Waves in Elastic Solids

Michael J. Frazier, Assistant Professor
Mechanical and Aerospace Engineering
University of California, San Diego
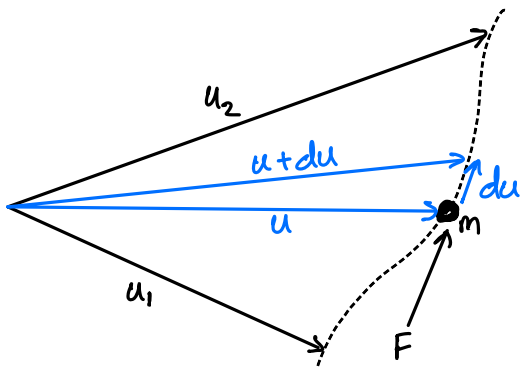
TOPIC 1:
Principles of Dynamics

kinetic energy (T): energy of motion

potential energy (V): energy of configuration

work (W): energy added/removed from a system that, necessarily, changes its kinetic and/or potential energy

Consider a particle moving under the action of a force.

incremental work: $dW = F \cdot du$

$$dW = F \cdot du = m\ddot{u} \cdot du = m\frac{d\dot{u}}{dt} \cdot \frac{du}{dt} dt = m\frac{d\dot{u}}{dt} dt \cdot \frac{du}{dt} = m\frac{du}{dt} \cdot d\dot{u} = d\left(\frac{1}{2} m\dot{u} \cdot \dot{u}\right) = dT$$

The work performed in moving a particle from u_1 to u_2 is responsible for a change in the kinetic energy

$$W = \int_{u_1}^{u_2} F \cdot du = \int_{\dot{u}_1}^{\dot{u}_2} d\left(\frac{1}{2} m\dot{u} \cdot \dot{u}\right) = \frac{1}{2} m\dot{u}_2 \cdot \dot{u}_2 - \frac{1}{2} m\dot{u}_1 \cdot \dot{u}_1 = \Delta T$$

The work performed in moving a particle from u_1 to u_2 under the influence of a conservative force, F_c, is independent of the path taken.

Consider the work done by a conservative force as the particle moves from u_1 to u_2 through a reference point, u_r:

$$W = \int_{u_1}^{u_2} F_c \cdot du = \int_{u_1}^{u_r} F_c \cdot du + \int_{u_r}^{u_2} F_c \cdot du = \underbrace{\int_{u_1}^{u_r} F_c \cdot du}_{V_1} - \underbrace{\int_{u_2}^{u_r} F_c \cdot du}_{V_2} = -\Delta V$$

The work done by a conservative force as the particle moves from u_1 to u_2 is equal to the negative of the change in potential energy.

The work done by non-conservative forces as a particle moves from u_1 and u_2 is responsible for a change in the total energy of the system.

$$dW = F_c \cdot du + F_{nc} \cdot du \longrightarrow dT = -dV + F_{nc} \cdot du \longrightarrow F_{nc} \cdot du = d(T+V) = dE$$

$$dW = \int_{u_1}^{u_2} dE = \Delta E$$

In the absense of non-conservative forces, $E = const.$

The principle of virtual work is, essentially, a statement of static equilibrium, i.e., no dynamics. From here, we develop principles of dynamics from an energy perspective.

Consider a body under load. Under load, we imagine the body deforms and displaces such that some imagined work is performed. The imagined displacements and work are virtual, and underpin the principle of virtual work, the first variational principle of mechanics.
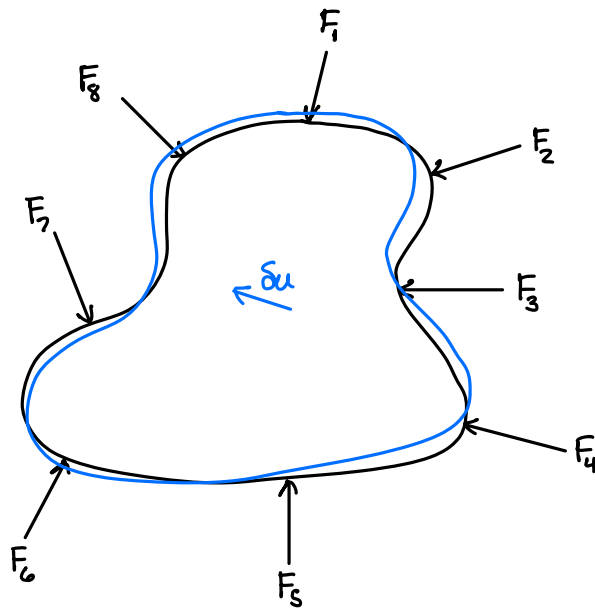
We are free to imagine any displacements ... so long as certain rules are obeyed:

1. instantaneous: imagining the virtual displacements does not require the passage of time. As an additional benefit, instantaneity ensures that the system conditions do not change

2. infinitesimal: virtual displacement behave as differentials. The symbols δ and d are used to distinguish virtual differentials from actual differentials that may occur over a time interval, dt.

3. kinematically admissible: virtual displacements must not violate known constraints of the problem lest the very essence of the problem be altered.

$$\delta W = F_1 \cdot \delta u_1 + F_2 \cdot \delta u_2 + \cdots F_n \cdot \delta u_n = \left(\sum_{i=1}^{n} F_i \right) \cdot \delta u \qquad \text{virtual work}$$

For a system in equilibrium, $\sum_{i=1}^{n} F_i = 0$, thus: $\delta W = 0$

Since forces at the system constraints do no work, they need not be considered in statics problems.

Consider the system below. When the bar is horizontal, the spring is unstretched. Determine the equilibrium configuration using the principle of virtual work.

$F_1 = -ku_1 \hat{\imath}$ $\qquad u_1 = x\hat{\imath}$

$F_2 = -mg\hat{\jmath}$ $\qquad u_2 = y\hat{\jmath}$
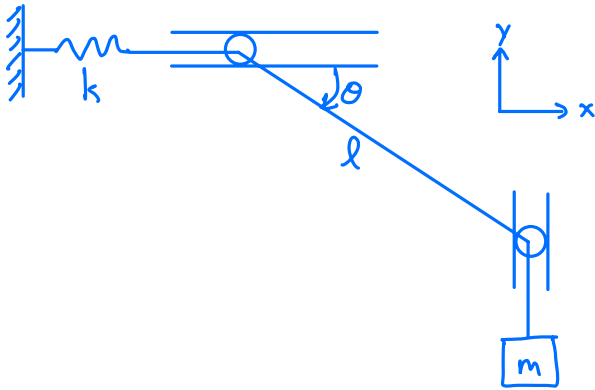
$\delta W = \sum\limits_{i=1}^{2} F_i \cdot \delta u_i = -kx\delta x + mg\,\delta y = 0$

→ At this point, we can go no further because x and y are not independent; they are linked by constraint equations and/or a generalized coordinate:
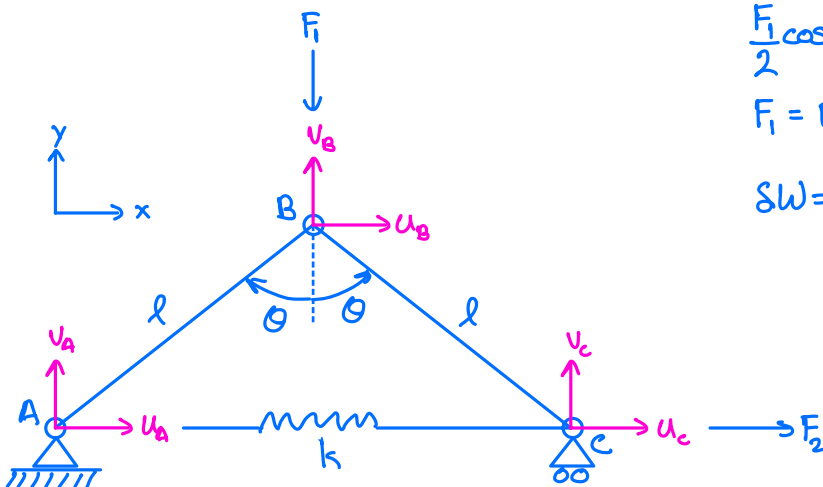
$x = l(1-\cos\theta)$ $\qquad y = -l\sin\theta$

$\delta x = l\sin\theta\,\delta\theta$ $\qquad \delta y = -l\cos\theta\,\delta\theta$

$[-kl(1-\cos\theta)\sin\theta - mg\cos\theta]\,l\,\delta\theta = 0$

$\therefore \quad -kl(1-\cos\theta)\tan\theta = mg$

Consider the system below. Absent the loading, the spring is unstretched. Determine the equilibrium configuration using the principle of virtual work.

reaction forces at A and C do no work

$\dfrac{F_1}{2}\cos\theta + F_2 = -k(u_c - u_A)\hat{\imath}$ $\qquad u_A = x_A\hat{\imath}$ $\quad u_c = x_c\hat{\imath}$

$F_1 = F_1\hat{\jmath}$ $\qquad u_B = y_B\hat{\jmath}$

$\delta W = -k(x_c - x_A)\delta x_c - F_1\delta y_B = 0$

$x_A = 0$ $\quad x_c = 2l\sin\theta$ $\quad y_B = l(1-\sin\theta)$

$\delta x_A = 0$ $\quad \delta x_c = 2l\cos\theta\,\delta\theta$ $\quad \delta y_B = -l\cos\theta\,\delta\theta$

$(-4kl\sin\theta + F_1)\,l\cos\theta\,\delta\theta = 0$

$\therefore \quad F_1 = 4kl\sin\theta$

The principle of virtual work can be extended to dynamical systems via the principle of d'Alembert by incorporating inertial forces. Like the principle of virtual work, it treats the system as a whole without breaking the system up (i.e., method of joints/sections) or bothering with constraint forces. Where the principle of virtual work is a statement of static equilibrium, d'Alembert's principle may be regarded as a statement of dynamic equilibrium.

$$\sum_{i=1}^{n} (F_i - m_i \ddot{u}_i) \cdot \delta u_i = 0 \qquad \text{principle of d'Alembert}$$

A massless rigid bar is constrained to move illustrated. Determine the EOM using d'Alembert's principle.
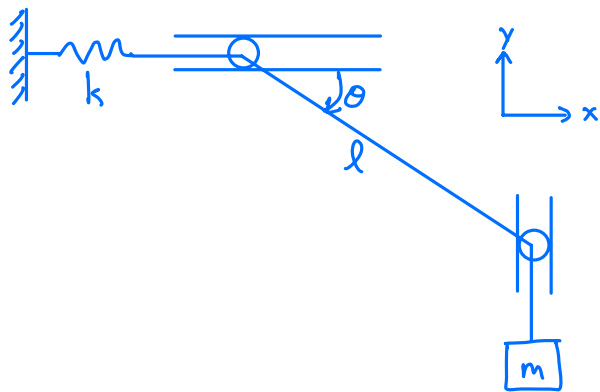
$$F_1 = -ku_1 \hat{i} \qquad u_1 = x \hat{i}$$

$$F_2 = -mg \hat{j} \qquad u_2 = y \hat{j}$$

$$\sum_{i=1}^{2} (F_i - m\ddot{u}_i) \cdot \delta u_i = -kx\,\delta x + m(g + \ddot{y})\delta y = 0$$

$$-[k\ell(1-\cos\theta)\sin\theta + m(g - \ell\ddot{\theta}\cos\theta + \ell\dot{\theta}^2\sin\theta)\cos\theta]\,\ell\delta\theta = 0$$

$$\therefore \quad k\ell(1-\cos\theta)\tan\theta + m(g - \ell\ddot{\theta}\cos\theta + \ell\dot{\theta}^2\sin\theta) = 0$$

$$x = \ell(1-\cos\theta) \qquad y = -\ell\sin\theta$$

$$\delta x = \ell\sin\theta\,\delta\theta \qquad \delta y = -\ell\cos\theta\,\delta\theta$$

$$\dot{y} = -\ell\dot{\theta}\cos\theta$$

$$\ddot{y} = -\ell\ddot{\theta}\cos\theta + \ell\dot{\theta}^2\sin\theta$$

Although the principles of virtual work and d'Alembert succeed Newton in treating the system as a whole and voiding constraint forces, they are still cumbersome in their vectorial mathematics and their use of physical coordinates which may not be independent, requiring a coordinate transformation. Casting the problem, from the start, in terms of independent, generalize coordinates simplifies the problem formulation in involving a minimum set of degrees of freedom.

$$n = d_s N - c$$

# of DOFs
# of bodies
constraints
of space dimensions

minimum # of DOF (e.g., equations) to describe a problem.

Hamilton's principle works directly with generalized coordinates in the form of scalar functions.

$$\frac{d}{dt} \sum_{i=1}^{n} m_i \dot{u}_i \cdot \delta u_i = \sum_{i=1}^{n} (m_i \ddot{u}_i \cdot \delta u_i + \underbrace{m_i \dot{u}_i \cdot \delta \dot{u}_i}_{})$$

$$\delta \left(\frac{1}{2} m_i \dot{u}_i \cdot u_i \right) = \delta T_i$$

$$\therefore \sum_{i=1}^{n} m_i \ddot{u}_i \cdot \delta u_i = \sum_{i=1}^{n} \left[\frac{d}{dt} (m_i \dot{u}_i \cdot \delta u_i) - \delta T_i \right]$$

$$\sum_{i=1}^{n} (F_i - m_i \ddot{u}_i) \cdot \delta u_i = \sum_{i=1}^{n} \left[\underbrace{F_i \cdot \delta u_i}_{\delta W_i} - \frac{d}{dt} (m_i \dot{u}_i \cdot \delta u_i) + \delta T_i \right] = \delta W + \delta T - \sum_{i=1}^{n} \frac{d}{dt} (m_i \dot{u}_i \cdot \delta u_i) = 0$$

For a system of particles in motion, as time evolves from t_1 to t_2, each particle will trace a particular path denoted the "true path". Nevertheless, we can imagine a "varied path" that still coincides with the true path at instances t_1 and t_2.
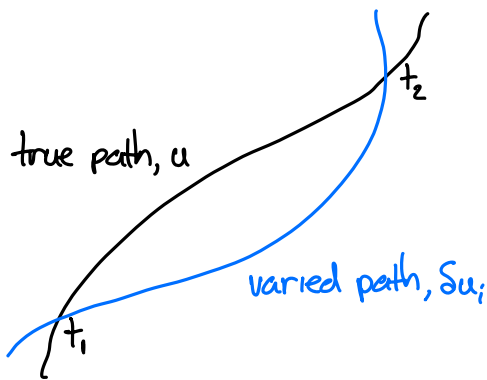
$$\int_{t_1}^{t_2} (\delta W + \delta T) dt = \int_{t_1}^{t_2} \sum_{i=1}^{n} \frac{d}{dt} (m_i \dot{u}_i \cdot \delta u_i) dt = \sum_{i=1}^{n} m_i \dot{u}_i \cdot \delta u_i \Big|_{t_1}^{t_2} = 0$$

true path, u

varied path, δu_i

$\delta u_i(t_2) = \delta u_i(t_1) = 0$ since virtual displacements vanish at the true path

$$\int_{t_1}^{t_2} (\delta W + \delta T) dt = \delta \int_{t_1}^{t_2} (W + T) dt = \delta \int_{t_1}^{t_2} \underbrace{(T - V)}_{\mathcal{L}: \text{Lagrangian}} dt = 0$$

Hamilton's principle: the variation that minimizes T-V coincides with the true path.

Since virtual displacements must be reversible, work due to non-conservative forces are not accounted for. Thus, $\delta W = -\delta V$.

Hamilton's principle is based on scalar (not vector) functions that may be written directly in terms of independent generalized coordinates.
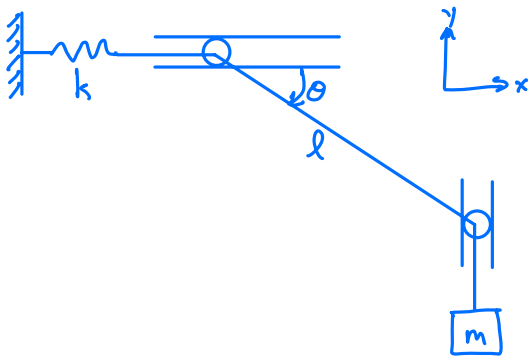
A massless bar is constrained to move as illustrated. Determine the EOM using Hamilton's principle.

$$T = \frac{1}{2}m\dot{y}^2$$

$$V = -mgy + \frac{1}{2}kx^2$$

$$\delta L = \delta T - \delta V = m\dot{y}\,\delta\dot{y} + mg\,\delta y - kx\,\delta x$$

$$\int_{t_1}^{t_2}\delta L = \int_{t_1}^{t_2}(m\dot{y}\,\delta\dot{y} + mg\,\delta y - kx\,\delta x)\,dt$$

$$= \int_{t_1}^{t_2}(-m\ddot{y}\,\delta y + mg\,\delta y - kx\,\delta x)\,dt$$

no variation at t_1 or t_2
$$\int_{t_1}^{t_2}m\dot{y}\,\delta\dot{y}\,dt = \cancel{m\dot{y}\,\delta y\Big|_{t_1}^{t_2}}^{0} - \int m\ddot{y}\,\delta y\,dt$$

$$\therefore\quad kx\,\delta x - m(g-\ddot{y})\,\delta y = 0 \quad \text{just as before if } \ddot{y} = 0$$

$$kl^2(1-\cos\theta)\sin\theta - mgl\cos\theta + ml^2(\ddot{\theta}\cos\theta - \dot{\theta}\sin\theta)\cos\theta = 0$$

$$ml(\ddot{\theta}\cos\theta - \dot{\theta}\sin\theta) - mg + kl(1-\cos\theta)\tan\theta = 0$$

Notice that, in the application of Hamilton's principle, we often perform integration by parts in order to eliminate the virtual velocities (i.e., by transferring the time derivative). The modest advancement that comes with Lagrange's equations is that this step is taken into account by construction.

This is achieved by considering a generic, rather than a specific, system:

$$T = T(q_1, q_2, \cdots, q_N, \dot{q}_1, \dot{q}_2, \cdots, \dot{q}_N)$$

kinetic energy is a function of generalized displacements and velocities.

$$W = -V(q_1, q_2, \cdots, q_N) + W_{nc}(q_1, q_2, \cdots, q_N)$$

work is a function of only generalized displacements

$$\delta T = \sum_{i=1}^{N}\left(\frac{\partial T}{\partial q_i}\delta q_i + \frac{\partial T}{\partial \dot{q}_i}\delta\dot{q}_i\right)$$

$$\delta W = \sum_{i=1}^{N}\left(-\frac{\partial V}{\partial q_i} + \frac{\partial W_{nc}}{\partial q_i}\right)\delta q_i$$

$$\int_{t_1}^{t_2}(\delta T + \delta W)\,dt = \int_{t_1}^{t_2}\sum_{i=1}^{N}\left(\frac{\partial T}{\partial q_i}\delta q_i + \frac{\partial T}{\partial \dot{q}_i}\delta\dot{q}_i - \frac{\partial V}{\partial q_i}\delta q_i + \frac{\partial W_{nc}}{\partial q_i}\delta q_i\right)dt = 0 \qquad [1]$$

The $\delta\dot{q}_i$ term prevents us from completing the derivation of the EOM, so we perform integration by parts.

$$\int_{t_1}^{t_2}\frac{\partial T}{\partial \dot{q}_i}\delta\dot{q}_i\,dt = \cancel{\frac{\partial T}{\partial \dot{q}_i}\delta q_i\Big|_{t_1}^{t_2}}^{0} - \int_{t_1}^{t_2}\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_i}\right)\delta q_i\,dt \qquad \text{substitute into } [1]$$

$$\int_{t_1}^{t_2} \sum_{i=1}^{N} \left(\frac{\partial T}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_i}\right) - \frac{\partial V}{\partial q_i} + \frac{\partial W_{nc}}{\partial q_i} \right) \delta q_i \, dt = 0$$

$$\therefore \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_i}\right) - \frac{\partial T}{\partial q_i} + \frac{\partial V}{\partial q_i} = \frac{\partial W_{nc}}{\partial q_i} \quad \text{or} \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = \frac{\partial W_{nc}}{\partial q_i} = Q_{nc,i}$$

Although Lagrange's equations apply to discrete and continuous systems alike, they are more convenient in the discrete context. Hamilton's principle is more convenient in continuous systems.
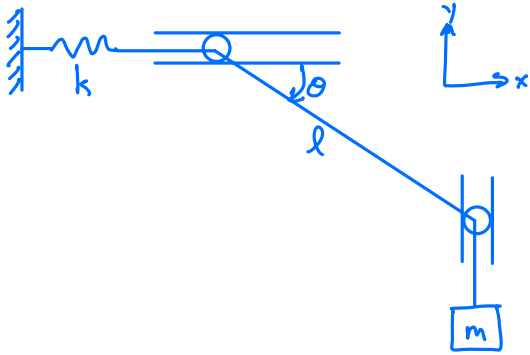
A massless bar is constrained to move as illustrated. Determine the EOM using d'Alembert's principle.

$$T = \frac{1}{2} m \dot{y}^2 = \frac{1}{2} m \ell^2 \cos^2\theta \, \dot{\theta}^2$$

$$V = mgy + \frac{1}{2} kx^2 = -mg\ell\sin\theta + \frac{1}{2} k\ell^2 (1-\cos\theta)^2$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_i}\right) - \frac{\partial T}{\partial q_i} + \frac{\partial V}{\partial q_i} = Q_{nc,i} = 0 \qquad q = \theta$$

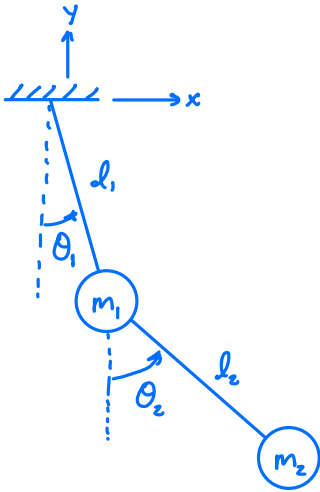$$\frac{\partial T}{\partial \dot{\theta}} = m\ell^2 \cos^2\theta \, \dot{\theta}$$

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\theta}}\right) = m\ell^2 \left(\cos^2\theta \, \ddot{\theta} - 2\sin\theta\cos\theta \, \dot{\theta}^2\right)$$

$$-\frac{\partial T}{\partial \theta} = m\ell^2 \sin\theta\cos\theta$$

$$\frac{\partial V}{\partial \theta} = -mg\ell\cos\theta + k\ell^2 (1-\cos\theta)\sin\theta$$

$$\therefore \ m\ell \left(\ddot{\theta}\cos\theta - \dot{\theta}^2\sin\theta\right) - mg + k\ell(1-\cos\theta)\tan\theta = 0$$

Hamilton's Principle Example (skipped)

$$T = \frac{1}{2}m_1(\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2}m_2(\dot{x}_2^2 + \dot{y}_2^2)$$

$$V = m_1 g y_1 + m_2 g y_2$$

$$\int_{t_1}^{t_2} \delta L \, dt = \int_{t_1}^{t_2} (m_1 \dot{x}_1 \delta \dot{x}_1 + m_1 \dot{y}_1 \delta \dot{y}_1 + m_2 \dot{x}_2 \delta \dot{x}_2 + m_2 \dot{y}_2 \delta \dot{y}_2 + m_1 g \delta y_1 + m_2 g \delta y_2) \, dt$$

$$= \int_{t_1}^{t_2} [-m_1 \ddot{x}_1 \delta x_1 - m_2 \ddot{x}_2 \delta x_2 + (-m_1 \ddot{y}_1 + m_1 g)\delta y_1 + (-m_2 \ddot{y}_2 + m_2 g)\delta y_2] \, dt$$

$$x_1 = \ell_1 \sin\theta_1 \qquad x_2 = \ell_1 \sin\theta_1 + \ell_2 \sin\theta_2$$
$$y_1 = -\ell_1 \cos\theta_1 \qquad y_2 = -\ell_1 \cos\theta_1 - \ell_2 \cos\theta_2$$

$$\dot{x}_1 = \ell_1 \cos\theta_1 \, \dot{\theta}_1 \qquad \dot{x}_2 = \ell_1 \cos\theta_1 \, \dot{\theta}_1 + \ell_2 \cos\theta_2 \, \dot{\theta}_2$$
$$\dot{y}_1 = \ell_1 \sin\theta_1 \, \dot{\theta}_1 \qquad \dot{y}_2 = \ell_1 \sin\theta_1 \, \dot{\theta}_1 + \ell_2 \sin\theta_2 \, \dot{\theta}_2$$

$$\ddot{x}_1 = -\ell_1 \sin\theta_1 \, \dot{\theta}_1^2 + \ell_1 \cos\theta_1 \, \ddot{\theta}_1 \qquad \ddot{x}_2 = -\ell_1 \sin\theta_1 \, \dot{\theta}_1^2 + \ell_1 \cos\theta_1 \, \ddot{\theta}_1 - \ell_2 \sin\theta_2 \, \dot{\theta}_2^2 + \ell_2 \cos\theta_2 \, \ddot{\theta}_2$$
$$\ddot{y}_1 = \ell_1 \cos\theta_1 \, \dot{\theta}_1^2 + \ell_1 \sin\theta_1 \, \ddot{\theta}_1 \qquad \ddot{y}_2 = \ell_1 \cos\theta_1 \, \dot{\theta}_1^2 + \ell_1 \sin\theta_1 \, \ddot{\theta}_1 + \ell_2 \cos\theta_2 \, \dot{\theta}_2^2 + \ell_2 \sin\theta_2 \, \ddot{\theta}_2$$

$$-m_1(-\ell_1 \sin\theta_1 \, \dot{\theta}_1^2 + \ell_1 \cos\theta_1 \, \ddot{\theta}_1)\ell_1 \cos\theta_1 \, \delta\theta_1 - m_2(-\ell_1 \sin\theta_1 \, \dot{\theta}_1^2 + \ell_1 \cos\theta_1 \, \ddot{\theta}_1 - \ell_2 \sin\theta_2 \, \dot{\theta}_2^2 + \ell_2 \cos\theta_2 \, \ddot{\theta}_2)(\ell_1 \cos\theta_1 \, \delta\theta_1 + \ell_2 \cos\theta_2 \, \delta\theta_2)$$

$$-m_1(\ell_1 \cos\theta_1 \, \dot{\theta}_1^2 + \ell_1 \sin\theta_1 \, \ddot{\theta}_1 - g)\ell_1 \sin\theta_1 \, \delta\theta_1 - m_2(\ell_1 \cos\theta_1 \, \dot{\theta}_1^2 + \ell_1 \sin\theta_1 \, \ddot{\theta}_1 + \ell_2 \cos\theta_2 \, \dot{\theta}_2^2 + \ell_2 \sin\theta_2 \, \ddot{\theta}_2 - g)\cdots$$

$$(\ell_1 \sin\theta_1 \, \delta\theta_1 + \ell_2 \sin\theta_2 \, \delta\theta_2)$$

Since $\delta\theta_1 \neq 0$, its coefficient must vanish:

$$(m_1 + m_2)\ell_1 \ddot{\theta}_1 + m_2 \ell_2 [\cos(\theta_1 - \theta_2)\ddot{\theta}_2 + \sin(\theta_1 - \theta_2)\dot{\theta}_2^2] + g(m_1 + m_2)\sin\theta_1 = 0$$

Notice the dual dependence on m_1 and m_2

Since $\delta\theta_2 \neq 0$, its coefficient must vanish:

$$\ell_2 \ddot{\theta}_2 + \ell_1[\ddot{\theta}_1 \cos(\theta_1 - \theta_2) - \dot{\theta}_1^2 \sin(\theta_1 - \theta_2)] + g\sin\theta_2 = 0$$

