Excited probe interacting with sample – nonlinearity, virial and dissipation
From the last lecture

- Introduction to tapping mode or amplitude modulated (AM-AFM)
- Introduction to frequency modulation AFM (FM-AFM)
- In the context of linear analysis of point mass oscillator interaction with sample
Limitations of the linearized analysis

Key assumptions were:
- Only valid when amplitude is much smaller than tip-sample gap \( A \ll d^* \)
- Usually requires \( A \ll 1\text{nm} \)

\[
F_{ts}^{CONS}(d) = F_{ts}^{CONS}(d^*) - k_{ts} \ddot{q}
\]

\[
F_{ts}^{Diss}(d, \dot{d}) = -c_{ts} \dot{q}
\]
Linear vs. nonlinear freq. response

Linear

Nonlinear - attractive

Nonlinear - att/rep

$A \propto \omega$

$\phi = 90^\circ$

$\omega = \omega_0$

$\omega$
Analytical theory of dynamic AFM

\[ m\ddot{q} + c\dot{q} + kq = F_{\text{ext}}(t) + F_{\text{ts}}^{\text{CONS}}(Z + q) + F_{\text{ts}}^{\text{DISS}}(Z + q, \dot{q}) \]

where \( F_{\text{ts}}^{\text{DISS}}(Z + q, \dot{q}) = F_{\text{ts}}^{\text{DISS}}(Z + q, -\dot{q}) \)

\[
\ddot{q} + \frac{1}{\omega_0^2} \dot{q} + q = \frac{F_0}{k} \sin(\omega t) + \frac{F_{\text{ts}}^{\text{CONS}}(Z + q) + F_{\text{ts}}^{\text{DISS}}(Z + q, \dot{q})}{k}
\]

with \( \omega_0 = \sqrt{\frac{k}{m}} \), \( Q = \frac{m\omega_0}{c} \)

Assume steady state solution (neglecting \( q^* \))

\( q(t) = A\sin(\omega t - \phi) \)

\( \dot{q}(t) = A\omega \cos(\omega t - \phi) \)

Define \( \theta = \omega t - \phi \), then

\( q = A\sin(\theta) \)

\( \dot{q} = A\omega \cos(\theta) \)  \( (2) \)
Analytical theory of dynamic AFM

$q = A \sin(\theta)$

$d = Z + A \sin(\theta)$

$d_{\text{max}} = Z + A$

$\theta = 0$

$\theta = \frac{3\pi}{2}$

$\theta = 2\pi$

Sample surface

Sample

$F_{ts}$

Dissipative force

Conservative force

Interaction time
Analytical theory of dynamic AFM

Substitute (2) in (1)

\[- \sin \theta + \frac{A}{Q} \cos \theta + A \sin(\theta) = \frac{F_0}{k} (\sin \theta \cos \phi + \cos \theta \sin \phi) + \frac{F_{\text{CONS}} + F_{\text{DISS}}}{k} \]

(2)

We define

\[V_{ts}(Z, A) = \left< F_{\text{CONS}} \cdot q \right> = \frac{1}{2\pi/\omega_0^2} \int_0^{2\pi/\omega_0^2} F_{\text{CONS}} \cdot q \, dt = \frac{1}{2\pi} \int_0^{2\pi} F_{\text{CONS}} \cdot q \, d\theta \]

\[E_{ts}(Z, A) = -\int_0^{2\pi/\omega_0^2} F_{\text{DISS}} \cdot \dot{q} \, dt = -\int_0^{2\pi} F_{\text{DISS}} \cdot A \cos(\theta) \, d\theta \]

(3)

Multiply (2) by \( q = A \sin(\theta) \), integrate from \( \theta = 0 \to 2\pi \), and divide by \( 2\pi \) we get (see Appendix)

\[V_{ts}(Z, A) = \frac{kA^2}{2} \left( 1 - \frac{\omega^2}{\omega_0^2} \right) - \frac{AF_0}{2} \cos \phi \] (Units of energy)

(4)

Multiply (2) by \( \dot{q} = A \omega \cos(\theta) \) and integrate from \( \theta = 0 \to 2\pi \), we get (see Appendix)

\[E_{ts}(Z, A) = \pi AF_0 \sin \phi - \pi kA^2 \frac{\omega}{Q\omega_0} \] (Units of energy)

