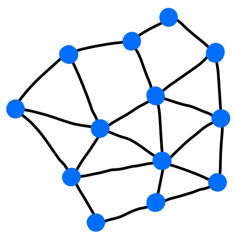
Lecture 1 Vibrational modes and rheology of generic networks

1. General discrete mechanical networks

How to describe vibrations of mechanical networks?



Elastic energy: $E = \frac{1}{2} \sum_{i,j} u_i D_{ij} u_j$

$(\underline{\underline{D}} = \underline{\underline{Q}} \cdot \underline{\underline{K}} \cdot \underline{\underline{C}})$

< Discussion: (1) Q: What simplifying assumptions did we make?

A: ① Mass can be lumped at sites

② Interactions are pairwise and linearized

(2) Q: what types of real systems can this model describe?

Which assumption may be violated in which systems?

A: open-ended

(3) Q: what type of matrix is D ?

A: symmetric (or hermitian in $\vec{q}$ space) if the system is conserved >

< Discussion: how to characterize interactions from observations?

Scenario 1: we can observe particles, can give them force, but can't see the springs

Solution :
$$F_i = D_{ij} u_j$$
$$u_i = (D^{-1})_{ij} F_j$$

Scenario 2 : we can observe particles, can't touch them, can't see the springs
The system is under thermal fluctuations

Solution :
$$\langle u_i u_j \rangle = \frac{\int \mathcal{D}u \, e^{-\beta E} u_i u_j}{\int \mathcal{D}u \, e^{-\beta E}} = k_B T \, (D^{-1})_{ij}$$

This has been used for colloidal glasses
(Andrea's paper in Ref list)

Generic dynamic response

Equation of motion :
$$m \ddot{u}_i = -\frac{\partial E}{\partial u_i} + F_i^{ext} - \eta \dot{u}_i = -D_{ij} u_j + F_i^{ext} - \eta \dot{u}_i$$

2. Eigenmodes of vibration

How to solve the EOM? It's easier to go to frequency space:

$$u_i(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} u_i(\omega)$$

EOM $\rightarrow$ (different ω components are orthogonal)

$$-m\omega^2 u_i(\omega) = -D_{ij} u_j(\omega) + F_i^{ext}(\omega) + i\eta\omega u_i(\omega)$$

$$\left[\underline{\underline{D}} - (m\omega^2 + i\eta\omega)\underline{\underline{I}}\right] \underline{u}(\omega) = \underline{F}^{ext}(\omega)$$

$$\underline{u}(\omega) = \underbrace{\left[\underline{\underline{D}} - (m\omega^2 + i\eta\omega)\underline{\underline{I}}\right]^{-1}}_{\equiv \underline{\underline{G}}(\omega)} \cdot \underline{F}^{ext}(\omega) \qquad (1)$$

$\equiv \underline{\underline{G}}(\omega)$: elasticity Green's function

This is a formal solution.

How to analyze the response? : use eigenstates

$$\underline{\underline{D}} = \underline{\underline{V}}^{+} \underline{\underline{\Lambda}} \underline{\underline{V}} \qquad \text{where} \qquad V^{+} = \begin{pmatrix} | & | & & | \\ \vdots & \vdots & \cdots & \vdots \\ | & | & & | \end{pmatrix}$$

or $\underline{\underline{\Lambda}} = \underline{\underline{V}}\,\underline{\underline{D}}\,\underline{\underline{V}}^{+}$ orthonormal eigenvectors of D

where U is $\begin{cases} \text{orthogonal} \\ \text{unitary} \end{cases}$ for D as $\begin{cases} \text{symmetric} \\ \text{hermitian} \end{cases}$ matrices

<Comment: when the network is a periodic lattice

eigenmodes = planewave states $\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{pmatrix} e^{i\vec{q}\cdot\vec{r}}$

eigenvel in unit cell

$\underline{\underline{D}}$ block diagonalize in $\vec{q}$ space

(consequence of translational invariance)

The Green's function takes the form

$$\underline{\underline{G}}(\omega) \to G_q(\omega) = \frac{1}{\Lambda_q - m\omega^2 - i\eta\omega}$$

3. Linear-responce theory of mechanical vibrations

Use these eigenmodes to simplify the response

(1) $\rightarrow$ $\underline{V} \cdot \underline{u}(\omega) = \underline{\underline{V}} \cdot \left[D - (m\omega^2 + i\eta\omega) I \right]^{-1} \cdot \underline{\underline{V}}^{\dagger} \cdot \underline{\underline{V}} \cdot \underline{F}^{ext}$

project F^{ext} to mode α

$$u_i(\omega) = \sum_{\alpha} \frac{V_i^{(\alpha)} V_j^{(\alpha)} F_j^{ext}(\omega)}{\Lambda_\alpha - m\omega^2 - i\eta\omega}$$

