Fundamentals of Atomic Force Microscopy
Part 2: Dynamic AFM Methods

Week 4, Lecture 2
Reconstruction of Interaction Force from Frequency Shift in FM-AFM

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From the last lecture

- Shape of total potential energy well of oscillator+sample system governs the natural frequency of the probe
  - For a quadratic well, frequency is independent of oscillation amplitude
  - Tip-sample interaction adds additional terms making the frequency shift depend on both Z and oscillation amplitude
  - How to convert freq. shift vs. Z into U_{ts} or F_{ts}^{CONS}?

Relation between frequency shift and interaction force

- Recall

$$\frac{\Delta\omega_0}{\omega_0} = -\frac{V_{ts}(Z,A)}{kA^2} \qquad (1)$$

where

$$V_{ts}(Z,A) = \left\langle F_{ts}^{CONS} \bullet q \right\rangle = \frac{1}{2\pi}\int_0^{2\pi} F_{ts}^{CONS}(Z + A\sin\theta) \bullet A\sin\theta \, d\theta$$

$$= \frac{1}{\pi}\int_{q=-A}^{+A} F_{ts}^{CONS}(Z+q) \bullet \frac{q}{\sqrt{A^2-q^2}}\, dq \qquad (2)$$

Let $u = \sin\theta, q = Au$ then (2) becomes

$$V_{ts}(Z,A) = \frac{A}{\pi}\int_{u=-1}^{+1} F_{ts}^{CONS}(Z+Au) \bullet \frac{u}{\sqrt{1-u^2}}\, du$$

Thus

$$\boxed{\frac{\Delta\omega_0}{\omega_0} = -\frac{1}{k\pi A}\int_{u=-1}^{+1} F_{ts}^{CONS}(Z+Au) \bullet \frac{u}{\sqrt{1-u^2}}\, du = -\frac{1}{k\pi A^2}\int_{q=-A}^{+A} F_{ts}^{CONS}(Z+q) \bullet \frac{q}{\sqrt{A^2-q^2}}\, dq \qquad (3)}$$

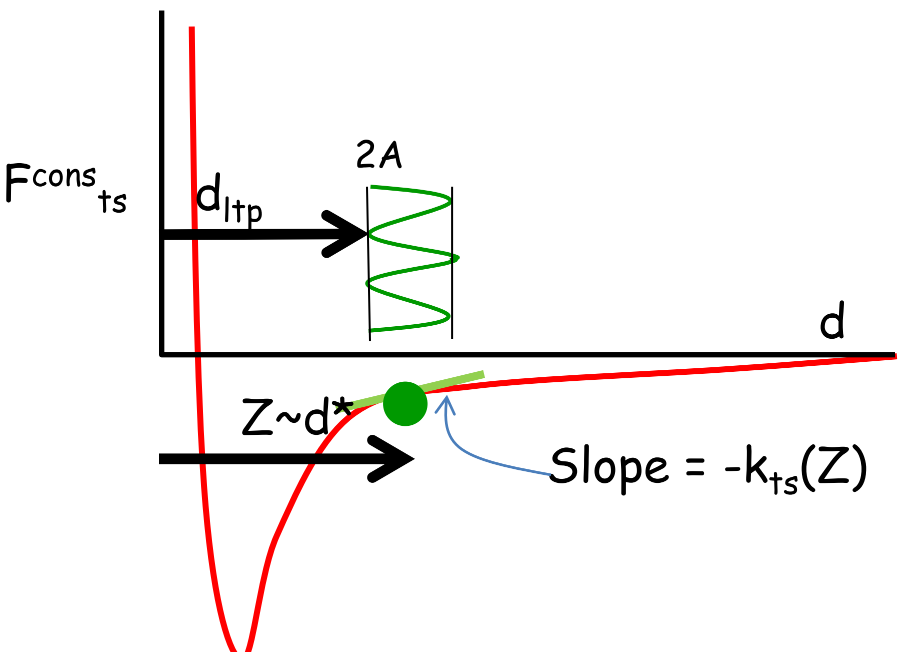
- Formula derived by F. J. Giessibl, Phys. Rev. B., 56, 16010, 1997.
- Key assumption is that Z=d* i.e. the mean deflection of the tip is considered negligible compared to oscillation amplitude