(5)
Physical meaning of $E_{ts}$

$$E_{ts}(Z,A) = - \int_0^{2\pi/\omega_0} F_{ts}^{\text{Diss}} \cdot \dot{q} \, dt = -\int_0^{2\pi} F_{ts}^{\text{Diss}} \cdot A\cos(\theta) \, d\theta = -2 \int_{-A}^{A} F_{ts}^{\text{Diss}} \cdot dq$$

- Irreversible work done in one oscillation cycle by tip on sample
- Or energy dissipated from vibrating tip into sample in one cycle of oscillation

$$F_{ts}(d,d') = F_{ts}^{\text{CONS}}(d) + F_{ts}^{\text{Diss}}(d,d')$$

Diagrams showing the force $F_{ts}$ and energy $E_{ts}$ at various stages of tip-sample interaction.
Physical meaning of $V_{ts}$

It can be shown that (See Appendix)

$$V_{ts}(Z,A) = \langle F_{ts}^{CONS} \cdot q \rangle = -\frac{A}{\pi} \int_{-A}^{+A} k_{ts}(Z + q) \sqrt{1 - \left(\frac{q}{A}\right)^2} dq = -\frac{1}{2} \left\{ \frac{1}{\pi} \int_{0}^{2\pi} k_{ts}(Z + A \sin \theta) \cos^2 \theta d\theta \right\} A^2$$

where $k_{ts}(d) = -\frac{\partial F_{ts}^{CONS}}{\partial d}$

- $V_{ts}$ is sometimes called the Virial of the tip-sample force
- Integrand is a weighted measure of tip-sample force gradients over the oscillation cycle
- In the limit of small amplitude i.e linear analysis (see Appendix)

$$V_{ts}(Z,A) \sim -\frac{k_{ts}(Z) A^2}{2}$$

i.e. the Virial is the negative of the stored energy in the conservative tip-sample interaction
### Appendix

**Alternate expressions for the virial**

\[
V_{\text{ts}} (Z, A) = \langle F_{\text{ts}}^{\text{CONS}} \cdot q \rangle = \frac{1}{2\pi} \int_{0}^{2\pi} F_{\text{ts}}^{\text{CONS}} (Z + A\sin \theta) \cdot A\sin \theta \, d\theta
\]  

(6)

\[q = A\sin \theta\]

\[\therefore dq = A\cos \theta \, d\theta\]

Rewriting (6) in terms of an integral in \( q \) we get (splitting the integral from 0 to \( 2\pi \) into \( 2\pi \) (the integral from \( q = -A \) to \( +A \)) and multiplying and dividing the integrand by \( \cos \theta \))

\[
V_{\text{ts}} (Z, A) = \frac{1}{\pi} \int_{-A}^{A} F_{\text{ts}}^{\text{CONS}} (Z + q) \cdot \frac{q}{\sqrt{A^2 - q^2}} \, dq
\]  

(7)
Appendix

- Eq (7) suggests that \( V_{ts} \) is the “weighted” work done by conservative forces as the tip moves from its lowest position to its highest position.

- The weight function \( \frac{q}{\sqrt{A^2 - q^2}} \) (shown in shaded blue) favors the work done at the extreme ends of the oscillation.
Appendix

Integrating (6) by parts

\[ V_{ts}(Z, A) = \frac{1}{2\pi} \int_0^{2\pi} F_{ts}^{CONS}(Z + A\sin\theta) \cdot A\sin\theta \, d\theta \]

\[ = \frac{1}{2\pi} \left[ -F_{ts}^{CONS}(Z + A\sin\theta) \cdot A\cos\theta \right]_0^{2\pi} + \frac{1}{2\pi} \int_0^{2\pi} \frac{\partial F_{ts}^{CONS}(Z + A\sin\theta)}{\partial \theta} \cdot A\cos\theta \, d\theta \quad (8) \]

The first term above is 0. The second term can be written as an integral in 'q' by recognizing that

\[ q = A\sin\theta, \]

\[ \therefore dq = A\cos\theta \, d\theta \]

and

\[ \frac{\partial F_{ts}^{CONS}}{\partial \theta} = \frac{\partial F_{ts}^{CONS}}{\partial q} \frac{\partial q}{\partial \theta} = \frac{\partial F_{ts}^{CONS}}{\partial q} A\cos\theta = \frac{\partial F_{ts}^{CONS}}{\partial q} A\sqrt{1 - \left(\frac{q}{A}\right)^2} \quad (9) \]

