Nanomechanical Oscillators
from Thermodynamics to Pattern Formation

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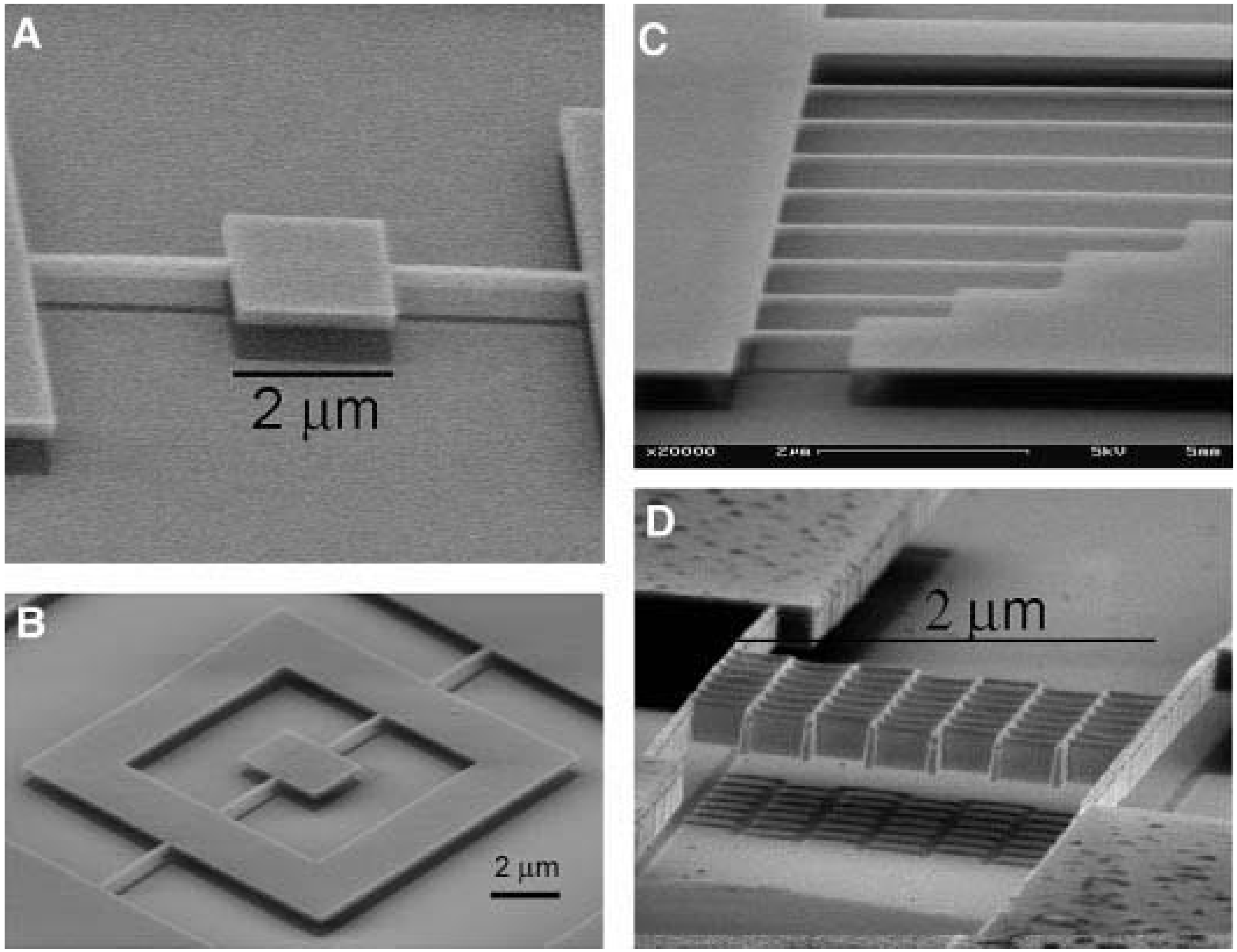
Support: DARPA, NSF, BSF, Nato and EU

Outline

- Motivation: MEMS and NEMS
- BioNEMS: Fluctuations in the linear regime
- Pattern formation: Nonlinear and collective effects in parametrically driven arrays



Single crystal silicon [From Craighead, Science **290**, 1532 (2000)]

MicroElectroMechanical Systems and NEMS

Arrays of tiny mechanical oscillators:

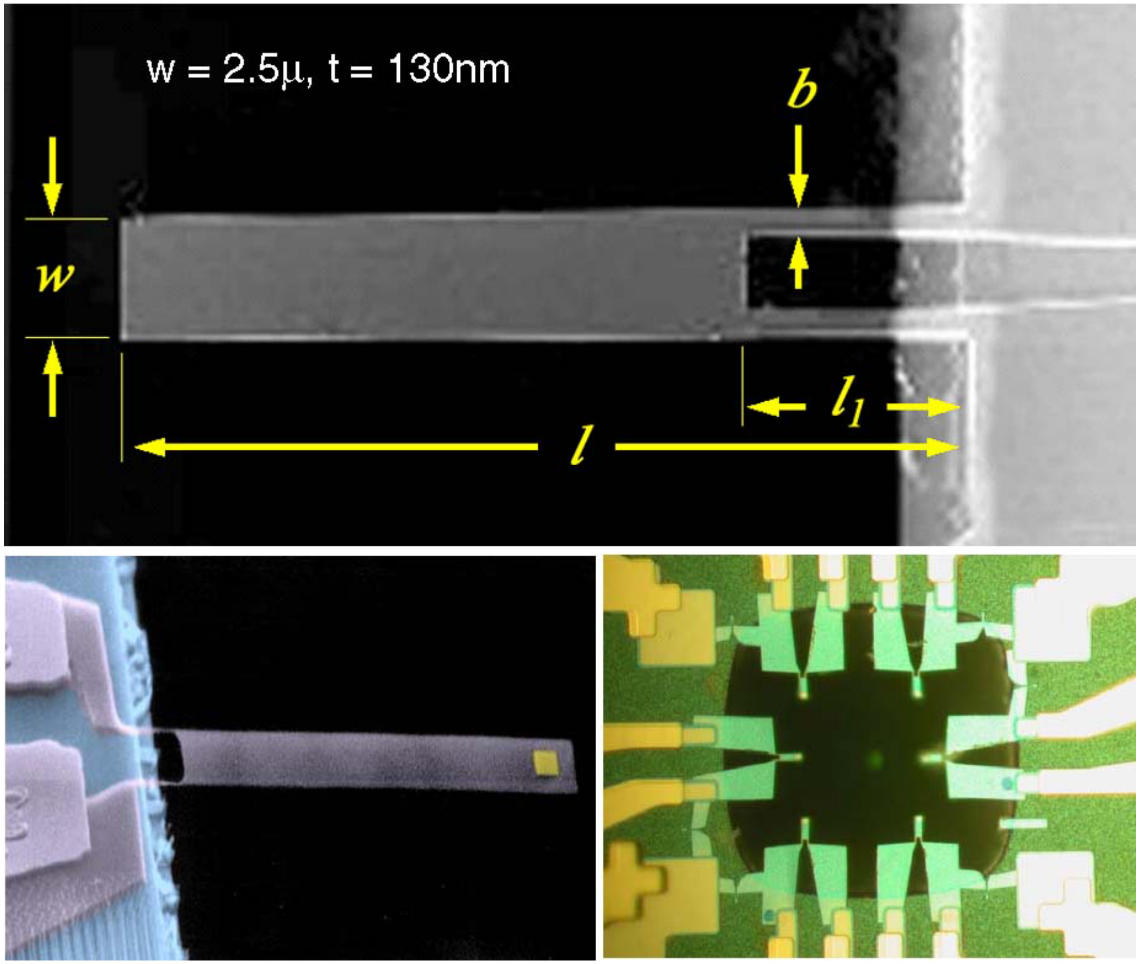
- driven, dissipative $\Rightarrow$ nonequilibrium
- nonlinear
- collective
- noisy
- (potentially) quantum

Goals

- Apply knowledge from statistical mechanics, nonlinear dynamics, pattern formation etc. to technologically important questions
- Investigate pattern formation and nonlinear dynamics in new regimes

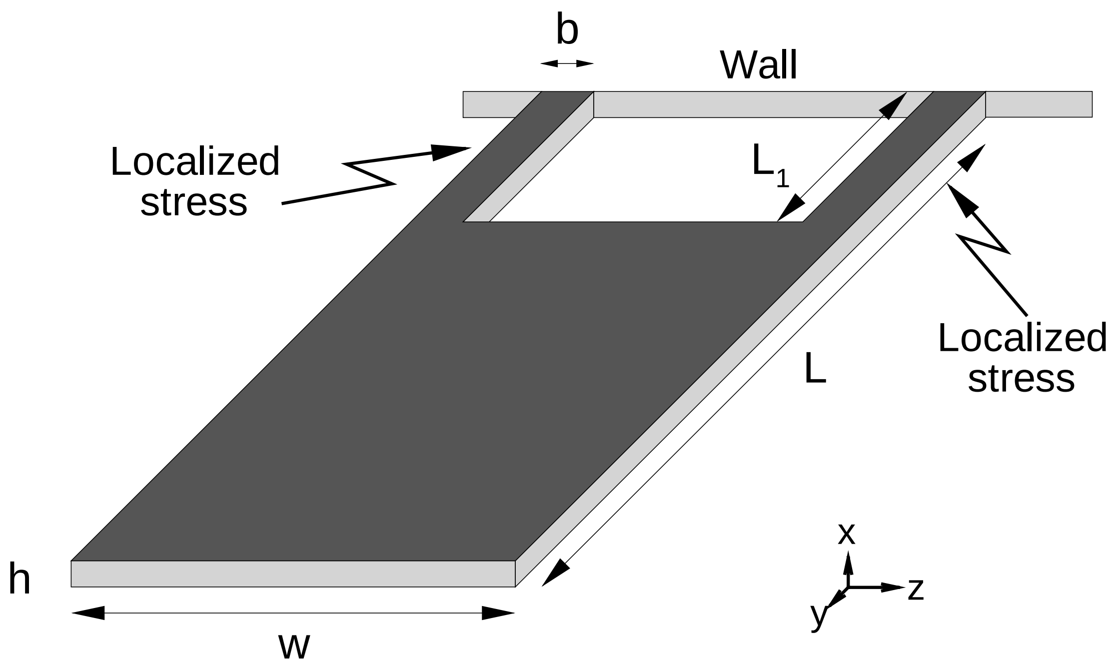
Part I: Fluctuations of micro-cantilevers in solution