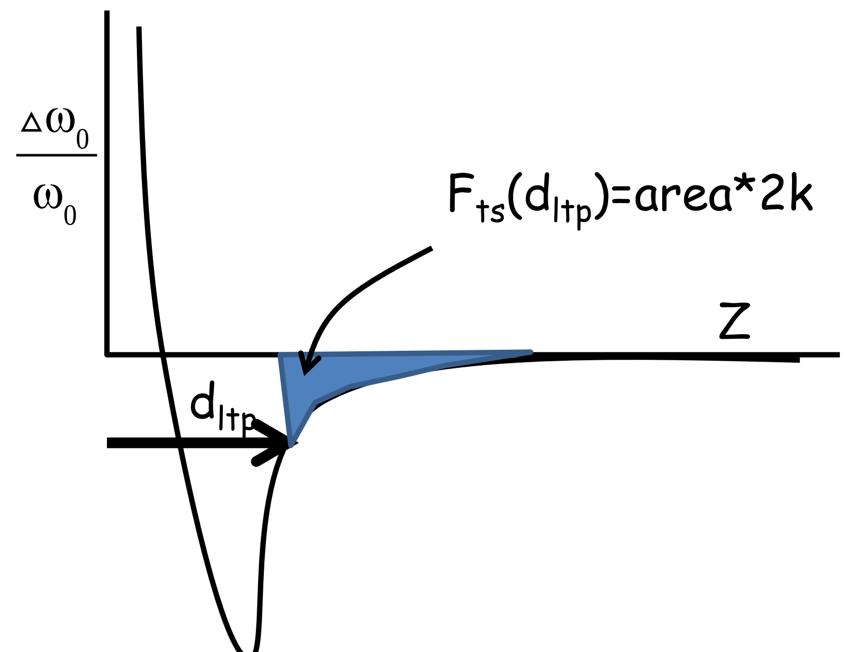
The small amplitude approximation

- In week 2, we showed that when A<< Z then $V_{ts}(Z,A) \sim -\frac{k_{ts}(Z)\,A^2}{2}$
- Apply this to Eq. (1) and we get $\Omega(Z) = \frac{\Delta\omega_0(Z)}{\omega_0} = \frac{1}{2}\frac{k_{ts}(Z)}{k}$
- From which the force can be reconstructed as follows

$$F_{ts}^{CONS}(d_{ltp}) = 2k\int_{d_{ltp}}^{\infty} \Omega(\xi)\, d\xi \qquad (4)$$

- Where d_{ltp}, "the lower turnaround point" is as shown below*





* In the small amplitude approximation d_{ltp} ~Z (or d*)

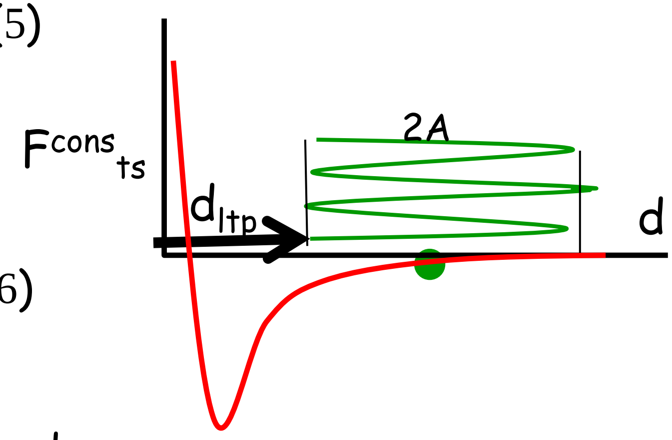
The large amplitude approximation

- When A>> Z then

This derivation is based on Giessibl and Bielefeldt, Phys. Rev. B, 61, 9968, 2000

Define a "normalized" frequency shift parameter into Eq. (3)

$$\gamma(Z,A)=kA^{3/2}\frac{\Delta\omega_0}{\omega_0}=-\frac{1}{\pi\sqrt{A}}\int_{q=-A}^{+A}F_{ts}^{CONS}(Z+q)\bullet\frac{q}{\sqrt{A^2-q^2}}\,dq \qquad (5)$$