Notice the lack of dependence on m_1

TOPIC 2: Vibration in Discrete Systems

Before considering the dynamics of waves, we briefly discuss the related topic of vibrations. Consider a cork bobbing on the surface of a liquid as a wave passes. The cork oscillates in time similar to a vibrating system, a characteristic shared by every point in a wave. The cork represents the vibration of a discrete system. A continuous system may exhibit oscillations in space and time, just like a wave. However, a vibration represents an exchange of energy at a point, while a wave represents the flow of energy from one point in a system to another.
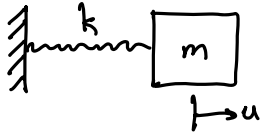
$$\sum F = m\ddot{u} = -ku \qquad \text{the force of the spring opposes the displacement of the mass}$$

$$m\ddot{u} + ku = 0$$

$$\ddot{u} + \omega_o^2 u = 0 \quad \longleftarrow \quad u = Ae^{dt} \qquad \omega_o^2 = k/m \quad \text{natural frequency}$$

$$(d^2 + \omega_o^2)u = 0 \qquad \therefore \qquad d = \pm i\omega_o$$

$$u = A_1 e^{i\omega_o t} + A_2 e^{-i\omega_o t} \qquad \text{since each value of } d \text{ is a solution, then the sum (i.e., superposition)}$$
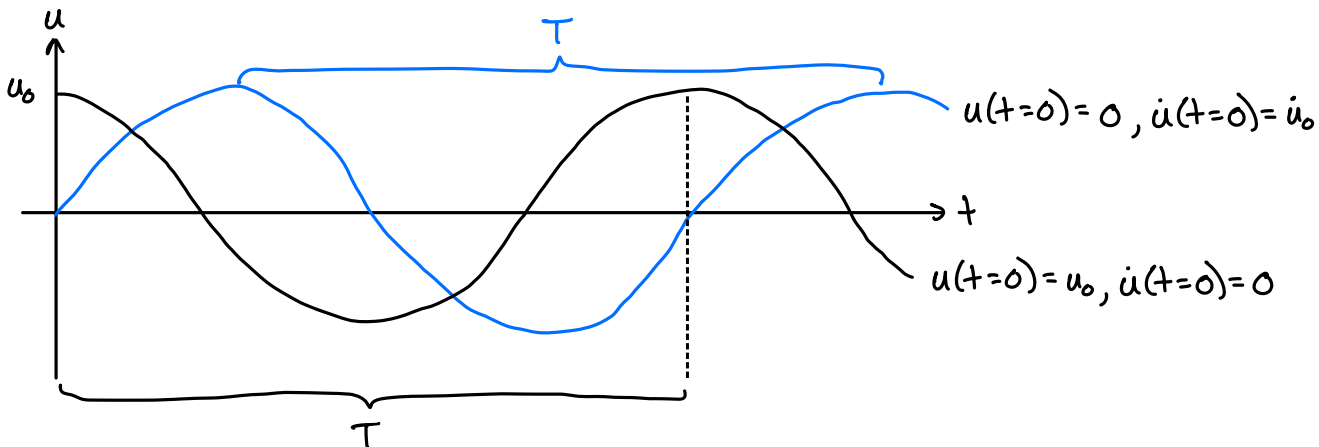$$\text{of each solution is also a solution}$$

$$u = A_1[\cos(\omega_o t) + i\sin(\omega_o t)] + A_2[\cos(\omega_o t) - i\sin(\omega_o t)] \qquad \text{Euler's formula: } e^{\pm i\phi} = \cos\phi \pm i\sin\phi$$

$$= (A_1 + A_2)\cos(\omega_o t) + (A_1 - A_2)i\sin(\omega_o t)$$

$$= C_1\cos(\omega_o t) + C_2\sin(\omega_o t) \qquad C_1, C_2 \text{ determined from initial conditions}$$

$$u(t=0) = C_1 = u_o$$

$$\dot{u}(t=0) = \omega_o C_2 = \dot{u}_o \qquad \therefore \qquad C_2 = \frac{\dot{u}_o}{\omega_o}$$

$$u(t=0) = 0, \ \dot{u}(t=0) = \dot{u}_o$$

$$u(t=0) = u_o, \ \dot{u}(t=0) = 0$$

$$\omega_o = \frac{2\pi}{T}$$

We've just solved an eigenvalue problem for the eigenvalue ω_0 (natural frequency). In MDOF systems, the concept of the mode shape (eigenvector) can be appreciated. Beyond the frequency the mode shape is the particular way in which a system vibrates: how the amplitude and phase of vibration of one DOF relates to that of others in the system. It is an expression of the efficient allocation of energy within a system.
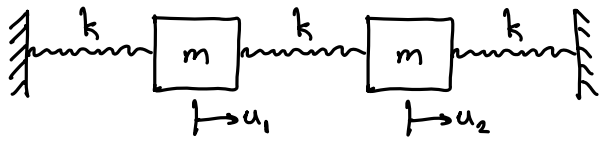
$$\sum F_1 = m\ddot{u}_1 = -2ku_1 + ku_2$$

$$\sum F_1 = m\ddot{u}_2 = ku_1 - 2ku_2$$

$$\begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix}\begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{bmatrix} + \begin{bmatrix} 2k & -k \\ -k & 2k \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \longleftarrow u = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}e^{i\omega t} = Xe^{i\omega t}$$

assume each mass oscillates with the same frequency.

$$M \quad \ddot{u} + \quad K \quad u = 0$$

$$-\omega^2\begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + \begin{bmatrix} 2k & -k \\ -k & 2k \end{bmatrix}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix}^{-1}\begin{bmatrix} 2k & -k \\ -k & 2k \end{bmatrix}}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \omega^2\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

D: dynamical matrix

A matrix transforms a vector (i.e., rotates and scales it). The EVP asks what vector X transforms into itself scaled by a factor ω.

$$|D| = m^2\omega^4 - 4km\omega^2 + 3k^2 = 0 \qquad \text{secular/characteristic equation}$$

$$\therefore \quad \omega^2 = \omega_1^2 = \frac{k}{m} \quad ; \quad \omega^2 = \omega_2^2 = \frac{3k}{m}$$

In general, a system with n discrete DOFs will possess n distinct natural frequencies, although in some cases, two natural frequencies may possess the same value (i.e., be degenerate). A mode shape is tied to each frequency.

$$\left(\frac{2k}{m} - \omega_n\right)X_1 - \frac{k}{m}X_2 = 0 \qquad \therefore \qquad \frac{X_2^{(n)}}{X_1^{(n)}} = \frac{2k - m\omega_n^2}{k} \longrightarrow \frac{X_2^{(1)}}{X_1^{(1)}} = 1 \quad ; \quad \frac{X_2^{(2)}}{X_1^{(2)}} = -1$$

mode n=1

mode n=2
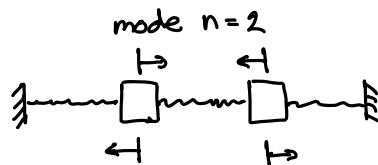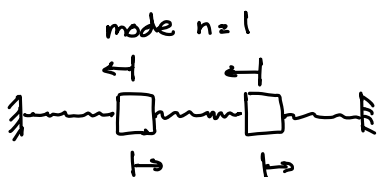
First mode: masses oscillate in phase.

Second mode: masses oscillate out-of-phase

$$E = T + V = \frac{1}{2}\dot{u}^T M \dot{u} + \frac{1}{2} u^T K u = \frac{1}{2} u^T (-\omega^2 M + K) u \longrightarrow dE = du^T(-\omega^2 M + K) u$$

Consider matching eigenvalue and eigenvector, e.g., ω_1^2 and $X^{(1)}$:

$$dE = du^T \underbrace{(-\omega_1^2 M + K) X^{(1)}}_{=0} e^{i\omega_1 t} = 0$$

The zero results from the EVP and indicates that no energy exchange is required to sustain a vibration in mode $X^{(1)}$ at ω_1.

Consider matching eigenvalue and eigenvector, e.g., ω_1^2 and $X^{(1)}$:

$$dE = du^T(-\omega_2^2 M + K) X^{(1)} e^{i\omega_2 t} = du^T \begin{bmatrix} \frac{2k}{m} - \frac{3k}{m} & -\frac{k}{m} \\ -\frac{k}{m} & \frac{2k}{m} - \frac{3k}{m} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} X_1^{(1)} e^{i\omega_2 t} = du^T \begin{bmatrix} -\frac{2k}{m} \\ -\frac{2k}{m} \end{bmatrix} X_1^{(1)} e^{i\omega_2 t} \neq 0$$

The non-zero indicates that a vibration in mode other than $X^{(1)}$ must be at a frequency ω_1 (and vice-versa); otherwise, energy must be (most likely) injected into the system (e.g., via forcing).

Eigenvalues and eigenvectors, ω_n^2 and $X^{(n)}$, occur in pairs and the $X^{(n)}$ are orthogonal to each other. Consider two $\omega_n, X^{(n)}$ pairs which satisfy the governing equations:

$$\omega_i^2 M \bar{X}^{(i)} = K \bar{X}^{(i)} \qquad \text{mode } i$$

$$\omega_j^2 M \bar{X}^{(j)} = K \bar{X}^{(j)} \qquad \text{mode } j$$

Premultiply the previous by the transpose of the opposite mode:

$$\omega_i^2 [\bar{X}^{(j)}]^T M \bar{X}^{(i)} = [\bar{X}^{(j)}]^T K X^{(i)} \equiv [\bar{X}^{(i)}]^T K X^{(j)}$$

$$- \omega_j^2 [\bar{X}^{(i)}]^T M \bar{X}^{(j)} \equiv \omega_j^2 [\bar{X}^{(j)}]^T M \bar{X}^{(i)} = [\bar{X}^{(i)}]^T K X^{(j)}$$

equivalence due to symmetry of M and K

$$(\omega_i^2 - \omega_j^2) [\bar{X}^{(j)}]^T M \bar{X}^{(i)} = 0$$

In general, $\omega_i^2 \neq \omega_j^2$, therefore $[X^{(j)}]^T M X^{(i)} = 0$ and, by extension, $[X^{(j)}]^T K X^{(i)} = 0$; thus $X^{(i)}$ and $X^{(j)}$ are orthogonal with respect to M and K. Similarly,

$$\omega_i^2 [X^{(j)}]^T X^{(i)} = [X^{(j)}]^T 0 X^{(i)} = [X^{(i)}]^T 0 X^{(j)}$$

$$- \omega_j^2 [X^{(i)}]^T X^{(j)} = \omega_j^2 [X^{(j)}]^T X^{(i)} = [X^{(i)}]^T 0 X^{(j)}$$

$$(\omega_i^2 - \omega_j^2)[X^{(j)}]^T X^{(i)} = 0 \qquad \text{orthogonality of normal modes}$$

Due to their orthogonality, the mode shapes (eigenvectors) form a basis in n-dimensional space, meaning that any other vector must be some linear combination of these vectors.

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = x\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + y\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + z\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

basis in 3D rectilinear space

If $\bar{u}$ is an arbitrary vector in n-dimensional space, it can be expressed as:

$$\bar{u} = \sum_{i=1}^{n} c_i \bar{X}^{(i)} \qquad c_i \text{ are constants ; this is the expansion theorem}$$

Premultiplying $\bar{u}$ by $[\bar{X}^{(i)}]^T M$ (or $[\bar{X}^{(i)}]^T K$) the value of c_i can be determined:

$$[\bar{X}^{(i)}]^T M \bar{u} = [\bar{X}^{(i)}]^T M \sum_{i=1}^{n} c_i \bar{X}^{(i)} = c_i [\bar{X}^{(i)}]^T M \bar{X}^{(i)} = c_i m_{ii} \qquad \therefore c_i = \frac{[\bar{X}^{(i)}]^T M \bar{u}}{m_{ii}}$$

drop the sum since $[\bar{X}^{(i)}]^T X^{(j)} = \delta_{ij}$ (orthogonality)

The expansion theorem is very useful in finding the response of MDOF systems subject to arbitrary forcing by decoupling the system of equations following a procedure called modal analysis.

Looking at $-\omega^2 M \bar{X} + K \bar{X} = 0$, it is apparent that the EOM are coupled by way of K. The coupling depends on the coordinates we use. It is possible to choose coordinates which uncouple the EOM.

$$\text{Let } \bar{u} = \sum_{i=1}^{n} c_i \bar{X}^{(i)} = \underbrace{[\bar{X}^{(1)} \ \bar{X}^{(2)} \ \bar{X}^{(3)} \ldots]}_{\text{transformation matrix}} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix} = X \bar{c}$$

coordinate vector (principal coordinates)

$$M\ddot{u} + Ku = MX\ddot{\bar{c}} + KX\bar{c} = \bar{F}$$

As we have seen, $[\bar{X}^{(i)}]^T M \bar{X}^{(i)} = m_{ii}$ and $[\bar{X}^{(i)}]^T K \bar{X}^{(i)} = k_{ii}$ diagonalize M and K. Let's premultiply the above by X^T.

modal mass   modal stiffness

$$X^T M X \ddot{\bar{c}} + X^T K X \bar{c} = M_D \ddot{\bar{c}} + K_D \bar{c} = m_{ii}\ddot{c}_i + k_{ii} c_i = f_i$$

since the equations are uncoupled, we can solve them one-by-one... no complicated inverse or determinant needed.

$$m_{ii}\ddot{c}_i + k_{ii} c_i = f_i = 0 \quad \longleftarrow \quad \bar{c} = \bar{C}e^{i\omega t}$$

$$(-\omega^2 m_{ii} + k_{ii}) c_i = 0 \qquad \therefore \omega^2 = \frac{k_{ii}}{m_{ii}} = \omega_i^2$$

Recall our previous problem. Let's apply the expansion theorem / modal analysis.

$$\bar{X}^{(1)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \; ; \; \bar{X}^{(2)} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad \therefore \; \underline{X} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\underline{X}^T M \underline{X} \ddot{\bar{c}} + \underline{X}^T K \underline{X} \bar{c} = \begin{bmatrix} 2m & 0 \\ 0 & 2m \end{bmatrix} \begin{bmatrix} \ddot{c}_1 \\ \ddot{c}_2 \end{bmatrix} + \begin{bmatrix} 2k & 0 \\ 0 & 6k \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \longrightarrow \begin{cases} -2m\omega^2 c_1 + 2kc_1 = 0 & \therefore \; \omega^2 = \omega_1^2 = \dfrac{k}{m} \\ -2m\omega^2 c_2 + 6kc_2 = 0 & \therefore \; \omega^2 = \omega_2^2 = \dfrac{3k}{m} \end{cases}$$

just as before

# TOPIC 3:
Vibration in Continuous Systems

Although most of the course is presented from the perspective of discrete systems with finite degrees of freedom, it is still worthwhile to, at times, consider continuous systems of infinite degrees of freedom.

degrees of freedom (DOFs): count the minimum number of independent coordinates necessary to describe the state of all parts of the system over time.
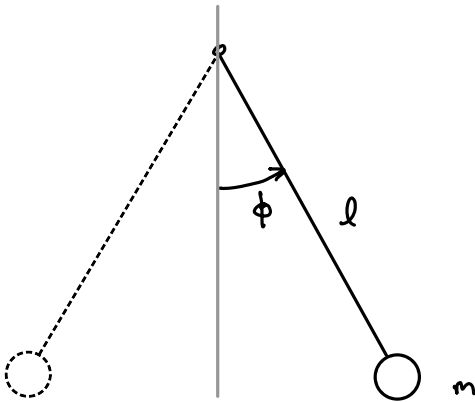
The pendulum is a SIDOF system provided the tether is inextensible, then $\phi(t)$ is the only DOF (polar/cylindrical coordinates).

In Cartesian coordinates, $x(t)$ and $y(t)$ are not independent, but related (i.e., constrained) by $x^2 + y^2 = l^2$; thus one coordinate sets the other.
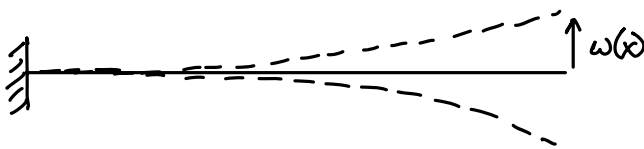
$\uparrow w(x)$ The cantilever is a continuous system

| Discrete	Continuous
finite # DOFs	infinite # DOFs
finite # natural freqs./shapes	infinite # natural freqs./mode shapes
formulated as Diff Eqs. (easy to solve)	formulated as PDEs (generally difficult to solve)
lumped/concentrated material parameters	distributed material parameters (i.e., functions of position)

We study vibration in continuous systems from the simplest 1D examples – rods, shafts, and strings – that share governing equations of identical form.

$\rightarrow u$
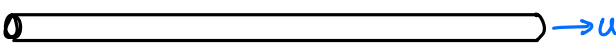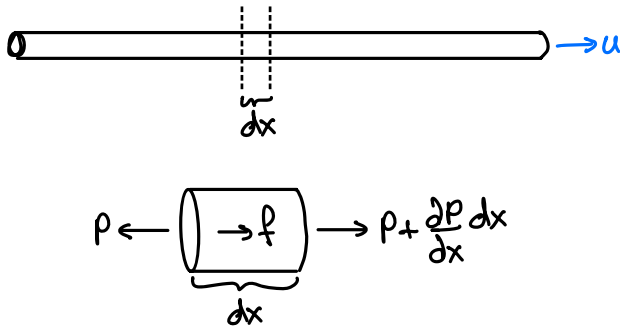
rod: longitudinal displacements, u, and loads, f
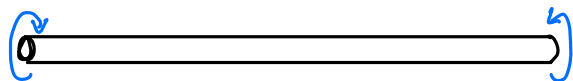
shaft: angular displacements, θ, and loads, τ

string: transverse displacements, w, and loads, f

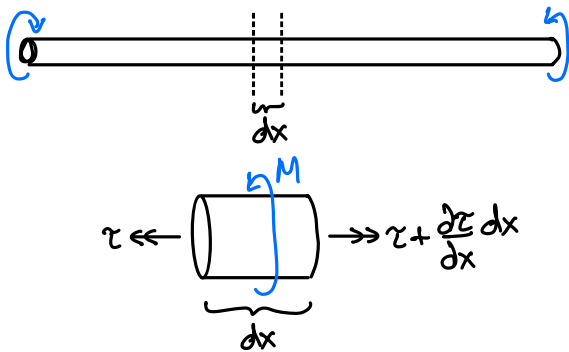**rod:** longitudinal displacements, u, and loads, f

$$\Sigma F_x = \rho A\, dx\, \frac{\partial^2 u}{\partial t^2} = -P + \left(P + \frac{\partial P}{\partial x}dx\right) + f\, dx$$

$$\therefore\ \rho A \frac{\partial^2 u}{\partial t^2} = \frac{\partial P}{\partial x} + f \quad\longleftarrow\quad P = \sigma_x A = EA\frac{\partial u}{\partial x}$$

$$\rho A \frac{\partial^2 u}{\partial t^2} = EA\frac{\partial^2 u}{\partial x^2} + f$$

shaft: angular displacements, θ, and loads, τ

$$\Sigma M = J\, dx\, \frac{\partial^2 \theta}{\partial t^2} = -\tau + \left(\tau + \frac{\partial \tau}{\partial x}dx\right) + M\, dx$$

$$\therefore\ J\frac{\partial^2 \theta}{\partial t^2} = \frac{\partial \tau}{\partial x} + M \quad\longleftarrow\quad \tau = k_\theta G\frac{\partial \theta}{\partial x}$$

$$J\frac{\partial^2 \theta}{\partial t^2} = k_\theta G\frac{\partial^2 \theta}{\partial x^2} + M$$

string: transverse displacements, ω, and loads, f

$$\Sigma F_y = \rho\, ds\, \frac{\partial^2 \omega}{\partial t^2} = -T\sin\theta + \left(T + \frac{\partial T}{\partial s}ds\right)\sin\left(\theta + \frac{\partial \theta}{\partial s}ds\right) + f\, ds$$

assume small θ such that $ds \approx dx$

$$\rho\, ds\, \frac{\partial^2 \omega}{\partial t^2} = -T\theta + \left(T + \frac{\partial T}{\partial x}dx\right)\left(\theta + \frac{\partial \theta}{\partial x}dx\right) + f\, dx$$

$$\rho\, ds\, \frac{\partial^2 \omega}{\partial t^2} = \theta\frac{\partial T}{\partial x}dx + T\frac{\partial \theta}{\partial x}dx + \underbrace{\frac{\partial T}{\partial x}\frac{\partial \theta}{\partial x}dx^2}_{\approx 0} + f\, dx$$

$$\rho\, dx\, \frac{\partial^2 \omega}{\partial t^2} = \theta\frac{\partial T}{\partial x}dx + T\frac{\partial \theta}{\partial x}dx = \frac{\partial}{\partial x}(\theta T)dx + f\, dx$$

$$\sin\theta = \frac{\partial \omega}{\partial x} \approx \theta$$

$$\rho\frac{\partial^2 \omega}{\partial t^2} = \frac{\partial}{\partial x}\left(T\frac{\partial \omega}{\partial x}\right) + f$$

$$\rho\frac{\partial^2 \omega}{\partial t^2} = T\frac{\partial^2 \omega}{\partial x^2} + f \qquad \text{For } T \text{ sufficiently large, small } \omega \text{ has a vanishing affect on } T; \text{ thus } T \approx \text{const.}$$

$\rho A, EA \longleftrightarrow J, k_\theta G \longleftrightarrow \rho, T$
rod   shaft   string

we continue with the rod system absent loading, but the results extend to the shaft and string systems

The standard method of solution employs the separation of variables, $u(x,t) = P(x) Q(t)$.

$$P\frac{\partial^2 Q}{\partial t^2} = c_0^2 Q \frac{\partial^2 P}{\partial x^2} \longrightarrow \frac{1}{Q}\frac{\partial^2 Q}{\partial t^2} = \frac{c_0^2}{P}\frac{\partial^2 P}{\partial x^2} \qquad c_0 = \sqrt{\frac{E}{\rho}} \quad \text{speed of sound}$$

Since the LHS is a function of t only and the RHS is a function of x only, then the equation can only be valid if each side is equal to a constant.

$$\underset{\downarrow}{\text{LHS}} \quad \underset{\downarrow}{c_0^2} \quad \underset{\downarrow}{\text{RHS}}$$
$$[1/s^2] = [m^2/s^2][1/m^2] \qquad \frac{1}{Q}\frac{\partial^2 Q}{\partial t^2} = -\omega^2 \; [1/s^2] \qquad \frac{1}{P}\frac{\partial^2 P}{\partial t^2} = -\kappa^2 \; [1/m^2] \qquad \left(\frac{\omega}{\kappa}\right)^2 = c_0^2$$

$$\frac{\partial^2 Q}{\partial t^2} + \omega^2 Q = 0 \qquad \frac{\partial^2 P}{\partial x^2} + \kappa^2 P = 0 \qquad$$

equations are of same form as a SDOF, $\ddot{u} + \omega_0^2 u = 0$; therefore, we can assume the same form of solution: $Q(t) = A e^{st}$ and $P(x) = B e^{rx}$.

$$s^2 + \omega^2 = 0 \quad \therefore \quad s = \pm i\omega \qquad Q(t) = A_1 e^{i\omega t} + A_2 e^{-i\omega t} \longrightarrow C_1 \cos(\omega t) + C_2 \sin(\omega t)$$

$$r^2 + \kappa^2 = 0 \quad \therefore \quad r = \pm i\kappa \qquad P(x) = B_1 e^{i\kappa x} + B_2 e^{-i\kappa x} \longrightarrow D_1 \cos(\kappa x) + D_2 \sin(\kappa x)$$

$$u(x,t) = P(x) Q(t) = [B_1 e^{i\kappa x} + B_2 e^{-i\kappa x}][A_1 e^{i\omega t} + A_2 e^{-i\omega t}]$$

$$= A_1 B_1 e^{i(\kappa x + \omega t)} + A_2 B_1 e^{i(\kappa x - \omega t)} + A_1 B_2 e^{-i(\kappa x - \omega t)} + A_2 B_2 e^{-i(\kappa x + \omega t)}$$

$$= C_1 e^{i(\kappa x + \omega t)} + C_2 e^{-i(\kappa x + \omega t)} + C_3 e^{i(\kappa x - \omega t)} + C_4 e^{-i(\kappa x - \omega t)}$$

$$= [W\cos(\kappa x) + X\sin(\kappa x)][Y\cos(\omega t) + Z\sin(\omega t)]$$

from initial conditions

from boundary conditions

Presently, the above represents an infinite system since x is unbounded. Vibration problems concern finite systems. Since the PDE is second-order in space and time, the solution $u(x,t)$ requires two boundary and two initial conditions:

$$u(x=a, t) = u_a(t) \quad \text{and} \quad \frac{\partial u}{\partial x}(x=b, t) = u_b(t) \qquad \text{boundary conditions} \qquad \forall t$$

$$u(x, t=0) = u_0(x) \quad \text{and} \quad \frac{\partial u}{\partial t}(x, t=0) = \dot{u}_0(x) \qquad \text{initial conditions} \qquad \forall x$$

If the rod is fixed at both ends, then $P(0) = P(\ell) = 0$

$P(0) = W = 0$; $P(\ell) = W\cos(k\ell) + X\sin(\kappa\ell) = 0$ $\quad \therefore \quad K_n\ell = n\pi \quad n = 0, 1, 2, \ldots$

$\omega = Kc_0 \quad \therefore \quad K_n\ell = \dfrac{\omega_n\ell}{c_0} = n\pi \quad \therefore \quad \omega_n = K_n c_0 \quad$ $n=1$: fundamental mode $\quad$ (n=0: rigid body mode)
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ ω_1: fundamental frequency
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ K_1: fundamental wavenumber

$\qquad\qquad\qquad\qquad XY \qquad\qquad\qquad\quad XZ$
$\qquad\qquad\qquad\qquad \downarrow \qquad\qquad\qquad\quad \downarrow$
$u_n(x,t) = \sin(k_n x)\left[C_n \cos\left(\dfrac{nc_0\pi}{\ell}t\right) + D_n \sin\left(\dfrac{nc_0\pi}{\ell}t\right)\right] \qquad$ nth solution is called the nth harmonic/normal mode

$u(x,t) = \displaystyle\sum_{n=1}^{\infty} u_n(x,t) \qquad$ general solution; gives all possible vibrations via superposition; the particular
$\qquad\qquad\qquad\qquad\qquad$ vibration that occurs is uniquely determined by initial conditions

Consider the mode shapes $P_n(x)$
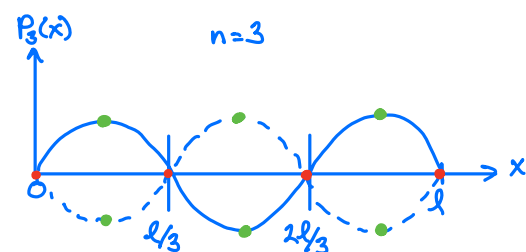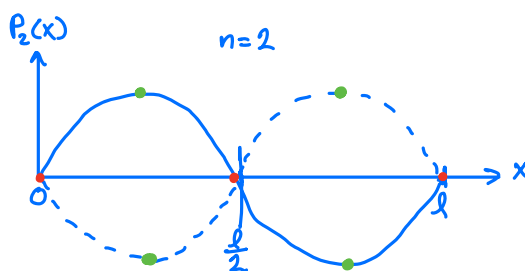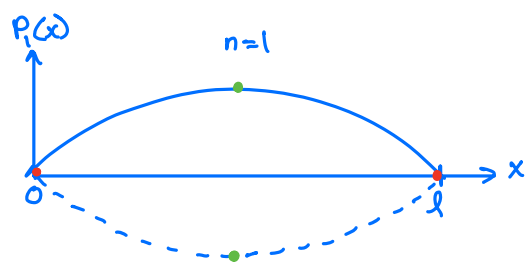
The points $P_n(x) = 0$ are the nodes

$P_n(x) = 0$ if $K_n x = \dfrac{n\pi}{\ell}x = m\pi \quad \therefore \quad x = \dfrac{m\ell}{n}; \ m = 0, 1, 2 \ldots (x \le \ell)$

The points $P_n(x)$ is maximal are the anti-nodes

$\max[P_n(x)]$ if $K_n x = \dfrac{n\pi}{\ell}x = m\dfrac{\pi}{2} \quad \therefore \quad x = \dfrac{m\ell}{2n}$

The orthogonality of normal modes in discrete systems extends to continuous systems as well, although it is most simply proven in 1D. For continuous systems, boundary conditions must be explicitly accounted for (they are automatically accounted for in discrete systems). Consider a rod:

$\dfrac{\partial^2 u}{\partial t^2} = c_0^2 \dfrac{\partial^2 u}{\partial x^2} \quad \longleftarrow \quad u_n(x,t) = P_n(x)[Y_n\cos(\omega_n t) + Z_n\sin(\omega_n t)]$

$-\omega_n^2 P_n(x) = c_0^2 P_n''(x)$

$-K_n^2 P_n(x) = P_n''(x)$

Let's consider the eigenfunctions $P_i(x)$ and $P_j(x)$ corresponding to ω_i and ω_j.

$P_i'' = -K_i^2 P_i \quad \underrightarrow{\text{multiply by } P_j \text{ and integrate}} \quad \displaystyle\int_0^\ell P_i'' P_j \, dx = -K_i^2 \int_0^\ell P_i P_j \, dx$

$P_j'' = -K_j^2 P_j \quad \underrightarrow{\text{multiply by } P_i \text{ and integrate}} \quad \displaystyle\int_0^\ell P_j'' P_i \, dx = -K_j^2 \int_0^\ell P_j P_i \, dx$

$$\int_0^\ell P_i'' P_j \, dx = P_i' P_j \Big|_0^\ell - \int_0^\ell P_i' P_j' \, dx = -\kappa_i^2 \int_0^\ell P_i P_j \, dx$$

$$\int_0^\ell P_j'' P_i \, dx = P_j' P_i \Big|_0^\ell - \int_0^\ell P_j' P_i' \, dx = -\kappa_j^2 \int_0^\ell P_j P_i \, dx$$

For a fixed end, $P = 0$; for a free end, $P' = 0$. Let's assume either both ends fixed or both ends free, then

$$\int_0^\ell P_i' P_j' \, dx = \kappa_i^2 \int_0^\ell P_i P_j \, dx$$

$$- \int_0^\ell P_j' P_i' \, dx = \kappa_j^2 \int_0^\ell P_j P_i \, dx$$

$$(\kappa_i^2 - \kappa_j^2) \int_0^\ell P_i P_j \, dx = 0 \qquad \text{For } \kappa_i \neq \kappa_j, \text{ then } \int_0^\ell P_i P_j \, dx = 0$$

Just as the orthogonality of eigenvectors supports the expansion theorem in discrete systems, orthogonal eigenfunctions support the expansion theorem for continuous systems. Any set of functions that form an orthogonal basis has a corresponding Fourier series including sines and cosines that are easy to handle.