BioNEMS Prototype



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

Example Design Parameters

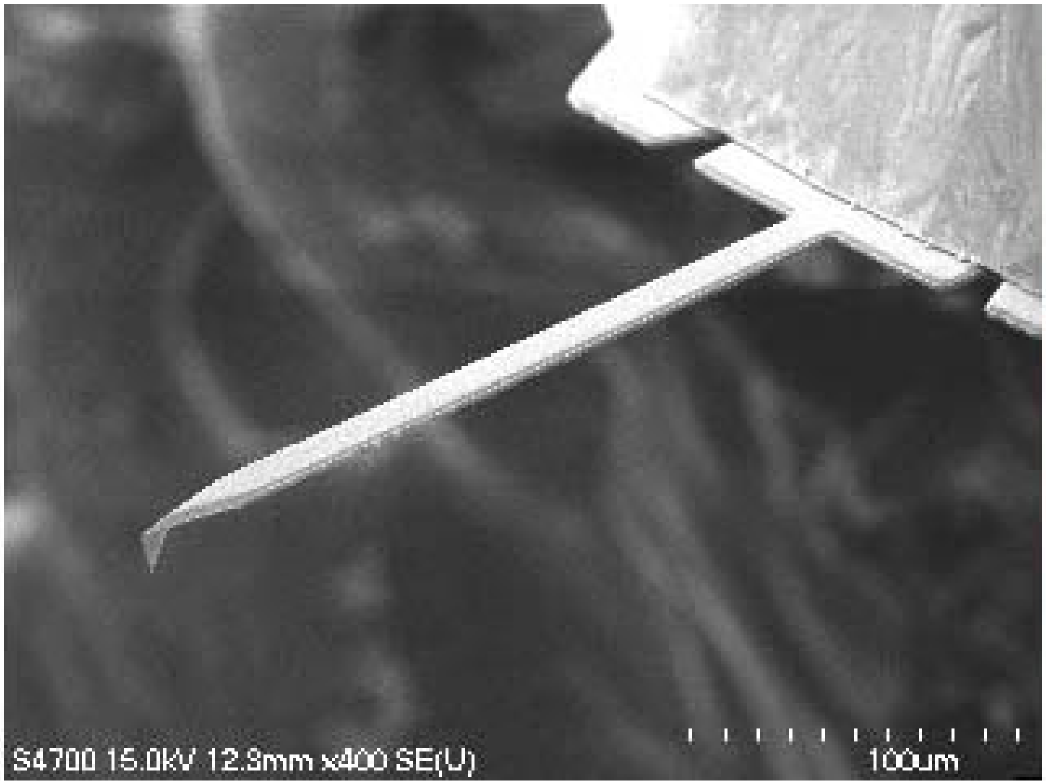


Dimensions: $L = 3\mu$, $w = 100$nm, $t = 30$nm, $L_1 = 0.6\mu$, $b = 33$nm

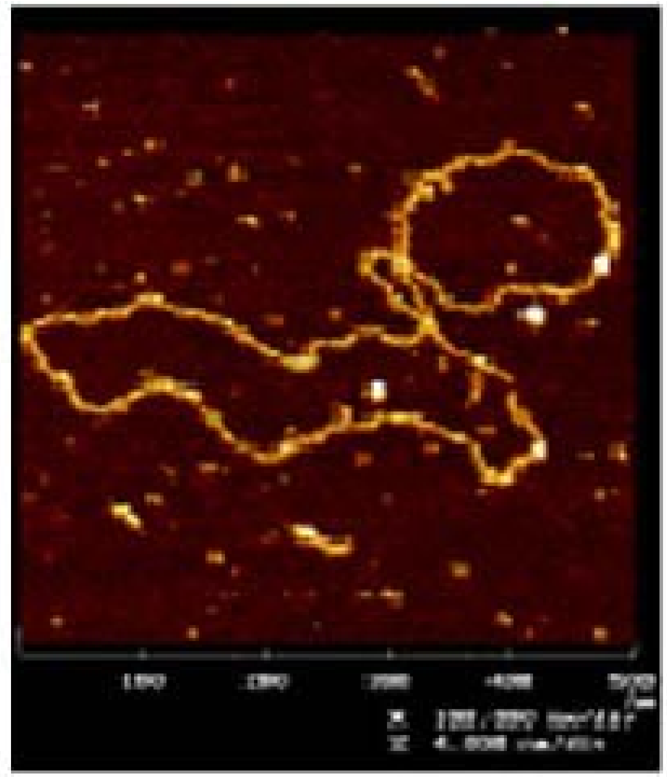
Material: $\rho = 2230$Kg/m^3, $E = 1.25 \times 10^{11}$N/m^2

Results: Spring constant $K = 8.7$mN/m; vacuum frequency $\nu_0 \sim 6$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

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{u} = -\vec{\nabla} p + \nu \nabla^2 \vec{u},$$
$$\vec{\nabla} \cdot \vec{u} = 0$$

with ν the kinematic viscosity η/ρ.

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

For typical BioNEMS/AFM:

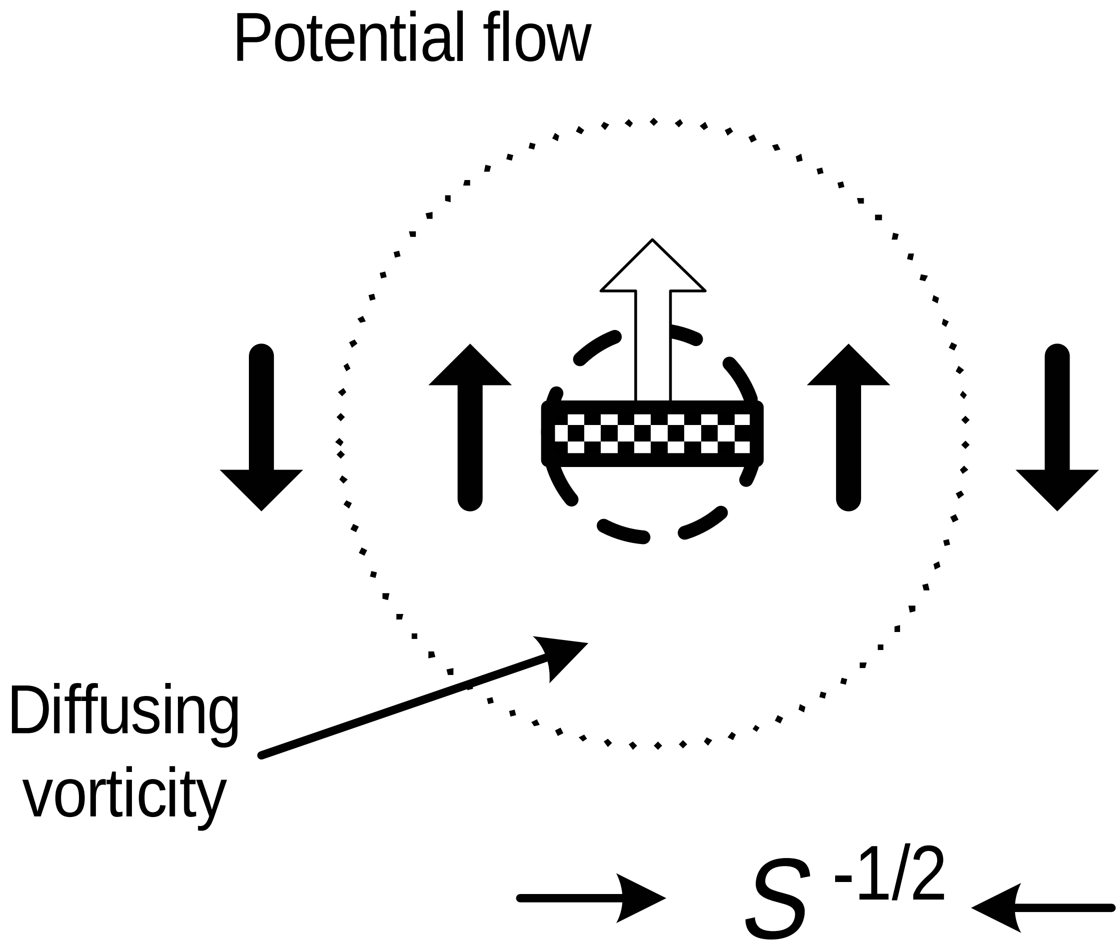
- $\vec{u} \cdot \vec{\nabla} \vec{u} = O(u^2)$ is negligible because of tiny oscillation amplitudes
- Important parameter is the Strouhal number

$$\boxed{\mathcal{S} = \frac{\omega w^2}{4\nu} \approx 1.6}$$

ω	frequency	$2\pi \times 1$ MHz
w	width	1μ
ν	kinematic viscosity	10^{-6} m^{2}s^{-1}

Low Reynolds number flow: linear …but can't take $\mathcal{S} = 0$

Simple Picture (Sader)



Stokes Theory

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

$$F/v = 6\pi\rho\nu a$$

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

$$\gamma = F/v = \pi\rho\nu \times \mathcal{S}\,\mathrm{Im}\,\Gamma(\mathcal{S})$$

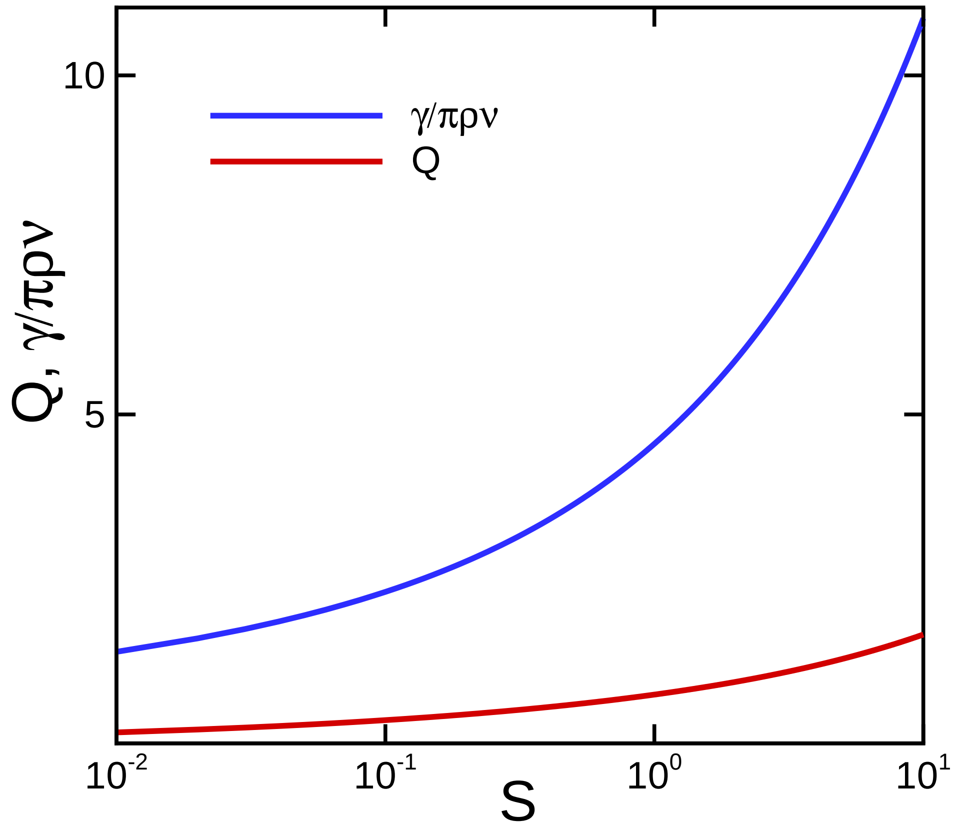
with

$$\Gamma(\mathcal{S}) = 1 + \frac{4iK_1(-i\sqrt{i\mathcal{S}})}{\sqrt{i\mathcal{S}}K_0(-i\sqrt{i\mathcal{S}})}$$

Effective mass per unit length from fluid

$$M = \pi a^2\rho\,\mathrm{Re}\,\Gamma(\mathcal{S}) \Longrightarrow Q \simeq \frac{\mathrm{Re}\,\Gamma(\mathcal{S})}{\mathrm{Im}\,\Gamma(\mathcal{S})}$$

(Other parameter $\mathcal{T} = \frac{\pi}{4}\frac{\rho}{\rho_s}\frac{w}{t} = \frac{\text{mass of cylinder of fluid}}{\text{mass of cantilever}} \sim 2$)



For small $\mathcal{S}$: $$\mathcal{S}\Gamma(\mathcal{S}) \to \frac{-4i}{\frac{1}{2}\log\left(\frac{4}{\mathcal{S}}\right) - C_E + i\,\frac{\pi}{4}}$$

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 …(see eg. *Chandler*)

