Lecture 16
Analytical descriptions of AM-AFM, theory of phase contrast

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Eigenmodes

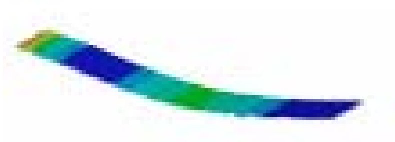
1st eigenmode

$$(\beta L)_1 = 1.875, (\beta L)_2 = 4.694, (\beta L)_3 = 7.855 \ldots\ldots$$

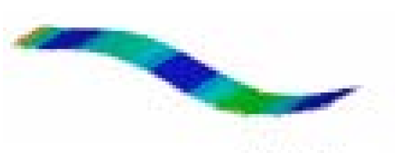
Thus

$$\omega_1 : \omega_2 : \omega_3 : .... = 1 : 6.26 : 17.55 : ...$$

for a uniform rectangular lever with negligible tip mass



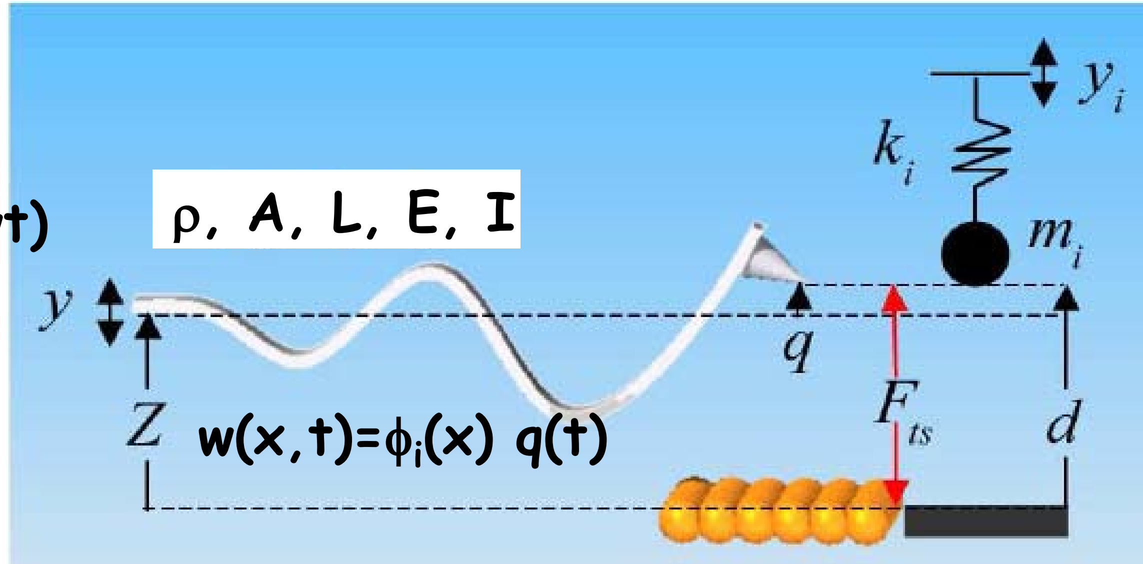
2nd eigenmode



3rd eigenmode

Equivalent point mass oscillator

$y(t)=Y\cos(wt)$



$y_i(t)=Y_i\cos(wt)$

- Energy based equivalence principle

$$\frac{1}{2}k_i q^2 = \frac{1}{2}\int_{x=0}^{x=L} EI\left(\frac{d^2\phi_i}{dx^2}\right)^2 dx \quad \frac{1}{2}m_i q^2 = \frac{1}{2}\int_{x=0}^{x=L} \rho A\left(\phi_i\right)^2 dx \quad Y_i = Y\left(\frac{\omega}{\omega_i}\right)^2 \frac{\int_0^L \phi_i(x)dx}{\int_0^L \left(d^2\phi_i \big/ dx^2\right) dx}$$