Units of $\gamma(Z,A)$ are $Nm^{0.5}$. Rewriting (5)

$$\gamma(Z,A)==\frac{1}{\sqrt{2\pi}}\int_{q=-A}^{+A}\frac{F_{ts}^{CONS}(Z+q)}{\sqrt{A+q}}\bullet\frac{-\frac{q}{A}}{\sqrt{\frac{1}{2}-\frac{q}{2A}}}\,dq \qquad (6)$$

In the large amplitude limit, two approximations can be made:

1. The second term in the integrand ~1 when q~-A i.e. for the duration that tip-sample forces are active
2. The upper limit on the integral can be changed from +A to +∞ since the interaction forces vanish by the time the tip reaches its top-most position

Using these it can be shown (See Appendix) that

$$F_{ts}^{CONS}(d_{ltp})=-2k\int_{d_{ltp}}^{\infty}\frac{A^{3/2}}{\sqrt{2(\xi-d_{ltp})}}\frac{\partial\Omega}{\partial\xi}\,d\xi \qquad (7)$$

Unifying approaches

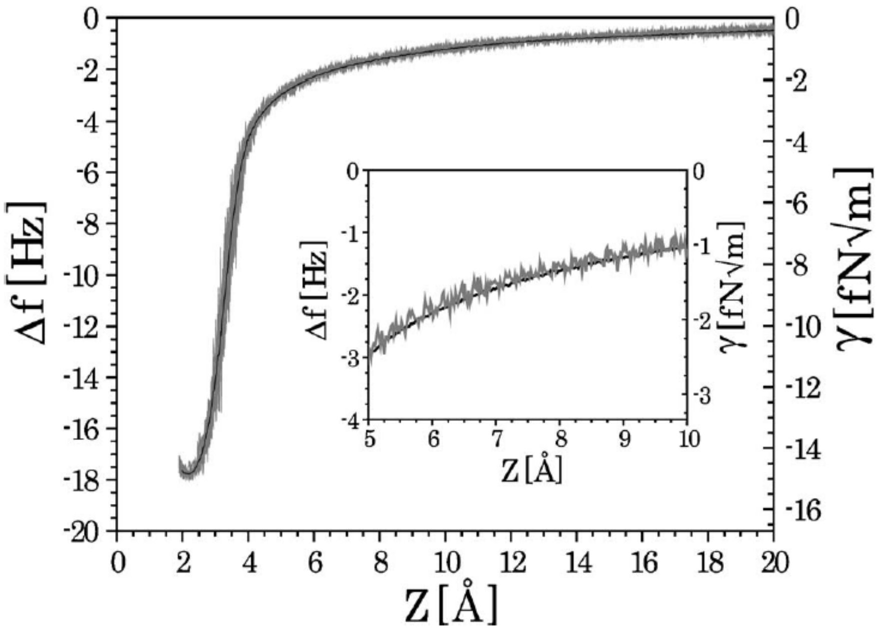
- For arbitrary amplitudes there are two approaches
- The first (Sader and Jarvis, App. Phys. Lett, 84, 10, 2004) shows (see appendix)

