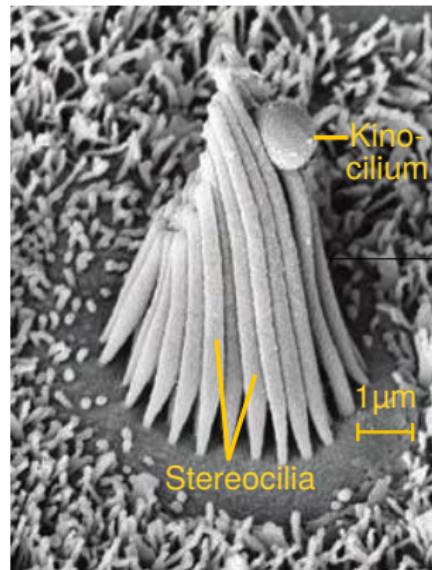
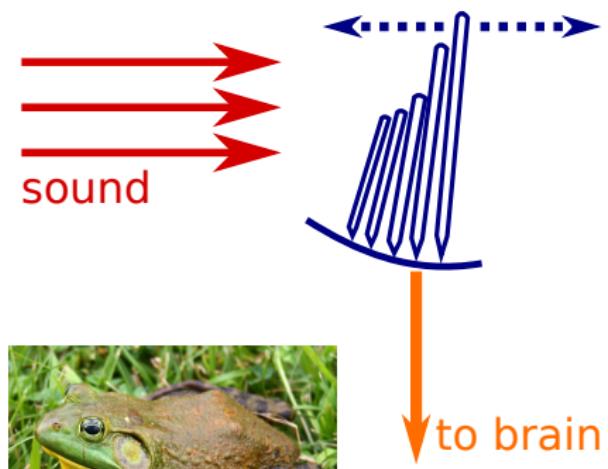
Active hair-bundle motility