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)] \qquad \text{Fourier approximation of } f(x)$$

$$\left. \begin{array}{l} \displaystyle\int_{-\pi}^{\pi} \sin(mx) \sin(nx) \, dx = \pi \delta_{mn} \\[2em] \displaystyle\int_{-\pi}^{\pi} \cos(mx) \cos(nx) \, dx = \pi \delta_{mn} \\[2em] \displaystyle\int_{-\pi}^{\pi} \sin(mx) \cos(nx) \, dx = 0 \end{array} \right\} \text{orthogonality of trigonometric functions}$$

To extract the a_n and b_n components of a Fourier expansion, simply multiply $f(x)$ by $\cos(nx)$ and $\sin(nx)$, respectively, and integrate $x \in [-\pi, \pi]$.

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) \, dx = \frac{a_0}{2\pi} \int_{-\pi}^{\pi} \cos(nx) \, dx + \frac{a_n}{\pi} \int_{-\pi}^{\pi} \cos(nx) \cos(nx) \, dx + \frac{b_n}{\pi} \int_{-\pi}^{\pi} \sin(nx) \cos(nx) \, dx$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(nx) \, dx = \frac{a_0}{2\pi} \int_{-\pi}^{\pi} \sin(nx) \, dx + \frac{a_n}{\pi} \int_{-\pi}^{\pi} \cos(nx) \sin(nx) \, dx + \frac{b_n}{\pi} \int_{-\pi}^{\pi} \sin(nx) \sin(nx) \, dx$$

$$\frac{a_0}{2} = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x)\,dx \qquad \text{average of } f(x) \text{ over } x \in [-\pi, \pi]$$

For 1D vibration problems, the problem domain is typically in the range $x \in [0, \ell]$, not $x \in [-\pi, \pi]$. Let's use $\eta \in [0, \ell]$ as our problem domain variable, then:

$$x = \frac{2\pi}{2\ell}\eta = \frac{\pi}{\ell}\eta \qquad \therefore \quad dx = \frac{\pi}{\ell}d\eta$$

↖ recall that the fundamental mode is only half a wavelength

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x)\cos(nx)\,dx \longrightarrow \left(\frac{1}{\pi}\right)\left(\frac{2\pi}{\ell}\right)\int_0^\ell f(\eta)\cos\left(n\frac{2\pi}{\ell}\eta\right)d\eta$$

The particular vibration that occurs is determined by the initial conditions which provide an initial distribution of energy within the system. For the rod problem, consider the following initial conditions:
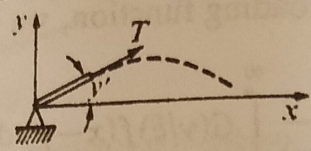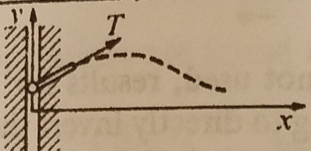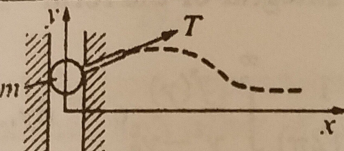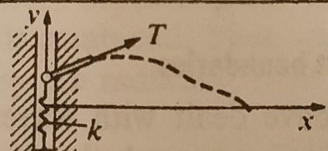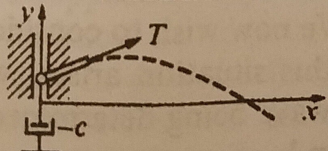
initial displacement: $u(x, t=0) = u_0(x) = \sum_{n=1}^{\infty} C_n \sin(k_n x)$

initial velocity: $\dot{u}(x, t=0) = \dot{u}_0(x) = \sum_{n=1}^{\infty} D_n \underbrace{\left(\frac{n\pi c_0}{\ell}\right)}_{\omega_n} \sin(k_n x) = \sum_{n=1}^{\infty} D_n \omega_n \sin(k_n x)$

Using the orthogonality of trigonometric functions:

$$C_n = \frac{2}{\ell} \int_0^\ell u_0(x)\sin(k_n x)\,dx \qquad D_n = \left(\frac{1}{\omega_n}\right)\left(\frac{2}{\ell}\right)\int_0^\ell \dot{u}_0(x)\sin(k_n x)\,dx \qquad n = 1, 2, 3, \ldots$$

TABLE 1.1

Type	Diagram	Equation
Fixed		$y(0,t)=0$
Free		$\dfrac{\partial y(0,t)}{\partial x}=0$
Mass		$m\ddot{y}(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$
Spring		$ky(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$
Dashpot		$c\dot{y}(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$

TOPIC 4:
Properties of Waves

A wave is a disturbance within a medium that propagates at a characteristic speed and, in doing so, transmits energy (and information) from one location to another. Waves are ubiquitous in nature and engineering; thus the import of their study. In this course, we focus on waves in elastic media.

$$\frac{\partial^2 u}{\partial t^2} = c_0^2 \frac{\partial^2 u}{\partial x^2} \qquad \text{wave equation}$$

$$u(x,t) = P(x)Q(t) = [B_1 e^{ikx} + B_2 e^{-ikx}][A_1 e^{i\omega t} + A_2 e^{-i\omega t}]$$

$$= C_1 e^{i(kx+\omega t)} + C_2 e^{-i(kx+\omega t)} + C_3 e^{i(kx-\omega t)} + C_4 e^{-i(kx-\omega t)} \qquad \text{general solution}$$

Consider a typical term of the general solution:

$$u(x,t) = Ce^{i(kx-\omega t)} = Ce^{i\phi} \qquad \phi \text{ is the phase}$$
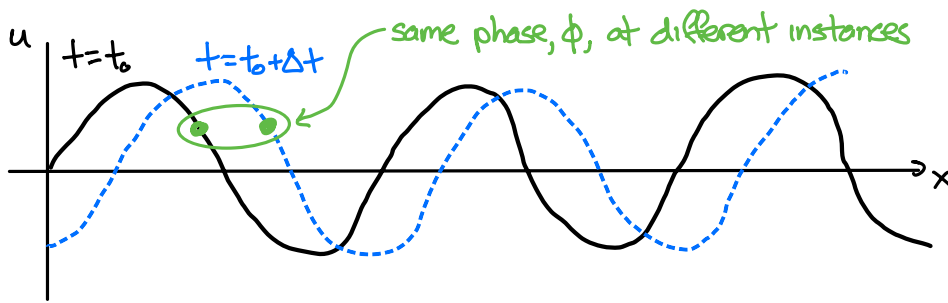
In order for the disturbance to propagate without a change to its profile (i.e., shape), all phases must move with the same velocity, v_p.

$$\phi = kx \pm \omega t \qquad \text{phase at arbitrary initial } x \text{ and } t$$

$$= k(x+\Delta x) \pm \omega(t+\Delta t) \qquad \text{phase after } \Delta t$$

$$= kx \pm \omega t + \underbrace{k\Delta x \pm \omega \Delta t}_{=0} \qquad \therefore \qquad \frac{\Delta x}{\Delta t} = \mp \frac{\omega}{k} = \mp c_0$$

For arbitrary Δt, in order to prevent distortion, Δx ensures $k\Delta x \pm \omega \Delta t = 0$. Each phase moves with velocity $v_p = \pm \frac{\omega}{k} = \pm c_0$. The +/- indicates propagation to the left/right.

Although, we have represented the disturbance with a sinusoidal profile, in general, the behavior of an arbitrary continuous profile (which can be decomposed in Fourier series) is the same: no distortion is observed since each of the Fourier components propagates with the same v_p.

Apparently, the general solution comprises both left- and right-propagating waves. If a vibration represents energy confined to a particular region, then it may be expected that, without imposed boundary conditions, the general solution represents the dynamics of an infinite medium in which energy cannot be confined in the form of a vibration. However, vibration in the form of a standing wave (i.e., $v_p = 0$) results from two counter-propagating waves of equal amplitude:

$$u(x,t) = A e^{i(kx+\omega t)} + A e^{i(kx-\omega t)}$$

$$= A\cos(kx+\omega t) + iA\sin(kx+\omega t) + A\cos(kx-\omega t) + iA\sin(kx-\omega t)$$

$$= 2A\cos(kx)\cos(\omega t) + 2iA\sin(kx)\cos(\omega t)$$

In considering the propagation of energy, we must derive an expression for the energy per element, dx, of the rod, i.e., the energy density.

$$dT = \frac{1}{2}(\rho A dx)\dot{u}^2 \qquad \text{differential kinetic energy}$$

$$dV = \frac{1}{2}\sigma_x \varepsilon_x A dx = \frac{1}{2}EA\varepsilon_x^2 dx = \frac{1}{2}EA\left(\frac{du}{dx}\right)^2 dx \qquad \text{differential potential energy}$$

$$\frac{\partial T}{\partial x} = \frac{1}{2}\rho A \dot{u}^2 \qquad \frac{\partial V}{\partial x} = \frac{1}{2}EA\left(\frac{du}{dx}\right)^2 \qquad \frac{\partial E}{\partial x} = \frac{\partial T}{\partial x} + \frac{\partial V}{\partial x} \left.\right\} \begin{array}{l}\text{kinetic, potential, and total}\\ \text{energies per unit length}\end{array}$$

Consider the effect of a waveform, $u(x,t) = f(kx-\omega t) = f(\phi)$, propagating to either the left or right in terms of energy:

$$\frac{\partial T}{\partial x} = \frac{1}{2}\omega^2 \rho A \frac{\partial^2 f}{\partial \phi^2} = \frac{1}{2}k^2 c_0^2 \rho A \frac{\partial^2 f}{\partial \phi^2} = \frac{1}{2}k^2 EA\frac{\partial^2 f}{\partial \phi^2} \qquad \frac{\partial V}{\partial x} = \frac{1}{2}k^2 EA\frac{\partial^2 f}{\partial \phi^2}$$

$\frac{\partial T}{\partial x} = \frac{\partial V}{\partial x}$ indicates that the wave energy is equally-divided among kinetic and potential components

Recall: $F = -\frac{\partial V}{\partial \varepsilon} = -EA\frac{du}{dx} \qquad v = \frac{du}{dt} \qquad P = Fv = -EA\frac{du}{dx}\frac{du}{dt} \quad$ power flow

Consider the power flow associated with left- and right-propagating waves, $f_1 = f(\kappa x + \omega t)$ and $f_2 = f(\kappa x - \omega t)$, crossing a boundary at $x = x_0$.
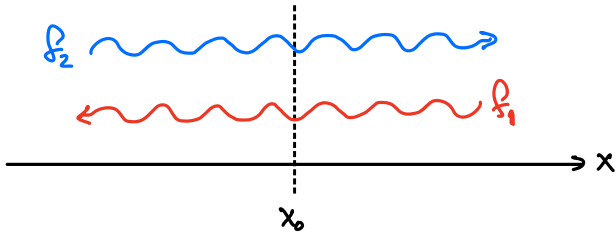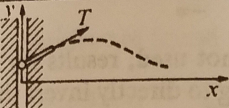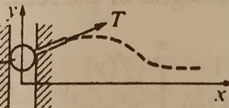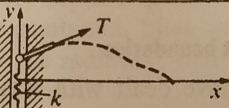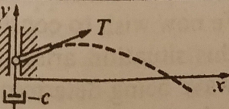

energy flows in the direction of propagation

$$P = -EA \frac{\partial u}{\partial x} \frac{\partial u}{\partial t}\Big|_{x=x_0} = -\kappa\omega EA \left(\frac{\partial f_1}{\partial \phi}\right)^2\Big|_{x=x_0} = -\kappa^2 c_0 EA \left(\frac{\partial f_1}{\partial \phi}\right)^2\Big|_{x=x_0}$$

energy leaving the region $x \geq x_0$

$$P = -EA \frac{\partial u}{\partial x} \frac{\partial u}{\partial t}\Big|_{x=x_0} = \kappa\omega EA \left(\frac{\partial f_2}{\partial \phi}\right)^2\Big|_{x=x_0} = \kappa^2 c_0 EA \left(\frac{\partial f_2}{\partial \phi}\right)^2\Big|_{x=x_0}$$

energy entering the region $x \geq x_0$

Let $u = f_1 + f_2$, then:
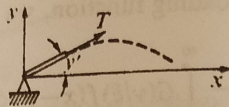
$$P = -EA \frac{\partial u}{\partial x} \frac{\partial u}{\partial t}\Big|_{x=x_0} = \kappa\omega EA \left[\left(\frac{\partial f_2}{\partial \phi}\right)^2 - \left(\frac{\partial f_1}{\partial \phi}\right)^2\right]\Big|_{x=x_0}$$

if f_1 and f_2 are of different amplitudes, then $P \neq 0$; thus energy either enters or leaves the region $x \geq x_0$

if f_1 and f_2 are of equal amplitude, then $P = 0$; thus no energy flows under vibration

The solution to problems of vibration in finite structures includes the imposition of boundary conditions. For the finite rod, these are traditionally: fixed-fixed, free-free, and fixed-free. However, other conditions are possible.

TABLE 1.1

Type	Diagram	Equation
Fixed		$y(0,t)=0$
Free		$\dfrac{\partial y(0,t)}{\partial x}=0$
Mass		$m\ddot{y}(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$
Spring		$ky(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$
Dashpot		$c\dot{y}(0,t)=T\dfrac{\partial y(0,t)}{\partial x}$

For a semi-infinite rod, there is only one boundary to consider and wave may approach this boundary and interact with it.

The reflection of an incident wave from a fixed boundary represents the simplest type of boundary interaction. Consider a disturbance, $u_i = f(\kappa x - \omega t)$, propagating to the right and incident on a fixed boundary. Since the wave energy is not transmitted across or dissipated/stored at the boundary, we may expect the wave energy to be reflected back in the form, $u_r = g(\kappa x + \omega t)$, toward the origin of the incident wave.

u_r

u_i
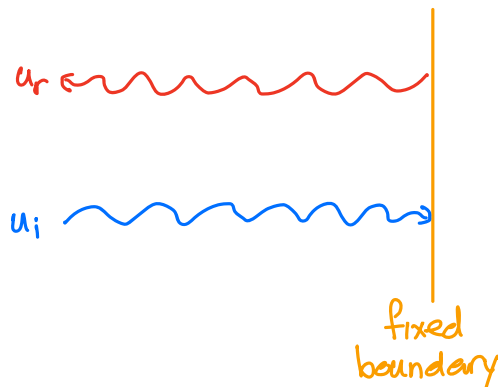
fixed
boundary

$\left. \begin{array}{l} u_i + u_r = 0 \\ \dot{u}_i + \dot{u}_r = 0 \end{array} \right\}$ at the fixed boundary, we expect the displacement and velocity to be zero

Let $u_i = f(\kappa x - \omega t) = f(\phi)$ and $u_r = g(\kappa x + \omega t) = g(\theta)$

$\dot{u}_i + \dot{u}_r = -\omega\left(\dfrac{\partial f}{\partial \phi} - \dfrac{\partial g}{\partial \theta}\right) = 0$ $\quad \therefore \quad$ $\dfrac{\partial g}{\partial \theta} = \dfrac{\partial f}{\partial \phi}$ $\quad$ this establishes that the reflected wave is identical to the incident wave
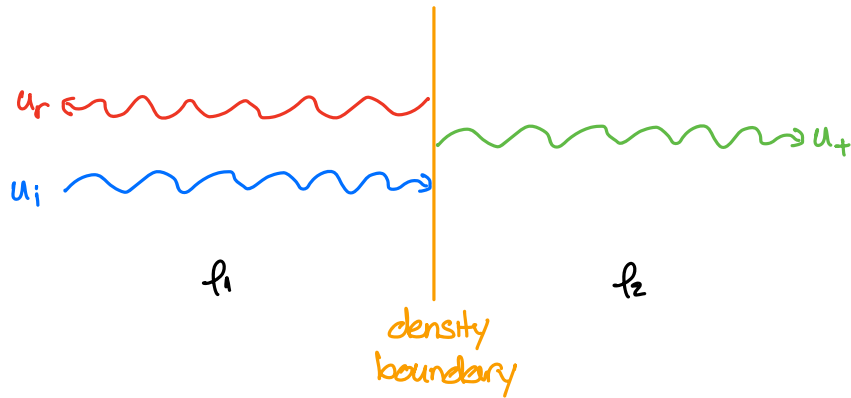
density boundary

Consider a disturbance, $u_i = f_1(\kappa_1 x - \omega_1 t) = f(\phi)$, incident on a material boundary separating two densities, ρ_1 and ρ_2. Such a scenario is capable of producing a reflected wave, $u_r = g(\kappa_1 x + \omega_1 t) = g(\theta)$, within the same medium that propagates with velocity, $c_1 = \omega_1/\kappa_1 = \sqrt{E/\rho_1}$, as well as permitting some energy transmission via $u_+ = f_2(\kappa_2 x - \omega_2 t) = f_2(\gamma)$ that propagates with velocity, $c_2 = \omega_2/\kappa_2 = \sqrt{E/\rho_2}$.

$\dot{u}_i + \dot{u}_r = u_+$

$\cancel{EA}\left(\dfrac{\partial u_i}{\partial x} + \dfrac{\partial u_r}{\partial x}\right) = \cancel{EA}\dfrac{\partial u_+}{\partial x}$ $\left.\right\}$ this scenario requires continuity of displacement (or velocity) and force at the boundary

$\dot{u}_i + \dot{u}_r = \dot{u}_+ \longrightarrow \omega_1\left(\dfrac{\partial f_1}{\partial \phi} - \dfrac{\partial g}{\partial \theta}\right) = \omega_2\dfrac{\partial f_2}{\partial \gamma} \left.\right\}$

$\dfrac{\partial u_i}{\partial x} + \dfrac{\partial u_r}{\partial x} = \dfrac{\partial u_+}{\partial x} \longrightarrow \kappa_1\left(\dfrac{\partial f_1}{\partial \phi} + \dfrac{\partial g}{\partial \theta}\right) = \kappa_2\dfrac{\partial f_2}{\partial \gamma}$
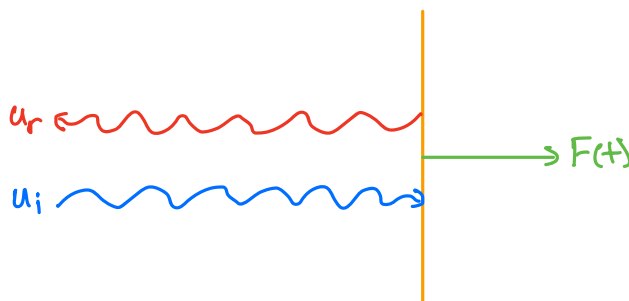
$\dfrac{\partial g}{\partial \theta} = \left(\dfrac{\kappa_2\omega_1 - \kappa_1\omega_2}{\kappa_2\omega_1 + \kappa_1\omega_2}\right)\dfrac{\partial f_1}{\partial \phi}$; $\quad$ $\dfrac{\partial f_2}{\partial \gamma} = \dfrac{2\kappa_1\omega_1}{\kappa_2\omega_1 + \kappa_1\omega_2}\dfrac{\partial f_1}{\partial \phi}$

R: reflection coefficient $\qquad$ T: transmission coefficient

$R = \left(\dfrac{\kappa_2\omega_1 - \kappa_1\omega_2}{\kappa_2\omega_1 + \kappa_1\omega_2}\right)\left(\dfrac{\kappa_1\kappa_2}{\kappa_1\kappa_2}\right) = \dfrac{c_1 - c_2}{c_1 + c_2}$ $\qquad$ $T = \left(\dfrac{2\kappa_1\omega_1}{\kappa_2\omega_1 + \kappa_1\omega_2}\right)\left(\dfrac{\kappa_1\kappa_2}{\kappa_1\kappa_2}\right) = \dfrac{\kappa_1 c_1}{(c_1 + c_2)\kappa_2}$

Let $c_2 \to \infty$ and we recover results similar to the fixed boundar scenario: $\lim\limits_{c_2 \to \infty} R = -1$ and $\lim\limits_{c_2 \to \infty} T = 0$.

Assuming the form of $\dfrac{\partial f_1}{\partial \phi}$ is known, then the reflected and transmitted waves may be determined.

Now, instead of the boundary separating two regions of different mass density, consider a wave propagation across a boundary separating regions of different elasticity/cross-sectional area which affects the force balance.

$$\dot{u}_i + \dot{u}_r = \dot{u}_t \qquad \longrightarrow \qquad \omega_1\left(\frac{\partial f_1}{\partial \phi} - \frac{\partial g}{\partial \theta}\right) = \omega_2 \frac{\partial f_2}{\partial \gamma}$$

$$A_1\left(\frac{\partial u_i}{\partial x} + \frac{\partial u_r}{\partial x}\right) = A_2 \frac{\partial u_t}{\partial x} \qquad \longrightarrow \qquad A_1 \kappa_1\left(\frac{\partial f_1}{\partial \phi} + \frac{\partial g}{\partial \theta}\right) = A_2 \kappa_2 \frac{\partial f_2}{\partial \gamma}$$
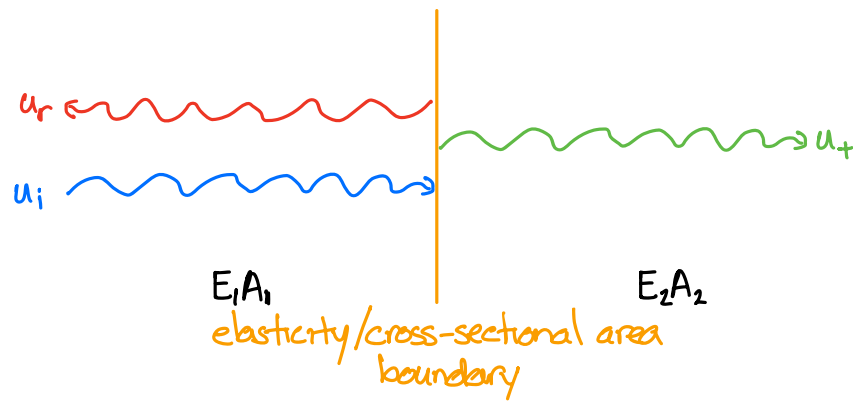
$$\left.\begin{array}{c} \end{array}\right\} \text{solve simultaneously}$$

$$\frac{\partial g}{\partial \theta} = \left(\frac{A_2 \kappa_2 \omega_1 - A_1 \kappa_1 \omega_2}{A_2 \kappa_2 \omega_1 + A_1 \kappa_1 \omega_2}\right)\frac{\partial f_1}{\partial \phi} = \underbrace{\left(\frac{A_2 c_1 - A_1 c_2}{A_2 c_1 + A_1 c_2}\right)}_{R}\frac{\partial f_1}{\partial \phi}$$

$$\frac{\partial f_2}{\partial \gamma} = \left(\frac{2 A_1 \kappa_1 \omega_1}{A_2 \kappa_2 \omega_1 + A_1 \kappa_1 \omega_2}\right)\frac{\partial f_1}{\partial \phi} = \underbrace{\left(\frac{2 A_1 c_1}{A_2 c_1 + A_1 c_2}\right)\left(\frac{\kappa_1}{\kappa_2}\right)}_{T}\frac{\partial f_1}{\partial \phi}$$

Problems involving transmission across boundaries often include mention of mechanical impedance. The impedance (Z) expresses the ratio of the amplitude of the driving force at a point to that of the resulting velocity. Note that "driving force" is not necessarily that of an external driver and may stem from the internal stress that accompanys a propagating wave.

Let's adopt a more general view by replacing the response of the right half-space with a forcing, F(t).

$$U(t) = \dot{u}_i + \dot{u}_r = -\omega\left(\frac{\partial f}{\partial \phi} - \frac{\partial g}{\partial \theta}\right) = -\kappa_1 \sqrt{\frac{E}{\rho}}\left(\frac{\partial f}{\partial \phi} - \frac{\partial g}{\partial \theta}\right)$$

$$\Sigma F_x = F(t) + AE\left(\frac{\partial u_i}{\partial x} + \frac{\partial u_r}{\partial x}\right) = 0 \qquad \text{applied to interface}$$

$$F(t) = -\kappa AE\left(\frac{\partial f}{\partial \phi} + \frac{\partial g}{\partial \theta}\right)$$

$$Z = \left|\frac{F}{V}\right| = AE\sqrt{\frac{\rho}{E}} = A\sqrt{\rho E} = \frac{AE}{C_0} \qquad \text{impedance for a semi-infinite rod}$$

Upon applying this result to R and T of two half-spaces with different elasticity/cross-sectional area, we get:

$$R = \frac{\left(E_1/E_2\right)\left(Z_1/Z_2\right) - 1}{\left(E_1/E_2\right)\left(Z_1/Z_2\right) + 1} \qquad\qquad T = \frac{2A_1 E_1 Z_2}{A_2 E_1 Z_2 + A_2 E_2 Z_1}$$

A procedure that is frequently used in the study of reflection and transmission at boundaries is to consider the incident wave to be a pure harmonic; thus, general, frequency-dependent relationships for the amplitude and phase of the reflected and transmitted waves are obtained.

Consider the incident wave of known amplitude, $u_i = Ae^{i(k_1 x - \omega_1 t)}$, and the reflected and transmitted waves of unknown amplitude, $u_r = Be^{i(-k_1 x - \omega_1 t)}$ and $u_t = Ce^{i(k_2 x - \omega_2 t)}$ in two half-spaces of different density.

$$\dot{u}_i + \dot{u}_R = \dot{u}_t \qquad\qquad\qquad \frac{\partial u_i}{\partial x} + \frac{\partial u_r}{\partial x} = \frac{\partial u_t}{\partial x}$$

$$i\omega_1 Ae^{i(k_1 x + \omega_1 t)} + i\omega_1 Be^{i(-k_1 x + \omega_1 t)} = i\omega_2 Ce^{i(k_2 x + \omega_2 t)} \qquad i k_1 Ae^{i(k_1 x + \omega_1 t)} - i k_1 Be^{i(-k_1 x + \omega_1 t)} = i k_2 Ce^{i(k_2 x + \omega_2 t)}$$

The location of the boundary between the two media is arbitrarily set to $x=0$. Similarly, since no energy is exchanged with the system, we expect our finding to hold for all time; thus $t=0$ is as appropriate as any other instant.

$$\omega_1(A+B) = \omega_2 C \qquad\qquad\qquad k_1(A-B) = k_2 C$$

$$\frac{B}{A} - \frac{\omega_2}{\omega_1}\frac{C}{A} = -1 \qquad\qquad\qquad \frac{B}{A} + \frac{k_2}{k_1}\frac{C}{A} = 1$$

$$\frac{B}{A} = -\frac{k_2/k_1 - \omega_2/\omega_1}{k_2/k_1 + \omega_2/\omega_1} = -\frac{1 - c_2/c_1}{1 + c_2/c_1} = \frac{c_1 - c_2}{c_1 + c_2} = R$$

$$\frac{C}{A} = \frac{2}{k_2/k_1 + \omega_2/\omega_1} = 2\frac{k_1/k_2}{1 + c_2/c_1} = \frac{2k_1 c_1}{(c_1 + c_2)k_2} = T$$

Consider the wave incident on a fixed end:

$$\dot{u}_i + \dot{u}_r = 0$$

$$i\omega e^{i\omega t}(Ae^{ikx} + Be^{-ikx}) = 0$$

$$Ae^{ikx} + Be^{-ikx} = 0 \qquad \therefore \qquad \frac{B}{A} = -1 = (1)e^{i\pi}$$

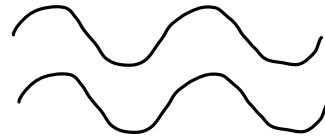the reflected and incident waves are of equal amplitude, but 180° out of phase
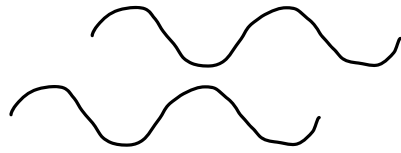
Consider the wave incident on a free end:

$$\frac{du_i}{dx} + \frac{du_r}{dx} = 0$$

$$ike^{i\omega t}(Ae^{ikx} - Be^{-ikx}) = 0$$

$$Ae^{ikx} - Be^{-ikx} = 0 \qquad \therefore \qquad \frac{B}{A} = 1 = (1)e^{i0}$$

the reflected and incident waves are of equal amplitude and in phase

Let's consider a wave propagating in a homogeneous rod where we earlier considered vibration. Recall:

$$\frac{\partial^2 u}{\partial t^2} = c_0^2 \frac{\partial^2 u}{\partial x^2} \qquad \text{(governing equation)}$$

$$u = P(x)\,Q(t) \qquad \text{where } P(x) = Ae^{\pm ikx} \text{ and } Q(t) = Be^{\pm i\omega t} \qquad \text{(solution)}$$
$$= ABe^{\pm i(kx \mp \omega t)}$$
$$= [Ce^{i(kx - \omega t)} + c.c.] + [Ce^{i(kx + \omega t)} + c.c.]$$

If we apply the solution $u = Ce^{i(kx + \omega t)}$, we obtain a familiar result: $\omega^2 = c_0^2 k^2$ $\therefore \left(\frac{\omega}{k}\right)^2 = c_0^2$

$\omega = c_0 k$
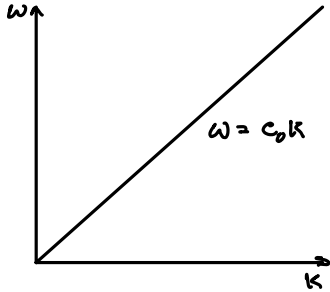
ω is linearly proportional to k via c_0. Waves of different freqs. all travel at the same velocity:
$$v_p = \frac{\omega}{k} = c_0 \quad \text{(phase velocity)}.$$

Now, let's consider the propagation of a wave in a rod in an elastic sleeve.

elastic sleeve

rod

elastic sleeve

$$\frac{\partial^2 u}{\partial t^2} = c_0^2 \frac{\partial^2 u}{\partial x^2} - \frac{ku}{\rho} \qquad \longleftarrow \quad u = Ce^{i(kx + \omega t)}$$

$$\omega^2 = (kc_0)^2 + \frac{k}{\rho}$$

$$\omega = \sqrt{(kc_0)^2 + \frac{k}{\rho}}$$

$\sqrt{k}$
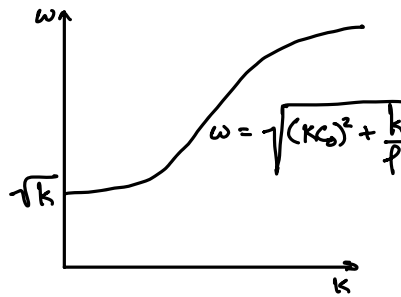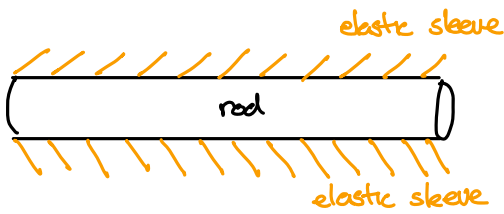
ω is not linearly proportional to k; waves of different freqs. travel at different velocities (hallmark of dispersion):
$$v_p = \frac{\omega(k)}{k}$$

Dispersion in metamaterials

Go to Mathematica: Group Velocity

For simplicity, consider two pure harmonic waves of equal amplitude but of frequencies that differ by a differential amount traveling through the same medium:

$$u = A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t) \qquad\qquad k_2 = k_1 + dk, \quad \omega_2 = \omega_1 + d\omega$$

$$= 2A\cos\left[\frac{1}{2}(k_2 - k_1)x - \frac{1}{2}(\omega_2 - \omega_1)t\right]\cos\left[\frac{1}{2}(k_2 + k_1)x + \frac{1}{2}(\omega_2 + \omega_1)t\right]$$

$$= 2A\cos\left(\frac{1}{2}dk\,x - \frac{1}{2}d\omega\,t\right)\cos\left[\frac{1}{2}(2k_1 + dk)x - \frac{1}{2}(2\omega_1 + d\omega)t\right]$$

$d\omega$ ignorable since $\omega_1 \gg d\omega$

dk ignorable since $k_1 \gg dk$

$$= 2A\cos(k_1 x + \omega_1 t)\cos\left[\frac{1}{2}(dk\,x - d\omega\,t)\right]$$

The first cosine term describes the high-frequency carrier wave. The second cosine term varies slowly and acts to modulate the carrier; enveloping it such that the high-frequency oscillations appear to travel in packets (or groups).