For negligible tip mass

$$k_1 = 1.03k,\ k_2 = 40.5k,\ k_3 = 317k$$

$$m_1 = m_2 = m_3 = ... = 0.249\ \rho AL$$

$$Y_1 \sim 1.5Y$$

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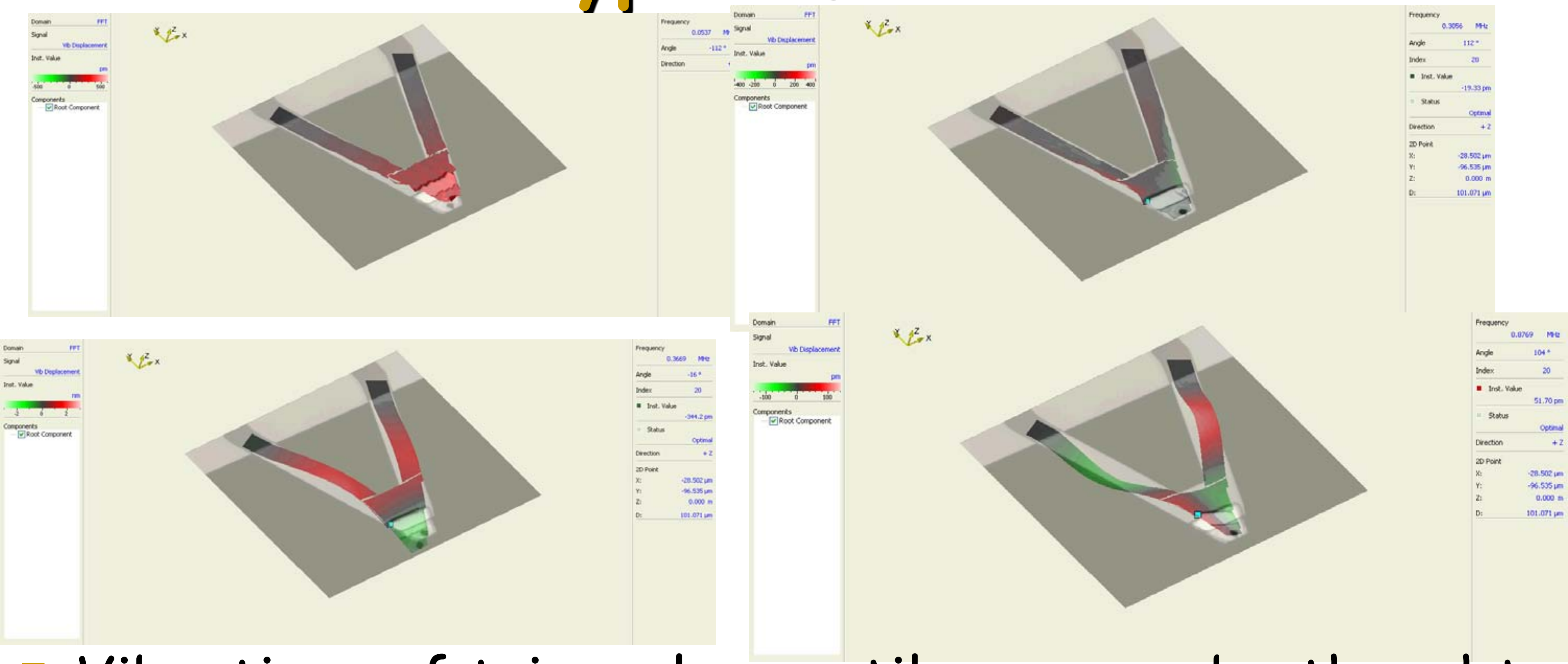
Melcher *et al*, App. Phys. Lett. 91(5), 2007