Hair bundle

Hudspeth, 2014

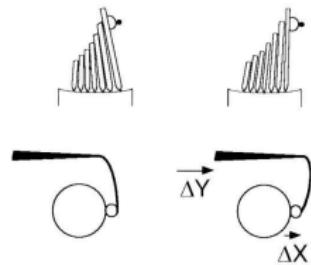
Active hair-bundle motility



Hair bundle

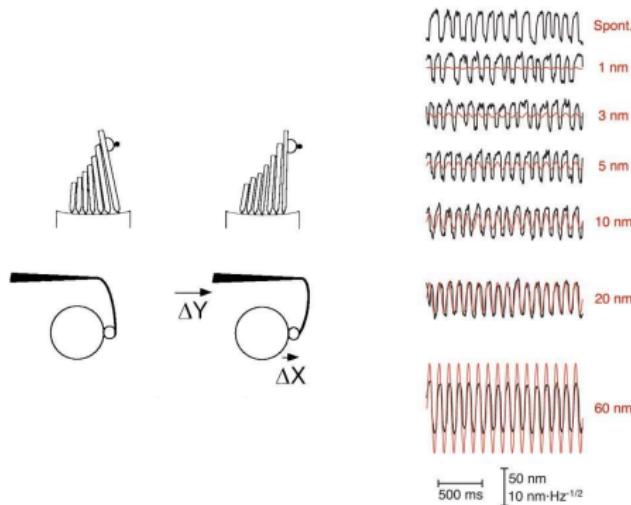
Hudspeth, 2014

Experimental setup and testing linear response



Experimental Setup
Benser et al., 1996

Experimental setup and testing linear response

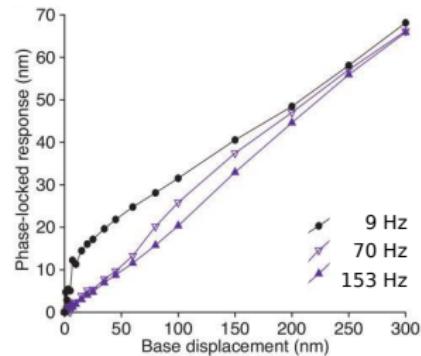
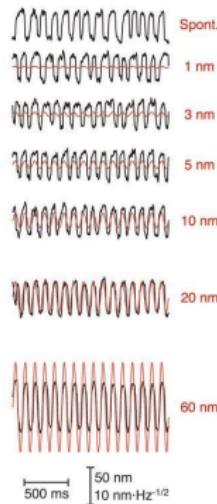
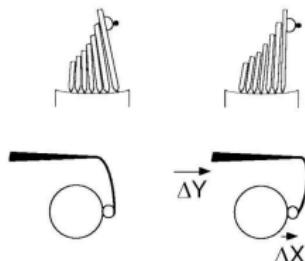


Experimental Setup
Benser et al., 1996

Applying force

Martin & Hudspeth, 2001

Experimental setup and testing linear response



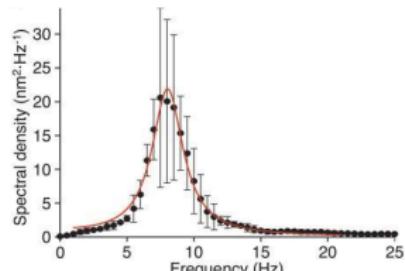
Experimental Setup
Benser et al., 1996

Applying force

Linear Response
Martin & Hudspeth, 2001

Experimental results

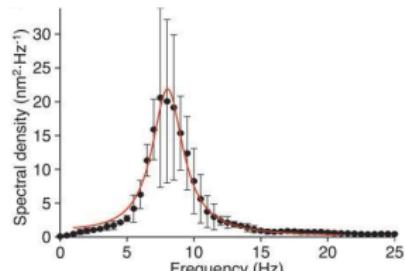
Martin et al., 2001



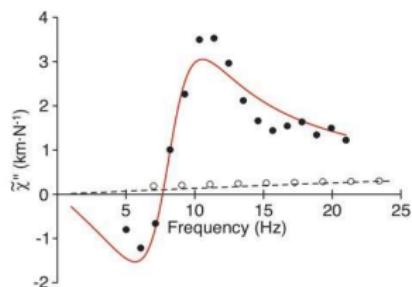
Power Spectrum

Experimental results

Martin et al., 2001



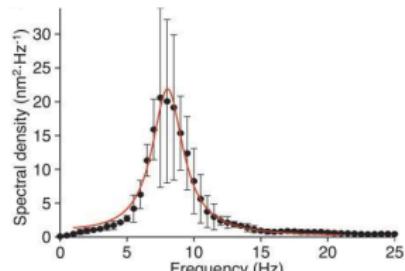
Power Spectrum



Response function

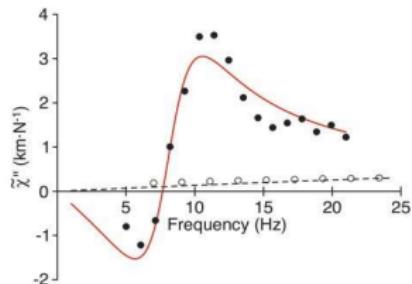
Experimental results

Martin et al., 2001



Power Spectrum

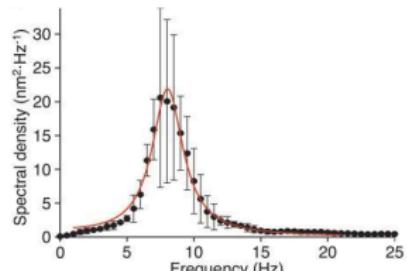
$$T_{\text{eff}}(\omega) = \frac{\omega}{2k} \frac{S(\omega)}{\chi''(\omega)}$$