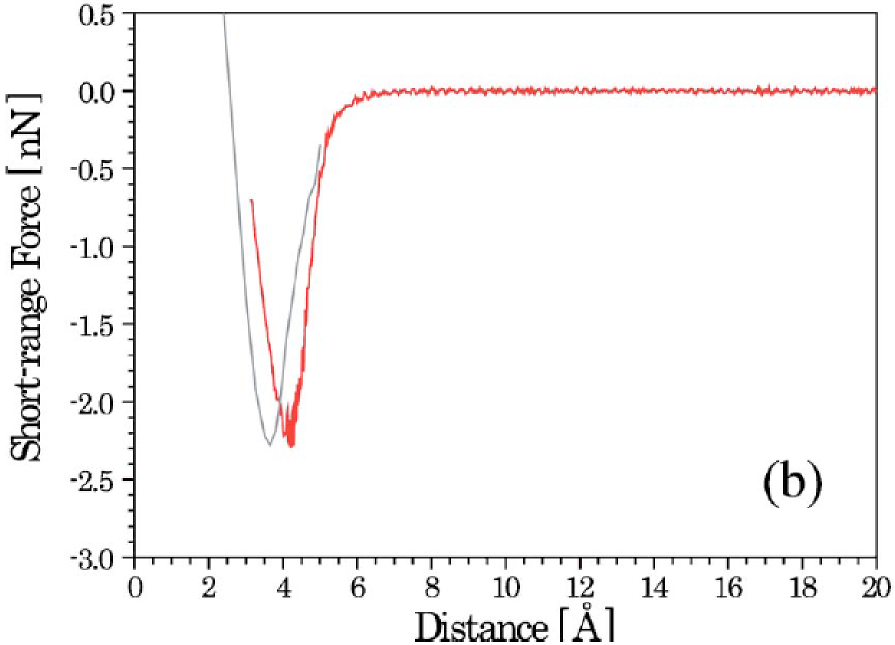
$$F_{ts}^{CONS}(d_{ltp}) = 2k \int_{d_{ltp}}^{\infty} \left\{ \Omega(\xi) + \frac{\Omega(\xi)\sqrt{A}}{8\sqrt{\pi\left(\xi - d_{ltp}\right)}} - \frac{A^{3/2}}{\sqrt{2(\xi - d_{ltp})}} \frac{\partial \Omega}{\partial \xi} \right\} d\xi \qquad (8)$$

- First term is the small amplitude approximation, last term is the large amplitude approximation, the middle term comes from an interpolation based on fractional calculus
- In practice $\Omega(Z)$ is acquired at discrete points and also the 2nd and 3rd terms can introduce a singularity in the integral, which needs to be properly accounted for (http://www.ampc.ms.unimelb.edu.au/afm/bibliography.html)
- Giessibl, App. Phys. Lett, 78, 123-125, proposes another numerical approach based on matrix inversion

An example

- Abe, Custance, Morita et al, App. Phys. Lett, 87, 173503, 2005





Frequency shift vs tip-sample vertical displacement *f-Z characteristics* acquired over a Si111-7x7 corner adatom at room temperature. Ten of a total of eighty *f-Z curves* measured during the tracking of the adatom are superimposed gray. The average curve from these 80 *f-Z curves is shown in black. The inset is for* the comparison of a single *f-Z curve gray with the averaged one black.* The axes on the right side display the corresponding normalized frequency shift *A=282 Å, f0=162 295.8 Hz, and k=28.7 N/m.*

(Red) Experimental chemical interaction force obtained on the corner adatom red, and predicted short-range force gray for a Si tip interacting with an adatom of the Si111-5x5 surface from first-principles calculations

Appendix

To reconstruct force based on the large amplitude assumption, we started at

$$\gamma(Z,A)=kA^{3/2}\frac{\Delta\omega_0}{\omega_0}=kA^{3/2}\Omega \qquad (1)$$

and reached the approximation

$$\gamma(Z,A)\sim\frac{1}{\sqrt{2\pi}}\int_{q=-A}^{+\infty}\frac{F_{ts}^{CONS}(Z+q)}{\sqrt{A+q}}\,dq \qquad (2)$$

Recalling that q=d-Z we can rewrite above as

$$\gamma(Z,A)\sim\frac{1}{\sqrt{2\pi}}\int_{d=d_{ltp}}^{+\infty}\frac{F_{ts}^{CONS}(d)}{\sqrt{d-d_{ltp}}}\,\partial d$$

Durig (App.Phys.Lett,1999) suggests that this can be inverted using identities for Abelian integrals into the following

$$F_{ts}^{CONS}(d_{ltp})=-2k\int_{d_{ltp}}^{\infty}\frac{A^{3/2}}{\sqrt{2(Z-d_{ltp})}}\frac{\partial\Omega}{\partial Z}dZ$$

d_{ltp} is the gap coresponding to the "lower turnaround point"

$d_{ltp}=Z-A$