Other types of cantilevers

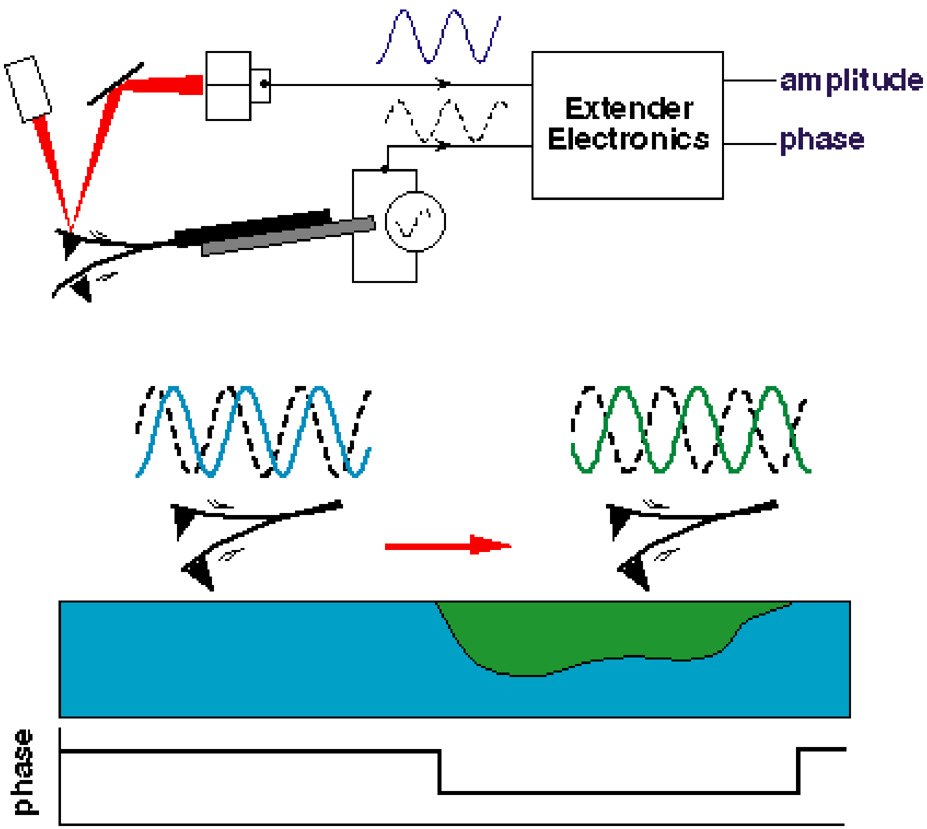


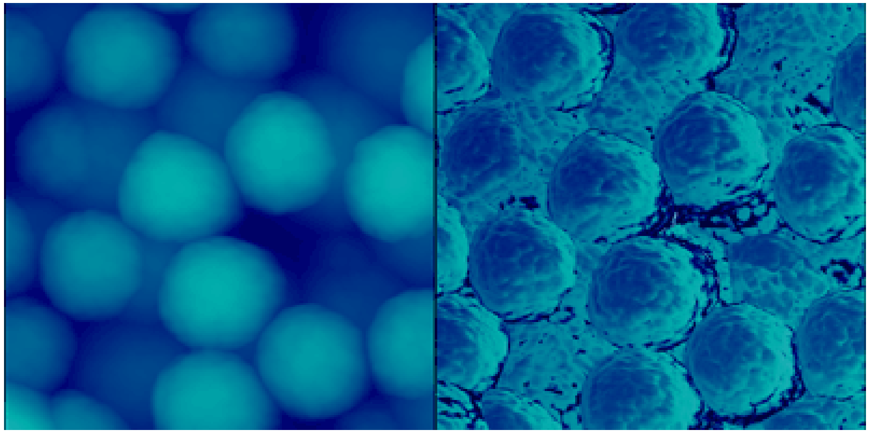
- Vibrations of triangular cantilevers can be thought of as two cantilevers joined together at their tip
- Leads to symmetric and anti-symmetric eigenmodes
- However the point mass oscillator equivalence holds

Analytical descriptions of AM-AFM

- So far we have resorted to numerical simulations (VEDA) of the point mass model or linearized the equations
- Perturbation methods are quite useful too to help understand
  - Origin of phase contrast
  - Origin of amplitude reduction
  - Average forces while tapping