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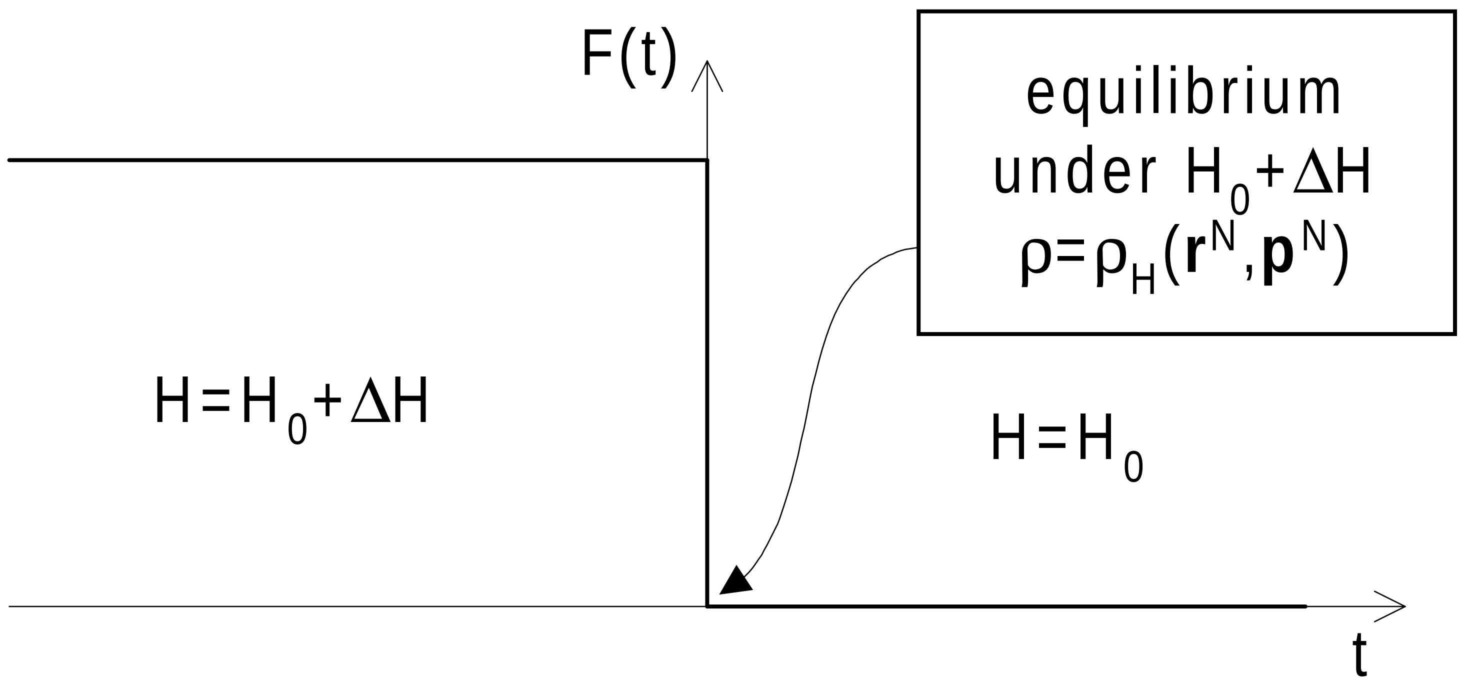
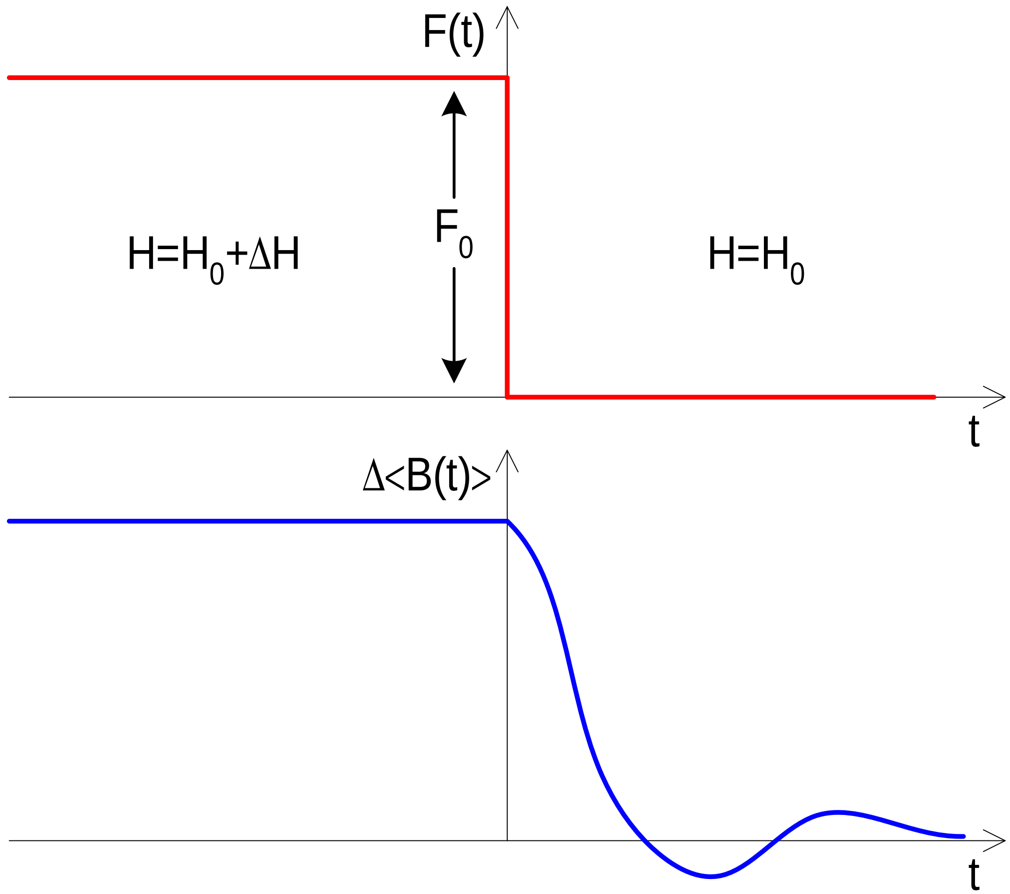
Consider Hamiltonian

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

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


F(t)
equilibrium
under $H_0+\Delta H$
$\rho=\rho_H(\mathbf{r}^N,\mathbf{p}^N)$
$H=H_0+\Delta H$
$H=H_0$
t



$$\langle \delta B(t)\delta A(0)\rangle_{\mathrm{e}} = k_B T\,\frac{\Delta\,\langle B(t)\rangle}{F_0}$$

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

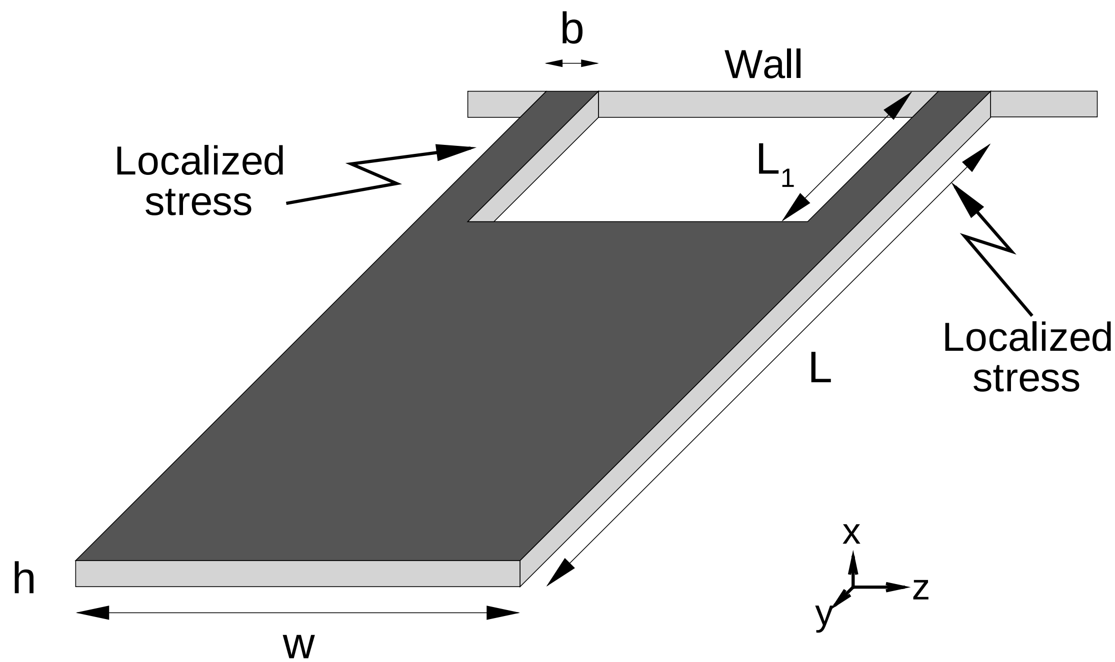
$$C_{XX}(t) = \langle \delta X(t) \delta X(0) \rangle_e = k_B T \frac{\Delta X(t)}{F_0}$$

- 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



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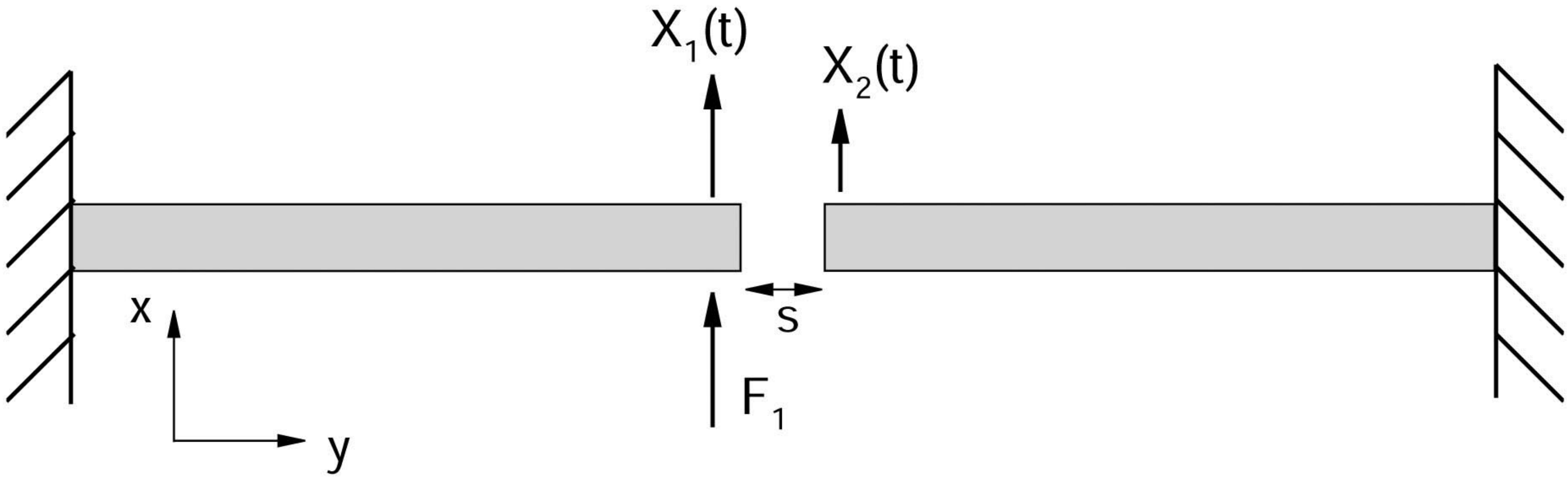
Adjacent cantilevers

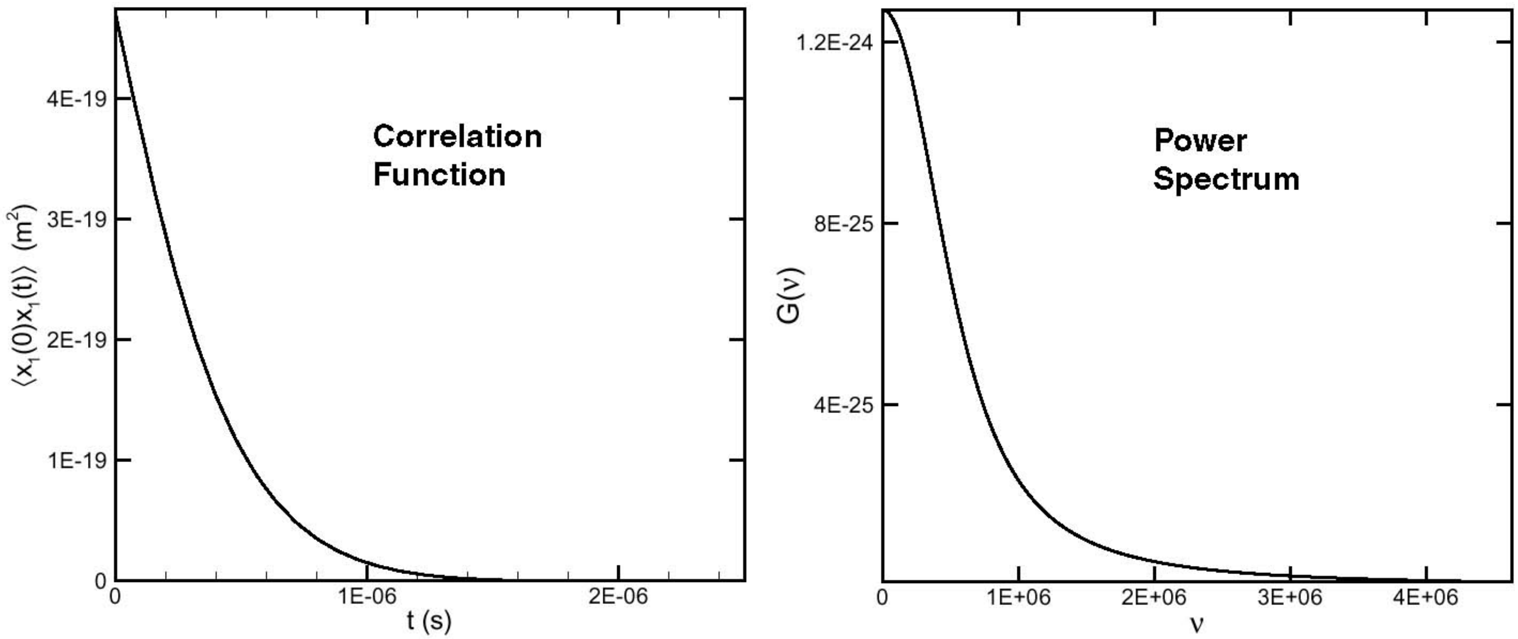


Correlation of Brownian fluctuations

$$\langle \delta X_2(t) \delta X_1(0) \rangle_e = k_B T \frac{\Delta X_2(t)}{F_1}$$