$v_p = \dfrac{\omega}{k_1}$ phase velocity of the carrier

$v_g = \dfrac{d\omega}{dk}$ phase velocity of the envelope; group velocity

$v_p > v_g$: the carrier oscillations will appear to originate from behind the group and travel forward before disappearing.

$v_p < v_g$: the carrier oscillations will appear to originate from the front of the group and travel aft before disappearing.

$v_p = v_g$: the carrier oscillations and envelope exhibit no relative motion; therefore, the oscillations do not move within the group.

Now, we show that the group velocity is also the velocity of energy transported by a propagating wave.

Consider the total energy density of a rod in an elastic sleeve:

$$\frac{\partial E}{\partial x} = \frac{\partial T}{\partial x} + \frac{\partial V}{\partial x} = \frac{1}{2}\rho A \dot{u}^* \dot{u} + \frac{1}{2}EA\left(\frac{du}{dx}\right)^*\left(\frac{du}{dx}\right) + \frac{1}{2}kAu^*u$$

$$= \frac{1}{2}\rho\omega^2 A + \frac{1}{2}EA\kappa^2 + \frac{1}{2}kA \qquad \longleftarrow \qquad \omega^2 = (\kappa c_0)^2 + \frac{k}{\rho}$$

$$= \frac{1}{2}\rho\left[(\kappa c_0)^2 + \frac{k}{\rho}\right]A + \frac{1}{2}EA\kappa^2 + \frac{1}{2}kA$$

imaginary κ

$e^{i(\kappa x + \omega t)}$

$e^{i\kappa x}e^{i\omega t}$

$e^{i(\kappa_R + i\kappa_I)x}e^{i\omega t}$

$e^{-\kappa_I x}e^{i\kappa_R x}e^{i\omega t}$

$v_0 = 0$

The corresponding power flow is:

$$P(x_0,t) = -EA\frac{du}{dx}\frac{du}{dt}\Big|_{x=x_0} = EA\,\omega\kappa = EA\left[(\kappa c_0)^2 + \frac{k}{\rho}\right]^{\frac{1}{2}}\kappa$$

The velocity of the energy, $v_e = P\left(\dfrac{\partial E}{\partial x}\right)^{-1} = \dfrac{c_0^2\kappa}{\left[(\kappa c_0)^2 + \frac{k}{\rho}\right]^{\frac{1}{2}}} = \dfrac{d\omega}{dk}$

TOPIC 5:
Lattice Waves

Our objective is to learn about the wave nature of lattice vibrations. Although we focus on 1D systems, the basic concepts presented extend to 3D systems, as well. Because there are infinite DOFs in an infinite system, there are as many natural frequencies and modes. The dispersion diagram summarizes the dynamic characteristics of the system.
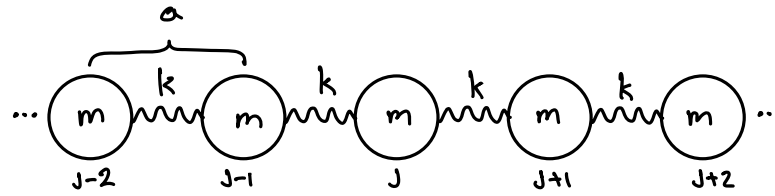
Method I: we consider the motion of degrees of freedom within an arbitrary unit cell – the fundamental repeating unit – and those freedoms to which they are coupled. We then impose the wave solution

$$u_{j+n} = U e^{i(\kappa x + \omega t)} = U e^{i[\kappa(j+n)a + \omega t]} = U e^{i(\kappa j a + \omega t)} e^{i \kappa n a}$$

which accounts for the discrete nature of the system.
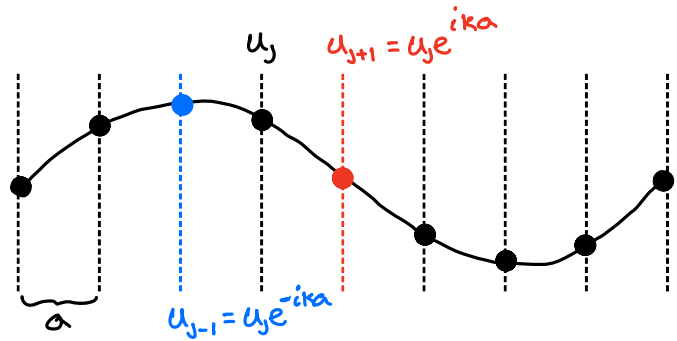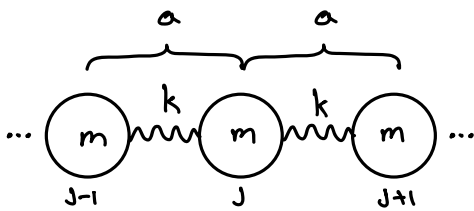
$$\sum F_x = m \ddot{u}_j = -k(2u_j - u_{j+1} - u_{j-1})$$

$$\therefore \quad m \ddot{u}_j + k(2u_j - u_{j+1} - u_{j-1}) = 0$$

$$-\omega^2 m + k(2 - e^{i\kappa a} - e^{-i\kappa a}) = 0$$

$$\omega = \left[\frac{2k}{m}(1 - \cos \kappa a)\right]^{\frac{1}{2}}$$
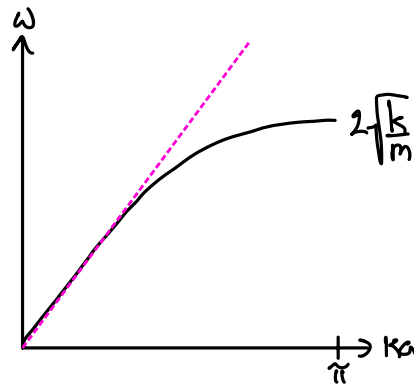
Discrete systems are inherently dispersive due to the different length scales involved: that of the system (i.e., the unit cell period, a) and that of the wave. For $\lambda \approx a$ ($\kappa a \approx \pi$), discreteness affects dominate; for $\lambda \gg a$, average affects dominate. Waves in homogeneous continua do not suffer dispersion.

Consider the phase velocity in the long-wavelength limit (i.e., $\kappa a \approx 0$)

$$\omega(\kappa a) = \left[\frac{2k}{m}(1 - \cos \kappa a)\right]^{\frac{1}{2}} \approx \left[\frac{2k}{m}\left(1 - 1 + \frac{(\kappa a)^2}{2}\right)\right]^{\frac{1}{2}} = \sqrt{\frac{k}{m}} \kappa a \qquad \therefore \qquad v_p = \frac{\omega(\kappa a)}{\kappa a} = \sqrt{\frac{k}{m}}$$

Long Wavelength ($\kappa a = \frac{1}{10}$)

Short Wavelength ($\kappa a = \frac{9}{10}$)
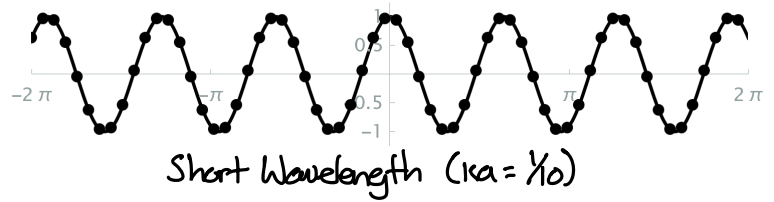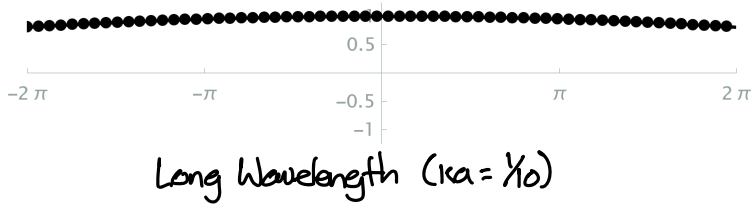
If a wave of very long wavelength is introduced to a linear lattice, the displacement of each mass will only vary by an infinitesimal amount over a great number of lattice points. On the scale of the wavelength, the lattice points are so densely packed that they effectively constitute a continuous medium.

Consider the continuum model via Taylor expansion: $u_{j\pm 1} \approx u(0) \pm a \left.\frac{du}{dx}\right|_{x=0} + \frac{a^2}{2}\left.\frac{d^2u}{dx^2}\right|_{x=0} + O(a^3)$

$m\ddot{u}_j + k(2u_j - u_{j+1} - u_{j-1})$

$\ddot{u}_j + \frac{k}{m}(2u_j - u_{j+1} - u_{j-1}) \approx \ddot{u} + \frac{k}{m}\left[2u - \left(u + a\frac{du}{dx} + \frac{a}{2}\frac{d^2u}{dx^2}\right) - \left(u - a\frac{du}{dx} + \frac{a}{2}\frac{d^2u}{dx^2}\right)\right] = \ddot{u} - \underbrace{\frac{ka^2}{m}\frac{d^2u}{dx^2}}_{\text{wave equation}} = 0$

$\ddot{u} - \frac{ka^2}{m}\frac{d^2u}{dx^2} = 0 \longleftarrow u = Ue^{i(\kappa x + \omega t)} \qquad \therefore \quad \omega^2 = \frac{k}{m}(\kappa a)^2 \qquad \therefore \quad v_p = \frac{\omega(\kappa a)}{\kappa a} = \sqrt{\frac{k}{m}}$

Since sound waves can propagate in crystalline solids comprising atoms/molecules arranged in a lattice and their wavelengths are much longer than the lattice spacing, the above-calculated phase velocities are associated with the sound speed and denotes the "acoustic" frequency band.
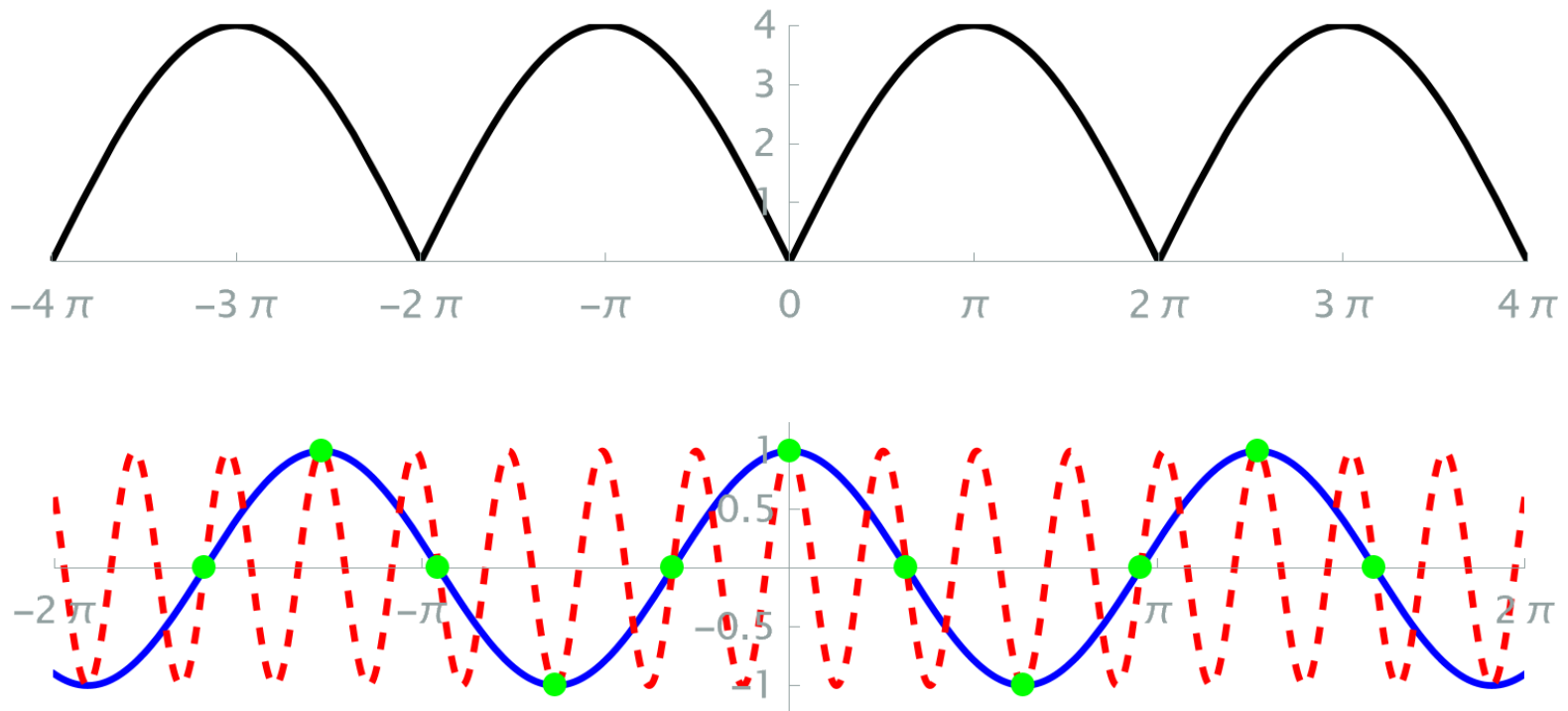
Brillouin_Zone.m

```matlab
clear;clc;

%% Setup - User Input
k=pi/1.5;
N=3;

x_min=-1*pi;
x_max=1*pi;
x_pts=201;

%% Calculations
x=linspace(x_min,x_max,x_pts);
x_int=round(x_min,0):round(x_max,0);

for j=1:N
    for phi=linspace(0,2*pi,101)
        plot(x,cos((k+2*pi)*x-phi),'r:',x,cos(k*x-phi),'b',...
            x_int,cos(k*x_int-phi),'k.',...
            'LineWidth',2,'MarkerSize',30);
        xlabel('Position, x');ylabel('Displacement, u');
        axis([x_min x_max -1.25 1.25]);
        legend('\kappa''=\kappa+2\pi',['\kappa=',num2str(k)],...
            'mass','Location','northoutside','NumColumns',3);
        daspect([1 1 1]);
        drawnow;
    end
end
```

In the wave representation of lattice vibrations, the wave function evaluated at each lattice point is the displacement. The wave function between lattice points is non-physical and, therefore irrelevant. Nevertheless, waves of different wavelengths can be constructed to describe the same lattice vibration as seen by $\omega(\kappa a) = \omega(\kappa' a)$ for $\kappa' a > |\pi|$.

Waves of shorter wavelength outside the first Brillouin zone that produce the same displacement have a lower v_p than those inside the Brillouin zone.

In the lattice, each atom is related to its neighbor through the propagation constant, $e^{i\kappa na}$, where $n = 0, \pm 1, \pm 2, \cdots$. To examine whether κa and $\kappa' a$ are truly equivalent for the same ω, we need only to compare the value of the propagation constant lattice point by lattice point:

$$e^{i\kappa na} = e^{i\kappa' na} = e^{i(\kappa + \Delta\kappa)na} = e^{i\kappa na} e^{i\Delta\kappa na} \qquad \therefore \quad e^{i\Delta\kappa na} = 1 \qquad \therefore \quad \Delta\kappa a = 2\pi$$

Any κ in the 1st BZ is independent; any κ' outside the 1st BZ is not and $\pm 2\pi/a$ can always be added to bring κ' within the 1st BZ.

Interestingly, $\kappa a = \pi$ and $\kappa' a = -\pi$ also satisfy $e^{i\kappa na} = e^{i\kappa' na}$ and may exist in the lattice simultaneously. While each mass oscillates according to $e^{i\omega t}$, each is always $180°$ out-of-phase with its neighbor — $\kappa a = \pi$ and $\kappa' a = -\pi$ represent standing waves.

The group velocity, $\partial\omega/\partial\kappa$, is zero at $\kappa a = \pm\pi$. For a physical explanation, consider a wave packet formed around $\kappa a = \pi$ with component waves symmetrically distributed in the range $(\pi - \Delta\kappa a) \leq \kappa a \leq (\pi + \Delta\kappa a)$. Components with $\kappa a > \pi$ will reflect into opposite-going waves with $(-\pi + \Delta\kappa a) \geq \kappa a \geq -\pi$. Now, for each left-going wave, there is a matching right-going wave of equal amplitude, which form a standing wave. Since the component standing waves do not propagate, neither does the wave packet; thus $v_g = 0$. Naturally, the same conclusion can be reach in considering a wave packet formed around $\kappa a = -\pi$.

Alternatively, consider a wave packet formed asymmetrically about $\kappa a = \pi$, e.g., $(\pi + \varepsilon - \Delta\kappa a) \leq \kappa a \leq (\pi + \varepsilon + \Delta\kappa a)$. For $\varepsilon = 0$, we reach the same conclusion as above. For $\varepsilon > 0$, more wave components are reflected back and the imbalance leads to $v_g \neq 0$; for $\varepsilon < 0$, fewer components are reflected back.
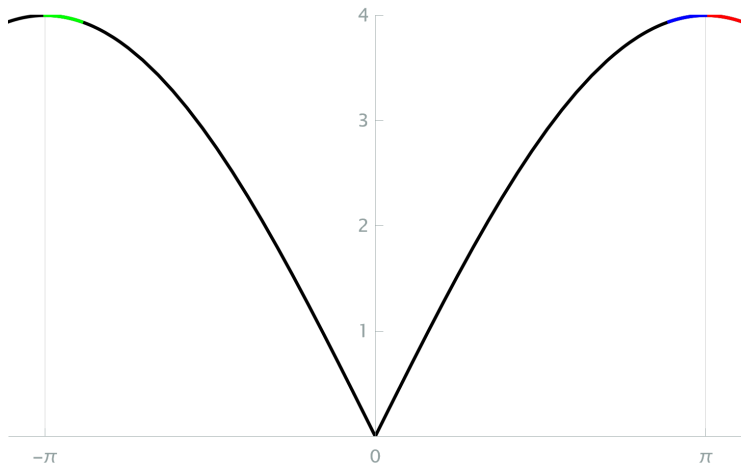
wave packet symmetric around $\kappa a = \pi$. waves of $\pi \leq \kappa a \leq (\kappa a + \Delta \kappa a)$ are reflected into $-\pi \leq \kappa a \leq (-\pi + \Delta \kappa a)$. The balance of left- and right-going waves is responsible for $v_g = 0$.
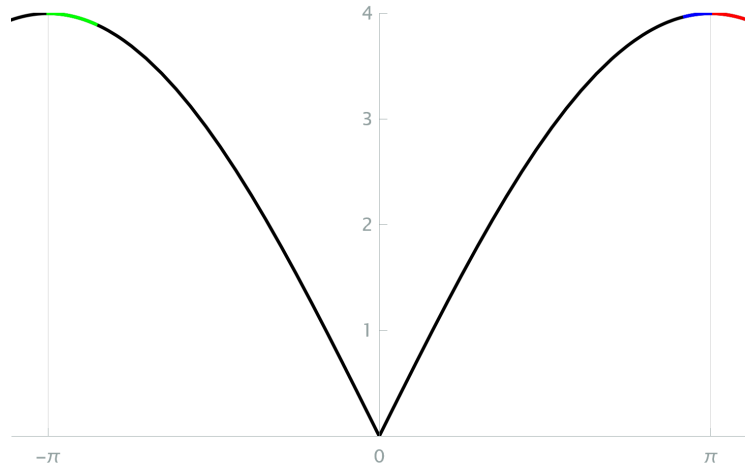
wave packet asymmetric around $\kappa a = \pi$. waves of $\pi \leq \kappa a \leq (\kappa a + \varepsilon + \Delta \kappa a)$ are reflected into $-\pi \leq \kappa a \leq (-\pi + \Delta \kappa a + \varepsilon)$. The imbalance of left- and right-going waves is responsible for $v_g \neq 0$.

Method II: we consider an isolated unit cell and apply the Bloch boundary conditions. This method is amenable to complex FE models comprising M and K matrices.
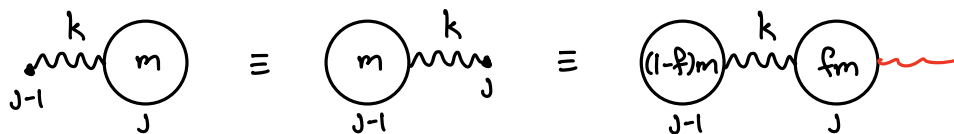
note: the total mass of the unit cell is m, thus $(1-f)m + fm = m$

$$
\left.\begin{array}{l}
(1-f)m\ddot{u}_{J-1} + k(u_{J-1} - u_J) = f_{J-1} \\
fm\ddot{u}_J + k(u_J - u_{J-1}) = f_J
\end{array}\right\} \rightarrow
\underbrace{\begin{bmatrix} (1-f)m & 0 \\ 0 & fm \end{bmatrix}}_{M_S}
\underbrace{\begin{bmatrix} \ddot{u}_{J-1} \\ \ddot{u}_J \end{bmatrix}}_{\ddot{u}_S}
+
\underbrace{\begin{bmatrix} k & -k \\ -k & k \end{bmatrix}}_{K_S}
\underbrace{\begin{bmatrix} u_{J-1} \\ u_J \end{bmatrix}}_{u_S}
=
\underbrace{\begin{bmatrix} f_{J-1} \\ f_J \end{bmatrix}}_{f_S}
$$

T: Bloch transformation matrix

$$
\underbrace{\begin{bmatrix} u_{J-1} \\ u_J \end{bmatrix}}_{u_S: \text{ full freedoms}}
=
\begin{bmatrix} e^{-i\kappa a} \\ 1 \end{bmatrix} u_J
=
\overbrace{\begin{bmatrix} \gamma \\ 1 \end{bmatrix}}^{T}
\underbrace{u_J}_{u_R: \text{ reduced/essential freedoms}}
$$

In using u_R, we must ensure energy consistancy:

$$KE = \frac{1}{2} \ddot{u}_s^T M_s \ddot{u}_s = \frac{1}{2}(T\ddot{u}_R)^H M_s T\ddot{u}_R = \frac{1}{2}\ddot{u}_R^H \underbrace{T^H M_s T}_{M_R} \ddot{u}_R$$

$$PE = \frac{1}{2} u_s^T K_s u_s = \frac{1}{2}(Tu_R)^H K_s T u_R = \frac{1}{2} u_R^H \underbrace{T^H K_s T}_{K_R} u_R$$

$$W = u_s^T f_s = (Tu_R)^H f_s = u_R^H \underbrace{T^H f_s}_{f_R} = 0 \quad \text{no work done on unit cell}$$

$$T^H(-\omega^2 M + K)Tu_R = 0$$

$$|T^H(-\omega^2 M + K)T| = A\gamma + B + \frac{A}{\gamma} = 0 \qquad A\gamma^2 + B\gamma + A = 0 \qquad A = -k \;;\; B = 2k - m\omega^2$$

$$\gamma(\omega) = \frac{-B \pm \sqrt{B^2 - 4A^2}}{2A} \qquad\qquad \kappa a = \kappa_R a + i\kappa_I a \qquad \kappa_R a = |Re[i\ln(\gamma)]| \qquad \kappa_I a = |Im[i\ln(\gamma)]|$$

$$\omega(\kappa a) = \left[-\frac{k(\gamma-1)^2}{m\gamma}\right]^{1/2} = \left[\frac{2k}{m}(1-\cos\kappa a)\right]^{1/2}$$
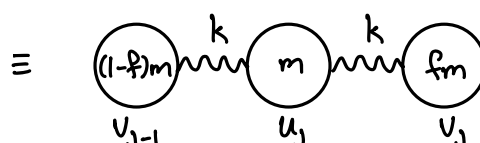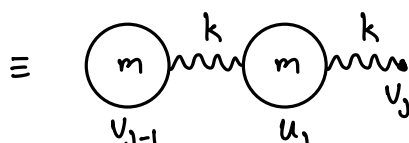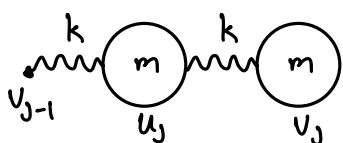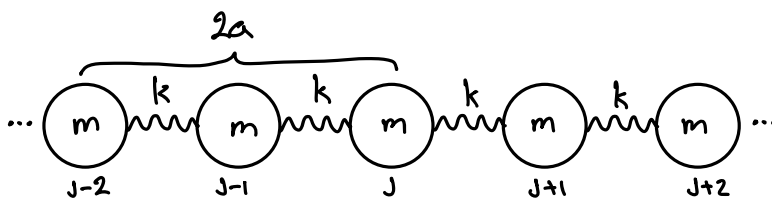
note: the total mass of the unit cell is $2m$, thus $(1-f)m + m + fm = 2m$. The fraction, f, applies to the boundaries only in order to maintain periodicty and avoid the redistribution of mass.

$$\left.\begin{array}{l} 0\ddot{v}_{j-1} + k(v_{j-1} - u_j) = f_{j-1} \\ m\ddot{u}_j + k(2u_j - v_{j-1} - v_j) = 0 \\ m\ddot{v}_j + k(v_j - u_j) = f_j \end{array}\right\} \rightarrow \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{bmatrix}}_{M_s} \underbrace{\begin{bmatrix} \ddot{v}_{j-1} \\ \ddot{u}_j \\ \ddot{v}_j \end{bmatrix}}_{\ddot{u}_s} + \underbrace{\begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix}}_{K_s} \underbrace{\begin{bmatrix} v_{j-1} \\ u_j \\ v_j \end{bmatrix}}_{u_s} = \underbrace{\begin{bmatrix} f_{j-1} \\ 0 \\ f_j \end{bmatrix}}_{f_s} \qquad \begin{bmatrix} v_{j-1} \\ u_j \\ v_j \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & \gamma \\ 1 & 0 \\ 0 & 1 \end{bmatrix}}_{T} \begin{bmatrix} u_j \\ v_j \end{bmatrix}$$

$$|T^H(-\omega^2 M_s + K_s)T| = 2k^2 - 4km\omega^2 + m^2\omega^4 - \frac{k^2}{\gamma} - k^2\gamma = 0 \qquad \gamma = e^{-2ika}$$
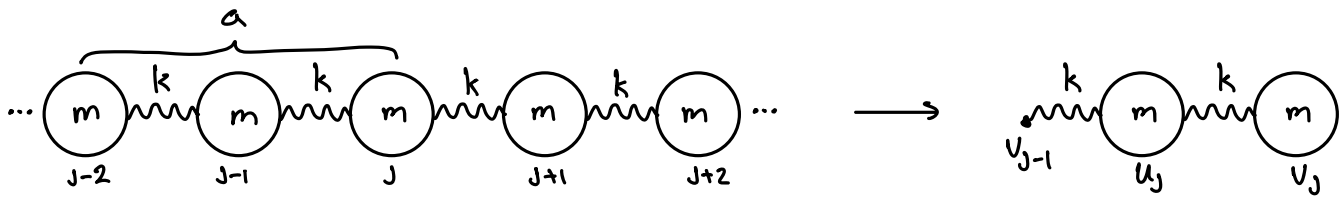
$$\omega_1 = \sqrt{\frac{2k}{m}\left(1 - \sqrt{\cos^2 ka}\right)} \qquad \omega_2 = \sqrt{\frac{2k}{m}\left(1 + \sqrt{\cos^2 ka}\right)}$$
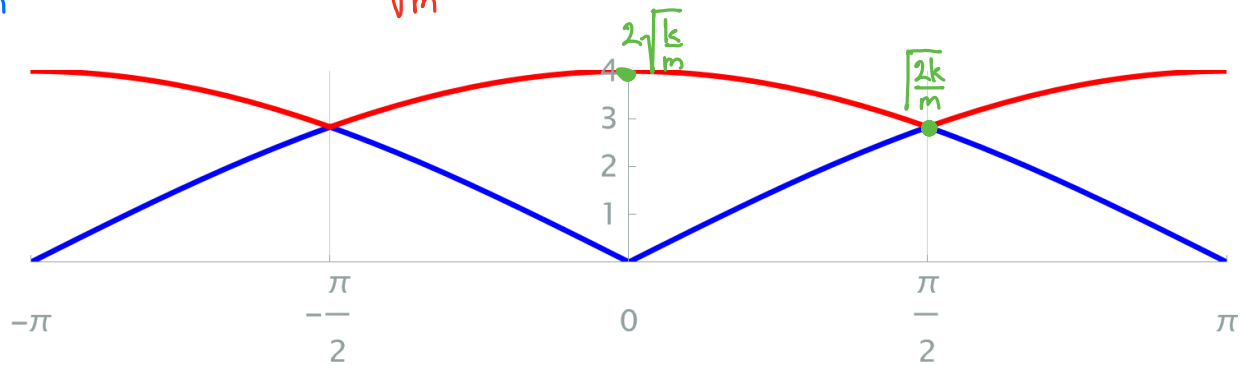
The lattice is the same as before, but the dispersion diagram looks different because of our choice of expanded unit cell (i.e., one which is larger than the actual spatial period, a). The frequency range is unchanged, but the wave number range is shortened by a factor N, where N is the length of the extended unit cell. This results in band folding.

$$e^{i\kappa nNa} = e^{i\kappa' nNa} = e^{i(\kappa + \Delta\kappa)nNa} = e^{i\kappa nNa}e^{i\Delta\kappa nNa} \quad \therefore \quad e^{i\Delta\kappa nNa} = 1 \quad \therefore \quad \Delta\kappa a = \frac{2\pi}{N}$$

M_s, K_s, u_R, u_R, and T are the same as above, except $\gamma = e^{-ika}$

$$\omega_1 = \left(\frac{k}{m}\left[2 - \sqrt{2(1+\cos ka)}\right]\right)^{1/2} \qquad \omega_2 = \left(\frac{k}{m}\left[2 + \sqrt{2(1+\cos ka)}\right]\right)^{1/2}$$
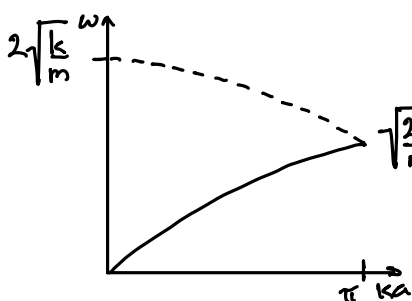
Once again, the band diagram has changed. Although the frequency and wavenumber range is consistent with the first case, niether $|v_g|$ nor v_p agree with the previous case.