Phase Contrast



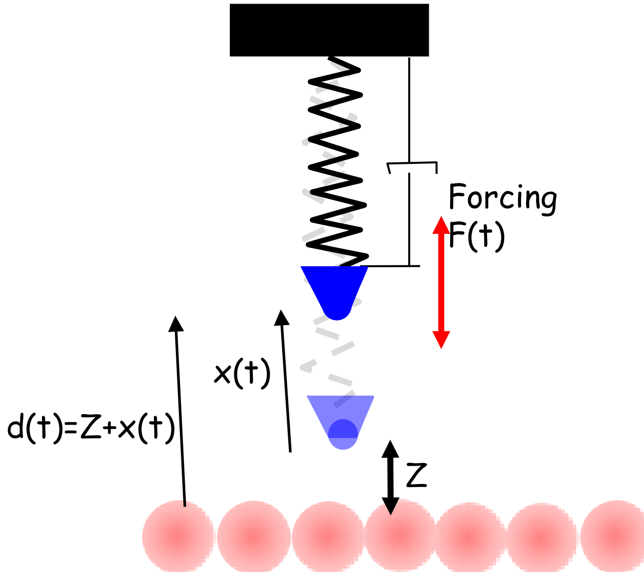


AFM height (left) and phase (right) images of poly(methylmethacrylate)

(Veeco, Inc.)

- Regular tapping mode implemented but signal phase monitored
- But what does a phase contrast image mean really?

Analytical description of AM-AFM



$$m\ddot{x} = -kx - c\dot{x} + F_0 \cos(\omega t) + F_{ts}(d, \dot{d})$$

$$\frac{\ddot{x}}{\omega_0^2} + x + \frac{1}{\omega_0 Q}\dot{x} = \frac{1}{k}\left(F_0 \cos(\omega t) + F_{ts}(d, \dot{d})\right) \quad where \qquad (1)$$

$$with \quad \omega_0 = \sqrt{\frac{k}{m}}, \; Q = \frac{m\omega_0}{c}$$

$$Let \quad x(t) = A\cos(\omega t - \phi) \quad so\ that \quad \dot{x}(t) = \dot{d}(t) = -A\omega\sin(\omega t - \phi) \qquad (2)$$

$$Substitute\ (2)\ in \quad (1), we\ get$$

$$-\left(\left(\frac{\omega}{\omega_0}\right)^2 - 1\right)\cos(\omega t - \phi) - \left(\frac{\omega}{\omega_0 Q}\right)\sin(\omega t - \phi) = \frac{1}{kA}\left\{F_0 \cos(\omega t) + F_{ts}(d, \dot{d})\right\} \qquad (3)$$

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Analytical description of AM-AFM

$$x(t) = A\cos(\omega t - \phi) \quad \textit{so that} \quad \dot{x}(t) = \dot{d}(t) = -A\omega\sin(\omega t - \phi) \qquad (1)$$

$$-\left(\left(\frac{\omega}{\omega_0}\right)^2 - 1\right)\cos(\omega t - \phi) - \left(\frac{\omega}{\omega_0 Q}\right)\sin(\omega t - \phi) = \frac{1}{kA}\left\{F_0 \cos(\omega t) + F_{ts}(d, \dot{d})\right\} \qquad (2)$$

$$\int_{t=0}^{2\pi/\omega} \sin(\omega t - \phi)\times(\bullet)\,dt \Rightarrow -\left(\frac{\omega}{\omega_0 Q}\right)\frac{\pi}{\omega} = -\frac{1}{kA}\frac{\pi}{\omega}F_0\sin(\phi) + \frac{1}{kA}\int_{t=0}^{2\pi/\omega}\sin(\omega t - \phi)\times F_{ts}(d, \dot{d})\,dt$$

$$Or,\ \sin(\phi) = \frac{kA}{F_0}\left\{\frac{\omega}{Q\omega_0} - \frac{1}{\pi kA^2}\int_{t=0}^{2\pi/\omega}\left(-A\omega\sin(\omega t - \phi)\right)\times F_{ts}(d, \dot{d})\,dt\right\} = \frac{kA}{F_0}\left\{\frac{\omega}{Q\omega_0} - \frac{1}{\pi kA^2}E_{diss}\right\}$$