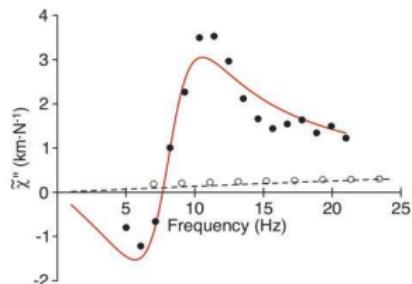
Response function

Experimental results

Martin et al., 2001

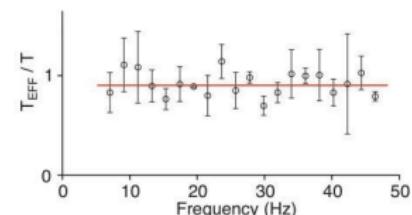
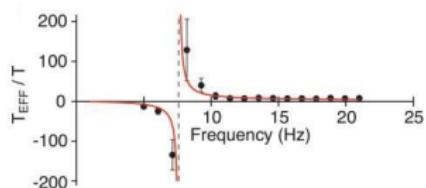


Power Spectrum

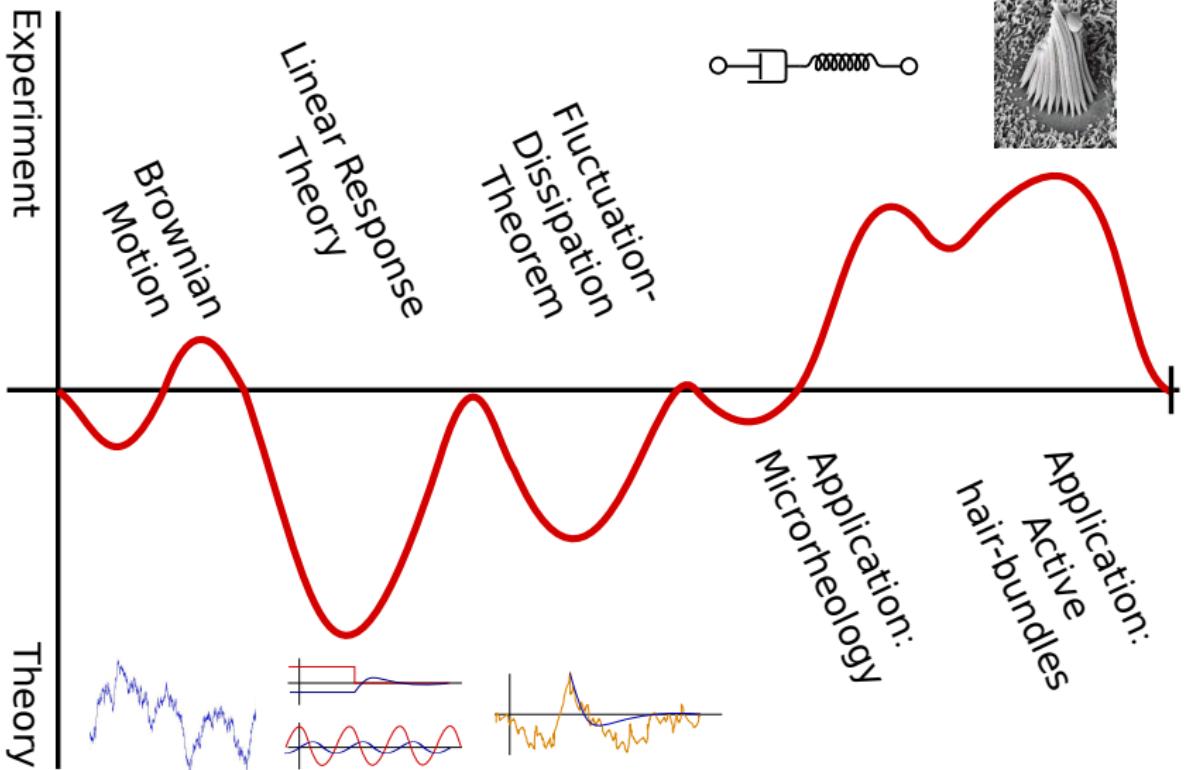


Response function

$$T_{\text{eff}}(\omega) = \frac{\omega}{2k} \frac{S(\omega)}{\chi''(\omega)}$$



Effective temperature



Conclusion

$$\begin{array}{ccccccc} \text{perturbed system} & \iff & \text{response function} & \iff & \text{autocorrelation} \\ \delta A & \stackrel{1.}{\iff} & \chi & \stackrel{2.}{\iff} & \chi'' & \stackrel{3.}{\iff} & S \end{array}$$