Consider a unit cell with two DOFs of mass m_1 and m_2, respectively.
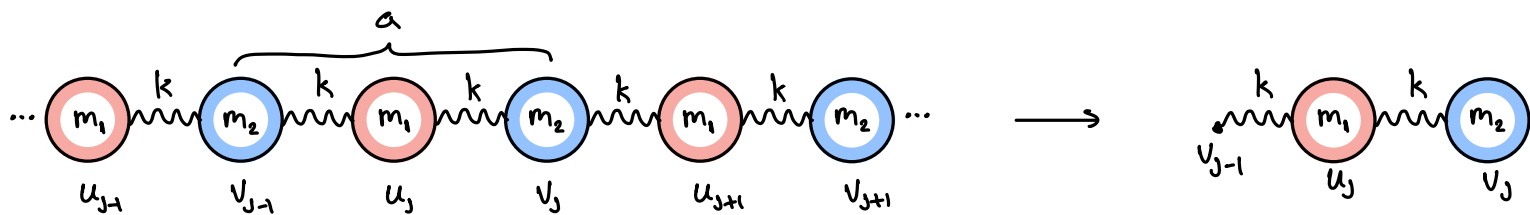
$$
\begin{bmatrix} 0 & 0 & 0 \\ 0 & m_1 & 0 \\ 0 & 0 & m_2 \end{bmatrix} \begin{bmatrix} \ddot{v}_{j-1} \\ \ddot{u}_j \\ \ddot{v}_j \end{bmatrix} + \begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix} \begin{bmatrix} v_{j-1} \\ u_j \\ v_j \end{bmatrix} = \begin{bmatrix} f_{j-1} \\ 0 \\ f_j \end{bmatrix}
\qquad
\begin{bmatrix} v_{j-1} \\ u_j \\ v_j \end{bmatrix} = \begin{bmatrix} 0 & \gamma \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_j \\ v_j \end{bmatrix}
$$

$\underbrace{}_{M_s}$ $\underbrace{}_{\ddot{u}_s}$ $\underbrace{}_{K_s}$ $\underbrace{}_{u_s}$ $\underbrace{}_{f_s}$ $\qquad \underbrace{}_{u_s} \quad \underbrace{}_{T} \quad \underbrace{}_{u_R}$

$$
T^H(-\omega^2 M_s + K_s) T u_R = \begin{bmatrix} 2k - \omega^2 m_1 & -k(1+\gamma) \\ -k\left(1 + \dfrac{1}{\gamma}\right) & 2k - \omega^2 m_2 \end{bmatrix} \begin{bmatrix} u_j \\ v_j \end{bmatrix} = 0
\qquad
\color{magenta}{\frac{v}{u} = \frac{2k - \omega^2 m_1}{k(1+\gamma)}}
$$

$\underbrace{}_{D}$

$$
|D| = -\frac{k^2}{\gamma} - k^2 \gamma + 2k^2 - 2k(m_1 + m_2)\omega^2 + m_1 m_2 \omega^4 = 0
$$

$$
\omega_1 = \left(\frac{k(m_1 + m_2)}{m_1 m_2} - \frac{k}{m_1 m_2} \left[\frac{(m_2 + m_1 \gamma)(m_1 + m_2 \gamma)}{\gamma} \right]^{1/2} \right)^{1/2}
$$

$$
= \left(\frac{k(m_1 + m_2)}{m_1 m_2} - \frac{k}{m_1 m_2} \sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos ka} \right)^{1/2}
$$

$$
\omega_2 = \left(\frac{k(m_1 + m_2)}{m_1 m_2} + \frac{k}{m_1 m_2} \left[\frac{(m_2 + m_1 \gamma)(m_1 + m_2 \gamma)}{\gamma} \right]^{1/2} \right)^{1/2}
$$

$$
= \left(\frac{k(m_1 + m_2)}{m_1 m_2} + \frac{k}{m_1 m_2} \sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos ka} \right)^{1/2}
$$
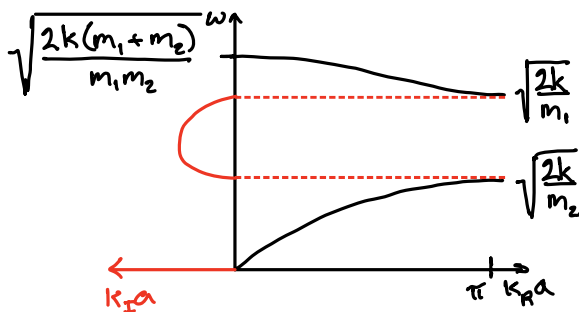
Once again, we have two frequency bands following the 2DOFs per unit cell; however, this time, there is a gap between the bands. In the band gap, no propagating wave solution exists; thus, no energy transfer. Instead, in the band gap, there is a standing wave with an exponentially-decreasing amplitude.

DiAtomic_Waveform.m

```matlab
1  clear;clc;
2  i=sqrt(-1);
3  syms gamma w
4
5  %% Setup - User Input
6  m1=1;
7  m2=2;
8  k=1;
9
10 w_min=0;w_max=2;
11 w_div=1001;
12
13 w_target=1.68;
14
15 n_cells=20;
16
17 %% Mass and Stiffness Matrices
18 M=diag([0 m1 m2]);
19 K=k*[1 -1 0;-1 2 -1;0 -1 1];
20
21 %% Calculations
22 T=[0 gamma;1 0;0 1];
23 Th=[0 1 0;1/gamma 0 1];
24
25 D=solve(det(Th*(-(w^2)*M+K)*T)==0,gamma);
26 str=strcat('@(w)',string(D(1)));
27
28 g=str2func(str);
29
30 %% Dispersion
31 clear w;
32
33 ka_real=nan(1,w_div+1);
34 ka_imag=nan(1,w_div+1);
35 [w,indx]=sort([w_target,linspace(w_min,w_max,w_div)]);
36
37 indx=max((indx==1).*(1:(w_div+1)));
```

```matlab
for j=1:(w_div+1)
    ka_real(j)=abs(real(i*log(g(w(j)))));
    ka_imag(j)=abs(imag(i*log(g(w(j)))));

    if j==indx
        ka_target=ka_real(j)+i*ka_imag(j);
    end
end

%% Waveform
U=[1;(2*k-m1*w_target^2)/(k*(1+g(w(indx))))]; % mode shape

u=nan(2,n_cells);u(:,1)=U;
for j=2:n_cells
    u(:,j)=U.*exp(i*(j-1)*ka_target);
end
u=u./max(real(u),[],'all');

%% Plotting
figure(1);
plot(-ka_imag,w,'r',ka_real,w,'k',...
    [0 0],[0 w_max],'k','LineWidth',2);
xlabel('Wavenumber, \kappaa');ylabel('Frequency, \omega');
axis([-pi/2 pi 0 w_max]);
legend('Im(\kappaa)','Re(\kappaa)');

figure(2);
plot(1:n_cells,real(u(1,:)),'r:.',...
    1:n_cells,real(u(2,:)),'b:.',...
    'MarkerSize',15);
xlabel('Cell No.');ylabel('Displacement, u');
title(['\omega = ',num2str(w_target)]);
axis([1 n_cells -1 1]);
legend('m_1','m_2');
```
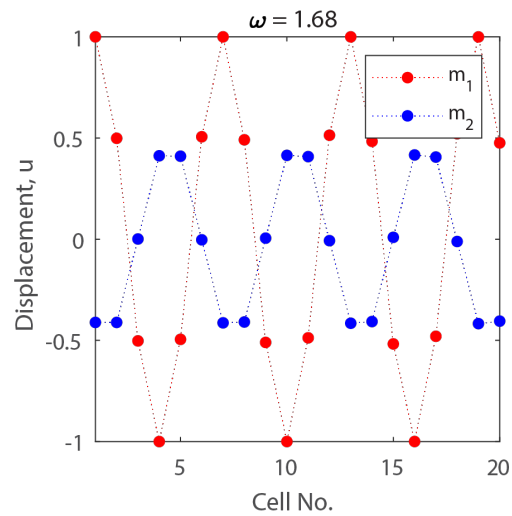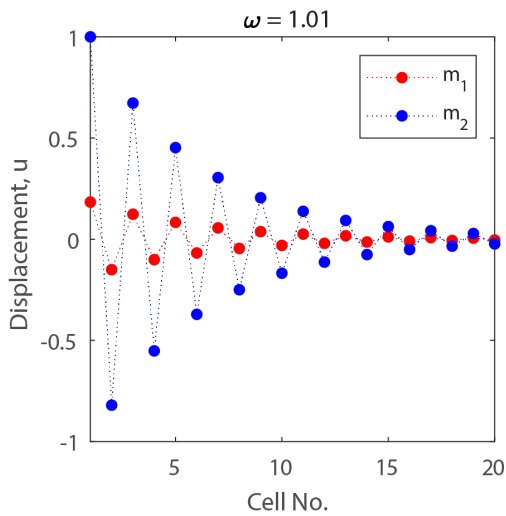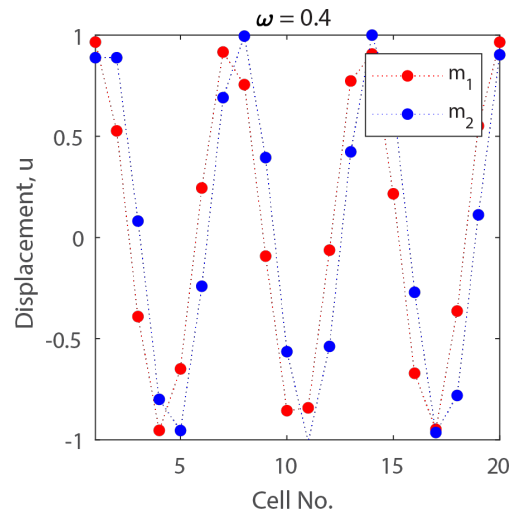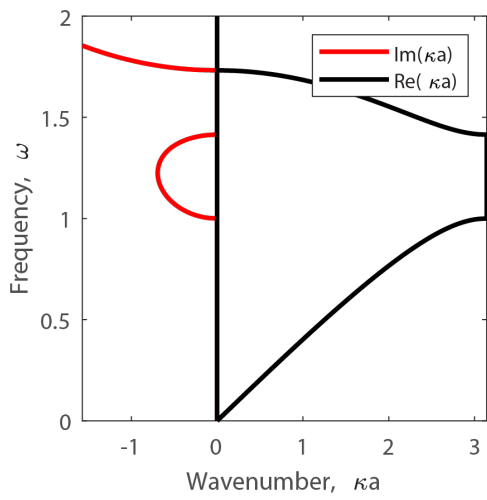
The relation between u_j and v_j can be shown to be $v/u = (2k - \omega^2 m_1)/k(1+g)$. Consider the Taylor expansion of ω_1^2 and ω_2^2 about $\kappa a = 0$ up to the first non-zero term, which are the square frequencies in the long wavelength limit:

$$\omega_1^2 \approx \omega_1^2(0) + \left[\frac{d\omega_1^2}{d\kappa a}\Big|_{\kappa a = 0}\right](\kappa a) + \frac{1}{2}\left[\frac{d^2\omega_1^2}{d(\kappa a)^2}\Big|_{\kappa a = 0}\right](\kappa a)^2 = \frac{k}{2(m_1+m_2)}(\kappa a)^2 \qquad \omega_2^2 = \frac{2k(m_1+m_2)}{m_1 m_2}$$

Now, if we substitute the long wavelength frequencies, $\omega^2 = \omega_{1,2}^2$, then we find

$\omega = \omega_1:$ $\quad \dfrac{v}{u} \approx \dfrac{2k - \omega^2 m_1}{2k} = 1 - \dfrac{m_1(\kappa a)^2}{4(m_1+m_2)} \approx 1$ $\quad$ masses oscillate in phase and with similar amplitude; atoms in a solid exhibit a similar motion during the passage of a sound wave, thus ω_1 is denoted the "acoustic mode".

$\omega = \omega_2:$ $\quad \dfrac{v}{u} \approx \dfrac{2k - \omega^2 m_1}{2k} = -\dfrac{m_1}{m_2}$ $\quad$ masses oscillate out of phase and with different amplitude; atoms in an ionic solid exhibit a similar motion during the passage of an oscillating electric field (as in an EM wave), thus ω_2 is denoted the "optical mode".

TOPIC 6:
Crystal Structure

The atom or group of atoms in crystalline solids appears to reproduce itself periodically throughout the sample as if attached to an underlying set of points with the corresponding periodicity. These points – an analytical construction – represent a lattice and the atoms/molecules represent a basis. Togethe the lattice plus basis constitute the crystal structure.

Due to translation invariance, the system appears identical when viewed from any arbitrary lattice point.

square lattice   +   diatomic basis   =   crystal structure

1D lattice   +   diatomic (mass-spring) basis
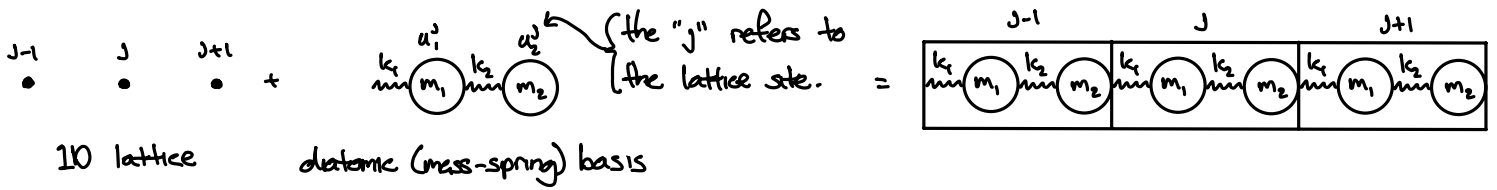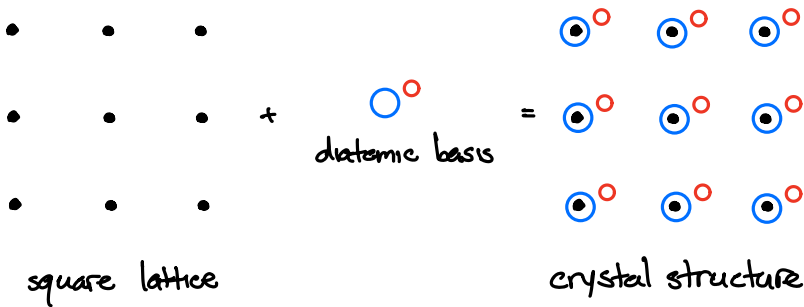
A lattice vector, $R = n_1 a_1 + n_2 a_2 + n_3 a_3$, points from the origin (an arbitrarily chosen lattice site) to a lattice point; where the a_i are unit vectors not all necessarily in the same plane. The volume occupied by $a_1 \cdot (a_2 \times a_3)$ is the smallest building block that can fill the whole space. This cell is the primitive cell and the a_i are the primitive lattice vectors. The primitive cell contains one lattice point regardless of how the primitive cell is positioned with the lattice.

$R = n_1 a_1$

primitive cell

$R = n_1 a_1 + n_2 a_2$

primitive cell

primitive cell

$R = n_1 a_1 + n_2 a_2$
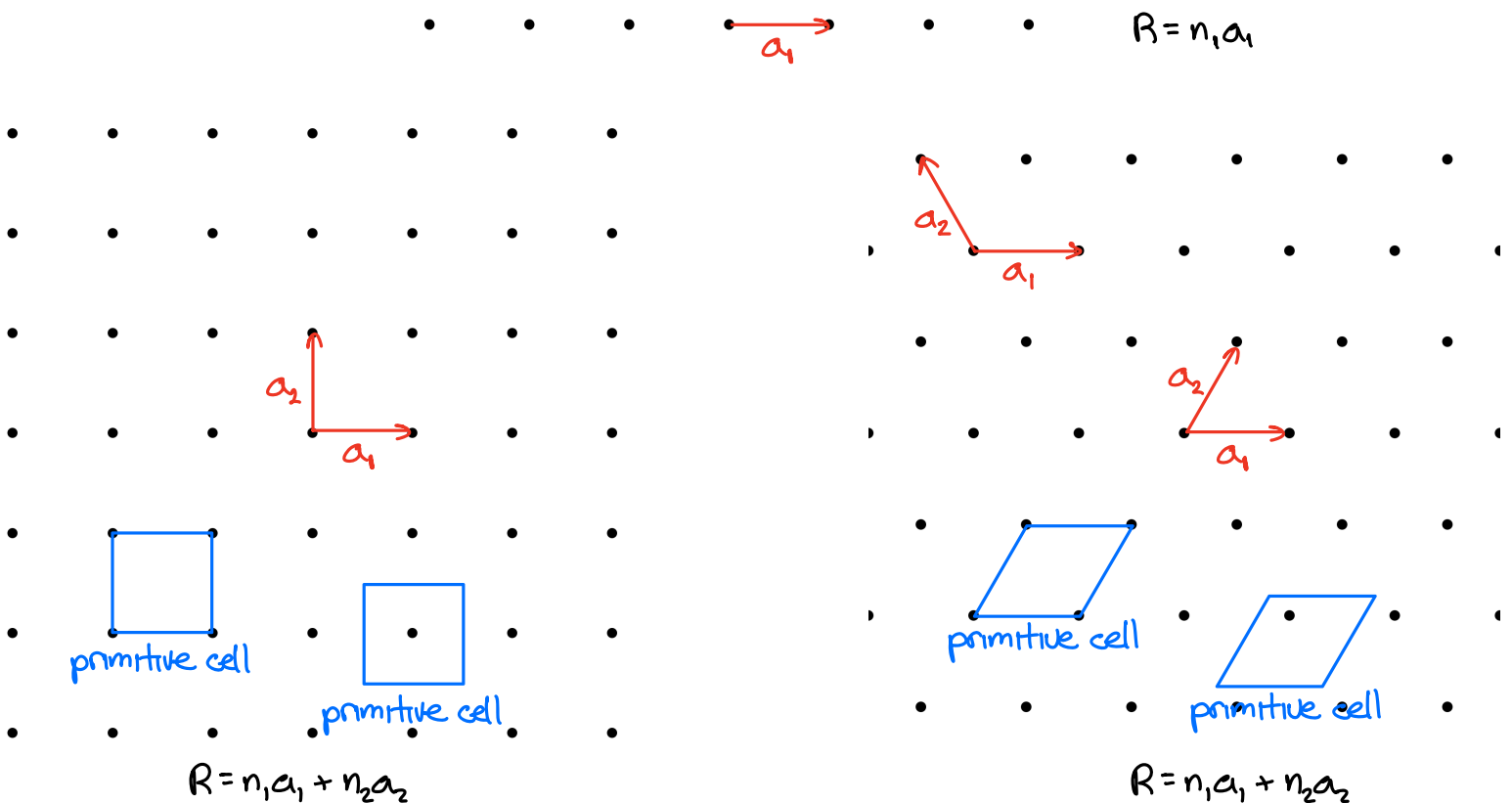
In addition to translation symmetry, a lattice can have rotation symmetry; a square lattice looks the same even after a rotation of $\pi/2$. Translation moves the origin to another location from an initial reference position; rotation keeps the origin in place.

Because of the pre-requisite of translation symmetry, crystals cannot have rotation symmetry for arbitrary angles. If the lattice is invariant under a rotation, θ, then it must also be invariant under a rotation, $-\theta$; otherwise directionality is introduced. Moreover, successive rotations should return the lattice to its original configuration, i.e., $m\theta = 2\pi$.
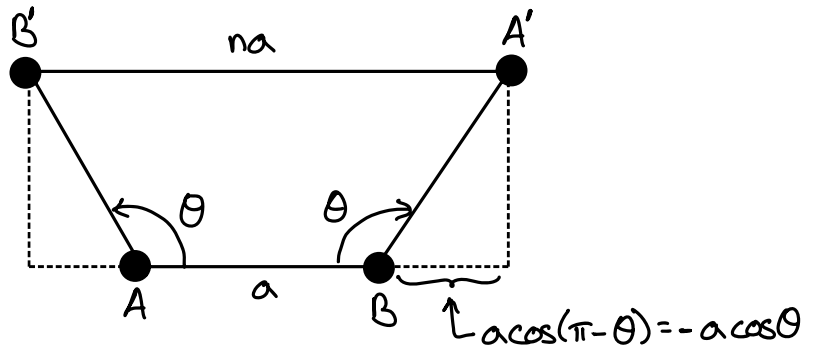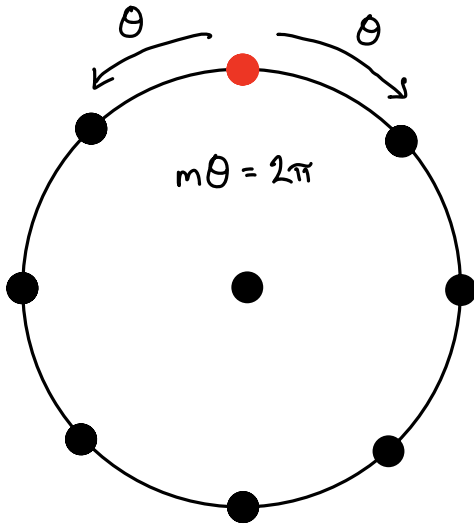
Consider two representative lattice points, A and B, separated by a primitive lattice spacing a. As required by translation symmetry, the lattice looks the same from the perspective of either A or B. If the lattice is invariant under a rotation θ about A, then it is also invariant under a rotation $-\theta$ about B. Translation symmetry requires any two lattice points be separated by a lattice vector. The lattice vector separating A' and B' is an integer multiple of a, i.e., na. Simultaneously, geometry requires the separation between A' and B' equal $a - 2a\cos\theta$:

$$\underbrace{a - 2a\cos\theta}_{\substack{\text{rotation} \\ \text{condition}}} = \underbrace{na}_{\substack{\text{translation} \\ \text{condition}}} \longrightarrow 1 - 2\cos\theta = n$$

The only possible integer solutions are $n = \{-1, 0, 1, 2, 3\}$ which correspond to $\theta = \left\{ \pm\frac{2\pi}{1}, \pm\frac{2\pi}{6}, \pm\frac{2\pi}{4}, \pm\frac{2\pi}{3}, \pm\frac{2\pi}{2} \right\}$; thus, there are only 1-, 2-, 3-, 4-, and 6-fold rotation symmetries. Other angles do not simultaneously satisfy translation symmetry.

It is the sum of translation, rotation, and other symmetries (i.e., inversion, reflection) that gives rise to the variety in crystal structure. There are a total of 14 different lattice types called Bravais lattices that exhaust all possible space lattices for building single crystals.

Bravais lattice:

(i) a periodic, infinite array of discrete points. From any of these points, the array looks exactly the same.   qualitative definition

(ii) consists of all points generated by $R = n_1 a_1 + n_2 a_2 + n_3 a_3$.   quantitative definition

There are 14 Bravais lattice types, i.e., variations under 7 crystal classes:
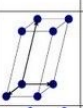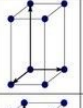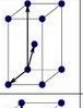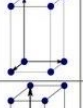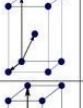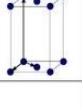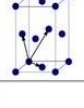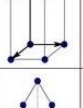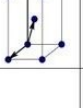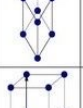
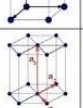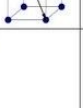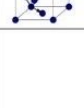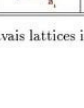| Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Table 1.1: Bravais lattices in three-dimensions.

3 independent interior angles

1 independent interior angle

orthogonal sides; all unequal lengths

orthogonal sides; 2 equal lengths

equal interior angles < 120°; all equal lengths

orthogonal sides; all equal lengths

SC: $a_1 = a \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ $a_2 = a \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ $a_3 = a \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

BCC alternative: $a_1 = \frac{a}{2} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}$ $a_2 = \frac{a}{2} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$ $a_3 = \frac{a}{2} \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$

FCC alternative (also diamond): $a_1 = \frac{a}{2} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$ $a_2 = \frac{a}{2} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ $a_3 = \frac{a}{2} \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$

Triangular/Hexagonal honeycomb: $a_1 = a \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $a_2 = \frac{a}{2} \begin{bmatrix} -1 \\ \sqrt{3} \end{bmatrix}$

At first glance, the hexagonal honeycomb appears to be a Bravais lattice; however, it is instructive to investigate this supposition. Closer examination shows that points b and c are not equivalent because the orientation of neighboring lattice sites around them are 180° apart; consequently, translation symmetry is broken.

From the above primitive lattice vectors, we claim to be able to generate the hexagonal honeycomb; however, if we attempt to generate only b and c lattice sites, we fail since an extra lattice since an extra lattice site appears at the center of each hexagonal cell, yielding a triangular lattice instead of the honeycomb.