(3)

$$But\ \frac{kA_0}{F_0} = \sqrt{\left(1 - \left(\frac{\omega}{\omega_0}\right)^2\right)^2 + \left(\frac{\omega}{\omega_0 Q}\right)^2} \quad \textit{so we get}$$

$$\sin(\phi) = \frac{1}{\sqrt{\left(1 - \left(\frac{\omega}{\omega_0}\right)^2\right)^2 + \left(\frac{\omega}{\omega_0 Q}\right)^2}}\left\{\frac{\omega}{Q\omega_0}\frac{A}{A_0} - \frac{1}{\pi kAA_0}E_{diss}\right\} \qquad (4)$$

$$If\ \ \omega = \omega_0\ \ then\ \sin(\phi) = \left\{\frac{A}{A_0} - \frac{Q}{\pi kAA_0}E_{diss}\right\}$$

- A/A_0 = constant in tapping mode scan
- Phase contrast = energy dissipation contrast!

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Anczykowski et al App. Surf. Sci., **140**, 376, 1999

Analytical description of AM-AFM

- Conversely

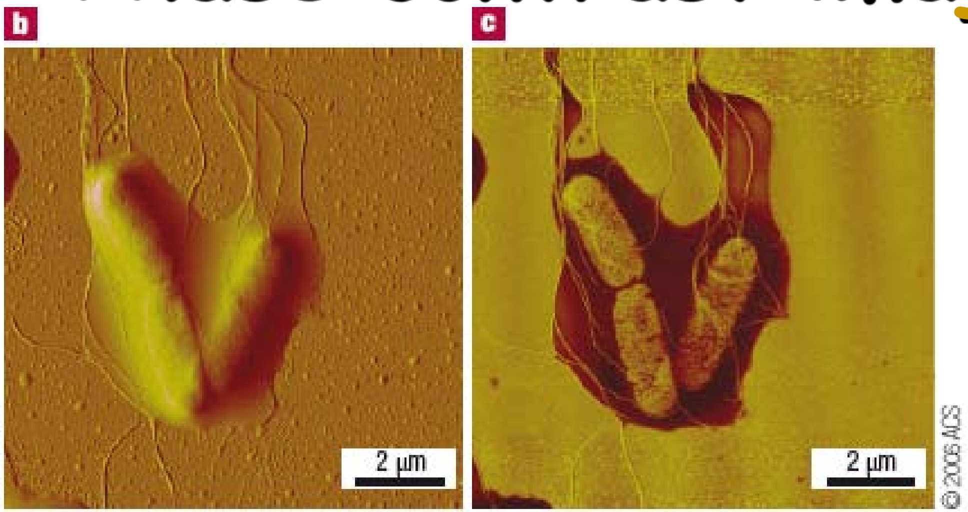
$$E_{diss} = \pi k A A_0 \left\{ \frac{\omega}{Q\omega_0} \frac{A}{A_0} - \sin(\phi) \sqrt{\left(1 - \left(\frac{\omega}{\omega_0}\right)^2\right)^2 + \left(\frac{\omega}{\omega_0 Q}\right)^2} \right\} \quad (1)$$

$$If \quad \omega = \omega_0$$

$$E_{diss} = \frac{\pi k}{Q} \left\{ A^2 - A_0 A \sin(\phi) \right\} \quad (2)$$

- Eq. (7) relates the energy dissipated per cycle due to tip-sample interaction to observables
- By quantitative knowledge of Q, k, A, A0, and f it becomes possible to know in an experiment the energy dissipated in eV or pJ per cycle

Phase contrast imaging in air/vacuum



(ϕ). **b**,**c**, The above considerations are illustrated by comparing the topography an aggregate of three *Salmonella typhimurium* cells covered by an extracellula polymeric capsule (**b**) and the phase image (**c**), that is acquired simultaneously the topography, reveals the inner structure of the cell as well as the continuity flagellae. (R. Avci *et al.* ref. 49 © 2007 American Chemical Society).