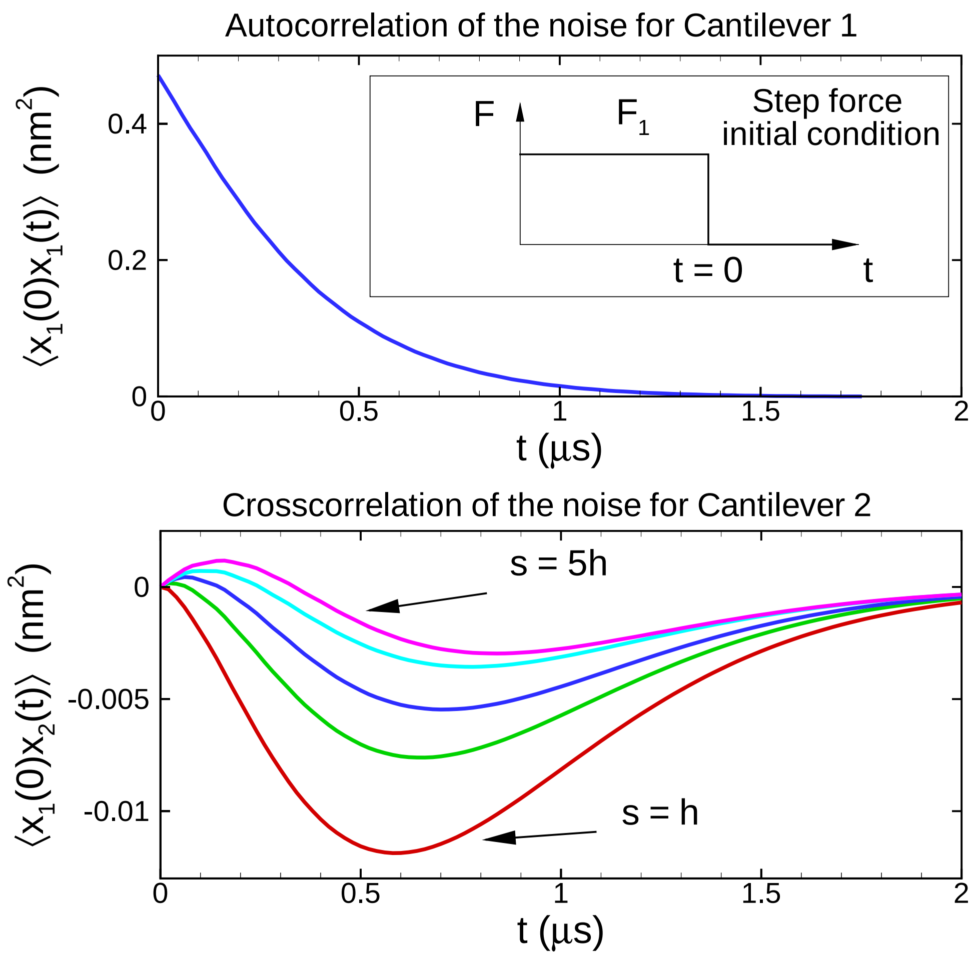
Results: single cantilever

3d Elastic-fluid code from CFD Research Corporation

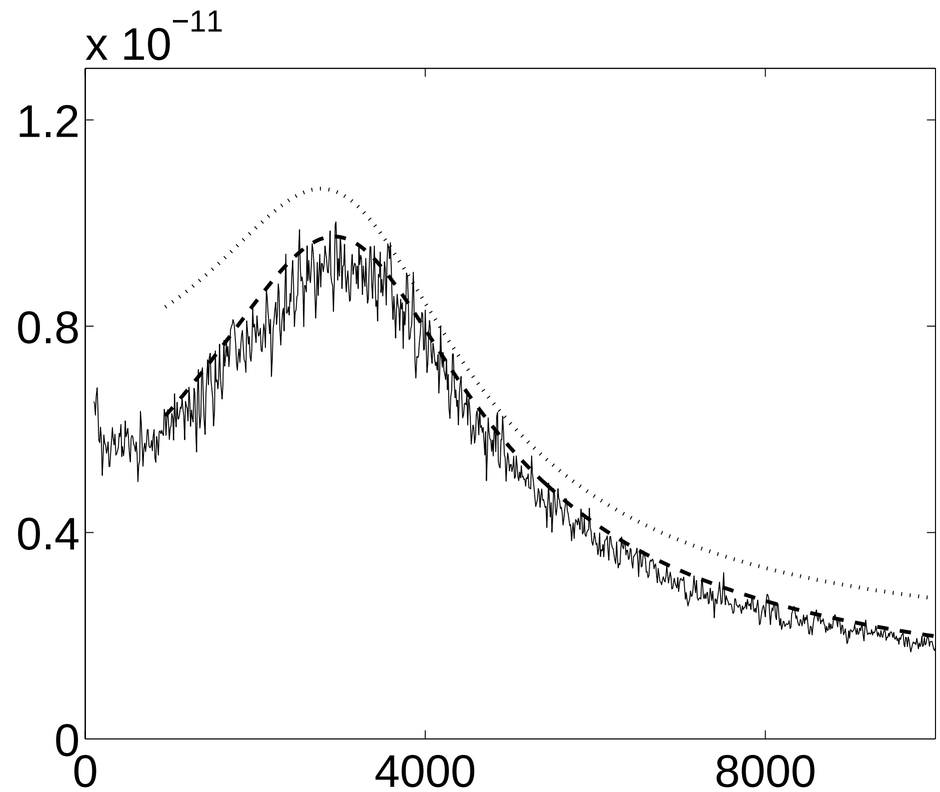


1μs force sensitivity: $K\sqrt{G_X(\nu)\times 1MHz}\sim 7pN$

Results: adjacent cantilevers



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

Part II: Pattern formation in parametrically driven arrays

Modelling high Q oscillators

$$0 = \ddot{x}_n + x_n$$

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n &+ x_n \\
&+ \gamma \dot{x}_n \qquad \text{linear damping}
\end{aligned}
$$

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n + x_n \\
+ \gamma \dot{x}_n \\
+ \delta_n x_n
\end{aligned}
$$

with δ_n taken from distribution $g(\delta_n)$

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n + x_n \\
+ \gamma \dot{x}_n \\
+ \delta_n x_n \\
+ \sum_m D_{nm}(x_m - x_n)
\end{aligned}
$$

reactive coupling

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n + x_n \\
+ \gamma \dot{x}_n \\
+ \delta_n x_n \\
+ \sum_m D_{nm}(x_m - x_n) \\
+ x_n^3 \qquad \text{nonlinear stiffening}
\end{aligned}
$$

Modelling high Q oscillators

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\begin{aligned}
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&+ \gamma \dot{x}_n \\
&+ \delta_n x_n \\
&+ \sum_m D_{nm}(x_m - x_n) \\
&+ x_n^3
\end{aligned}
$$

$$+\eta\left[(x_{n+1} - x_n)^2(\dot{x}_{n+1} - \dot{x}_n) - (x_n - x_{n-1})^2(\dot{x}_n - \dot{x}_{n-1})\right]$$ nonlinear damping

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+\eta \left[(x_{n+1} - x_n)^2 (\dot{x}_{n+1} - \dot{x}_n) - (x_n - x_{n-1})^2 (\dot{x}_n - \dot{x}_{n-1}) \right] \\
- g_E \dot{x}_n (1 - x_n^2) \qquad \text{energy input}
\end{aligned}
$$

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n + x_n \\
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\end{aligned}
$$

$$+g_P \cos\left[(2 + \delta\omega_P)t\right] x_n$$ parametric drive

Modelling high Q oscillators

$$
\begin{aligned}
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&+ \delta_n x_n \\
&+ \sum_m D_{nm}(x_m - x_n) \\
&+ x_n^3 \\
+\eta \big[(x_{n+1} - x_n)^2 (\dot{x}_{n+1} - \dot{x}_n) &- (x_n - x_{n-1})^2 (\dot{x}_n - \dot{x}_{n-1}) \big] \\
&+ g_P \cos[(2 + \delta\omega_P)t]\, x_n \\
&+ 2 g_D \cos[(1 + \delta\omega_D)t] \qquad \text{signal}
\end{aligned}
$$

Modelling high Q oscillators

$$
\begin{aligned}
0 = \ddot{x}_n + x_n \\
+ \gamma \dot{x}_n \\
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+g_P \cos\left[(2 + \delta\omega_P)t\right] x_n \\
+ 2g_D \cos\left[(1 + \delta\omega_D)t\right] \\
+ \text{Noise}
\end{aligned}
$$

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+ 2 g_D \cos\left[(1 + \delta\omega_D) t \right] \\
+ \text{Noise}
\end{aligned}
$$

Theoretical approach

- Oscillators at frequency unity + small corrections
- Assume dispersion, coupling, damping, driving, noise, and nonlinear terms are small.
- Introduce small parameter ε with ε^p characterizing the size of these various terms.
- Then with the "slow" time scale $T = \varepsilon t$

$$x_n(t) = \varepsilon^{1/2}\left[A_n(T)e^{it} + c.c.\right] + \varepsilon^{3/2}x_n^{(1)}(t) + \cdots$$

derive equations for $dA_n/dT = \cdots$.

Example: single Duffing oscillator

$$\ddot{x} + \gamma\dot{x} + x + x^3 = 2g_D\cos(\omega_D t)$$

Parameters:

γ	damping
g_D	drive strength
ω_D	drive frequency

Spring gets *stiffer* with increasing displacement.

We can calculate behavior close to the sinusoidal oscillation $\propto e^{it}$:

- oscillator driving near resonance $\omega_D \simeq 1$
- small damping
- small driving g_D of oscillation implies the effect of the nonlinearity will be small

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To implement these “smallnesses” write

$$\omega_D = 1 + \varepsilon \Omega_D$$

$$g_D = \varepsilon^{3/2} g$$

$$\gamma = \varepsilon \Gamma$$

with $\varepsilon \ll 1$ and g, Γ, Ω_D considered to be of order unity.

(For these scalings the different effects that perturb the oscillator away from $e^{\pm it}$ are comparable. If there is a different scaling of the small parameters, one or more effects may not be important in the dynamics.)

Introduce the WKB-like *ansatz* for the displacement

$$x(t) = \varepsilon^{1/2} A(T) e^{it} + \text{c.c.} + \varepsilon^{3/2} x_1(t) + \cdots$$

- $A(T)$ is a *complex* amplitude that gives the slow modulation
- $T = \varepsilon t$ is a *slow* time variable:

$$\frac{d}{dt} A = \varepsilon A'(T) \ll 1$$

- $x_1(t)$ and $\cdots$ give corrections to the ansatz that are required to be small

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Substitute into the equation of motion using

$$\dot{x} = \varepsilon^{1/2}(iA + \varepsilon A')e^{it} + \text{c.c.} + \varepsilon^{3/2}\dot{x}_1 + \cdots$$

$$\ddot{x} = \varepsilon^{1/2}(-A + 2i\varepsilon A' + \varepsilon^2 A'')e^{it} + \text{c.c.} + \varepsilon^{3/2}\ddot{x}_1 + \cdots$$

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$$\ddot{x} = \varepsilon^{1/2}(-A + 2i\varepsilon A' + \varepsilon^2 A'')e^{it} + \text{c.c.} + \varepsilon^{3/2}\ddot{x}_1 + \cdots$$

and collect terms to give at $O(\varepsilon^{3/2})$

$$\ddot{x}_1 + x_1 = (-2iA' - i\Gamma A - 3\,|A|^2\, A + g e^{i\Omega_D T})e^{it} - A^3 e^{3it} + \text{c.c.} + \cdots$$

For x_1 to be small, the resonant driving terms on the right hand side must be zero.