Conclusion

$$\begin{array}{ccccccc} \text{perturbed system} & \iff & \text{response function} & \iff & \text{autocorrelation} \\ \delta A & \stackrel{1.}{\iff} & \chi & \stackrel{2.}{\iff} & \chi'' & \stackrel{3.}{\iff} & S \end{array}$$

1. Linear response theory
2. Kramers-Kronig relations
3. Fluctuation-dissipation theorem

Conclusion

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1. Linear response theory
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3. Fluctuation-dissipation theorem

► Microrheology:

$$r(t) \implies S(\omega) \implies \chi''(\omega) \implies \chi(\omega) \implies G^*(\omega)$$

Conclusion

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1. Linear response theory
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► Microrheology:

$$r(t) \implies S(\omega) \implies \chi''(\omega) \implies \chi(\omega) \implies G^*(\omega)$$

► Active hair-bundles:

$$S(\omega), \chi(\omega) \implies T_{\text{eff}} \neq T \implies \text{actively driven}$$

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Thank you for
your attention!



Appendix

Heisenberg picture

All time dependency carried by operators, while $\rho = \rho_{eq}$ constant.
Operators:

$$A(t) = U^{-1}(t, t_0)AU(t, t_0),$$

following the equations of motion

$$i\hbar\partial_t A(t) = [H(t), A(t)].$$

Average measurements:

$$\langle A(t) \rangle_{ne} = \text{Tr } \rho_{eq} A(t).$$

Deduction FDT

Start with correlation function

$$\bar{S}_{AB}(t - t') = \langle A(t)B(t') \rangle .$$

Using $A(t) = e^{itH/\hbar} A(t) e^{-itH/\hbar}$, one shows that

$$\begin{aligned}\bar{S}_{AB}(t - t') &= \frac{1}{Z} \text{Tr } e^{-\beta H} A(t) B(t') \\ &= \frac{1}{Z} \text{Tr } e^{+i(t+i\beta\hbar)H/\hbar} A e^{-i(t+i\beta\hbar)H/\hbar} e^{-\beta H} B(t') \\ &= \frac{1}{Z} \text{Tr } A(t + i\beta\hbar) e^{-\beta H} B(t') \\ &= \frac{1}{Z} \text{Tr } e^{-\beta H} B(t') A(t + i\beta\hbar) \\ &= \bar{S}_{BA}(t' - t - i\beta\hbar) .\end{aligned}$$

Then, with $\tau := t - t'$,

$$\begin{aligned}\bar{S}_{AB}(\omega) &= \int e^{i\omega\tau} \bar{S}_{AB}(-\tau - i\beta\hbar) d\tau \\ &= \int e^{i\omega\tau} \left(\int \bar{S}_{AB}(\omega') e^{-i\omega'(-\tau - i\beta\hbar)} \frac{d\omega'}{2\pi} \right) d\tau \\ &= \int e^{-\beta\hbar\omega'} \bar{S}_{AB}(\omega') 2\pi\delta(\omega + \omega') \frac{d\omega'}{2\pi} \\ &= \bar{S}_{AB}(-\omega) e^{+\beta\hbar\omega}.\end{aligned}$$

And inserting yields

$$\begin{aligned}\chi''_{AB}(t - t') &= \frac{1}{2\hbar} \langle [A(t), B(t')] \rangle \\ &= \frac{1}{2\hbar} \langle \bar{S}_{AB}(\tau) - \bar{S}_{BA}(-\tau) \rangle, \\ \Rightarrow \quad \chi''_{AB}(\omega) &= \frac{1}{2\hbar} (\bar{S}_{AB}(\omega) - \bar{S}_{BA}(-\omega)) = \frac{1 - e^{-\beta\hbar\omega}}{2\hbar} \bar{S}_{AB}(\omega).\end{aligned}$$