Noise, AFMs, and Nanomechanical Biosensors

with Mark Paul (Virginia Tech), and the Caltech BioNEMS Collaboration

Support: DARPA
Outline

- Motivation: MEMS and NEMS
- BioNEMS: Fluctuations in the linear regime
[From M. R. Roukes, Caltech]
Single crystal silicon [From Craighead, Science 290, 1532 (2000)]
Diamond Film [From Sekaric et al., Appl. Phys. Lett. 81, 4445 (2002)]
Array of $\mu$-scale oscillators

[From Buks and Roukes J. MEMS. 11, 802 (2002)]
Self-Oscillations

[Zalalutdinov et al., Appl. Phys. Lett. 79, 695 (2001)]
MicroElectroMechanical Systems and NEMS

Tiny mechanical oscillators:

- driven, dissipative $\Rightarrow$ nonequilibrium
- nonlinear
- collective (arrays)
- noisy
- (potentially) quantum

Goals

- Apply knowledge from statistical mechanics, nonlinear dynamics, pattern formation etc. to technologically important questions
- Investigate stochastic and nonlinear dynamics, and pattern formation in new regimes
BioNEMS - Single BioMolecule Detector/Probe
BioNEMS Prototype

(Arlett et. al, Nobel Symposium 131, August 2005)
Example Design Parameters

**Dimensions:** $L = 3\mu, w = 100\text{nm}, t = 30\text{nm}, L_1 = 0.6\mu, b = 33\text{nm}$

**Material:** $\rho = 2230\text{Kg/m}^3, E = 1.25 \times 10^{11}\text{N/m}^2$

**Results:** Spring constant $K = 8.7\text{mN/m};$ vacuum frequency $\nu_0 \sim 6\text{MHz}$
Atomic Force Microscopy (AFM)

Commercial AFM cantilever (Olympus)  DNA molecule in water
Noise in micro-cantilevers

Thermal fluctuations (Brownian motion) important for:

- BioNEMS: detection scheme
- AFM: calibration

Goals:

- Correct formulation of fluctuations for analytic calculations
- Practical scheme for numerical calculations of realistic geometries
Previous approach (Sader 1998)

- Model molecular collisions with cantilever as white noise force uniformly distributed along cantilever

- Calculate modal response $\tilde{x}_n(\omega)$ for periodic driving force $\tilde{F}(\omega)$ (resonance curves)
  - interesting frequency dependent mass loading and damping from coupling to fluid

- Calculate fluctuation of tip displacement as sum of mode responses for constant $|\tilde{F}(\omega)|^2$
Problems

This approaches is formally incorrect and hard to implement for realistic geometries and strong damping:

- Noise force is not white
- Noise force is not uniformly distributed along surface
- Mode fluctuations are not in general independent
- Difficult to calculate coupled elastic-fluid modes, and many needed for strong damping
Fluid Dynamics Issues

\[
\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \nu \nabla^2 \vec{u},
\]

\[
\nabla \cdot \vec{u} = 0
\]

with \( \nu \) the kinematic viscosity \( \eta/\rho \).

Fluid dynamics is (relatively) easy if we can neglect the inertial terms.

For typical BioNEMS/AFM:

- \( \vec{u} \cdot \nabla \vec{u} = O(u^2) \) is negligible because of tiny oscillation amplitudes
- Important parameter is the Strouhal number

\[
S = \frac{\omega w^2}{4\nu} \approx 1.6
\]

| \( \omega \) | frequency | \( 2\pi \times 1 \text{ MHz} \) |
| \( w \) | width | \( 1 \mu \) |
| \( \nu \) | kinematic viscosity | \( 10^{-6} \text{ m}^2\text{s}^{-1} \) |

Low Reynolds number flow: linear …but can’t take \( S = 0 \)
Simple Picture (Sader)

Potential flow

Diffusing vorticity

\[ S^{-1/2} \]
**Stokes Theory**

Viscous force on sphere of radius $a$ moving with speed $v$ is

$$ F/v = 6\pi \rho va $$

Viscous force per unit length of cylinder of radius $a$ is given by

$$ \gamma = F/v = \pi \rho v \times S \Im \Gamma(S) $$

with

$$ \Gamma(S) = 1 + \frac{4i K_1(-i\sqrt{iS})}{\sqrt{iSK_0(-i\sqrt{iS})}} $$

Effective mass per unit length from fluid

$$ M = \pi a^2 \rho \Re \Gamma(S) \implies Q \approx \frac{\Re \Gamma(S)}{\Im \Gamma(S)} $$