This gives

$$\frac{d}{dT}A = -\frac{\Gamma}{2}A + i\frac{3}{2}|A|^2 A - i\frac{g}{2}e^{i\Omega_D T}$$

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This gives

$$\frac{d}{dT}A = -\frac{\Gamma}{2}A + i\frac{3}{2}|A|^2 A - i\frac{g}{2}e^{i\Omega_D T}$$

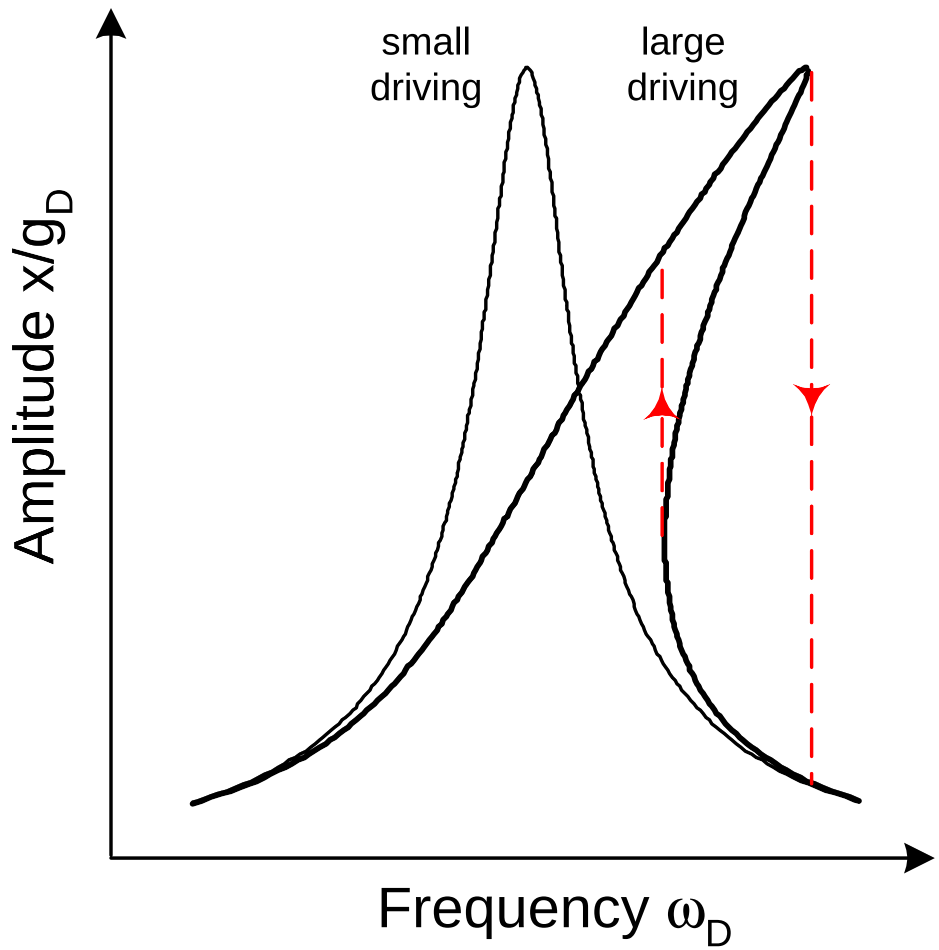
After transients the solution is $A = ae^{i\Omega_D T}$ with

$$|a|^2 = \frac{(g/2)^2}{(\Omega_D - \frac{3}{2}|a|^2)^2 + (\Gamma/2)^2}$$

or

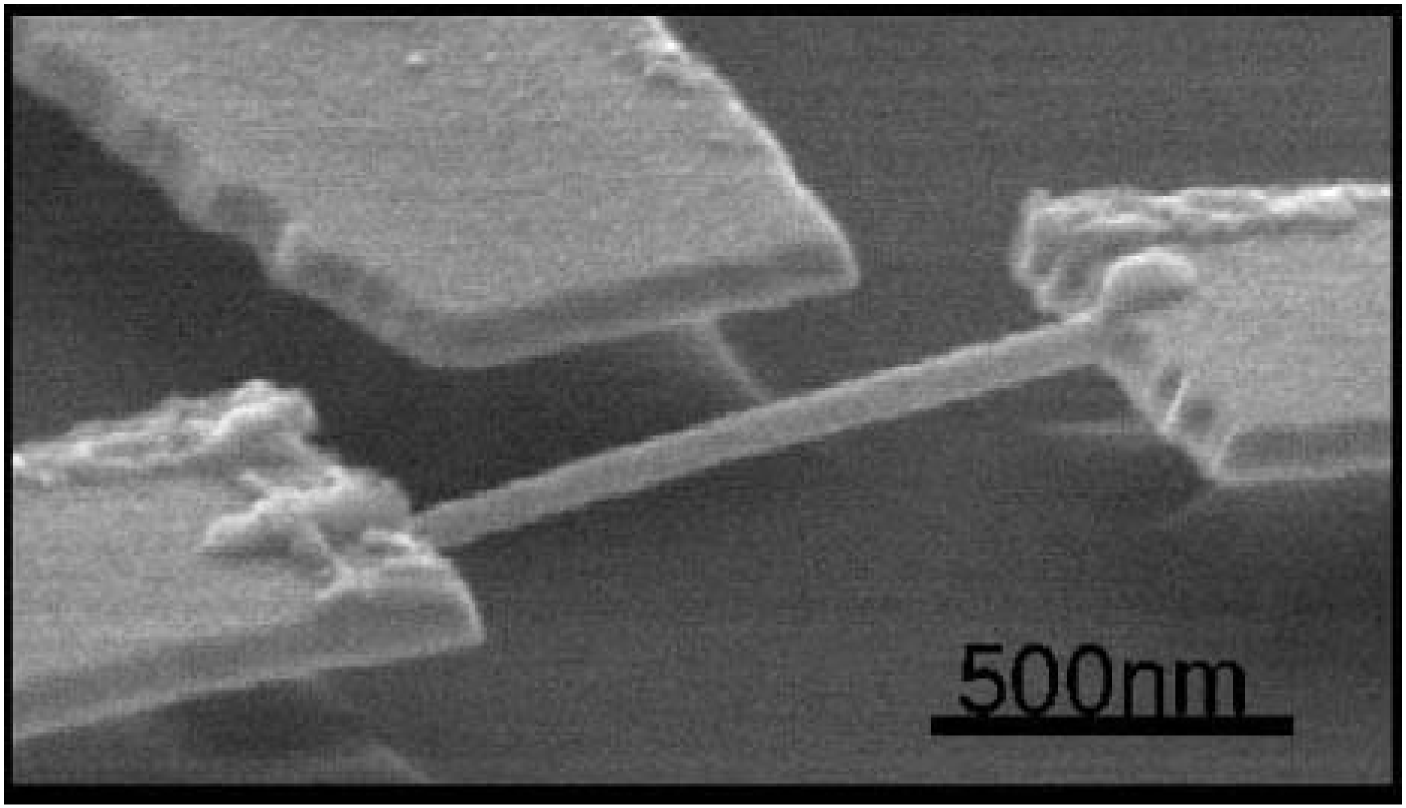
$$|x|^2 = \frac{(g_D/2)^2}{\left[\omega_D - \left(1 + \frac{3}{2}|x|^2\right)\right]^2 + (\gamma/2)^2}$$

Nonlinearity: Frequency pulling



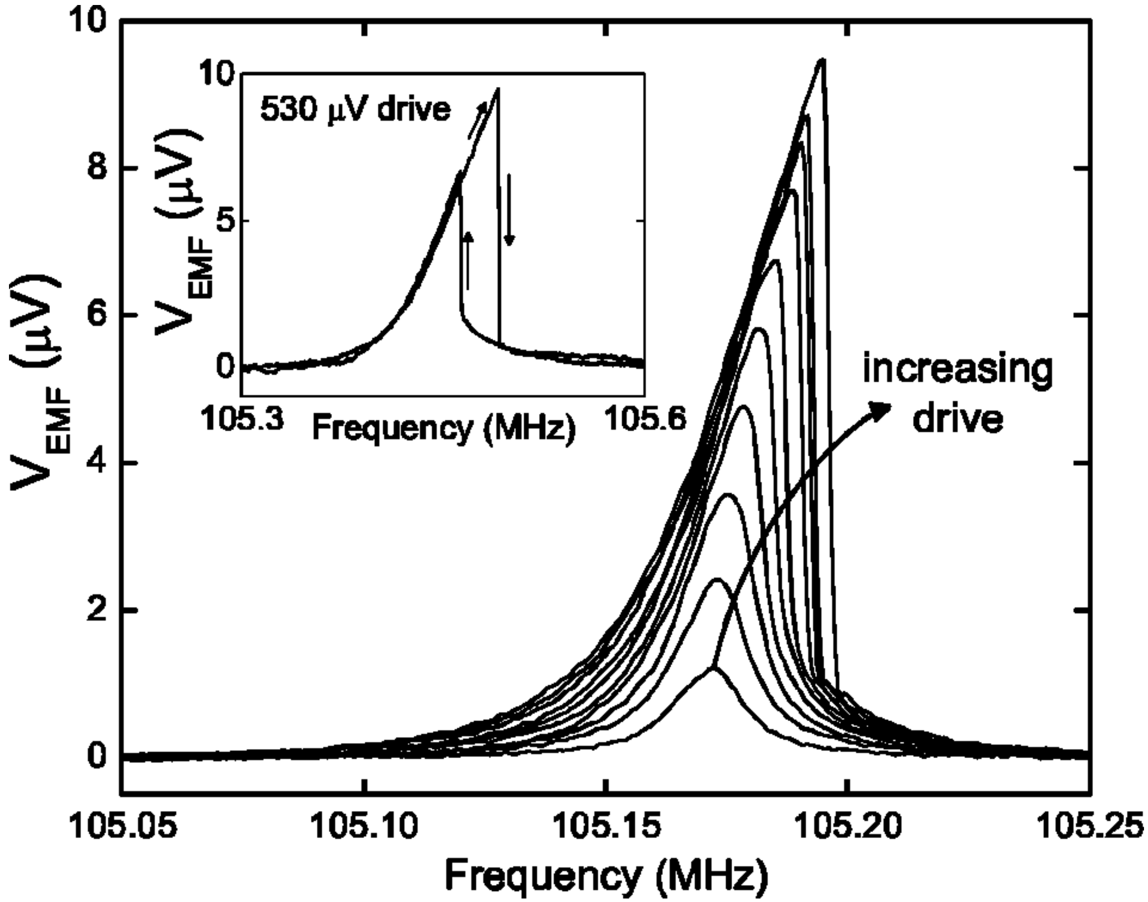
$$\ddot{x} + \gamma\dot{x} + x + x^3 = g_D \cos(\omega_D t)$$

Experiment



Platinum Wire [Husain et al., Appl. Phys. Lett. **83**, 1240 (2003)]

Results



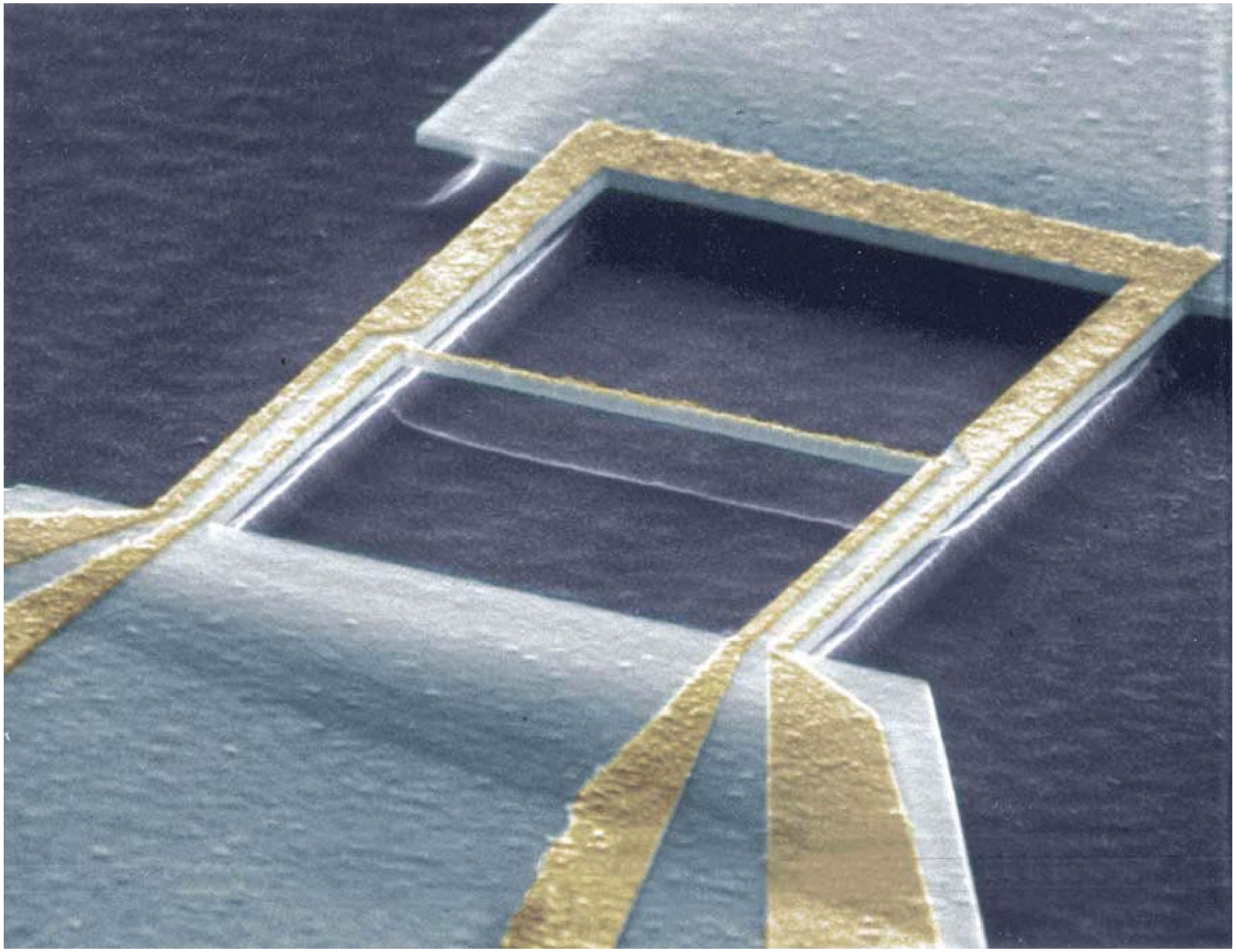
10
8
6
4
2
0
V_{EMF} (μV)
105.05
105.10
105.15
105.20
105.25
Frequency (MHz)
increasing
drive
10
5
0
V_{EMF} (μV)
530 μV drive
105.3
Frequency (MHz)
105.6