Figure 4 Complex microdomain structure of a block copolymer. The AFM images are rendered into three-dimensions using the height image as height-field and the phase image as contrast. The images show the formation of terraces in a thin film of SBS block copolymer and the systematic change of microdomain structures along the changes in film thickness from 32 nm at the lowest terrace to 57 nm at the higher terrace. Reprinted with permission from ref. 54.

- *From Garcia et al Nature Materials, 6, 2007*

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Origin of amplitude reduction

$$x(t) = A\cos(\omega t - \phi) \text{ so that } \quad d(t) = Z + A\cos(\omega t - \phi) \text{ and } \dot{x}(t) = \dot{d}(t) = -A\omega\sin(\omega t - \phi) \quad (1)$$

$$-\left(\left(\frac{\omega}{\omega_0}\right)^2 - 1\right)\cos(\omega t - \phi) - \left(\frac{\omega}{\omega_0 Q}\right)\sin(\omega t - \phi) = \frac{1}{kA}\left\{F_0 \cos(\omega t) + F_{ts}(d, \dot{d})\right\} \quad (2)$$

$$\int_{t=0}^{2\pi/\omega} \sin(\omega t - \phi) \times (\bullet)\, dt \Rightarrow$$

$$\frac{1}{kA} F_0 \sin(\phi) = \left(\frac{\omega}{\omega_0 Q}\right) + \frac{\omega}{\pi kA} \int_{t=0}^{2\pi/\omega} \sin(\omega t - \phi) \times F_{ts}(d, \dot{d})\, dt = \left(\frac{\omega}{\omega_0 Q_{eff}}\right) \quad (3)$$

$$\text{with } \frac{1}{Q_{eff}} = \frac{1}{Q} + \frac{\omega_0}{\pi kA} \int_{t=0}^{2\pi/\omega} \sin(\omega t - \phi) \times F_{ts}(d, \dot{d})\, dt$$

$$\int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi) \times (\bullet)\, dt \Rightarrow$$

- L. Wang et al App. Phys. Lett., **73**, 3781, 1998

$$\frac{F_0 \cos(\phi)}{kA} = \omega_{eff}^2 - \left(\frac{\omega}{\omega_0}\right)^2 \quad (4)$$

$$\text{with } \omega_{eff}^2 = 1 - \frac{\omega}{\pi kA} \int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi) \times F_{ts}(d, \dot{d})\, dt$$

Combining (1) (2)

$$A = \frac{F_0 / k}{\sqrt{\left(\left(\frac{\omega}{\omega_0}\right)^2 - \omega_{eff}{}^2\right)^2 + \left(\frac{\omega}{\omega_0 Q_{eff}}\right)^2}} \quad (5)$$

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Origin of amplitude reduction

$$x(t) = A\cos(\omega t - \phi) \text{ so that } \quad d(t) = Z + A\cos(\omega t - \phi) \text{ and } \dot{x}(t) = \dot{d}(t) = -A\omega \sin(\omega t - \phi) \quad (1)$$

$$A = \frac{F_0 / k}{\sqrt{\left(\left(\frac{\omega}{\omega_0}\right)^2 - \omega_{eff}{}^2\right)^2 + \left(\frac{\omega}{\omega_0 Q_{eff}}\right)^2}}$$

$$\text{with } \frac{1}{Q_{eff}} = \frac{1}{Q} + \frac{\omega_0}{\pi k A} \int_{t=0}^{2\pi/\omega} \sin(\omega t - \phi) \times F_{ts}(d, \dot{d}) dt = \quad \frac{1}{Q} - \frac{\omega_0}{\omega \pi k A^2} E_{diss}$$

$$\text{and } \quad \omega_{eff}^2 = 1 - \frac{\omega}{\pi k A} \int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi) \times F_{ts}(d, \dot{d}) d\ t$$