Def: $\chi_\alpha(\omega) = \dfrac{1}{\Lambda_\alpha - m\omega^2 - i\eta\omega}$ retarded Green's function of mode α

$$u_i(\omega) = \sum_\alpha \chi_\alpha(\omega) V_i^{(\alpha)} V_j^{(\alpha)} F_j^{ext}(\omega)$$

F.T. back to time domain

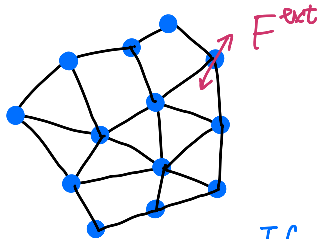
$$u_i(t) = \sum_\alpha \int dt' \underbrace{\chi_\alpha(t-t')}_{\text{real}} V_i^{(\alpha)} V_j^{(\alpha)} F_j^{ext}(t')$$

$\chi(\omega) \leftrightarrow \chi(t)$ using linear-responce theory $\rightarrow$

$$\begin{cases} \chi_\alpha(t) \text{ real} \Rightarrow \chi_\alpha(\omega) = \chi_\alpha^*(-\omega) \\ \chi_\alpha(t) = 0 \text{ for } t<0 \text{ (causality)} \Rightarrow \text{Kramers-Krönig relation} \end{cases}$$

< Discussion : What do we learn ?

① Responce to F^{ext}



$\rightarrow$ decompose into modes

coefficient $\dfrac{\langle V^\alpha | F^{ext} \rangle}{\Lambda_\alpha - m\omega^2 - i\eta\omega}$

- If $\eta = 0$ (no damping)

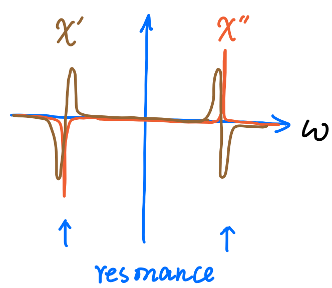
  $\dfrac{1}{\Lambda_\alpha - m\omega^2}$ diverge when $m\omega^2 = \Lambda_\alpha$ for any mode α : "resonance"

  $\rightarrow$ divergent responce

- If $\eta > 0$: broadened response : a range of modes are excited

$$\chi'_\alpha(\omega) = \frac{\Lambda_\alpha - m\omega^2}{(\Lambda_\alpha - m\omega^2)^2 + (\eta\omega)^2}$$

$$\chi''_\alpha(\omega) = \frac{\eta\omega}{(\Lambda_\alpha - m\omega^2)^2 + (\eta\omega)^2}$$



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② Dissipation

Consider periodic force $F^{ext}(t) = f \cos \omega_0 t$

$$\to F^{ext}(\omega) = \frac{f}{2}\left[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)\right]$$

$$\to u_i(\omega) = \sum_\alpha \left(\chi_\alpha'(\omega)+i\chi''(\omega)\right) V_i^{(\alpha)} V_j^{(\alpha)} \frac{f_j}{2}\left[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)\right]$$

$$\to u_i(t) = \sum_\alpha V_i^{(\alpha)} V_j^{(\alpha)} \frac{f_j}{2}\Big[\underset{\substack{\uparrow \\ \text{in-phase}}}{\chi_\alpha'(\omega_0)\cos\omega_0 t} + \underset{\substack{\uparrow \\ \text{out of phase}}}{\chi_\alpha''(\omega_0)\sin\omega_0 t}\Big]$$

$$= \sum_\alpha V_i^{(\alpha)} V_j^{(\alpha)} \frac{f_j}{2}\left|\chi_\alpha(\omega)\right| \cos\big(\omega_0 t - \overset{\substack{\text{phase lag} \\ \downarrow}}{\delta_\alpha(\omega_0)}\big)$$

where $\tan \delta_\alpha(\omega_0) = \dfrac{\chi_\alpha''(\omega_0)}{\chi_\alpha'(\omega_0)}$