Parametric drive in MEMS

$$\ddot{x} + \gamma \dot{x} + (1 + g_P \cos \omega_P t)x + x^3 = 0$$

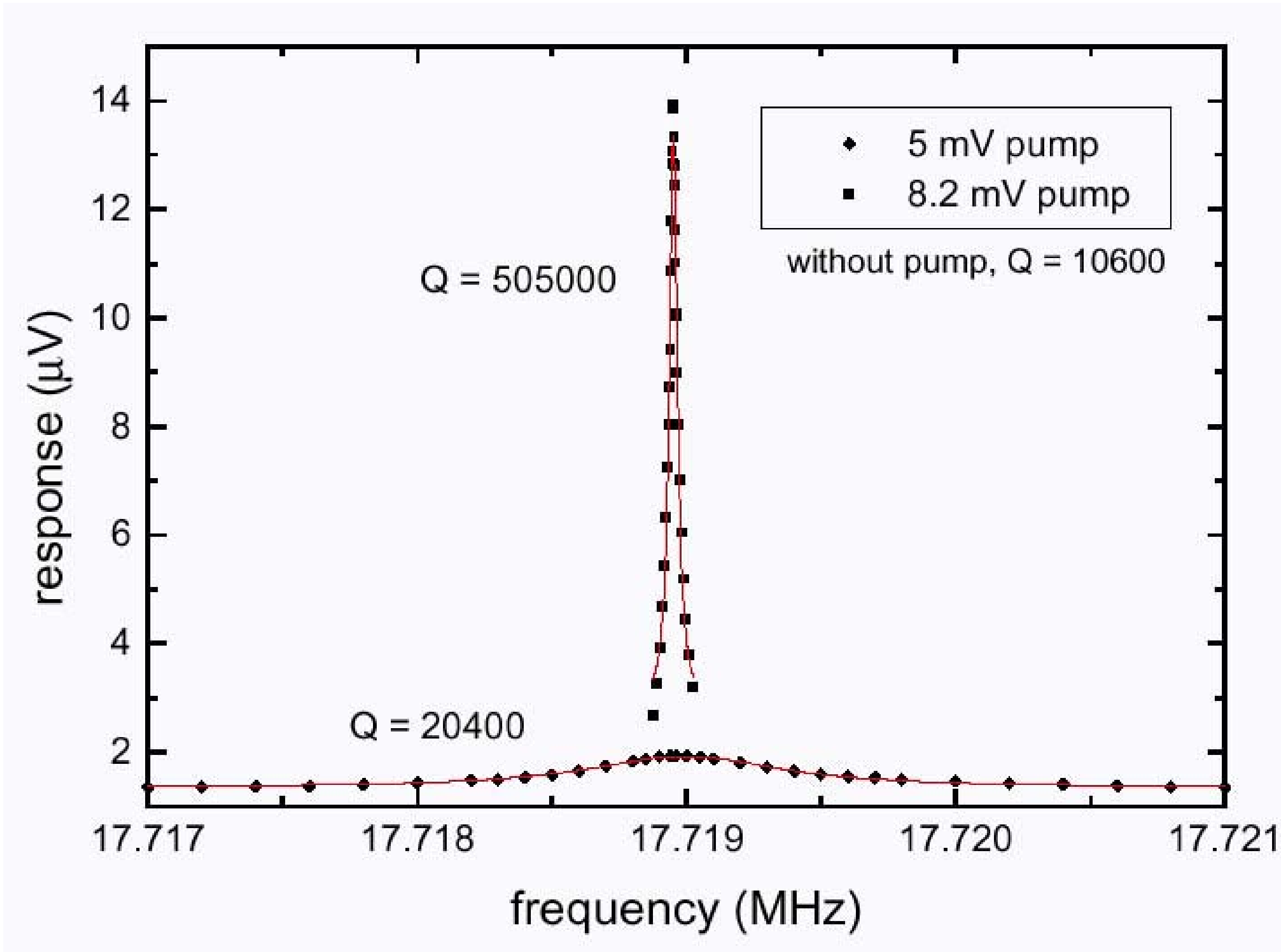
- oscillation of *parameter* of equation—here the spring constant
- $x = 0$ remains a solution in the absence of noise
- parametric drive decreases effective dissipation (for one quadrature of oscillations)
  - ⋆ amplification for small drive amplitudes
  - ⋆ instability for large enough drive amplitudes
- strongest response for $\omega_p = 2$

MEMS Elastic parametric drive



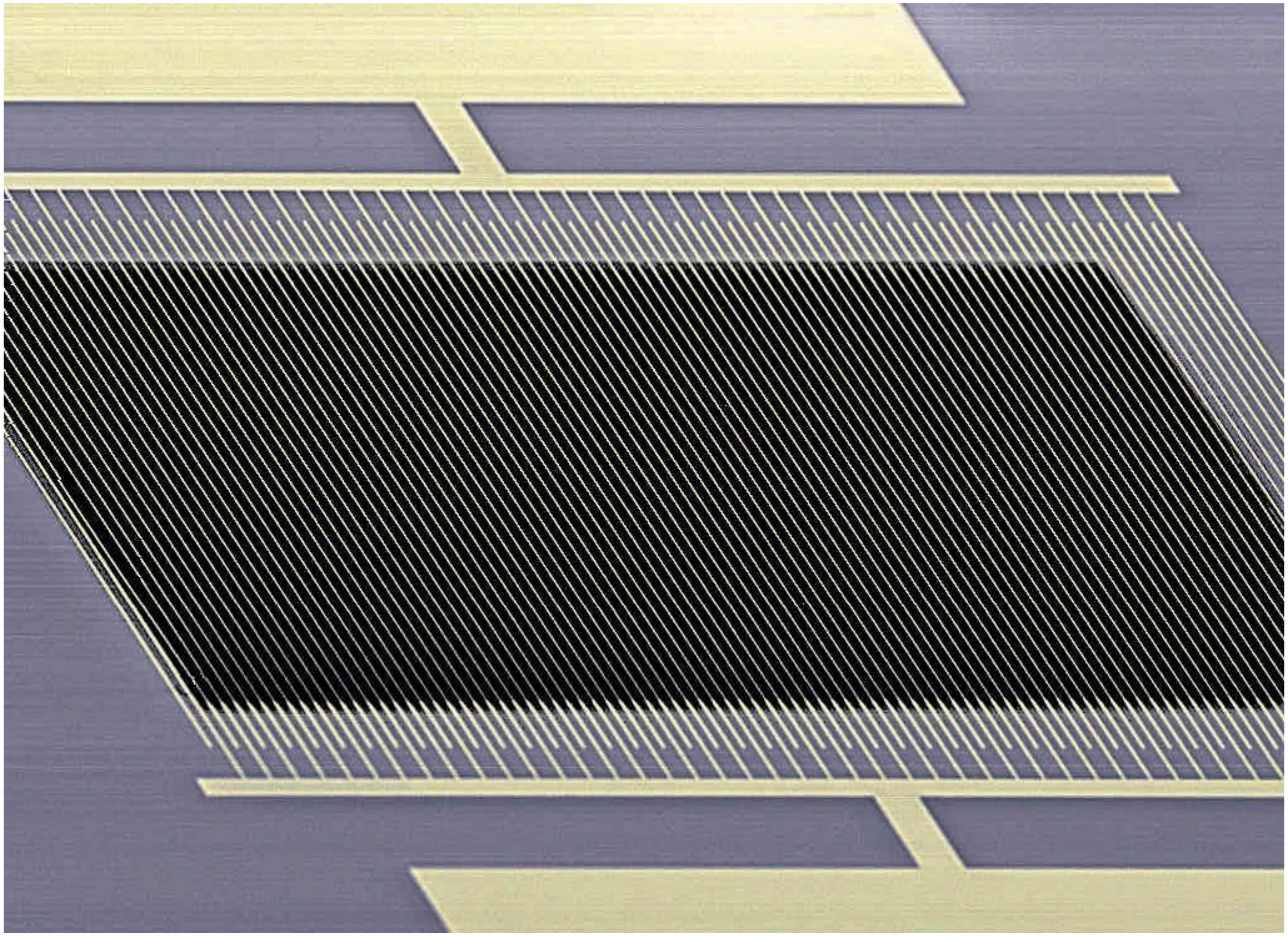
[Harrington and Roukes]

Amplification



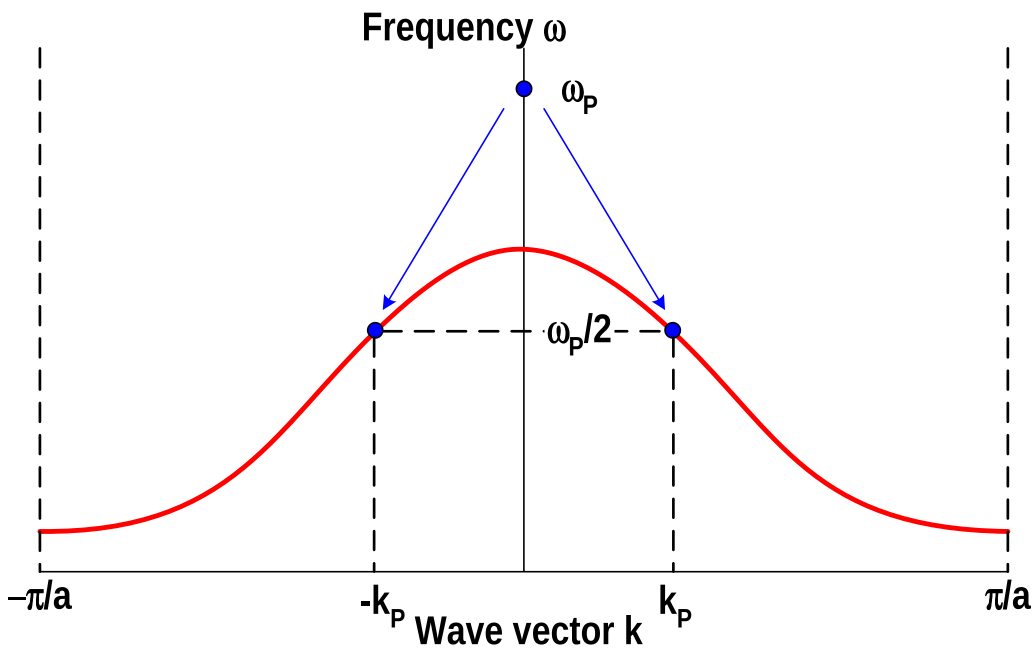
[Harrington and Roukes]

Parametric instability in arrays of oscillators



$270\mu \times 1\mu \times 0.25\mu$ gold beams [Buks and Roukes, 2001]