(Other parameter $T = \frac{\pi \rho}{4 \rho_s} \frac{w}{t} = \frac{\text{mass of cylinder of fluid}}{\text{mass of cantilever}} \sim 2$)
For small $S$: \[ S \Gamma(S) \to \frac{-4i}{\frac{1}{2} \log \left( \frac{4}{S} \right) - C_E + i \frac{\pi}{4}} \]
New approach: fluctuation-dissipation theorem

(Paul and MCC, 2004)

Equilibrium fluctuations can be related to the decay of a prepared initial condition

• (near equilibrium) thermodynamics: Onsager regression hypothesis

• statistical mechanics: fluctuation-dissipation theorem, linear response theory, Kubo formalism …
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Consider Hamiltonian

\[ H = H_0 - F(t)A \]

- \( H_0 \) unperturbed Hamiltonian
- \( A(\mathbf{r}_1 \ldots \mathbf{r}_N, \mathbf{p}_1 \ldots \mathbf{p}_N) \) system observable
- \( F(t) \) (small) time dependent force
\[ H = H_0 + \Delta H \]

Equilibrium under \( H_0 + \Delta H \):

\[ \rho = \rho_H (r^N, p^N) \]
\[ H = H_0 + \Delta H \]

\[ F(t) \]

\[ \Delta \langle B(t) \rangle \]

\[ \langle \delta B(t) \delta A(0) \rangle_e = k_B T \frac{\Delta \langle B(t) \rangle}{F_0} \]
Derivation

(e.g. see “Introduction to Modern Statistical Mechanics” by Chandler)
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To calculate the change in a measurement $\langle B(t) \rangle$ due to the application of a small field $F(t)$ that gives a perturbation to the Hamiltonian $\Delta H = -F(t) A$. 
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We can calculate averages in terms of the known distribution $\rho(r^N, p^N)$ at $t = 0$:

$$\langle B(t) \rangle = \int d^r N d^p N \rho(r^N, p^N) B(r^N(t), p^N(t))$$

where $r^N(t)$ is the phase space coordinate that evolves from the value $r^N$ at $t = 0$. 
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$$\langle B(t) \rangle = \int d^N r \, d^N p \, \rho (r^N, p^N) \, B (r^N(t), p^N(t))$$

where $r^N(t)$ is the phase space coordinate that evolves from the value $r^N$ at $t = 0$.

We could equivalently follow the time evolution of $\rho$ through Liouville’s equation and instead evaluate

$$\langle B(t) \rangle = \int d^N r \, d^N p \, \rho (r^N, p^N, t) \, B (r^N, p^N)$$

but the first form is more convenient.
Derivation (cont.)

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For $t \leq 0$ the distribution is the equilibrium one for the perturbed Hamiltonian $H (r^N, p^N) = H_0 + \Delta H$

$$
\rho(r^N, p^N) = \frac{e^{-\beta(H_0+\Delta H)}}{\int d r^N d p^N e^{-\beta(H_0+\Delta H)}}
$$

so that

$$
\langle B(0) \rangle = \frac{Tr e^{-\beta(H_0+\Delta H)} B (r^N, p^N)}{Tr e^{-\beta(H_0+\Delta H)}}
$$

writing $Tr \equiv \int d r^N d p^N$. 

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writing $Tr \equiv \int d r^N d p^N$.

For $t \geq 0$ we let $r^N(t), p^N(t)$ for each member of the ensemble evolve under the Hamiltonian, now $H_0$, from its value $r^N, p^N$ at $t = 0$, so that

$$\langle B(t) \rangle = \frac{Tr e^{-\beta (H_0 + \Delta H)} B (r^N(t), p^N(t))}{Tr e^{-\beta (H_0 + \Delta H)}}.$$ 

Note that the integral is over $r^N, p^N \equiv r^N (0), p^N (0)$, and $\Delta H = \Delta H (r^N, p^N)$ etc.
**Derivation (cont.)**

It is now a simple matter to expand the exponentials to first order in $\Delta H$ ($F_0$ small!)

$$
\langle B(t) \rangle \simeq \frac{Tr e^{-\beta H_0} (1 - \beta \Delta H) B \left( r^N(t), p^N(t) \right)}{Tr e^{-\beta H_0} (1 - \beta \Delta H)}
$$

to give

$$
\langle B(t) \rangle = \langle B \rangle_0 - \beta \left[ \langle \Delta H B(t) \rangle_0 - \langle B \rangle_0 \langle \Delta H \rangle_0 \right] + O (\Delta H)^2
$$

where $\langle \rangle_0$ denotes the average over the ensemble for an unperturbed system i.e. using $\rho_0 = e^{-\beta H_0} / Tr e^{-\beta H_0}$. 
Derivation (cont.)