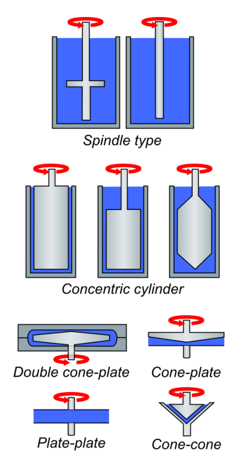
→ dissipation

$$P = \int f_i(t)\, \dot{u}_i(t) \to \sum_\alpha V_i^{(\alpha)} V_j^{(\alpha)} \frac{f_j^2}{2}\, \omega_0\, \underline{\underline{\chi_\alpha''(\omega_0)}}$$

4. Rheology of soft disordered materials

Rheology ↓ flow & deformation of matter

Cartoon picture of a rheometer:



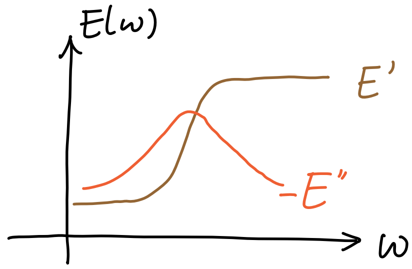
What is measured?

$$\underset{\substack{\uparrow \\ \text{strain}}}{\varepsilon(\omega)} \longleftrightarrow \underset{\substack{\uparrow \\ \text{stress}}}{\sigma(\omega)}$$

Complex elastic modulus

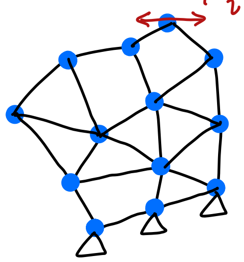
$$E(\omega) = \frac{\sigma(\omega)}{\varepsilon(\omega)}$$

Typical curve:



Can we understand rheology using these vibrational modes?

Extremely simplified toy model



$$E(\omega) \sim \frac{F_i^{ext}(\omega)}{u_i(\omega)}$$

$$\sim \frac{F_i^{ext}(\omega)}{\sum_\alpha \frac{V_i^{(\alpha)} V_j^{(\alpha)} F_j^{ext}(\omega)}{\Lambda_\alpha - m\omega^2 - i\eta\omega}}$$

$$\sim \left[\sum_\alpha \frac{1}{\Lambda_\alpha - m\omega^2 - i\eta\omega}\right]^{-1} \sim \left[\sum_\alpha \chi_\alpha(\omega)\right]^{-1}$$

Let's be a little more specific:

- Typical soft solids (e.g. gels) $\quad m\omega^2 \ll \eta\omega$

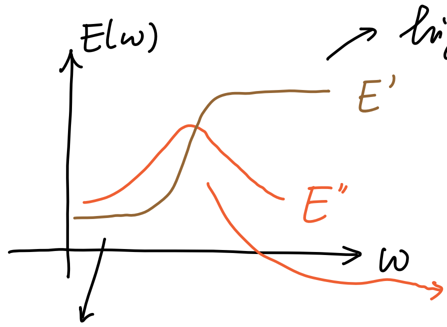
  inertia $\ll$ viscous force

  (low Reynolds number)

- Damping is relative to the fluid instead of space

  $-\eta \dot{u}_i$ should be $-\eta(\dot{u}_i - \dot{u}_i^{(affine)})$

$\Rightarrow$



high ω plateau: $i\eta\omega$ large
affine response

peak of dissipation:
$i\eta\omega \sim \Lambda_\alpha$ of soft modes

low ω plateau

$$E \sim \left(\sum_\alpha \frac{|V_i^{(\alpha)}|^2}{\Lambda_\alpha} \right)^{-1}$$: nonaffine response

Similar to χ', χ'':

E' : "storage modulus" in-phase, elastic response

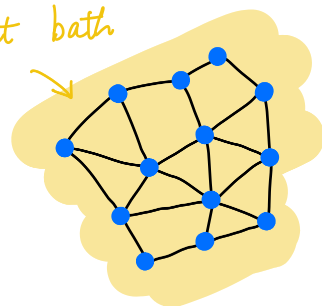
E'' : "loss modulus" out-of-phase, viscoelastic response.

Backup

4. Thermal fluctuations and

Fluctuation – Dissipation – Response relations

If the network is in a heat bath at temperature T



$\langle \vec{u}_i \, \vec{u}_j \rangle_{thermal} = ?$

Apply equilibrium canonical ensemble

$$Z = \int \prod_m du_m \, e^{-\beta E} = \int \prod_m du_m \, e^{-\frac{1}{2k_BT} u \cdot D \cdot u}$$

$$\langle \vec{u}_i \, \vec{u}_j \rangle = \frac{1}{Z} \int \prod_m du_m \; u_i \, u_j \, e^{-\frac{1}{2k_BT} u \cdot D \cdot u}$$