If the b and c sites are bundled into pairs, then the asymmetry is eliminated and the honeycomb lattice emerges. The honeycomb structure can be viewed as a Bravais lattice only under the condition that the primitive cell is one with a basis of two points, b and c.
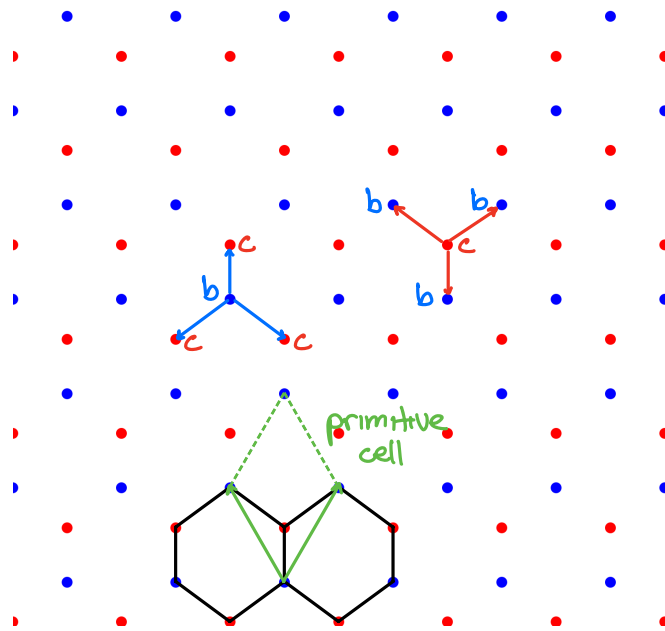
There are many ways to define the primitive cell in a Bravais lattice. We can draw the lattice vectors from one lattice point to all the others and then draw the plane that bisects each of them. The smallest volume enclosed by a set of bisecting planes is a primitive cell called called the Wigner-Sertz cell. It contains only this lattice point (not to be confused for the basis). Due to translation symmetry, every lattice point is enclosed within a similar cell. In reciprocal (i.e., wavevector) space, the Wigner-Sertz cell is of great value for understanding wave propagation in crystals.
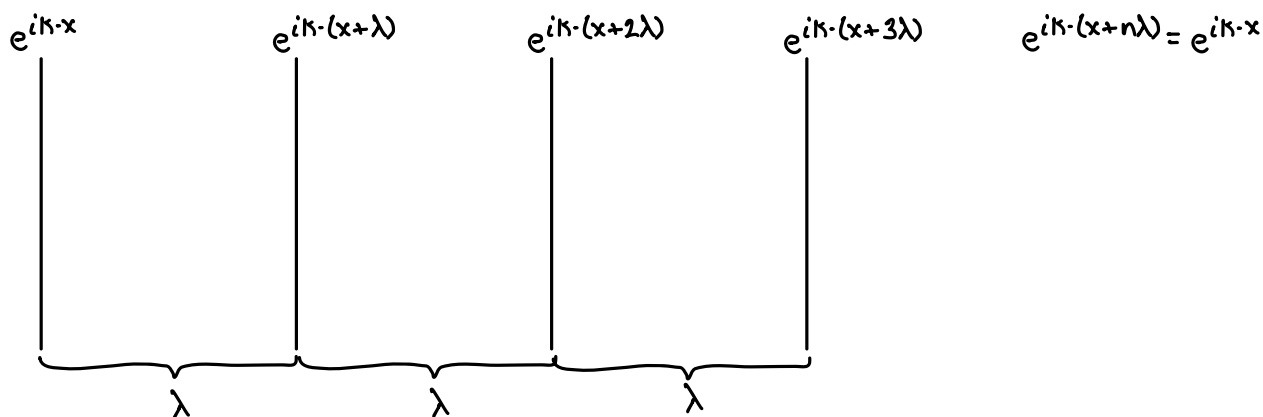

1st Brillouin Zone
2nd Brillouin Zone
3rd Brillouin Zone

−3π −2π −π   π 2π 3π
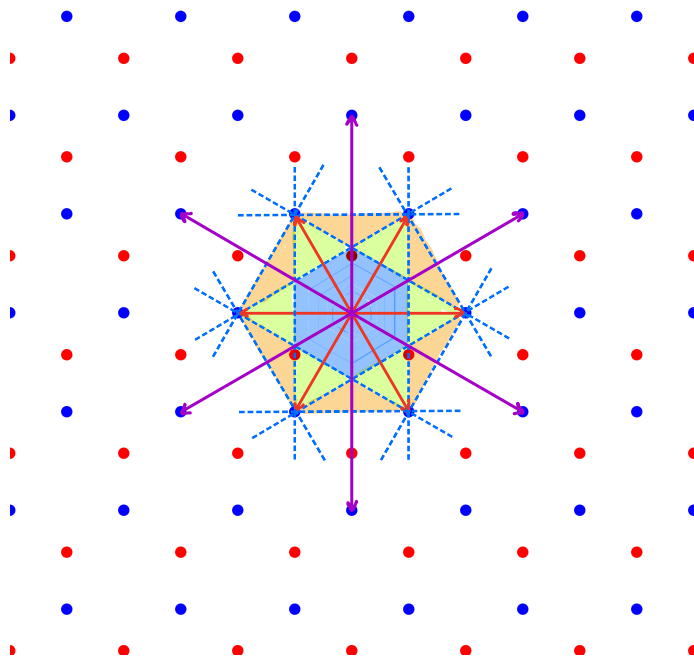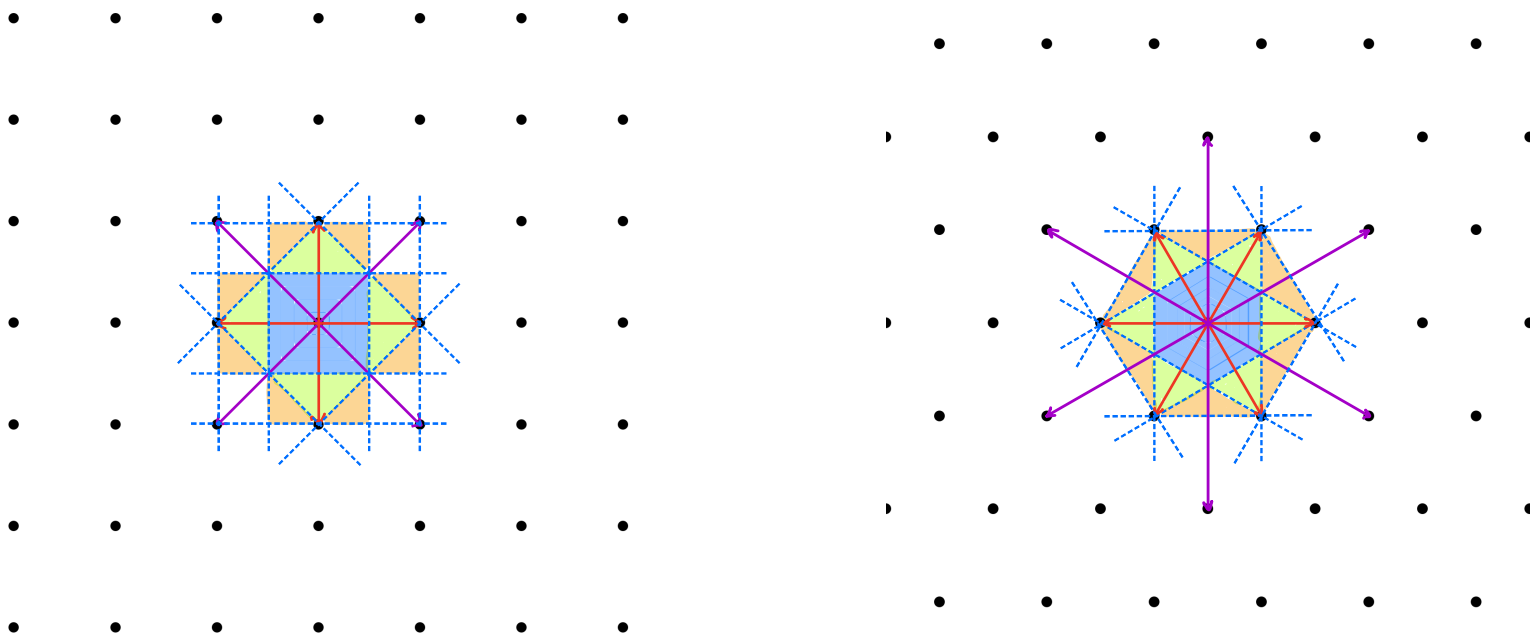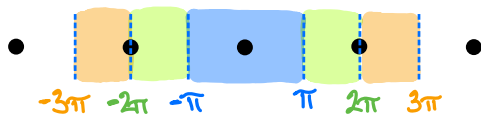
The most important characteristic of crystals is their periodicity stemming from the translational invariance. As a consequence, the physical properties are identical when view from any two lattice points, i.e., whether viewed from r or r+R.

Although, up to this point, we've largely focused on waves propagating in one dimension, we know wave propagation in higher dimensions is possible; thus, we may define the wave vector, $\kappa = \kappa_x \hat{i} + \kappa_y \hat{j} + \kappa_z \hat{k}$ where $|\kappa| = 2\pi/\lambda$ and, in $e^{i\kappa \cdot x}$, $\kappa \cdot x$ gives the wave phase.

Consider a plane wave propagating in a Bravais lattice. The wave amplitude is proportional to $e^{i\kappa \cdot x}$. On a plane perpendicular to κ, the wave phase is the same. This plane defines a wavefront.

$e^{i\kappa \cdot x}$ $\qquad$ $e^{i\kappa \cdot (x+\lambda)}$ $\qquad$ $e^{i\kappa \cdot (x+2\lambda)}$ $\qquad$ $e^{i\kappa \cdot (x+3\lambda)}$ $\qquad$ $e^{i\kappa \cdot (x+n\lambda)} = e^{i\kappa \cdot x}$

$\lambda \qquad \lambda \qquad \lambda$

For a given wavevector of arbitrary magnitude and direction, the phase factor, $e^{i\kappa \cdot x}$, of the wavefront at x may not necessarily be the same at x+R. However, there must be a special subset of κ (denoted G) that does have this periodicity, i.e.,

$$e^{i\kappa \cdot x} = e^{i\kappa \cdot (x+R)} = e^{i\kappa \cdot x} e^{i\kappa \cdot R} = e^{i\kappa \cdot x} \qquad \therefore \quad e^{i\kappa \cdot R} = 1 \qquad \therefore \quad \kappa \cdot R = 2\pi n$$

Let $G = m_1 b_1 + m_2 b_2 + m_3 b_3$ and $R = n_1 a_1 + n_2 a_2 + n_3 a_3$. $G \cdot R = 2\pi n$ requires that $a_i \cdot b_j = 2\pi \delta_{ij}$.

Since the set of G vectors is generated by all possible linear combinations of b_i with integer coefficients, G vectors also form a Bravais lattice in wavenumber space (κ-space), i.e., a reciprocal lattice. Its counterpart R creates the direct lattice in real space. While R has dimensions (m), G has dimensions (m⁻¹).
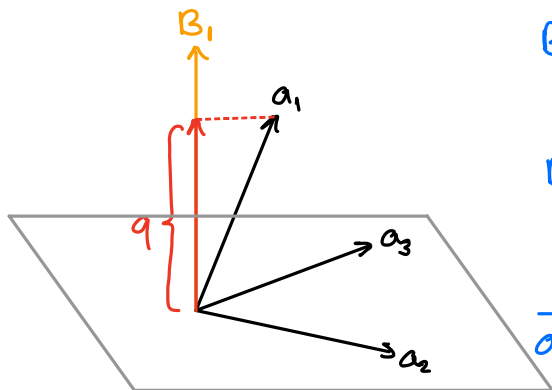
$B_1 = a_2 \times a_3$ $\qquad$ will give a vector $\perp$ to a_2 and a_3, but with a component in the a_1 direction

$B_1 \cdot a_1 = q \delta_{11}$ $\qquad$ will give a value q not necessarily 2π; must mult by $2\pi/q$

$$\frac{B_1 \cdot a_1}{a_1 \cdot (a_2 \times a_3)} = 2\pi \delta_{11} \quad \therefore \quad b_1 = \frac{B_1}{a_1 \cdot (a_2 \times a_3)} = \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}$$

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \qquad b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot (a_2 \times a_3)} \qquad b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot (a_2 \times a_3)} \qquad b_j = 2\pi \frac{area}{volume} = 2\pi \frac{1}{length}$$

SC:
$$b_1 = \frac{2\pi}{a} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad b_2 = \frac{2\pi}{a} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad b_3 = \frac{2\pi}{a} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

In 2D, we define B_j as the vector a_j rotated by $\pm \pi/2$ (direction doesn't matter due to the subsequent normalization).

$$B_j = \phi a_j \qquad \text{where } \phi = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Now, $a_i \cdot B_j = q \delta_{ij}$. Since, $\frac{2\pi}{q} a_i \cdot B_j = 2\pi \delta_{ij}$, we may define $b_j = \frac{2\pi}{q} B_j = 2\pi \frac{\phi a_i}{a_j^T \phi a_i}$

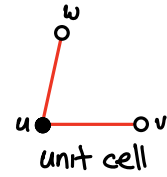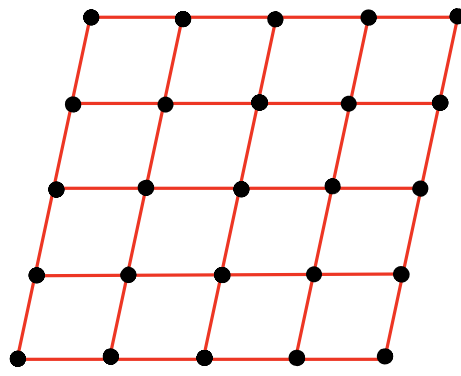$$b_1 = 2\pi \frac{\phi a_2}{a_1^T \phi a_2} \qquad b_2 = 2\pi \frac{\phi a_1}{a_2^T \phi a_1}$$

Square Lattice

$$b_1 = \frac{2\pi}{a} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad b_2 = \frac{2\pi}{a} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
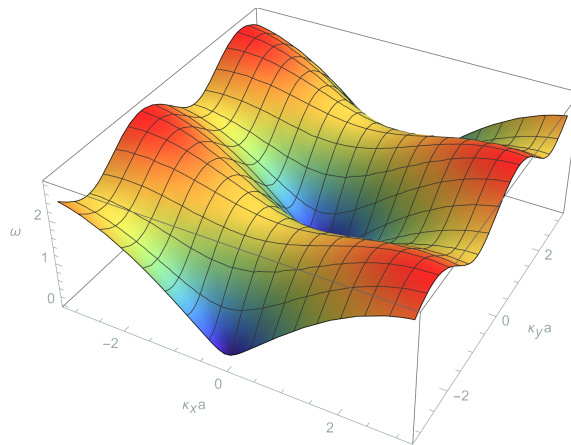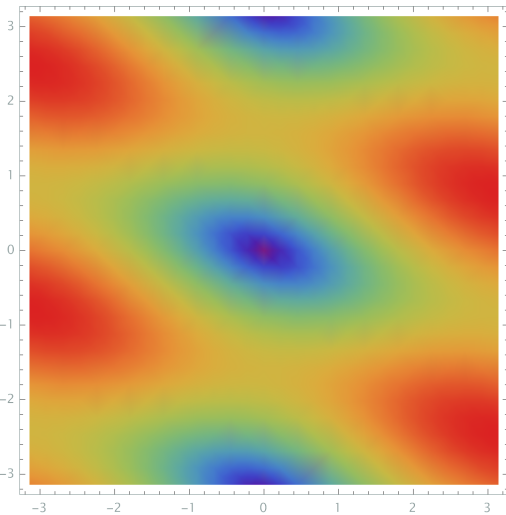
Tri-Honeycomb Lattice

$$b_1 = \frac{2\pi}{a} \begin{bmatrix} 1 \\ 1/\sqrt{3} \end{bmatrix} \qquad b_2 = \frac{2\pi}{a} \begin{bmatrix} 0 \\ 2/\sqrt{3} \end{bmatrix}$$

unit cell

$$m\ddot{u} + k(2u - v - w) = 0$$
$$0\ddot{v} + k(v - u) = 0$$
$$0\ddot{w} + k(w - u) = 0$$

$$m\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{M}\underbrace{\begin{bmatrix} \ddot{u} \\ \ddot{v} \\ \ddot{w} \end{bmatrix}}_{\ddot{x}} + k\underbrace{\begin{bmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}}_{K}\underbrace{\begin{bmatrix} u \\ v \\ w \end{bmatrix}}_{x} = 0$$

$$\underbrace{\begin{bmatrix} u \\ v \\ w \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} 1 \\ e^{i\kappa \cdot a_1} \\ e^{i\kappa \cdot a_2} \end{bmatrix}}_{T} u$$

$$\left| T^H (-\omega^2 M + K) T \right| = -\omega^2 + 4 - 2\cos(\kappa_x a) - 2\cos\left(\kappa_x a\sqrt{2-\sqrt{3}} + \kappa_y a\sqrt{2+\sqrt{3}}\right) = 0$$

$$b_1 = 2\pi \frac{\Phi a_2}{a_1^T \Phi a_2} = -\frac{2\pi}{\sqrt{2+\sqrt{3}}}\begin{bmatrix} -\sqrt{2+\sqrt{3}} \\ \sqrt{2-\sqrt{3}} \end{bmatrix}$$

$$b_2 = 2\pi \frac{\Phi a_1}{a_2^T \Phi a_1} = \frac{2\pi}{\sqrt{2+\sqrt{3}}}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

reciprocal lattice
Brillouin zone

$$a_1 = a\begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad a_2 = a\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$b_1 = \frac{2\pi}{a}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad b_2 = \frac{2\pi}{a}\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
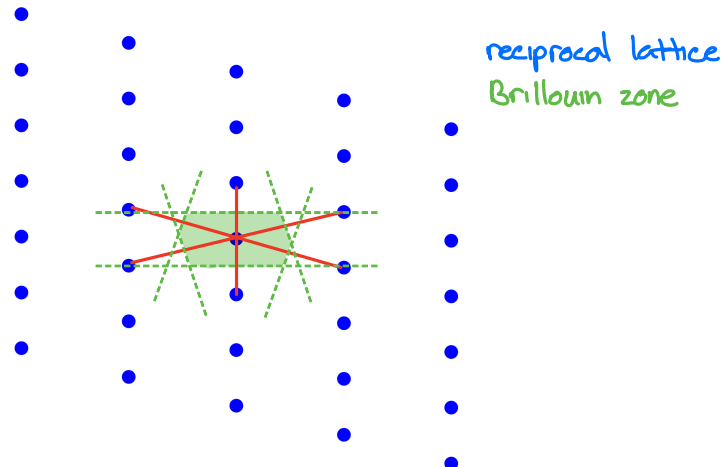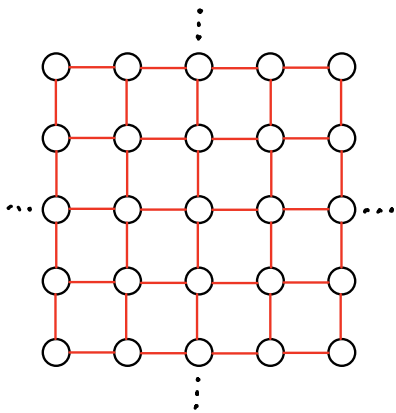
unit cell

square (direct) lattice
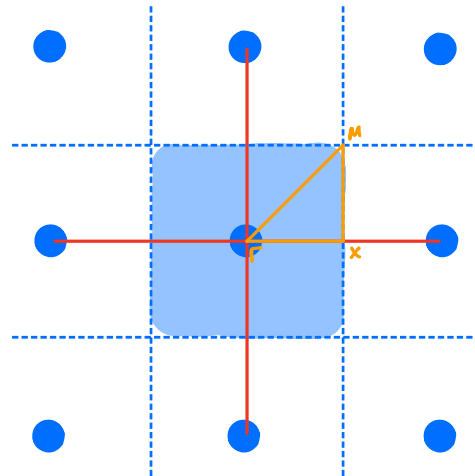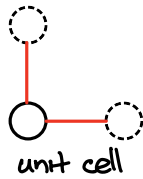
square (reciprocal) lattice

$$m\ddot{u}_{ij} = -2ku_{ij} + ku_{(i+1),j} + ku_{i,j+1} + f_{ij}$$
$$0\ddot{u}_{(i+1),j} = ku_{ij} - ku_{(i+1),j} + f_{(i+1),j}$$
$$0\ddot{u}_{i,j+1} = ku_{ij} - ku_{i,j+1} + f_{i,j+1}$$

$$\begin{bmatrix} m & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \ddot{u}_{ij} \\ \ddot{u}_{(i+1),j} \\ \ddot{u}_{i,j+1} \end{bmatrix} + \begin{bmatrix} 2k & -k & -k \\ -k & k & 0 \\ -k & 0 & k \end{bmatrix}\begin{bmatrix} u_{ij} \\ u_{(i+1),j} \\ u_{i,j+1} \end{bmatrix} = \begin{bmatrix} f_{ij} \\ f_{(i+1),j} \\ f_{i,j+1} \end{bmatrix}$$

$$u_{ij} = u_{ij}$$
$$u_{i+1,j} = u_{ij}e^{ik_x a}$$
$$u_{i,j+1} = u_{ij}e^{ik_y a}$$

$$\begin{bmatrix} u_{ij} \\ u_{i+1,j} \\ u_{i,j+1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 \\ e^{ik_x a} \\ e^{ik_y a} \end{bmatrix}}_{T} u_{ij}$$

$$|T^H(-\omega^2 M + K)T| = 4 - \omega^2 m - 2\cos(k_x a) - 2\cos(k_y a) = 0 \qquad \therefore \quad \omega = \sqrt{\frac{2k[2 - \cos(k_x a) - \cos(k_y a)]}{m}}$$
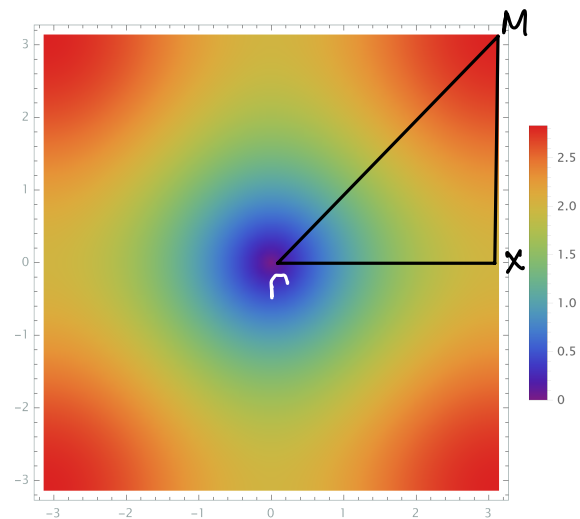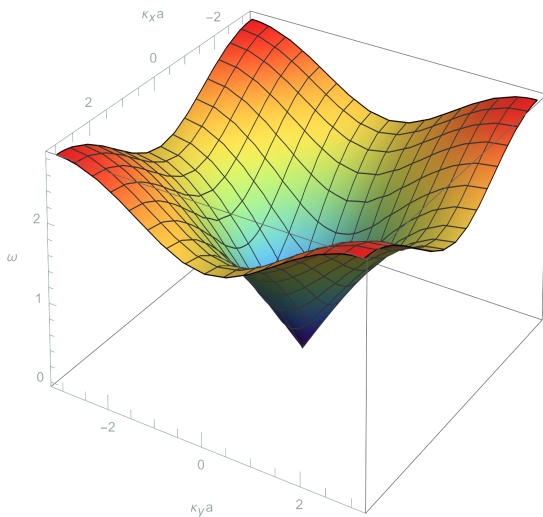
```
SQR_Lattice_Dispersion.m
```

```matlab
1  %%%% Nearest-neighbor coupling only.
2
3  clear;clc;
4
5  %% Setup-User Input
6  m=1;
7  k=1;
8
9  ka_div=51;
10
11 %% Calculations
12 [kxa,kya]=meshgrid(linspace(-pi,pi,ka_div));
13 w=sqrt(2*k*(2-cos(kxa)-cos(kya))/m);
14
15 [kxa_q,kya_q]=meshgrid(linspace(-pi,pi,21));
16 w_q=sqrt(2*k*(2-cos(kxa_q)-cos(kya_q))/m);
17
18 dwq_dkxa=(k*sin(kxa_q))./(m*w_q);
19 dwq_dkya=(k*sin(kya_q))./(m*w_q);
20
21 %% Plotting
22 figure(1);
23 surf(kxa,kya,w);
24 xlabel('\kappa_xa');ylabel('\kappa_ya');
25 zlabel('Frequency, \omega');
26 axis([-1 1 -1 1].*pi);axis square;
27 colormap(jet);
28
29 figure(2);
30 contour(kxa,kya,w,9,'k',...
31     'ShowText','on','LineWidth',1);hold on;
32 quiver(kxa_q,kya_q,dwq_dkxa,dwq_dkya,'b');hold off;
33 xlabel('\kappa_xa');ylabel('\kappa_ya');
34 axis square;
```

In addition to band gaps, the dispersion surfaces provide information on the propagation of energy within the lattice, which is defined by the group velocity vector:

$$\bar{v}_g = \nabla_k \omega(k) = (v_g)_x \hat{i} + (v_g)_y \hat{j}$$

$$= \frac{k}{m}\sin(k_x a)\left(\frac{2[2-\cos(k_x a)-\cos(k_y a)]}{m}\right)^{-\frac{1}{2}}\hat{i} + \frac{k}{m}\sin(k_y a)\left(\frac{2[2-\cos(k_x a)-\cos(k_y a)]}{m}\right)^{-\frac{1}{2}}\hat{j}$$

The identification of the direction of energy propagation through the analysis of the gradient of the dispersion surface [i.e., $\bar{v}_g = \nabla_k \omega(k)$] is illustrated before. The dispersion surface is represented by select iso-frequency contours, $\omega = \{0.5, 1.0, 1.5, 2.0, 2.5\}$, and the local gradient is represented by arrows magnitude-dependent color scaling.