- At high Q, amplitude decreases due to shift in nonlinear effective frequency

Average force

$$\frac{F_0\cos(\phi)}{kA} = \omega_{eff}^2 - \left(\frac{\omega}{\omega_0}\right)^2 \qquad (1)$$

$$\text{with } \omega_{eff}^2 = 1 - \frac{\omega}{\pi kA}\int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi)\times F_{ts}(d,\dot{d})dt$$

$$\text{Consider conservative forces only } F_{ts}(d)$$

$$\omega_{eff}^2 = 1 - \frac{\omega}{\pi kA}\int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi)\times F_{ts}(d)dt = 1 - \frac{\omega}{\pi kA^2}\int_{t=0}^{2\pi/\omega} A\cos(\omega t - \phi)\times F_{ts}(Z + A\cos(\omega t - \phi))dt$$

$$\sim 1 + \frac{\omega}{\pi kA}\frac{2\pi}{\omega}\langle F_{ts}(d)\rangle = 1 + \frac{2}{kA}\langle F_{ts}(d)\rangle \qquad (2\ \ )$$

$$\text{Valid when contact time} << \text{oscillation period}$$

$$\frac{2}{kA}\langle F_{ts}(d)\rangle = \frac{F_0\cos(\phi)}{kA} - 1 + \left(\frac{\omega}{\omega_0}\right)^2 \qquad (3)$$

San Paulo and Garcia PRB, **64**, 2001

$$\text{When } \omega = \omega_0$$

$$\langle F_{ts}(d)\rangle = \frac{F_0\cos(\phi)}{2} = \frac{F_0}{2}\sqrt{1-\sin^2\phi} = \frac{F_0}{2}\sqrt{1-\left(\frac{A}{A_0}\right)^2} = \frac{kA}{2Q}\sqrt{1-\left(\frac{A}{A_0}\right)^2} \qquad (4)$$

- Depends only on cantilever properties and operating conditions !!

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Analytical description of AM-AFM

$$x(t) = A\cos(\omega t - \phi) \quad so\ that \quad \dot{x}(t) = \dot{d}(t) = -A\omega\sin(\omega t - \phi) \qquad (1)$$

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$$Or,\ \sin(\phi) = \frac{kA}{F_0}\left\{\frac{\omega}{Q\omega_0} - \frac{1}{\pi kA^2}\int_{t=0}^{2\pi/\omega}\left(-A\omega\sin(\omega t - \phi)\right)\times F_{ts}(d,\dot{d})dt\right\} = \frac{kA}{F_0}\left\{\frac{\omega}{Q\omega_0} - \frac{1}{\pi kA^2}E_{diss}\right\}$$

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- Phase contrast = energy dissipation contrast!

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Anczykowski et al App. Surf. Sci., **140**, 376, 1999

Average force

$$\frac{F_0 \cos(\phi)}{kA} = \omega_{eff}^2 - \left(\frac{\omega}{\omega_0}\right)^2 \qquad (1)$$

$$\text{with } \omega_{eff}^2 = 1 - \frac{\omega}{\pi k A}\int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi) \times F_{ts}(d, \dot{d})dt$$

Consider conservative forces only $F_{ts}(d)$

$$\omega_{eff}^2 = 1 - \frac{\omega}{\pi k A}\int_{t=0}^{2\pi/\omega} \cos(\omega t - \phi) \times F_{ts}(d)dt = 1 - \frac{\omega}{\pi k A^2}\int_{t=0}^{2\pi/\omega} A\cos(\omega t - \phi) \times F_{ts}(Z + A\cos(\omega t - \phi))dt$$

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$$\frac{2}{kA}\langle F_{ts}(d)\rangle = \frac{F_0 \cos(\phi)}{kA} - 1 + \left(\frac{\omega}{\omega_0}\right)^2 \qquad (3)$$

San Paulo and Garcia PRB, 64, 2001

When $\omega = \omega_0$

$$\langle F_{ts}(d)\rangle = \frac{F_0 \cos(\phi)}{2} = \frac{F_0}{2}\sqrt{1 - \sin^2\phi} = \frac{F_0}{2}\sqrt{1 - \left(\frac{A}{A_0}\right)^2} = \frac{kA}{2Q}\sqrt{1 - \left(\frac{A}{A_0}\right)^2} \qquad (4)$$

- Depends only on cantilever properties and operating conditions !!

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Next time

- Peak forces
- Stiffness calibration methods