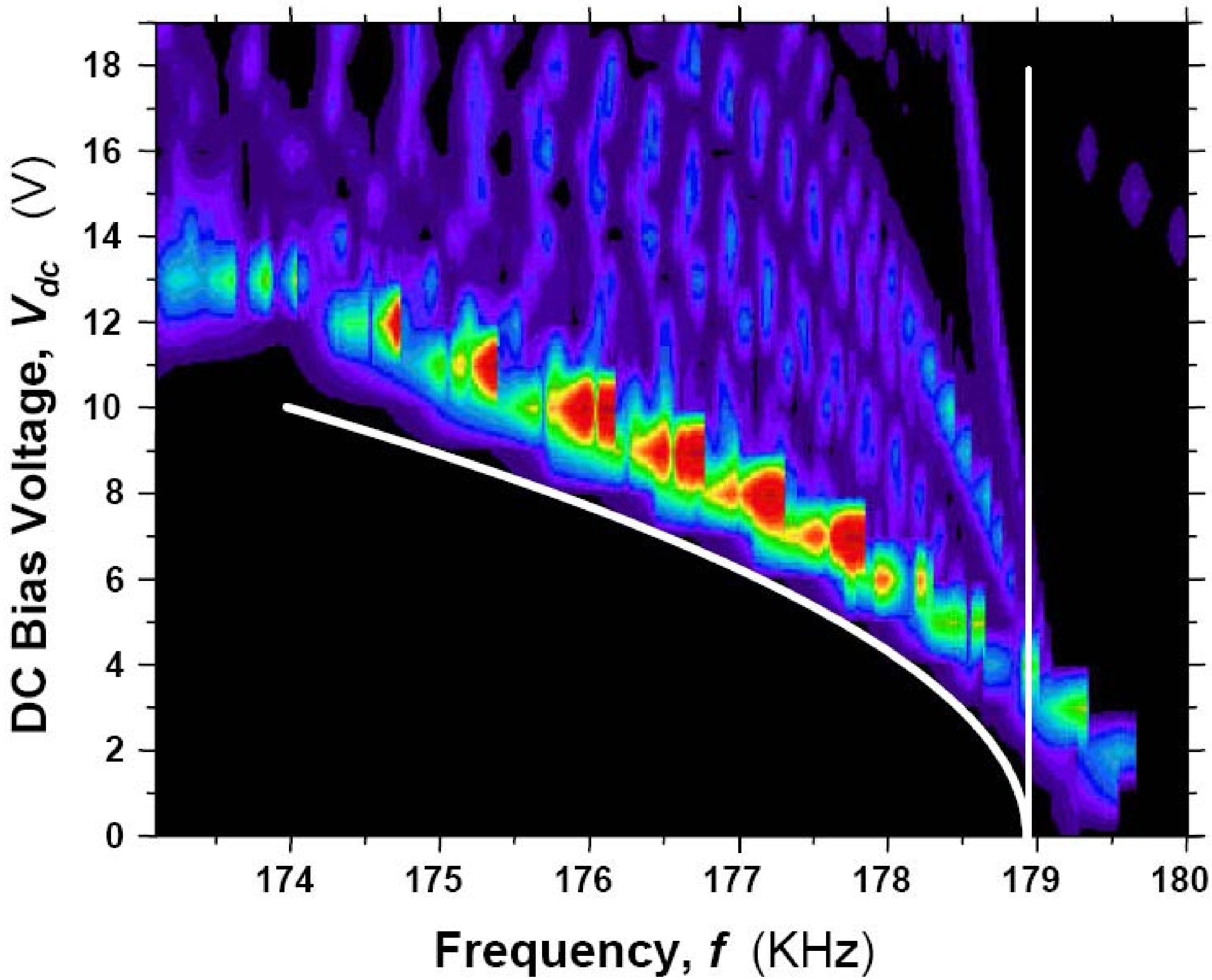
Simple intuition



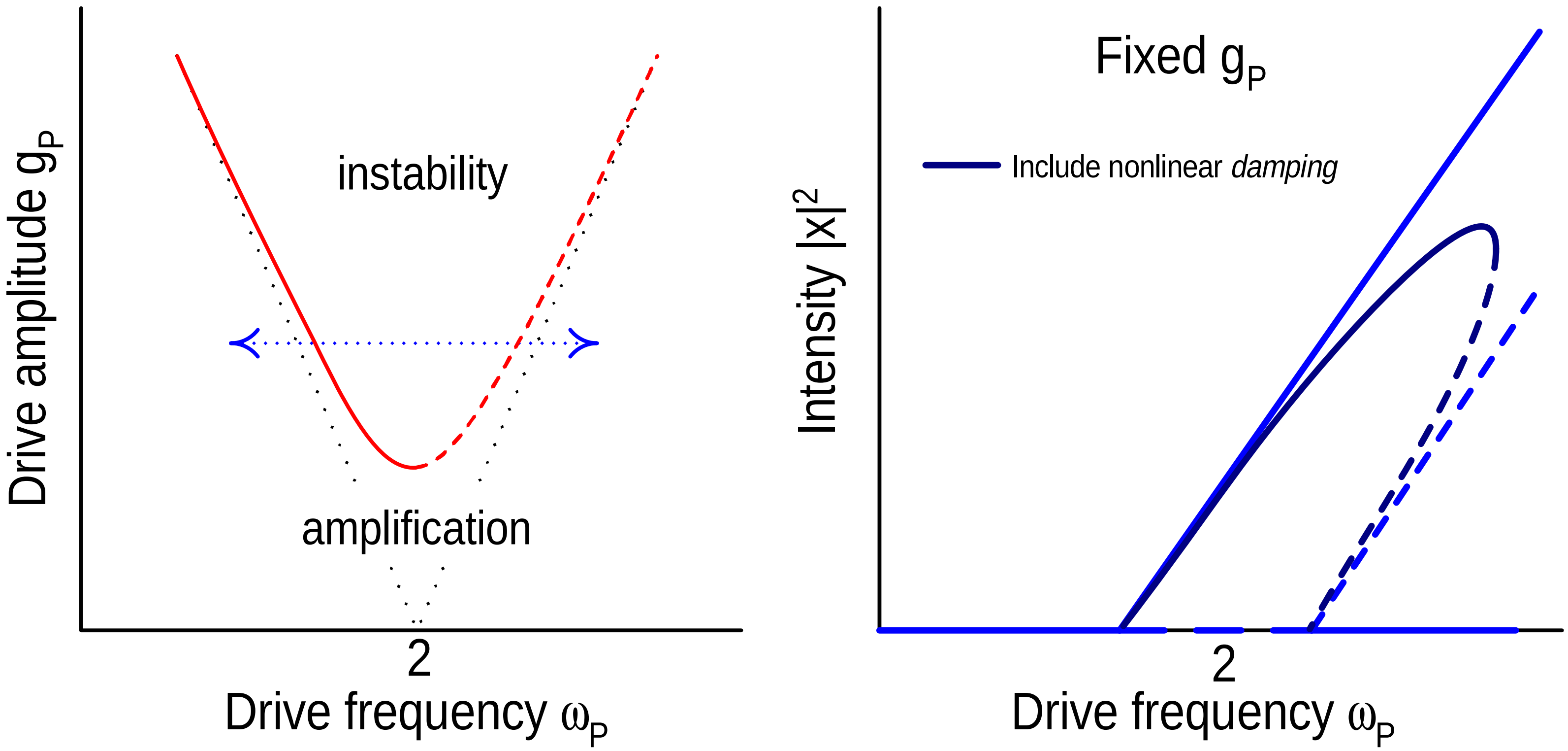
Above the parametric instability nonlinearity is essential to understand the oscillations.

- Mode Competition
- Pattern formation

Experimental results

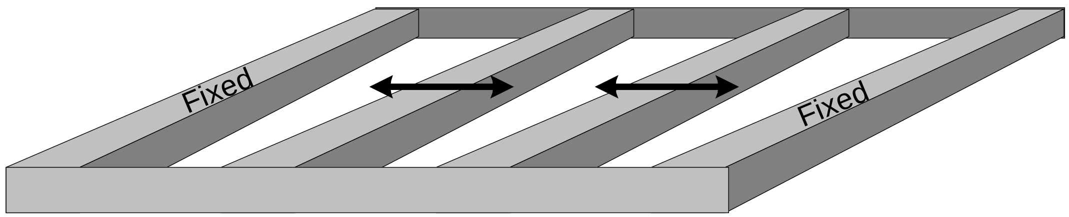


One beam theory



$$2i\frac{dA}{dT} - \frac{h}{2}A^* e^{i\Omega T} + i\gamma A + 3|A|^2 A + i\eta|A|^2 A = 0, \qquad A(T) \Rightarrow a e^{i\frac{\Omega}{2}T}$$

Many beam theory

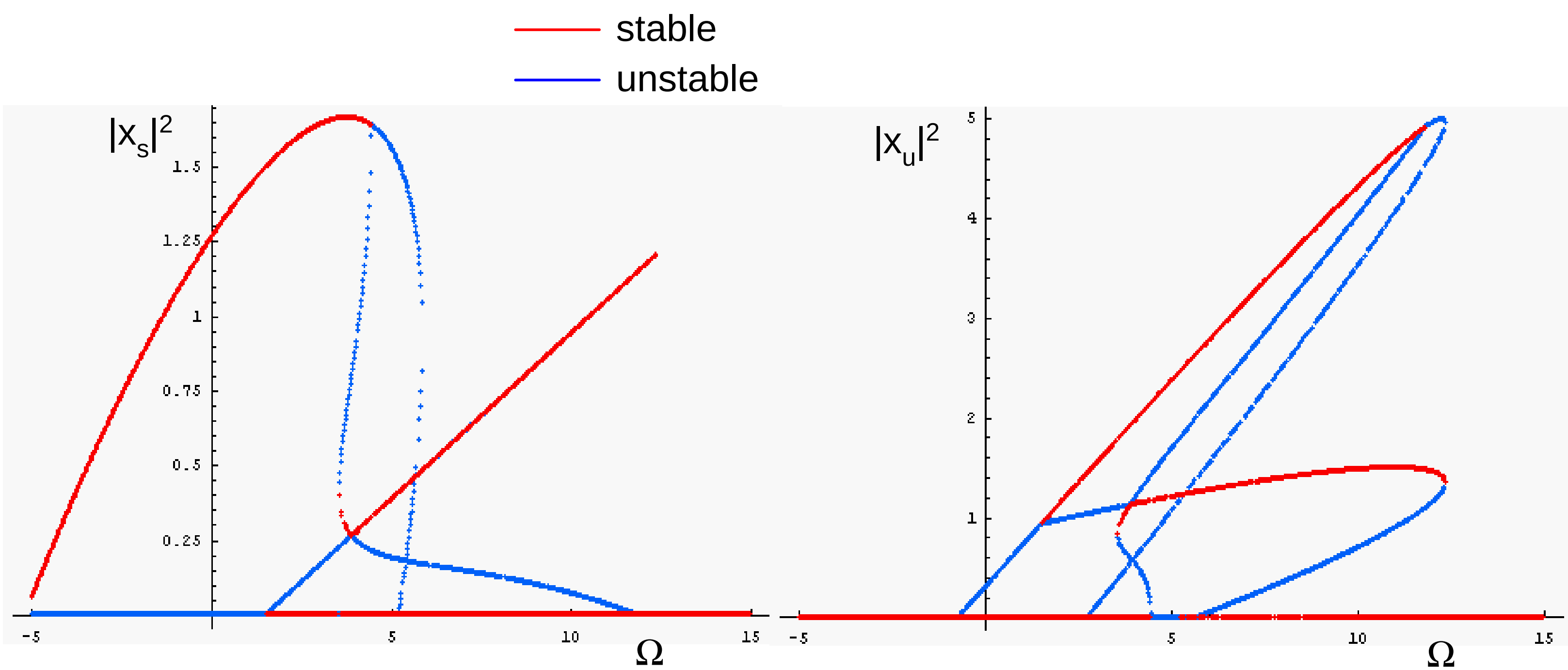


$$0 = \ddot{x}_n + x_n + x_n^3$$
$$+ \Delta^2(1 + g_P \cos[(2 + \varepsilon\Omega)t])(x_{n+1} - 2x_n + x_{n-1})$$
$$- \gamma(\dot{x}_{n+1} - 2\dot{x}_n + \dot{x}_{n-1})$$
$$+ \eta\left[(x_{n+1} - x_n)^2(\dot{x}_{n+1} - \dot{x}_n) - (x_n - x_{n-1})^2(\dot{x}_n - \dot{x}_{n-1})\right]$$

Local Duffing (elasticity) + Electrostatic Coupling (dc and modulated) + Dissipation (currents) + Nonlinear Damping (also currents)

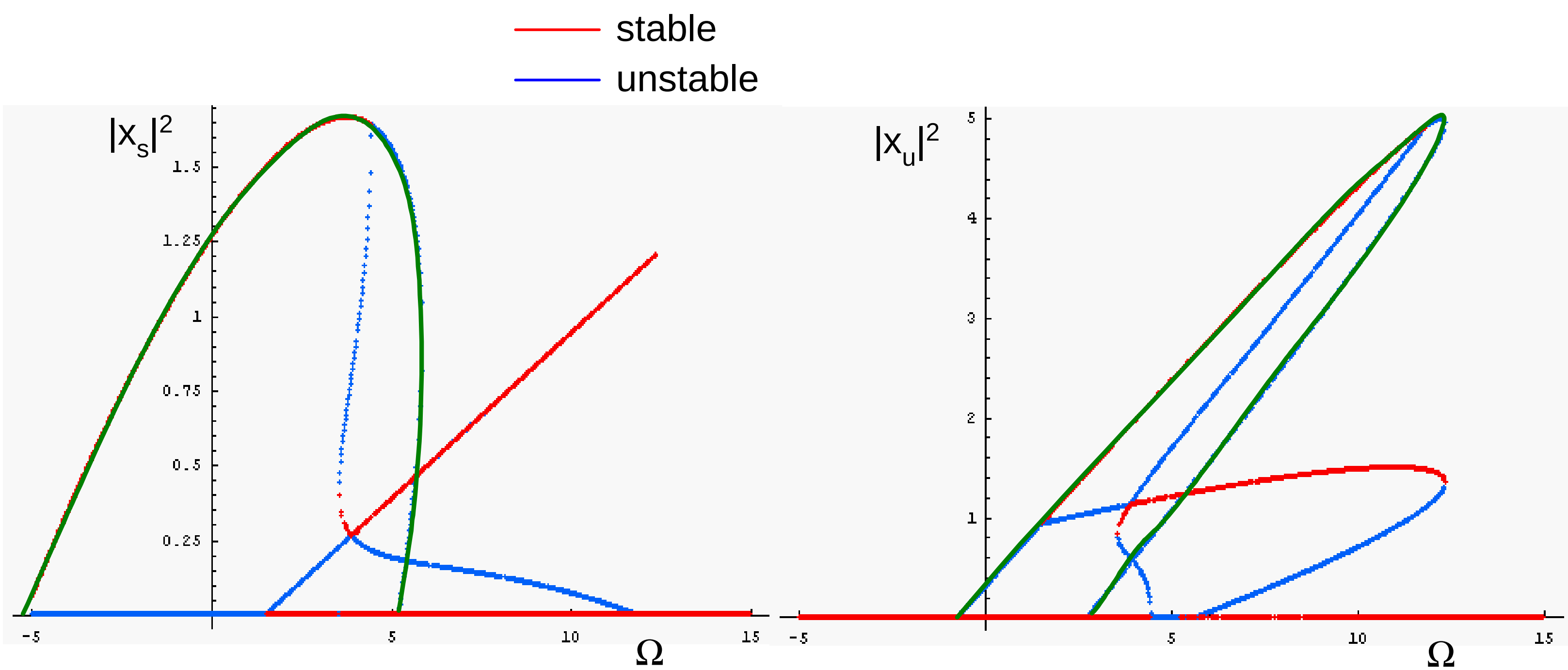
[Lifshitz and MCC Phys. Rev. B67, 134302 (2003)]