The iso-frequency contour at $\omega=1$ appears almost circular, which is indicative of isotropic wave energy propagation. The case for $\omega=2$ is markedly different as the iso-frequency contour comprises straight lines and all normal arrows are oriented along the $\pm\pi/4$ axes. This indicates that the wave energy is strongly confined to these directions.
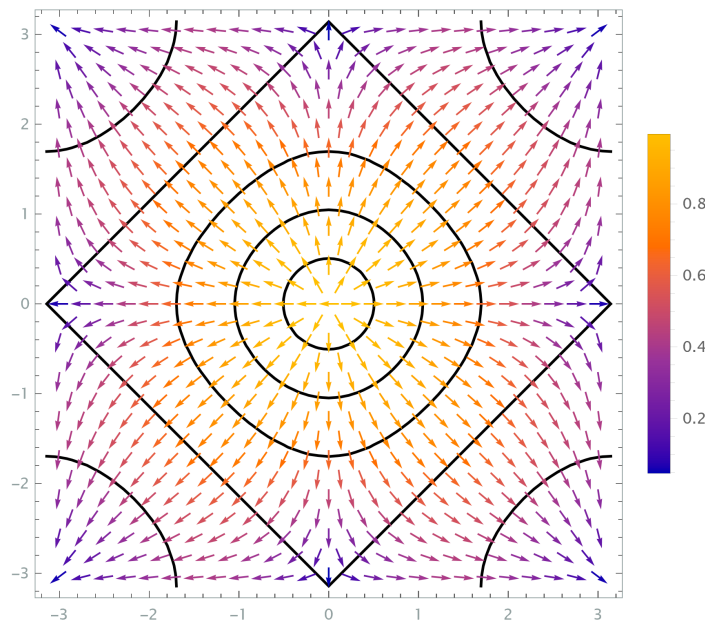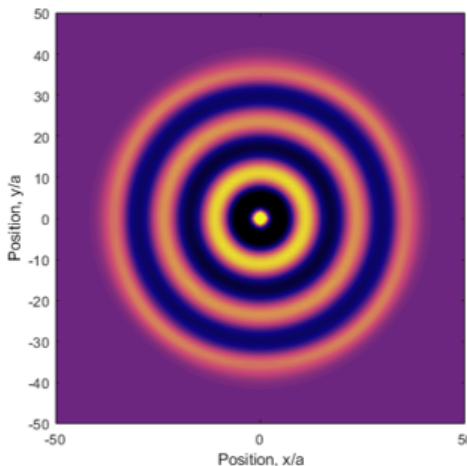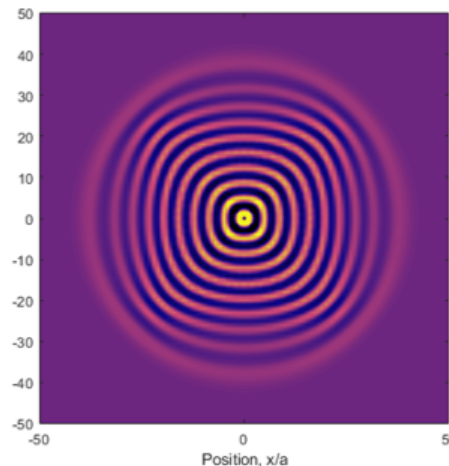
$\omega=1$ $\qquad$ $\omega=1.5$ $\qquad$ $\omega=2$
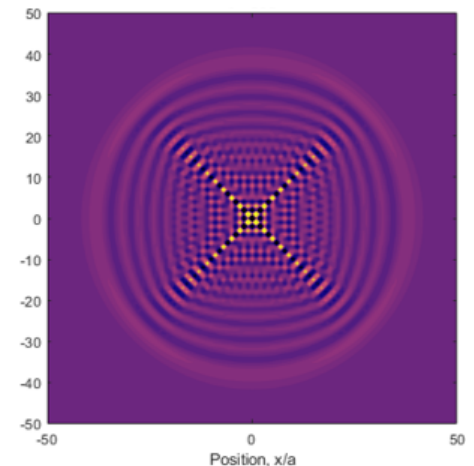
SQR_Lattice_Simulation.m

```matlab
1  clear;clc;
2
3  %% Setup-User Input
4  n_sites_x=101;
5  n_sites_y=101;
6
7  m=1;
8  k=1;
9
10 A=1/20;
11 w=2; %=3/4,2,2.5
12
13 dt=1e-1; % time increment
14 n_time_steps=4e2;
15
16 %% Connectivity
17 n_sites=n_sites_x*n_sites_y;
18
19 [x,y]=meshgrid(1:n_sites_x,1:n_sites_y);
20
21 LFT=(reshape(x,[1,n_sites])==1).*(1:n_sites);LFT(LFT==0)=[];
22 RGT=(reshape(x,[1,n_sites])==n_sites_x).*(1:n_sites);RGT(RGT==0)
     =[];
23 BTM=(reshape(y,[1,n_sites])==1).*(1:n_sites);BTM(BTM==0)=[];
24 TOP=(reshape(y,[1,n_sites])==n_sites_y).*(1:n_sites);TOP(TOP==0)
     =[];
25
26 N=repmat((1:n_sites)',[1 4]);
27 N(:,1)=N(:,1)+n_sites_y;
28 N(:,2)=N(:,2)+1;
29 N(:,3)=N(:,3)-n_sites_y;
30 N(:,4)=N(:,4)-1;
31
32 N(RGT,1)=RGT';
33 N(TOP,2)=TOP';
34 N(LFT,3)=LFT';
35 N(BTM,4)=BTM';
36
37 x=x-51;y=flipud(y)-51;
```

```matlab
%% Mass and Stiffness Matrices
M=sparse(1:n_sites,1:n_sites,m*ones(1,n_sites));
K=zeros(n_sites);
for j=1:n_sites
    K(j,N(j,:))=-k;
end
K=sparse(K+diag(-sum(K,2)));

%% Bathe Preliminaries
%%%% Integration parameters
p=0.54;q1=(1-2*p)/(2*p*(1-p));q2=1/2-p*q1;q0=1/2-q1-q2;
a0=p*dt;a3=(1-p)*dt;a1=(a0^2)/2;a2=a0/2;
a4=(a3^2)/2;a5=q0*a3;a6=(1/2+q1)*a3;a7=q2*a3;

%%%% Initial conditions
indx=round(n_sites/2);

un=spalloc(n_sites,1,n_sites); % displacement
vn=spalloc(n_sites,1,n_sites);vn(indx)=w*A; % velocity
an=spalloc(n_sites,1,n_sites); % acceleration

%% Bathe Scheme
for j=2:n_time_steps
    % First sub-step
    up=un+a0*vn+a1*an;

    fp=-K*up;

    ap=M\fp;
    vp=vn+a2*(an+ap);

    % Second sub-step
    un=up+a3*vp+a4*ap;
    un(indx)=A*sin(w*(j-1)*dt);

    ft=-K*un;

    an1=an;
    an=M\ft;
    an(indx)=-(w^2)*A*sin(w*(j-1)*dt);

    vn=vp+a5*an1+a6*ap+a7*an;
    vn(indx)=w*A*cos(w*(j-1)*dt);
end
```

```matlab
%% Plotting
figure(1);
contourf(x,y,reshape(un,[n_sites_y,n_sites_x]),...
    200,'EdgeColor','none');
xlabel('Position, x/a');ylabel('Position, y/a');
title(['\omega = ' num2str(w) '; t = ' num2str(floor((j-1)*dt)) '
    s']);
axis([-50 50 -50 50]);axis square;
colormap(jet);clim([-A A]./10);
```
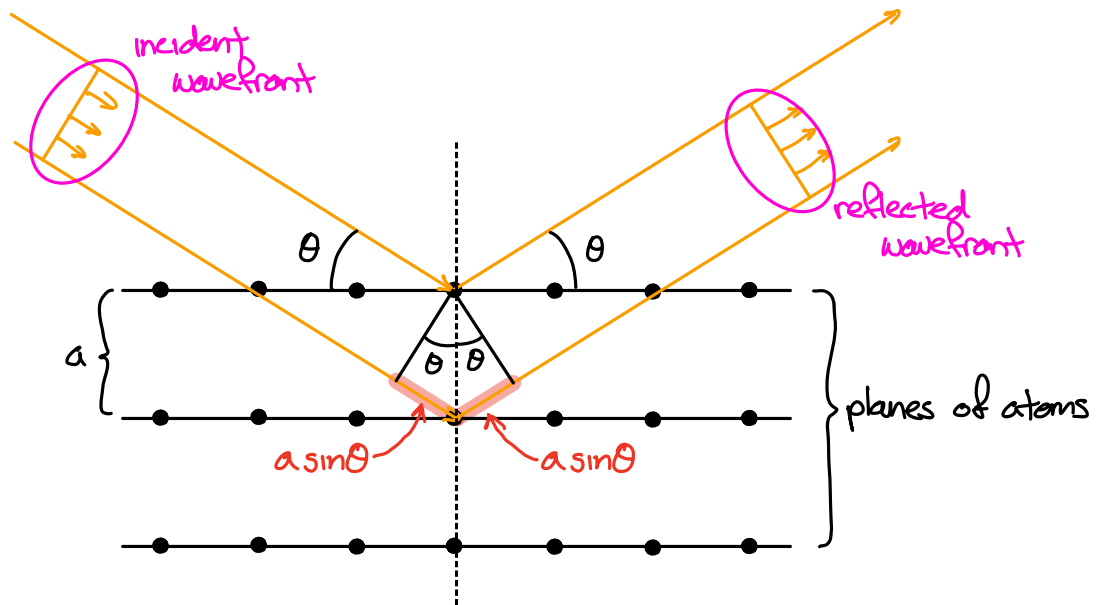
When an incident x-ray beam of sharply-defined wavelengths bounces off a crystal, intense reflection peaks are observed in certain directions. Atoms on parallel planes can reflect x-ray into either constructive or destructive interference depending upon the pathlength difference similar to the optical diffraction from a grating.

Consider the set of lattice planes above. An x-ray beam incident on a plane at an angle, θ, will reflect with the same angle and wavelength. Geometry gives a pathlength difference for two beams incident on planes separated by a distance, a, as $2a\sin\theta$.

If the pathlength difference is equal to an integer multiple of the wavelength, the two reflected waves will be in phase and constructive interference occurs, causing an intensity peak to be detected. This condition is the Bragg law of diffraction: $2a\sin\theta = n\lambda$.

Consider the case where the incident and reflected waves propagate along a single dimension, i.e., $\theta = \pi/2$; thus, $\lambda = 2a$ and $\kappa a = \frac{2\pi a}{2a} = \pi$. The boundaries of the 1st Brillouin zone represent satisfaction of the Bragg condition.

TOPIC 7:
The Transfer Matrix Method

The state vector at a point in an elastic system is a column vector containing the displacements and corresponding internal forces.
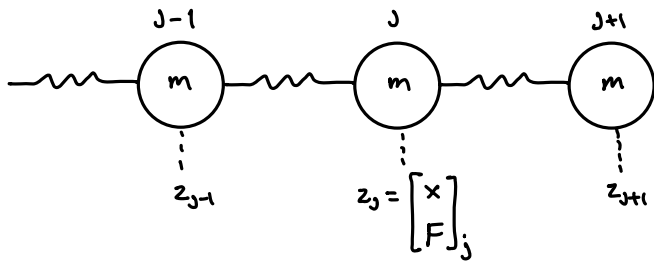
$$z_j = \begin{bmatrix} \phi \\ \tau \end{bmatrix}_j \quad \text{or} = \begin{bmatrix} \omega \\ T \end{bmatrix} \quad \text{or} = \begin{bmatrix} \omega \\ \phi \\ M \\ V \end{bmatrix}$$
shaft   string   beam

The transfer matrix method is a means of solving differential equations by discretizing the problem and assembling the building blocks. We will not go into depth here; instead, we will learn the basic idea in order to later use it in the study of Bragg scattering and local resonance.

Consider the spring between two masses. From equilibrium, we get:
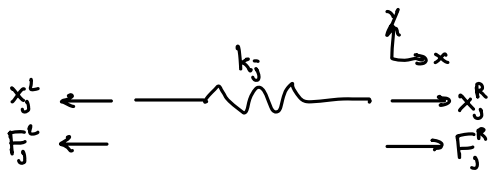
Sign Convention:
positive displacements coincide with positive directions of the coordinate system

$$F_j^R = F_j^L = k(x_j^R - x_j^L)$$

positive forces coincide with the outward normal

Collecting the displacements / forces associated with a point gives:

$$\left. \begin{array}{l} x_j^R = x_j^L + \dfrac{1}{k} F_j^L \\[2mm] F_j^R = F_j^L \end{array} \right\} \longrightarrow \begin{bmatrix} x \\ F \end{bmatrix}_j^R = \begin{bmatrix} 1 & 1/k \\ 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ F \end{bmatrix}_j^L$$

constitutive
equilibrium

$$z_j^R = T_f z_j^L \qquad T_f: \text{field transfer matrix}$$

Hence, by means of the transfer matrix T_f, we can express z_j^R in terms of z_j^L. At the moment, this method offers no special advantage.

Now, consider the mass between two springs. From equilibrium, we get:
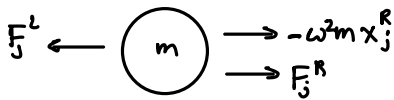
$$F_j^R - F_j^L - \omega^2 m x_j^R = 0 \qquad \therefore \quad F_j^L = F_j^R - \omega^2 m x_j^R$$

$$x = x_j^L = x_j^R$$

the mass is rigid and exists at a point, so the displacements to the left and right are the same.

$$\left. \begin{array}{l} x_j^L = x_j^R \\[2mm] F_j^L = F_j^R - \omega^2 m x_j^R \end{array} \right\} \longrightarrow \begin{bmatrix} x \\ F \end{bmatrix}_j^L = \begin{bmatrix} 1 & 0 \\ -\omega^2 m & 1 \end{bmatrix}\begin{bmatrix} x \\ F \end{bmatrix}_j^R$$

$$z_j^L = T_p z_j^R \qquad T_p: \text{point transfer matrix}$$

Bringing each together:

$x_J^L \leftarrow \text{---}\sim\sim\text{---} \rightarrow x_J^R$ $F_J^L \leftarrow \bigcirc_m \rightarrow \omega^2 m x_j^R$ $= \text{---}\sim\sim\bigcirc_m$
$F_J^L \leftarrow \qquad \rightarrow F_J^R$ $F_j^L \leftarrow \qquad \rightarrow F_j^R$

$$\begin{bmatrix} 1 & 1/k \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ F \end{bmatrix}_J^L = \begin{bmatrix} x \\ F \end{bmatrix}_J^R$$
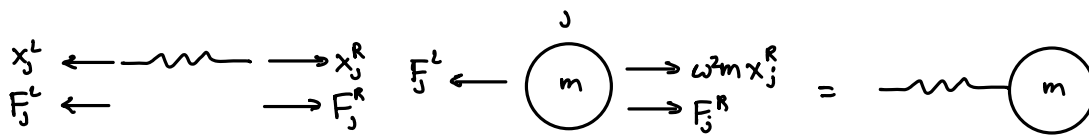
Compatibility requires $\begin{bmatrix} x \\ F \end{bmatrix}_J^R = \begin{bmatrix} x \\ F \end{bmatrix}_J^L$

(spring) (mass)

$$\begin{bmatrix} x \\ F \end{bmatrix}_J^L = \begin{bmatrix} 1 & 0 \\ -\omega^2 m & 1 \end{bmatrix} \begin{bmatrix} x \\ F \end{bmatrix}_J^R$$

$$\begin{bmatrix} 1 & 0 \\ -\omega^2 m & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1/k \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ F \end{bmatrix}_J^L = \begin{bmatrix} x \\ F \end{bmatrix}_J^R$$

$$\underbrace{\begin{bmatrix} 1 & 1/k \\ -\omega^2 m & 1 - \frac{\omega^2 m}{k} \end{bmatrix}}_{T} \begin{bmatrix} x \\ F \end{bmatrix}_J^L = \begin{bmatrix} x \\ F \end{bmatrix}_J^R$$

$z_J^L = z_J^R$ T: oscillator transfer matrix

Assume the system is fixed at the left end ($x_J^L = 0$) and free at the right end ($F_J^R = 0$), then:

$$x_J^R = \frac{1}{k} F_J^L \quad \text{and} \quad \left(1 - \frac{\omega^2 m}{k}\right) F_J^L = 0$$

Since $F_J^L \neq 0$, we recover the characteristic equation for the system's natural frequencies.

In general, the BCs are: $\begin{bmatrix} 0 \\ F \end{bmatrix}_J^L - \begin{bmatrix} 0 \\ F \end{bmatrix}_j^R$ $\begin{bmatrix} 0 \\ F \end{bmatrix}_J^L - \begin{bmatrix} x \\ 0 \end{bmatrix}_j^R$ $\begin{bmatrix} x \\ 0 \end{bmatrix}_J^L - \begin{bmatrix} x \\ 0 \end{bmatrix}_j^R$
   fixed – fixed   fixed – free   free – free

To append a second mass-spring system to the first, we recognize that compatibility requires $z_j^R = z_{j+1}^L$.

$x_1^L \leftarrow \text{---}\sim\sim\bigcirc_m \rightarrow \omega^2 m_1 x_1^R$ $x_2^L \leftarrow \text{---}\sim\sim\bigcirc_m \rightarrow \omega^2 m_2 x_2^R$
$F_1^L \leftarrow \qquad \rightarrow F_1^R$ $F_2^L \leftarrow \qquad \rightarrow F^R$
$T_1 z_1^L = z_1^R$ $T_2 z_2^L = z_2^R$
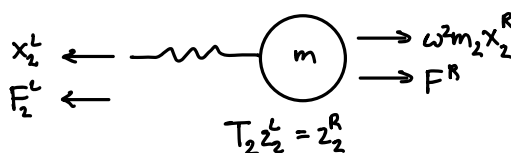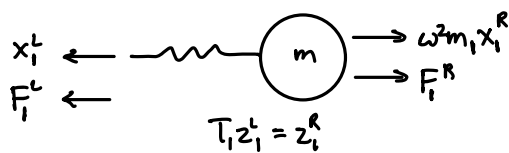
$T_1 z_1^L = z_1^R = z_2^L$

$T_2 z_2^L = T_2 T_1 z_1^L = z_2^R$ (two-mass system)

$\underbrace{T_N \cdots T_2 T_1}_{\text{cummulative transfer matrix}} z_1^L = z_N^R$ (general N-mass system)

Now, from the vibration of a finite system, let's consider wave propagation in the infinite system. In this case, Bloch BCs require that $z_j^R = e^{ika} z_j^L$:

$T z_j^L = z_j^R = e^{ika} z_j^L$ $\therefore$ $(T - e^{ika} I) z_j^L = 0$

Each layer is characterized by material properties $-E_j$ and ρ_j — and geometry $-\ell_j$

$u = (A_1 e^{i\kappa x} + A_2 e^{-i\kappa x}) e^{i\omega t}$
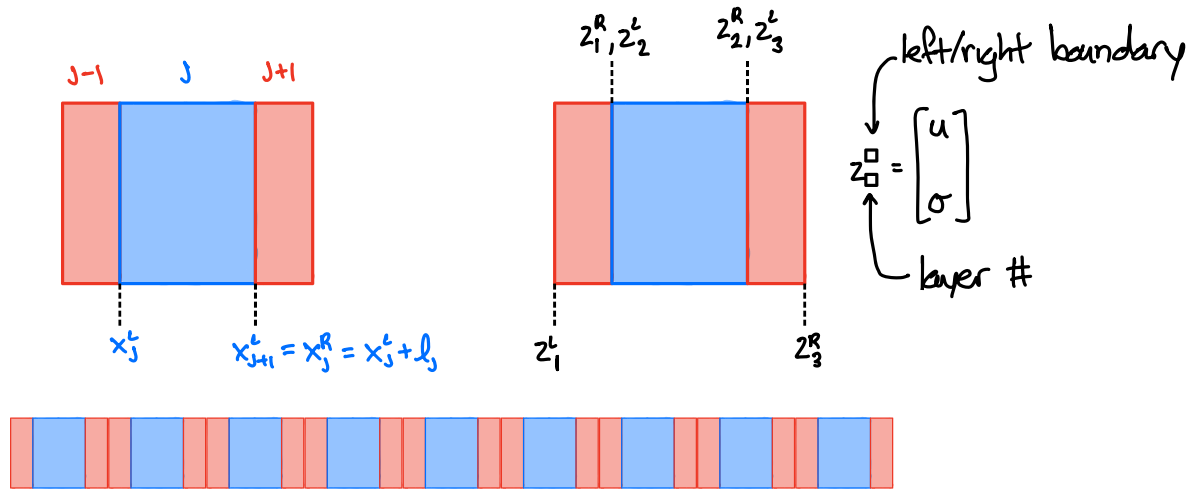
$\sigma = E \dfrac{du}{dx} = (i\kappa E A_1 e^{i\kappa x} - i\kappa E A_2 e^{-i\kappa x}) e^{i\omega t}$
$\qquad = (iZA_1 e^{i\kappa x} - iZA_2 e^{-i\kappa x}) e^{i\omega t}$

$$\begin{bmatrix} u \\ \sigma \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ iZ & -iZ \end{bmatrix}\begin{bmatrix} e^{i\kappa x} & 0 \\ 0 & e^{-i\kappa x} \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$$
$\underbrace{}_{z} = \underbrace{}_{B} \quad \underbrace{}_{C(x)} \ \underbrace{}_{a}$

$Z = \kappa E = \omega\sqrt{\rho E}$ since $\kappa = \omega/c$. Note that, at this point, κ is the wavenumber within a particular layer.

The transfer matrix is to relate the state at the boundary of one layer to the boundary of the next. To derive the transfer matrix, consider the state at x_i^L and $x_i^R = x_i^L + \ell_i$

$z_i^L = B\,C(x_i^L)\,a \qquad [1]$

$z_i^R = B\,C(x_i^R)\,a = B\,C(x_i^L + \ell_i)\,a = B\,C(x_i^L)\,C(\ell_i)\,a \qquad [2]$

$\color{blue}{e^{i\kappa x_i^R} = e^{i\kappa(x_i^L + \ell_i)} = e^{i\kappa x_i^L} e^{i\kappa \ell_i}}$

Let $x_i^L = 0$, then $C(0) = I$ and [1] becomes $z_i^L = Ba$ such that, from [1], the amplitude vector is $a = B^{-1} z_i^L$ and, from [2], $z_i^R = B\,C(\ell_i)\,a = \underbrace{B\,C(\ell_i)\,B^{-1}}_{T_1} z_i^L = T_1 z_i^L$

$$T_j = \begin{bmatrix} \cos(\kappa_j \ell_j) & \dfrac{1}{Z_j}\sin(\kappa_j \ell_j) \\[2mm] -Z_j \sin(\kappa_j \ell_j) & \cos(\kappa_j \ell_j) \end{bmatrix}$$

The transfer matrix can be applied recursively to relate the state at one boundary to any other in a multi-layered medium.

$$z_1^R = T_1 z_1^L = z_2^L \qquad [3]$$

$$z_2^R = T_2 z_2^L = T_2 T_1 z_1^L = z_3^L$$

$$z_3^R = T_3 z_3^L = T_3 T_2 T_1 z_1^L$$

in general: $z_n^R = \underbrace{T_n T_{n-1} T_{n-2} \cdots T_2 T_1}_{T: \text{ cummulative transfer matrix}} z_1^L = T z_1^L$

layer transfer matrix

recall $z_n^R = z_1^L e^{ika}$ where z is the wavenumber of the whole periodic, multi-layered medium and $a = \sum_j^n \ell_j$ is the spatial period. Consequently:

$$z_n^R = \underbrace{T z_1^L = z_1^L e^{ika}}_{\text{eigenvalue problem}} \qquad \therefore \qquad (T - \gamma I) z_1^L = 0 \qquad \text{where } \gamma = e^{ika}$$

While the eigenvalue, γ, delivers the dispersion relation, the eigenvector, z_1^L, yields the mode shape at a particular ω.

From [1], recall that $z_1^L = B_1 C(x_1^L) a_1$. Let $x_1^L = 0$ such that $C(0) = I$; therefore:

$$z_1^L = B_1 a_1 \qquad \therefore \qquad a_1 = B_1^{-1} z_1^L$$

Similarly, from [3], recall that:

$$z_1^R = T_1 z_1^L = z_2^L = B_2 C(x_2^L) a_2 \qquad \therefore \qquad a_2 = [B_2 C(x_2^L)]^{-1} T_1 z_1^L$$

Following this trend, we can find a_j for an arbitrary layer j:

$$a_j = [B_j C(x_j^L)]^{-1} T_{j-1} T_{j-2} \cdots T_2 T_1 z_1^L$$

Once all a_j have been determined, the portion of the displacement and stress mode shapes within each layer in the first unit cell can be computed from $z_j = B_j C_j(x) a_j$. Furthermore, Bloch's theorem, $z_n^R = \gamma z_1^L$, may be used to compute the displacement and stress mode shapes over as many subsequent unit cells as desired. A full mode shape is realized when the displacement/stress profile spans a complete wavelength, $\lambda = 2\pi / \kappa_R$.

TMM_Rod_Dispersion_and_Waveform.m

```matlab
1   clc;clearvars;
2   i=sqrt(-1);
3
4   %% Setup-User Input
5   d=[0.0025;0.005;0.0025];
6   E=[2e9;2e11;2e9]./(1e11);
7   rho=[1e3;3e3;1e3]./(1e11);
8
9   w_min=0.01;
10  w_max=20e5;
11  w_div=1e4;
12
13  w_target=309107/1;
14  n_period=5;
15  n_cell=29;
16  n_wavelength=1; % Supersedes n_cell unless set to 0
17
18  %% Transfer Matrix Solution
19  c0_sqrd=E./rho;
20  c0=sqrt(c0_sqrd);
21  d_cell=sum(d);
22
23  n_layer=length(d);
24
25  cnt=0;
26  krd=zeros(1,w_div);
27  kid=zeros(1,w_div);
28  for w=unique(sort([linspace(w_min,w_max,w_div) w_target]))
29      cnt=cnt+1;
30
31      %%%% T-Matrix %%%%
32      T=eye(2);
33      for j=n_layer:-1:1
34          k=w/c0(j);
35          Z=k*E(j);
36
37          T=T*[cos(k*d(j)) (1/Z)*sin(k*d(j));...
38              -Z*sin(k*d(j)) cos(k*d(j))];
39      end
40
41      [zL1,expkd]=eig(T,eye(2));expkd=diag(expkd);
```

```matlab
krd(cnt)=abs(real(-i*log(expkd(1,1))));
kid(cnt)=abs(imag(-i*log(expkd(1,1))));

if w==w_target
        krd_target=krd(cnt);
        kid_target=kid(cnt);
        kd_target=krd(cnt)+i*kid(cnt);
        zL1_target=zL1(:,1);
    end
end

%% Mode Shape
%%%% Amplitude
xL=cumsum([0,d(1:end-1)']);

T=eye(2);
A=zeros(2,n_layer);
B=zeros(2,2,n_layer);
k=zeros(1,n_layer);
for j=1:n_layer
    k(j)=w_target/c0(j);
    Z=k(j)*E(j);

    B(:,:,j)=[1 1;i*Z -i*Z];
    C=diag([exp(i*k(j)*xL(j)) exp(-i*k(j)*xL(j))]);
    A(:,j)=(B(:,:,j)*C)\T*zL1_target;

    T=[cos(k(j)*d(j)) (1/Z)*sin(k(j)*d(j));...
        -Z*sin(k(j)*d(j)) cos(k(j)*d(j))]*T;
end

%%%% Unit Cell Field
cnt=1;
u=B(:,:,1)*A(:,1);
x=0;
```

```matlab
for j=1:n_layer
    for m=linspace(0,d(j),100)
        if m~=0
            cnt=cnt+1;

            C=diag([exp(i*k(j)*(xL(j)+m)) exp(-i*k(j)*(xL(j)+m))
                ]);
            u(:,cnt)=B(:,:,j)*C*A(:,j);
            x(cnt)=xL(j)+m;
        end
    end
end

%%%% Waveform
lambda=0;
if n_wavelength>0
    lambda=2*pi*d_cell*n_wavelength/krd_target;
    n_cell=ceil(lambda/d_cell);
end

X=x;U=u;
for j=2:n_cell
    X=[X,x(2:end)+(j-1)*d_cell];
    U=[U,u(:,2:end).*exp(i*(j-1)*kd_target)];
end
if lambda>0
    X(X>lambda)=[];
    U=U(:,1:numel(X));
end

%% Plotting
w=unique(sort([linspace(w_min,w_max,w_div) w_target]));

figure(1);
plot(-kid,w,'r',krd,w,'k',...
    -kid_target,w_target,'ro',...
    krd_target,w_target,'ko',...
    [0 0],[0 w_max],'k','Linewidth',1);
xlabel('Wavenumber, \kappaa');ylabel('Frequency, \omega');
axis([-pi pi 0 w_max]);axis square

figure(2);
plot(X,real(U(1,:)),'k','LineWidth',1);
```

```matlab
dt=2*pi/(20*w_target);
T_end=2*pi*n_period/w_target;
for j=1:floor(T_end/dt)
    figure(3);
    plot(X,real(U(1,:).*exp(-i*w_target*(j-1)*dt)),'k','LineWidth',1);
    axis([min(X) max(X) -1 1]);
    axis square;
    drawnow;
end
```

Euler-Bernoulli Beam
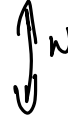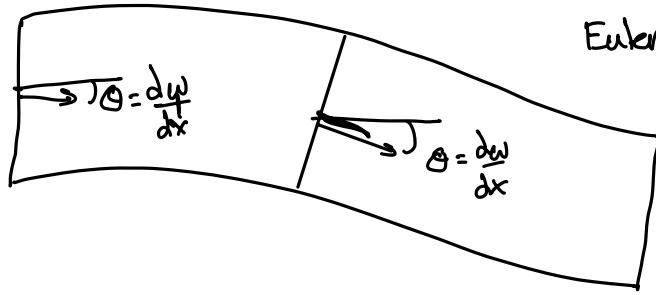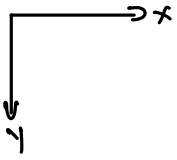
$$EI\frac{d^4 w}{dx^4} + \rho A\frac{d^2 w}{dt^2} = 0$$

$$c_0^2 \frac{d^4 w}{dx^4} + \frac{d^2 w}{dt} = 0 \qquad c_0^2 = \frac{EI}{\rho A} \qquad w = We^{i(kx - \omega t)}$$

$$\omega^2 = c_0^2 k^4 \qquad \omega = \pm k^2 c_0 \qquad k = \pm\sqrt{\pm\sqrt{\frac{\omega}{c_0}}}$$

Timoshenko Beam

$$kGA\left(\frac{d^2 w}{dx^2} - \frac{d\theta}{dx}\right) = \rho A\frac{d^2 w}{dt^2}$$

$$EI\frac{d^2 \theta}{dx^2} + kGA\left(\frac{dw}{dx} - \theta\right) = \rho I\frac{d^2 \theta}{dt^2}$$

$$\left. \right\}$$

$$\frac{EI}{\rho A}\frac{d^4 w}{dx^4} - \frac{I}{A}\left(1 + \frac{E}{kG}\right)\frac{d^4 w}{dx^2 dt^2} + \frac{d^2 w}{dt^2} + \frac{\rho I}{kGA}\frac{d^4 w}{dt^4} = 0$$

$$w = Be^{i(kx - \omega t)}$$

$$k^4 - \rho\frac{kG + E}{kGE}\omega^2 k^2 + \left(\frac{\rho^2}{kGE}\omega^2 - \frac{\rho A}{EI}\right)\omega^2 = 0$$

$$1 - \rho\frac{kG + E}{kGE}v_p^2 + \left(\frac{\rho^2}{kGE}v_p^2\right)v_p^2 = 0 \qquad \textcolor{red}{v_p \text{ is bounded} \quad k \to \infty}$$

$$\left(\frac{\rho^2}{kGE}\omega^2 - \frac{\rho A}{EI}\right)\omega^2 = 0 \qquad \textcolor{red}{\therefore \quad \omega = 0 \;; \; \sqrt{\frac{kGA}{\rho I}}}$$

$$w(x) = B_1 e^{ik_1 x} + B_2 e^{-ik_1 x} + B_3 e^{ik_2 x} + B_4 e^{-ik_2 x}$$

$$\theta(x) = C_1 e^{ik_1 x} + C_2 e^{-ikx} + C_3 e^{ik_2 x} + C_4 e^{-ik_2 x}$$

$$\frac{C_1}{B_1} = \frac{kGk^2 - \omega^2\rho}{kGk}$$

$$X_1 = \frac{kGk_1^2 - \omega^2\rho}{kGk_1} \qquad X_2 = \frac{kGk_2^2 - \omega^2\rho}{kGk_2}$$

$$M = -EI\frac{d\theta}{dx} \qquad V = kGA\left(\frac{dw}{dx} + \theta\right)$$

$$W_1 = EI\left(k_1^2 - \frac{\omega^2\rho}{kG}\right) \qquad W_2 = EI\left(k_2^2 - \frac{\omega^2\rho}{kG}\right)$$

$$Z_1 = EI\left(\underbrace{\frac{kGk_1^2 - \omega^2\rho}{kGk_1}}_{X_1}\right) \qquad Z_2 = EI\left(\underbrace{\frac{kGk_2^2 - \omega^2\rho}{kGk_2}}_{X_2}\right)$$

$$z = \begin{bmatrix} w \\ \theta \\ V \\ M \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 \\ X_1 & -X_1 & X_2 & -X_2 \\ W_1 & W_1 & W_2 & W_2 \\ Z_1 & -Z_1 & Z_2 & -Z_2 \end{bmatrix}}_{B} \underbrace{\begin{bmatrix} B_1 e^{ik_1 x} \\ B_2 e^{-ik_1 x} \\ B_3 e^{ik_2 x} \\ B_4 e^{-ik_2 x} \end{bmatrix}}_{C(x)\,a}$$

$$z_1^L = B_1 \overset{=I}{C(x_1^L)} a_1 \qquad x_1^L = 0$$

$$z_1^L = B_1 a_1 \qquad \therefore \quad a_1 = B_1^{-1} z_1^L$$

$$z_1^R = B_1 C(\ell) a_1 = \underbrace{B_1 C(\ell) B^{-1}}_{T} z_1^L$$

TOPIC 8:
Finite Differences and Numerical Integration

Last class, we covered Hamilton and Lagrange's energy-based methods for deriving the EOM of a system. Of course, we derive these equations with the intent to solve them in order to predict and analyse the evolution of the system at hand. However, an exact solution is often difficult to formulate except for specific or very simplified examples. Therefore, a number of approximate (numerical) schemes have been developed. Today, we consider the basics of the finite difference method.