Finally splitting the integral

from 0 to 2\(\pi\) into 2\(\pi\) (the integral from \(q=-A\) to +A) we can write

\[ V_{ts}(Z, A) = \frac{A}{\pi} \int_{-A}^{+A} k_{ts}(Z + q) \sqrt{1 - \left(\frac{q}{A}\right)^2} \, dq \]

where \(k_{ts}(d) = -\frac{\partial F_{ts}^{CONS}}{\partial d} = -\frac{\partial F_{ts}^{CONS}}{\partial q} \)

The physical significance of (9) was discussing in the main slides of this lecture
Expressions for virial and dissipation in terms of observables when $\omega \neq \omega_0$

\[
\frac{\ddot{q}}{\omega_0^2} + \frac{1}{\omega_0 Q} \dot{q} + q = \frac{F_0}{k} \sin(\omega t) + \frac{F_{\text{CONS}}(Z + q) + F_{\text{DISS}}(Z + q, q)}{k} \tag{10}
\]

Assume steady state solution

\[q(t) = A \sin(\omega t - \phi) = A \sin(\theta)\]
\[\dot{q}(t) = A \omega \cos(\omega t - \phi) = A \omega \cos(\theta)\]

Substituting this in (10) we get

\[-A \frac{\omega^2}{\omega_0^2} \sin \theta + A \frac{\omega}{\omega_0 Q} \cos \theta + A \sin(\theta) = \frac{F_0}{k} (\sin \theta \cos \phi + \cos \theta \sin \phi) + \frac{F_{\text{CONS}}(Z + A \sin(\theta)) + F_{\text{DISS}}(Z + A \sin(\theta), A \omega \cos \theta)}{k} \tag{11}\]

Multiply (11) by $q = A \sin(\theta)$ and integrate from $\theta = 0 \ldots 2\pi$, we get

\[V_\tau (Z, A) = \left< F_{\text{CONS}} \cdot q \right> = \frac{1}{2\pi} \int_0^{2\pi} F_{\text{CONS}}(Z + A \sin(\theta)) \cdot A \sin \theta \, d\theta = \frac{kA^2}{2} \left( 1 - \frac{\omega^2}{\omega_0^2} \right) - \frac{AF_0}{2} \cos \phi \tag{12}\]

Multiply (11) by $q = A \omega \cos(\theta)$ and integrate from $\theta = 0 \ldots 2\pi$, we get

\[E_\tau (Z, A) = -\int_0^{2\pi} F_{\text{DISS}}(Z + A \sin(\theta), A \omega \cos \theta) \cdot A \cos(\theta) \, d\theta = \pi AF_0 \sin \phi - \pi kA^2 \frac{\omega}{Q \omega_0} \tag{13}\]
Appendix

Expression for virial in the limit of small amplitude

As shown in this lecture the virial is defined as

\[ V_{ts}(Z,A) = \left\langle F_{ts}^{CONS} \cdot q \right\rangle = -\frac{A}{\pi} \int_{q=-A}^{+A} k_{ts}(Z+q) \sqrt{1-\left(\frac{q}{A}\right)^2} \ dq \]

where \( k_{ts}(d) = -\frac{\partial F_{ts}^{CONS}}{\partial d} \)

For \( q,A \ll Z \), we can write \( k_{ts}(Z+q) \) as a Taylor series expansion

\[ k_{ts}(Z+q) = k_{ts}(Z) + \frac{\partial k_{ts}}{\partial q} q + \frac{1}{2} \frac{\partial^2 k_{ts}}{\partial q^2} q^2 \]

Neglecting higher order terms, we have \( k_{ts}(Z+q) \sim \) so that

\[ V_{ts}(Z,A) \sim -\frac{A}{\pi} k_{ts}(Z) \int_{q=-A}^{+A} \sqrt{1-\left(\frac{q}{A}\right)^2} \ dq \]

Now let \( q = A\sin \theta, \ dq = A\cos \theta \ d\theta \)

\[ V_{ts}(Z,A) \sim -\frac{A^2}{\pi} k_{ts}(Z) \int_{\theta=-\pi/2}^{+\pi/2} \cos^2 \theta \ d\theta = -\frac{k_{ts}(Z)A^2}{2} \]

In this limit the virial measures the maximum potential energy stored in the tip-sample force