2 beam periodic solutions



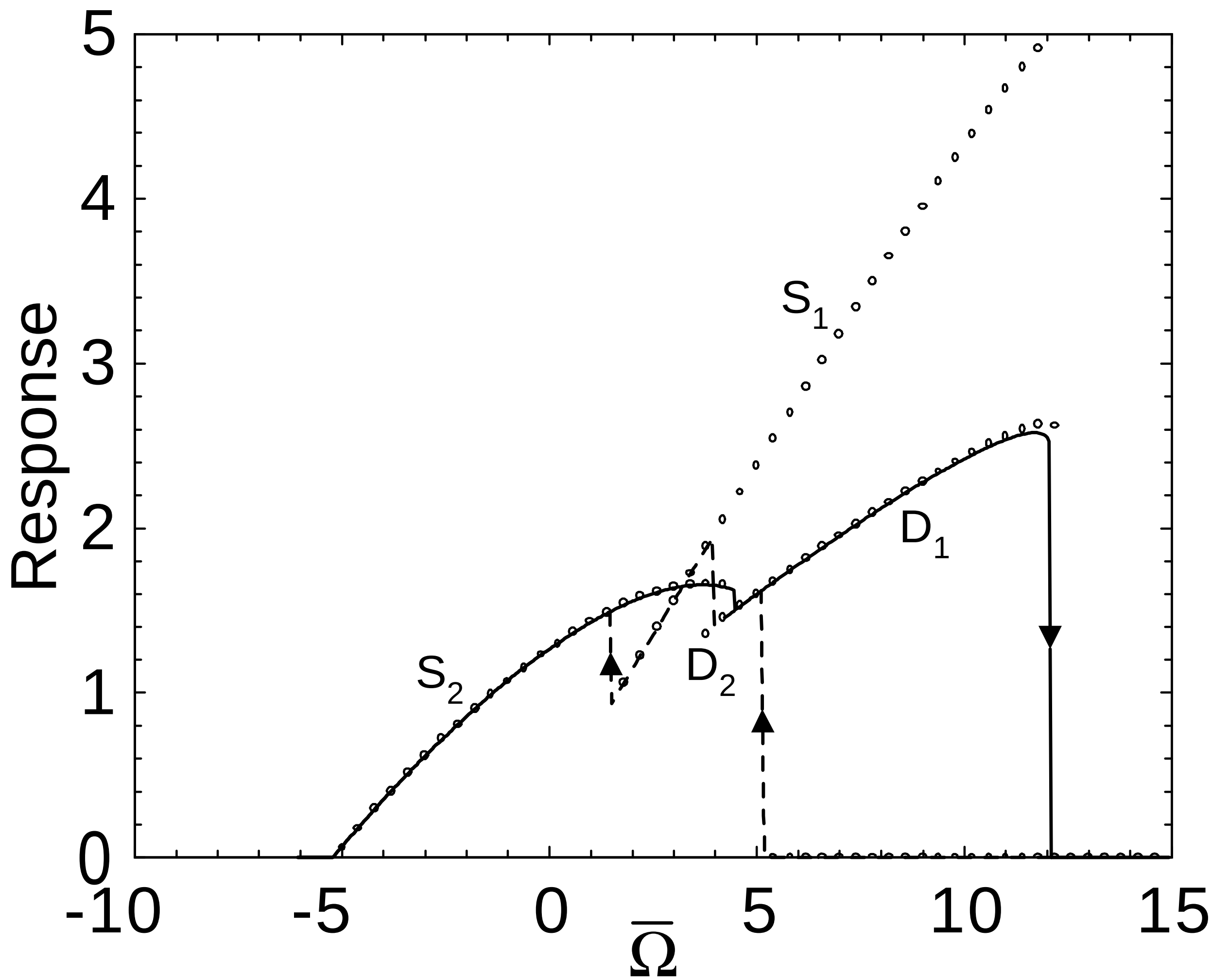
Intensity of symmetric mode $|x_s|^2$ and antisymmetric mode $|x_u|^2$ as frequency is scanned.

2 beam periodic solutions

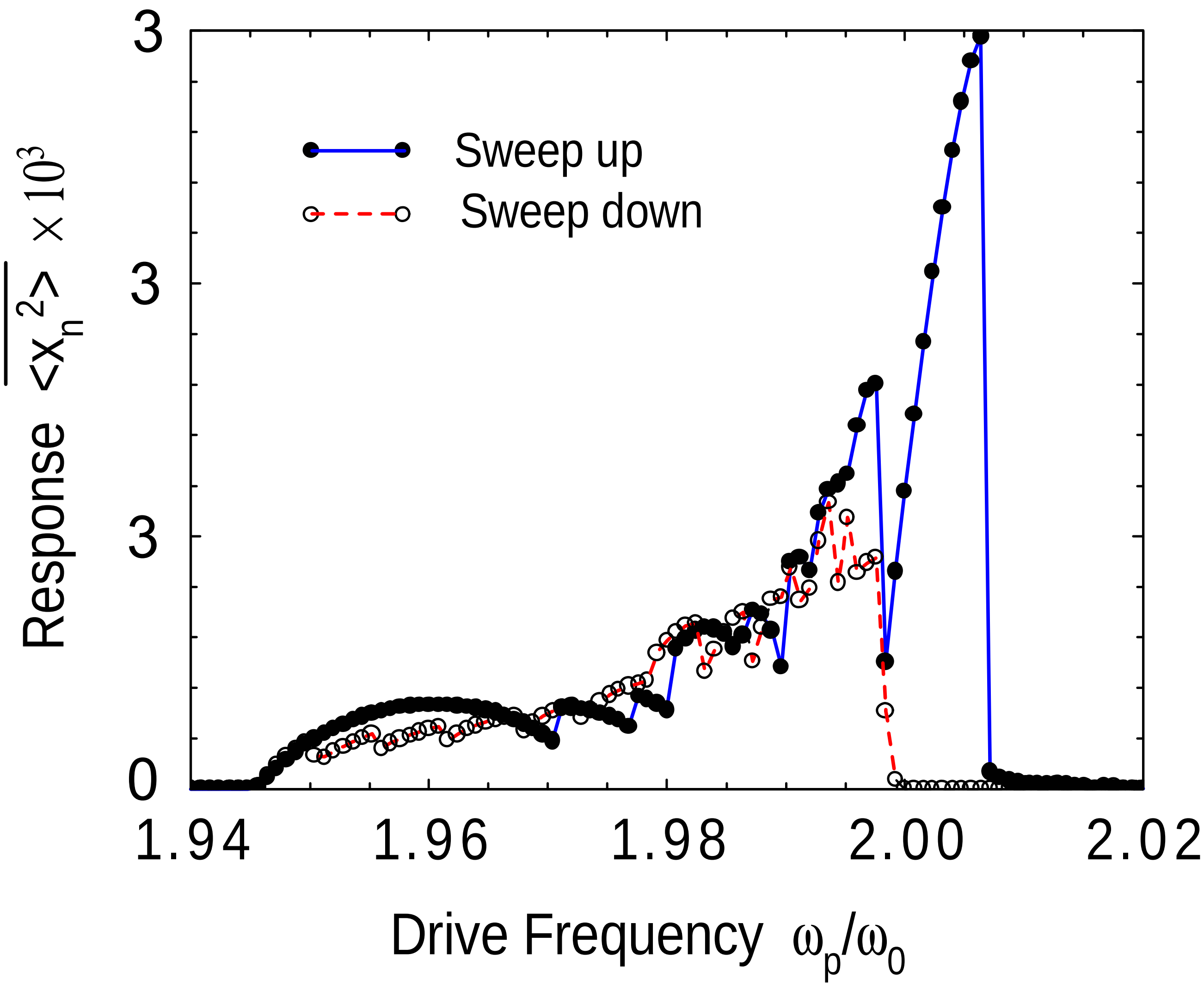


The green lines correspond to a single excited mode, the remainder to coupled modes.

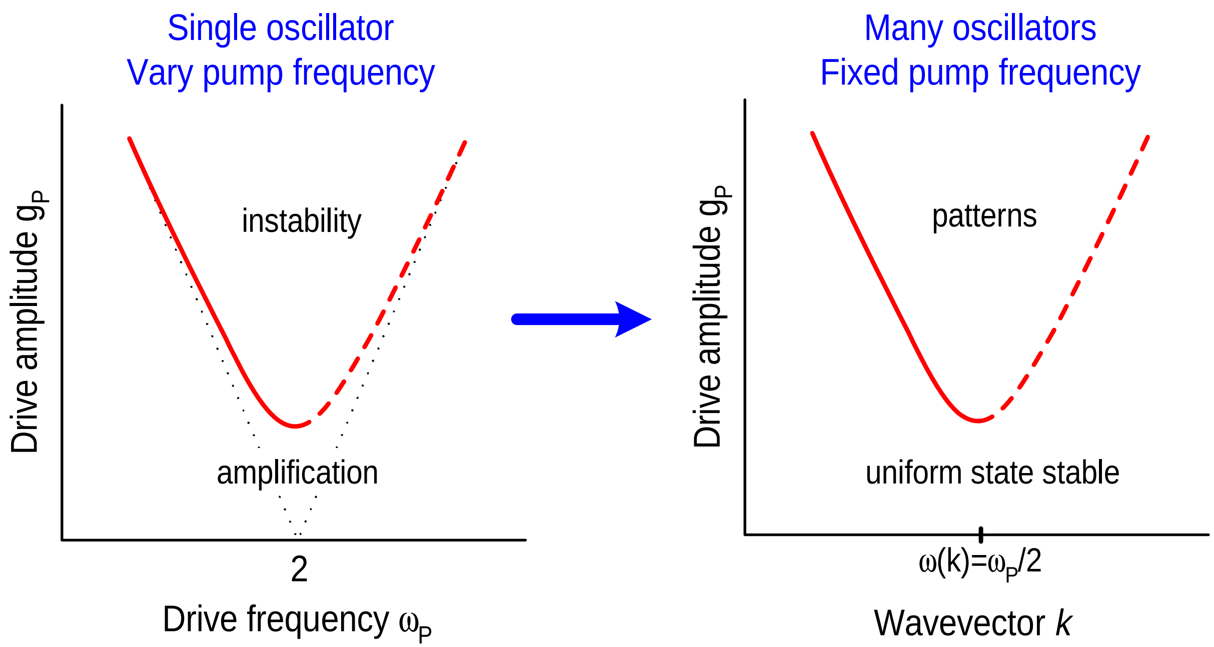
Hysteresis for two beams



Simulations of 67 Beams



Many beams



Continuum approximation: new amplitude equation

[Bromberg, MCC and Lifshitz (preprint, 2005)]

$$\frac{\partial A}{\partial T} = A + \frac{\partial^2 A}{\partial X^2} + i\frac{2}{3}\left(4|A|^2\frac{\partial A}{\partial X} + A^2\frac{\partial A^*}{\partial X}\right) - 2|A|^2 A - |A|^4 A$$

Conclusions

I've described two aspects of theoretically modelling micron and submicron scale oscillators

- Linear fluctuations in solution [Paul and MCC, Phys. Rev. Lett. **92**, 235501 (2004)]
- Nonlinear collective effects of parametrically driven high-Q arrays [Lifshitz and MCC, Phys. Rev. **B67**, 134302 (2003)]

Other areas of interest:

- 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 [cf. Aldridge and Cleland, Phys. Rev. Lett. **94**, 156403 (2005)]
  - ⋆ Collective states in arrays of oscillators
- Analysis of a QND scheme to measure the discrete levels in quantum harmonic oscillator [Santamore, Doherty, and MCC, Phys. Rev. **B70**, 144301 (2004)]