It is now a simple matter to expand the exponentials to first order in $\Delta H$ ($F_0$ small!)

$$\langle B(t) \rangle \approx \frac{Tr e^{-\beta H_0} (1 - \beta \Delta H) B (\mathbf{r}^N(t), \mathbf{p}^N(t))}{Tr e^{-\beta H_0} (1 - \beta \Delta H)}$$

to give

$$\langle B(t) \rangle = \langle B \rangle_0 - \beta \left[ \langle \Delta H B(t) \rangle_0 - \langle B \rangle_0 \langle \Delta H \rangle_0 \right] + O (\Delta H)^2$$

where $<>_0$ denotes the average over the ensemble for an unperturbed system i.e. using

$$\rho_0 = e^{-\beta H_0} / Tr e^{-\beta H_0}.$$

Finally writing $\delta B(t) = B(t) - \langle B \rangle_0$ etc., and noticing that putting in the form of $\Delta H$

$$\Delta H = -F_0 A (\mathbf{r}^N, \mathbf{p}^N) = -F_0 A (0)$$

gives for the change in the measurement $\Delta \langle B(t) \rangle = \langle B(t) \rangle - \langle B \rangle_0$

$$\Delta \langle B(t) \rangle = \beta F_0 \langle \delta A \rangle_0 \delta B(t) \rangle_0 .$$
Application to single cantilever

Assume observable is tip displacement $X(t)$

- Apply small step force of strength $F_0$ to tip
- Calculate or simulate deterministic decay of $\Delta X(t)$ for $t > 0$. Then

$$C_{XX}(t) = \langle \delta X(t) \delta X(0) \rangle_e = k_B T \frac{\Delta X(t)}{F_0}$$

- Fourier transform of $C_{XX}(t)$ gives power spectrum of $X$ fluctuations $G_X(\omega)$
Advantages

• Correct!

• Essentially no approximations in formulation
  ◦ assume $\Delta \langle X(t) \rangle$ given by deterministic calculation
  ◦ also in implementation assume continuum description

• Incorporates
  ◦ full elastic-fluid coupling
  ◦ non-white, spatially dependent noise
  ◦ no assumption on independence of mode fluctuations
  ◦ complex geometries

• Single numerical calculation over decay time gives complete power spectrum

• Can be modified for other measurement protocols by appropriate choice of conjugate force
  ◦ AFM: deflection of light (angle near tip)
  ◦ BioNEMS: curvature near pivot (piezoresistivity)
Single cantilever

Dimensions: $L = 3 \mu m$, $W = 100$nm, $L_1 = 0.6 \mu m$, $b = 33$nm

Material: $\rho = 2230$Kg/m$^3$, $E = 1.25 \times 10^{11}$N/m$^2$
Device schematic
Adjacent cantilevers

\[ \langle \delta X_2(t) \delta X_1(0) \rangle_c = k_B T \frac{\Delta X_2(t)}{F_1} \]
Device schematic
Results: single cantilever

3d Elastic-fluid code from CFD Research Corporation

$1 \mu s$ force sensitivity: $K \sqrt{G_X(v)} \times 1 MHz \sim 7 pN$
Results: adjacent cantilevers

Autocorrelation of the noise for Cantilever 1

Crosscorrelation of the noise for Cantilever 2
Comparison with AFM experiments

\[232.4\mu \times 20.11\mu \times 0.573\mu\] Asylum Research AFM (Clarke et al., 2005)

Dashed line: calculations from fluctuation-dissipation approach
Dotted line: calculations from Sader (1998) approach
Wall effects

![Graph showing amplitude vs. frequency with wall effects demonstrated. The graph plots amplitude on the y-axis and frequency on the x-axis, with data points and curves illustrating the effect of wall interactions.]
Conclusions

I’ve described one aspect of theoretically modelling micron and submicron scale oscillators


Other areas of interest:


- Analysis of a QND scheme to measure the discrete levels in quantum harmonic oscillator [Santamore, Doherty, and MCC, Phys. Rev. B70, 144301 (2004)]

- Synchronization due to nonlinear frequency pulling and reactive coupling [MCC, Zumdieck, Lifshitz, and Rogers, Phys. Rev. Lett. 93, 224101 (2004)]

- Noise induced transitions between driven (nonequilibrium) states
  - Single nonlinear oscillator
  - Collective states in arrays of oscillators