The goal of the FDM is the replacement of the differential equation by a system of algebraic ones. First, we discretize the problem domain, and then substitute the derivatives with finite difference approximations.
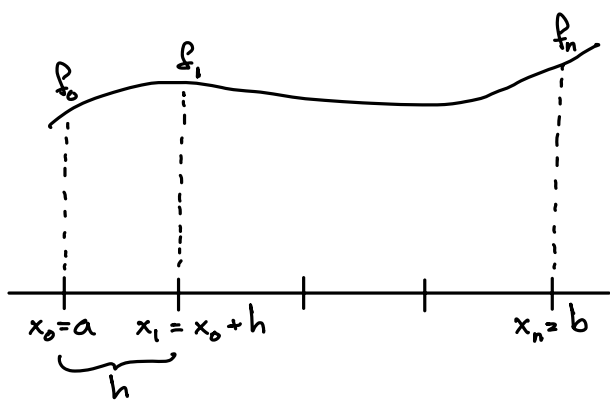
x_i are called pivot points. f_i are the unknown values of the solution.

In general, the domain does not need to be divided into even intervals, but it is most convenient.

If $f(x)$ varies significantly between pivot point, the interval h should be reduced as part of convergence study.

A number of methods may be applied to approximate the derivatives; we choose the Taylor expansion about $x = x_0$:

$$f(x_0 \pm h) = f(x_0) \pm h f'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{3!} f'''(x_0) + \cdots + \frac{h^n}{n!} f^{(n)}(x_0) + O(h^{n+1})$$

↖ truncation error

Thus, for 1st order Taylor expansion with, we have:

$$f(x_0+h) = f(x_0) + h f'(x_0) + O(h^2) \quad \therefore \quad f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} = \frac{f_1 - f_0}{h} \qquad \text{(forward difference)}$$

$$f(x_0-h) = f(x_0) - h f'(x_0) + O(h^2) \quad \therefore \quad f'(x_0) = \frac{f(x_0) - f(x_0-h)}{h} = \frac{f_0 - f_{-1}}{h} \qquad \text{(backward difference)}$$

$$f(x_0+h) - f(x_0-h) = 2h f'(x_0) + O(h^2) \quad \therefore \quad f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} = \frac{f_1 - f_{-1}}{2h} \qquad \text{(central difference)}$$

We can also formulate approximations at $O(h^4)$, but let's proceed with the central difference method to approximate $f''(x)$:

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + h^2 f''(x_0) + O(h^2) \quad \therefore \quad f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

For an arbitrary pivot point x_i: $(f'')_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$

Using any of the difference schemes, we can approximate a derivative at pivot point x_i with $i = 1, \ldots, N$. In general, we can use these schemes as formulated; however, the boundaries $i = 1, N$ require special attention to accommodate the possibility of (x_0, f_0) and (x_{N+1}, f_{N+1}).

$$f'(x_1) = \frac{f_2 - f_0}{2h} \qquad f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} \qquad f'(x_5) = \frac{f_6 - f_4}{2h}$$

$$\frac{f_2 - 2f_1 + f_0}{h^2}$$

f_1 f_2 f_3 f_4 f_5

x_1 x_2 x_3 x_4 x_5

boundary   interior   boundary
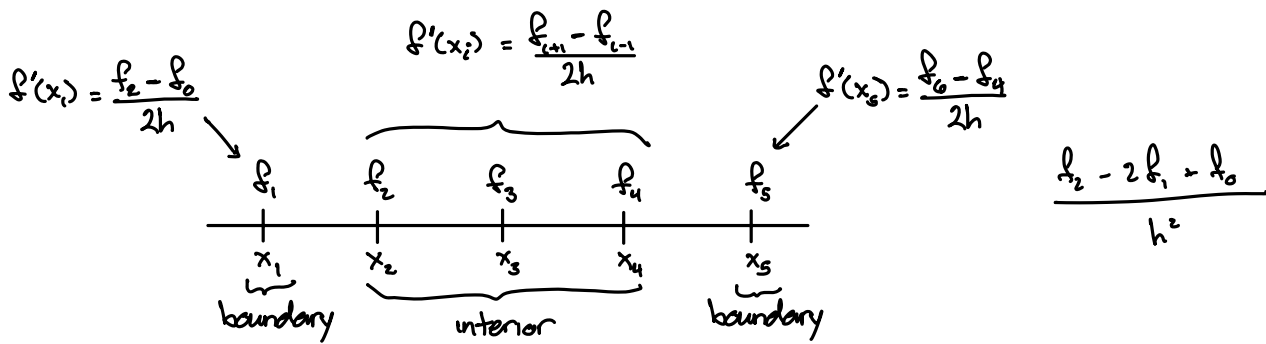
f_0 and f_6 do not exist (are beyond the domain). To accommodate them, we generally have three options: periodic, Dirichlet, and Neumann (note: these are numerical BCs, not physical BCs).

Periodic: $f_0 = f_5$ and $f_6 = f_1$

Dirichlet: $f_0 = 0$ and $f_6 = 0$ (assumes solution decays to zero from the interior)

Neumann: $f_0 = f_1$ and $f_6 = f_5$ (assumes function varies linearly beyond the boundary, therefore, second-order and higher derivatives vanish.)

Other custom BCs may be applied as well.

Use finite differences to solve $\frac{d^2 f}{dx^2} + xf - x = 0$ on the interval $x \in \overset{a,b}{[0,1]}$ with (physical) BCs $f(0) = 0$ and $f(1) = 0$.

$$\frac{d^2 f}{dx^2} + xf - x = 0 \longrightarrow \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + x_i f_i - x_i = 0 \qquad i = 1, \ldots, N$$

Let there be N pivot points, and so, $h = \frac{b-a}{N-1}$. Let $N = 5$, and so, $h = \frac{1}{4}$.

I took the negative of the proceeding equations for personal aesthetic reasons.

$i = 1:$ $(f_2 - 2f_1 + 0)(16) + (0)f_1 = 0$

$i = 2:$ $(f_3 - 2f_2 + f_1)(16) + (0.25)f_2 = 0.25$

$i = 3:$ $(f_4 - 2f_3 + f_2)(16) + (0.5)f_3 = 0.5$

$i = 4:$ $(f_5 - 2f_4 + f_3)(16) + (0.75)f_4 = 0.75$

$i = 5:$ $(0 - 2f_5 + f_4)(16) + (1)f_5 = 1$

$$\overbrace{\frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}}^{D_x^{(2)}} \overbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}}^{f} - \ldots$$

$$\frac{1}{4}\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{bmatrix}}_{C}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix} = -\frac{1}{4}\underbrace{\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}}_{b}$$

Applying the BCs $f_1 = f_5 = 0$ reduces the system of equations as follows

$$\left((16) \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} - \frac{1}{4} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \right) \begin{bmatrix} f_2 \\ f_3 \\ f_4 \end{bmatrix} = -\frac{1}{4} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad \therefore \quad \begin{bmatrix} f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} -0.0413 \\ -0.0663 \\ -0.0579 \end{bmatrix}$$

Note, do not mix schemes (e.g., central, forward, backward) when solving equation. Given, e.g., $\frac{d^2 f}{dx^2} + \frac{df}{dx} + f = 0$, use either scheme A for each derivative or scheme B for each derivative but not scheme A for $\frac{d^2 f}{dx^2}$ and scheme B for $\frac{df}{dx}$ ... this encourages errors.

The equation, $\frac{d^2 f}{dx^2} + x f - x = 0$, displays the typical components of a Diff Eq. — operators and functions.

Consider the more generic representation, $\frac{d^2 f(x)}{dx^2} + a(x) f(x) + b(x) = 0$.

The operators (i.e., derivatives, scaling functions) transform the function and, therefore, become matrices in the finite difference representation. The functions (i.e., unknown values, excitation functions) become column vectors in the FD representation.

For single-variable derivatives beyond second order and mixed derivatives of any order, there are a variety of alternative definitions. Consider, applying the first-order scheme twice in order to formulate a second order scheme.

$$\frac{d}{dx}\left(\frac{df}{dx}\right) = \frac{1}{2h}\left[\left(\frac{df}{dx}\right)_{i+1} - \left(\frac{df}{dx}\right)_{i-1}\right] = \frac{1}{2h}\left[\frac{df_{(i+1)}}{dx} - \frac{df_{(i-1)}}{dx}\right] = \frac{1}{4h}\left(f_{i+2} - 2f_i + f_{i-2}\right)$$

This scheme is less accurate than the one developed by Taylor series as function values further from the evaluation site are used to approximate the derivative. This hierarchal formulation is generally less accurate than the Taylor-derived version and becomes more so with increasing hierarchal levels. However, this is one option for mixed derivatives:

$$f(x_0+h, y_0+l) - f(x_0-h, y_0+l) = 2h f_x(x_0, y_0+l)$$

$$f(x_0+h, y_0-l) - f(x_0-h, y_0-l) = 2h f_x(x_0, y_0-l)$$

$$f_x(x_0, y_0+l) - f_x(x_0, y_0-l) = 2l f_{xy}(x_0, y_0)$$

$$\therefore f_{xy}(x_0, y_0) = \frac{f_x(x_0, y_0+l) - f_x(x_0, y_0-l)}{2l} = \frac{f(x_0+h, y_0+l) - f(x_0-h, y_0+l) - f(x_0+h, y_0-l) + f(x_0-h, y_0-l)}{4hl}$$

In other words $\frac{d}{dy}\left(\frac{df}{dx}\right) = \frac{1}{2l}\left[\left(\frac{df}{dx}\right)_{j+1} - \left(\frac{df}{dx}\right)_{j-1}\right] = \frac{1}{2l}\left[\frac{df_{(j+1)}}{dx} - \frac{df_{(j-1)}}{dx}\right] = \frac{1}{4hl}\left(f_{i+1,j+1} - f_{i-1,j+1} - f_{i+1,j-1} + f_{i-1,j-1}\right)$

Notice that FD approximations are, essentially, weighted sums of function values in the vicinity of the pivot point. We can use this condition in addition to the Taylor series expansion to describe a general procedure for developing a FD approximation.

STEP 1: Determine the function values you wish to use in the approximation.

$\qquad f_i \quad f_{i-1} \quad f_{i+1} \quad f_{i+2} \quad$ (stencil)

STEP 2: Determine the corresponding Taylor series expansion up to order n-1, where n = # function values.

$$f_i = f + 0\frac{\partial f}{\partial x} + 0\frac{\partial^2 f}{\partial x^2} + 0\frac{\partial^3 f}{\partial x^3}$$

$$f_{i-1} = f - h\frac{\partial f}{\partial x} + \frac{h^2}{2}\frac{\partial^2 f}{\partial x^2} - \frac{h^3}{6}\frac{\partial^3 f}{\partial x^3}$$

$$f_{i+1} = f + h\frac{\partial f}{\partial x} + \frac{h^2}{2}\frac{\partial^2 f}{\partial x^2} + \frac{h^3}{6}\frac{\partial^3 f}{\partial x^3}$$

$$f_{i+2} = f + (2h)\frac{\partial f}{\partial x} + \frac{(2h)^2}{2}\frac{\partial^2 f}{\partial x^2} + \frac{(2h)^3}{6}\frac{\partial^3 f}{\partial x^3}$$

$$\begin{bmatrix} f_i \\ f_{i-1} \\ f_{i+1} \\ f_{i+2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & -h & \frac{h^2}{2} & -\frac{h^3}{6} \\ 1 & h & \frac{h^2}{2} & \frac{h^3}{6} \\ 1 & 2h & 2h^2 & \frac{4h^3}{3} \end{bmatrix} \begin{bmatrix} f \\ \frac{\partial f}{\partial x} \\ \frac{\partial^2 f}{\partial x^2} \\ \frac{\partial^3 f}{\partial x^3} \end{bmatrix}$$

F — function   W — weights   D — derivatives

$$D = W^{-1}F \qquad \therefore \left(\frac{\partial f}{\partial x}\right)_i = \frac{-2f_{i-1} - 3f_i + 6f_{i+1} - f_{i+2}}{6h}$$

$$\left(\frac{\partial^3 f}{\partial x^3}\right)_i = \frac{-f_{i-1} + 3f_i - 3f_{i+1} + f_{i+2}}{h^3}$$

Formulate a difference approximation of the mixed derivative $\frac{\partial^2 f}{\partial x \partial y}$ using $f_{i,j}$, $f_{i-1,j-1}$, $f_{i+1,j-1}$, $f_{i+1,j+1}$, and $f_{i-1,j+1}$.

$$f_{i,j} = f$$

$$f_{i-1,j-1} = f - h\frac{\partial f}{\partial x} - \ell\frac{\partial f}{\partial y} + \frac{1}{2}\left(h^2\frac{\partial^2 f}{\partial x^2} + 2h\ell\frac{\partial^2 f}{\partial x \partial y} + \ell^2\frac{\partial^2 f}{\partial y^2}\right)$$

$$f_{i+1,j-1} = f + h\frac{\partial f}{\partial x} - \ell\frac{\partial f}{\partial y} + \frac{1}{2}\left(h^2\frac{\partial^2 f}{\partial x^2} - 2h\ell\frac{\partial^2 f}{\partial x \partial y} + \ell^2\frac{\partial^2 f}{\partial y^2}\right)$$

$$f_{i+1,j+1} = f + h\frac{\partial f}{\partial x} + \ell\frac{\partial f}{\partial y} + \frac{1}{2}\left(h^2\frac{\partial^2 f}{\partial x^2} + 2h\ell\frac{\partial^2 f}{\partial x \partial y} + \ell^2\frac{\partial^2 f}{\partial y^2}\right)$$

$$f_{i-1,j+1} = f - h\frac{\partial f}{\partial x} + \ell\frac{\partial f}{\partial y} + \frac{1}{2}\left(h^2\frac{\partial^2 f}{\partial x^2} - 2h\ell\frac{\partial^2 f}{\partial x \partial y} + \ell^2\frac{\partial^2 f}{\partial y^2}\right)$$

$$f_{i+1,j} = f + h\frac{\partial f}{\partial x} + \frac{h^2}{2}\frac{\partial^2 f}{\partial x^2}$$

$$\begin{bmatrix} f_{i,j} \\ f_{i-1,j-1} \\ f_{i+1,j-1} \\ f_{i+1,j+1} \\ f_{i-1,j+1} \\ f_{i+1,j} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -h & -\ell & \frac{h^2}{2} & h\ell & \frac{\ell^2}{2} \\ 1 & h & -\ell & \frac{h^2}{2} & -h\ell & \frac{\ell^2}{2} \\ 1 & h & \ell & \frac{h^2}{2} & h\ell & \frac{\ell^2}{2} \\ 1 & -h & \ell & \frac{h^2}{2} & -h\ell & \frac{\ell^2}{2} \\ 1 & h & 0 & \frac{h^2}{2} & 0 & 0 \end{bmatrix} \begin{bmatrix} f \\ \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial^2 f}{\partial x^2} \\ \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

$$\therefore \frac{\partial^2 f}{\partial x \partial y} = \frac{f_{i+1,j-1} - f_{i+1,j+1} + f_{i+1,j+1} - f_{i-1,j+1}}{4h\ell}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1,j+1} + f_{i-1,j+1} - 4f_i + 4f_{i+1,j} - f_{i+1,j-1} - f_{i+1,j+1}}{2h^2} \quad \color{red}{\text{why?}}$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{f_{i+1,j-1} - 2f_{i+1,j} + f_{i+1,j+1}}{\ell^2}$$

Consider the governing equation of a homogeneous string (or rod/bar):

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \qquad x \in (0, \ell) \quad \text{governing equation}$$

$$\left.\begin{array}{ll} u(0,t) = 0 & t \in [0,T] \\[2mm] u(\ell,t) = 0 & t \in [0,T] \end{array}\right\} \text{boundary conditions}$$

$$\left.\begin{array}{ll} u(x,0) = U(x) & x \in (0, \ell) \\[2mm] \dot{u}(x,0) = V(x) & x \in [0,\ell] \end{array}\right\} \text{initial conditions}$$

1. Discretize the problem domain in space and time.

We discretize space into N_x points and time into N_t points, thus $\Delta x = \frac{\ell}{N_x}$ and $x_i = i\Delta x$ where $i = 0, \ldots, N_x$; similarly, $\Delta t = \frac{T}{N_t}$ and $t_j = j\Delta t$ with $j = 0, \ldots, N_t$.

2. Approximate derivatives by finite differences.

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1}^j - 2u_i^j + u_{i+1}^j}{(\Delta x)^2} \qquad\qquad \frac{\partial^2 u}{\partial t^2} = \frac{u_i^{j-1} - 2u_i^j + u_i^{j+1}}{(\Delta t)^2}$$

$$u(0,t) = u_i^j = 0 \qquad (i=0) \qquad\qquad u(\ell,t) = u_i^j = 0 \qquad (i = N_x)$$

$$\left.\frac{\partial u}{\partial t}\right|_{(x_i, t_j)} = \frac{u_i^{j+1} - u_i^{j-1}}{2\Delta t} = V(x_i) \qquad u = u_i^j = U(x_i) \qquad (j=0)$$

3. Insert FD approximations into governing equation and rearrange for u_i^{j+1}.

$$u_i^{j+1} = \eta^2 \left(u_{i-1}^j - 2u_i^j + u_{i+1}^j\right) - u_i^{j-1} + 2u_i^j \qquad\qquad \eta = c\frac{\Delta t}{\Delta x} \quad \text{Courant number} \qquad (j=1, \ldots, N_t)$$

$$\left.\begin{array}{l} u_i^{-1} = u_i^1 - 2\Delta t\, V(x_i) \\[4mm] u_i^1 = \frac{\eta^2}{2}\left(U_{i-1} - 2U_i + U_{i+1}\right) + \Delta t\, V(x_i) + u_i \end{array}\right\} j = 0$$

$\Delta x/\Delta t$ is the "speed" limit of our numerical integration; therefore, it must be at least as fast as the physics of our problem (dictated by c), thus $\eta \leq 1$ (stability condition).

Explicit_FDTD.m

```matlab
1  clear;clc;
2
3  %% Setup - User Input
4  n_site=1001; % # sites
5
6  L=1; % domain size
7  c=26; % speed of sound
8
9  T=3/100; % total simulation time
10 eta=1/3; % Courant #
11
12 %% Mesh Definition
13 x=linspace(0,L,n_site); % mesh
14 dx=x(2); % space step
15
16 dt=eta*dx/c; % time step
17 Nt=floor(T/dt); % # time steps
18
19 i_indx=[1:n_site 1:(n_site-1) 2:n_site];
20 j_indx=[1:n_site 2:n_site 1:(n_site-1)];
21 value=[-2*ones(1,n_site) ones(1,n_site-1) ones(1,n_site-1)];
22 K=sparse(i_indx,j_indx,value); % coefficient matrix
23
24 %% Explicit Time Integration
25 u_init=sparse(n_site,1); % initial displacement
26 v_init=sparse(n_site,1);v_init(round(n_site/2),1)=1; % initial
      velocity
27
28 u=sparse(n_site,Nt+1);u(:,1)=u_init; % displacement matrix;
29
30 for k=1:Nt
31     if k==1
32         u(:,2)=(eta^2)*K*u(:,1)./2+u(:,1)+v_init*dt;
33     else
34         u(:,k+1)=(eta^2)*K*u(:,k)+2*u(:,k)-u(:,k-1);
35     end
```

```matlab
    %%%% Plotting
    if floor(k/15)==k/15 % plot every 15 time steps
        plot(x,u(:,k+1),'k-','LineWidth',1);
        xlabel('Position, x');ylabel('Displacement, u');
        title(['t/T = ',num2str(round(k/Nt,3))]);
        axis([0 L -1e-5 3e-5]);
        drawnow;
    end
end
```

$$\frac{u_{i,j}^{k-1} - 2u_{i,j}^{k} + u_{i,j}^{k+1}}{(\Delta t)^2} = c^2 \left[\frac{u_{i-1,j}^{k} - 2u_{i,j}^{k} + u_{i+1,j}^{k}}{(\Delta x)^2} + \frac{u_{i,j-1}^{k} - 2u_{i,j}^{k} + u_{i,j+1}^{k}}{(\Delta y)^2} \right]$$

$$u_{i,j}^{k+1} = c^2 (\Delta t)^2 \left[\frac{u_{i-1,j}^{k} - 2u_{i,j}^{k} + u_{i+1,j}^{k}}{(\Delta x)^2} + \frac{u_{i,j-1}^{k} - 2u_{i,j}^{k} + u_{i,j+1}^{k}}{(\Delta y)^2} \right] + 2u_{i,j}^{k} - u_{i,j}^{k-1}$$

$$\frac{u_{i,j}^{k+1} - u_{i,j}^{k-1}}{2\Delta t} = V(x_i, y_i) \qquad \therefore \qquad u_{i,j}^{k-1} = u_{i,j}^{k+1} - 2\Delta t\, V(x_i, y_i) \qquad \therefore \qquad u_{i,j}^{-1} = u_{i,j}^{1} - 2\Delta t\, V(x_i, y_i) \Bigg\}$$

$$\left. u_{i,j}^{1} = \frac{c^2 (\Delta t)^2}{2} \left[\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{(\Delta y)^2} \right] + u_{i,j} + \Delta t\, V(x_i, y_i) \right\} k=0$$

1 Explicit Time Integration

Over the past couple lectures, we have developed the basics of numerical integration via the method of finite differences and even applied this tool toward the solution (i.e., simulation) of a string with a propagating disturbance. This example was a demonstration of an *explicit* integration scheme, i.e., one in which the solution at a later time step (i.e., u^{j+1}, $\dot{u}^{j+1}$, $\ddot{u}^{j+1}$) depends on the current conditions (i.e., u^j, $\dot{u}^j$, $\ddot{u}^j$) or earlier. Now, let's consider a more general dynamic system than the string, one in which spatial discretization is accomplished via the finite element method, yielding:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{f}_{\text{int}}(\mathbf{u}) = \mathbf{f}_{\text{ext}}(t),$$

where $\mathbf{f}_{\text{int}}(\mathbf{u})$ and $\mathbf{f}_{\text{ext}}(t)$ are internal and time-depended (i.e., excitation) forces, respectively. Let's assume a linear force-displacement relation for the internal forces, $\mathbf{f}_{\text{int}}(\mathbf{u}) = \mathbf{K}\mathbf{u}$, thus:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}_{\text{ext}}(t). \tag{1}$$

2 Implicit Time Integration

2.1 Linear Acceleration Scheme

In the derivation of the previous explicit, time integration scheme, we replaced the derivatives $\dot{\mathbf{u}}$ and $\ddot{\mathbf{u}}$ with their finite difference approximations stemming from Taylor expansions. Now, let's try an alternative route. Assume the acceleration varies linearly over a given time increment, then:

$$\ddot{\mathbf{u}}(\tau) = \ddot{\mathbf{u}}^j + \frac{\tau - t_0}{\Delta t}(\ddot{\mathbf{u}}^{j+1} - \ddot{\mathbf{u}}^j) \quad t_0 \leq \tau \leq t_0 + \Delta t,$$

where τ is a dummy variable. Next, we integrate the dummy variable, τ, over the time step, i.e., from t_0 to $t_0 + \Delta t$. Just as in undergraduate dynamics, we integrate once to arrive at the velocity and a second time to determine the displacement:

$$\int_{t_0}^{t_0+\Delta t} \ddot{\mathbf{u}}(\tau)\mathrm{d}\tau = \dot{\mathbf{u}}^{j+1} - \dot{\mathbf{u}}^j = \ddot{\mathbf{u}}^j \Delta t + \frac{\Delta t}{2}(\ddot{\mathbf{u}}^{j+1} - \ddot{\mathbf{u}}^j) \tag{2a}$$

$$\int_{t_0}^{t_0+\Delta t} \int \ddot{\mathbf{u}}(\tau)\mathrm{d}\tau = \mathbf{u}^{j+1} - \mathbf{u}^j = \Delta t\dot{\mathbf{u}}^j + \frac{(\Delta t)^2}{6}(\ddot{\mathbf{u}}^{j+1} + 2\ddot{\mathbf{u}}^j), \tag{2b}$$

We could stop here and insert these definitions into the Eq. (1) to develop an implicit update rule, but lets continue.

2.2 Average Acceleration Scheme

Now, let's assume a constant, averaged acceleration over the time increment Δt given by

$$\ddot{\mathbf{u}}(\tau) = \frac{1}{2}(\ddot{\mathbf{u}}^{j+1} + \ddot{\mathbf{u}}^j) \quad t_0 \leq \tau \leq t_0 + \Delta t$$

Now, we integrate the dummy variable, τ, over the time step. Integrating once yields the velocity; yet again gives the displacement:

$$\int_{t_0}^{t_0+\Delta t} \ddot{\mathbf{u}}(\tau)\mathrm{d}\tau = \dot{\mathbf{u}}^{j+1} - \dot{\mathbf{u}}^j = \frac{\Delta t}{2}(\ddot{\mathbf{u}}^{j+1} + \ddot{\mathbf{u}}^j)$$

$$\int_{t_0}^{t_0+\Delta t} \int \ddot{\mathbf{u}}(\tau)\mathrm{d}\tau = \mathbf{u}^{j+1} - \mathbf{u}^j = \dot{\mathbf{u}}^j \Delta t + \frac{(\Delta t)^2}{4}(\ddot{\mathbf{u}}^{j+1} + \ddot{\mathbf{u}}^j),$$

or, by solving for $\dot{\mathbf{u}}^{j+1}$ and $\mathbf{u}^{j+1}$ in the previous:

$$\mathbf{u}^{j+1} = \mathbf{u}^j + \dot{\mathbf{u}}^j \Delta t + \frac{(\Delta t)^2}{4}(\ddot{\mathbf{u}}^{j+1} + \ddot{\mathbf{u}}^j) \tag{4a}$$

$$\dot{\mathbf{u}}^{j+1} = \dot{\mathbf{u}}^j + \frac{\Delta t}{2}(\ddot{\mathbf{u}}^{j+1} + \ddot{\mathbf{u}}^j) \tag{4b}$$

We could stop here and insert these definitions into the Eq. (1) to develop an implicit update rule, but lets continue.

2.3 The Newmark-β Scheme

For the Newmark-β scheme, we essentially combine the results of the linear and averaged acceleration techniques. Consider the displacement definitions in Eqs. (2a) and (4a). Each of these may be represented by a single equation with the aid of a tuning variable, $\beta \in [\frac{1}{3}, \frac{1}{2}]$:

$$\mathbf{u}^{j+1} = \mathbf{u}^j + \dot{\mathbf{u}}^j \Delta t + \frac{(\Delta t)^2}{2}\left[\beta \ddot{\mathbf{u}}^{j+1} + (1-\beta)\ddot{\mathbf{u}}^j\right], \tag{5}$$

where $\beta = 1/3$ and $\beta = 1/2$, respectively, yield the linear and averaged definitions. Intermediate values result in a scheme that is a little bit of both, and β determines whether the scheme is more of the linear acceleration assumption or the average acceleration assumption. Values outside this range are meaningless and may result in either an unstable or less accurate scheme.

For the velocity, equations (2b) and (4b) are identical; however, notice that if the $\ddot{\mathbf{u}}^{j+1}$ term were absent, then we would have an explicit scheme (since the updated condition depends on current or earlier conditions). Introducing the variable, $\gamma \in \{0, \frac{1}{2}\}$, we can combine the explicit and implicit definitions:

$$\dot{\mathbf{u}}^{j+1} = \dot{\mathbf{u}}^j + \Delta t\left[\gamma \ddot{\mathbf{u}}^{j+1} + (1-\gamma)\ddot{\mathbf{u}}^j\right], \tag{6}$$

where $\gamma = 0$ and $\gamma = \frac{1}{2}$, respectively, yield the explicit and implicit definitions.

- **Linear Acceleration**, $(\beta, \gamma) = \left(\frac{1}{3}, \frac{1}{2}\right)$

- **Average Acceleration**, $(\beta, \gamma) = \left(\frac{1}{2}, \frac{1}{2}\right)$

- **Explicit**, $(\beta, \gamma) = (0, 0)$

Ultimately, we are interested in the updated displacement, $\mathbf{u}^{j+1}$, when solving Eq. (1). We will accomplish this following a series of substitutions. First, let's solve Eq. (5) for $\ddot{\mathbf{u}}^{j+1}$:

$$\ddot{\mathbf{u}}^{j+1} = \frac{1}{\beta}\left[\frac{2}{(\Delta t)^2}(\mathbf{u}^{j+1} - \mathbf{u}^j - \Delta t \dot{\mathbf{u}}^j) - (1-\beta)\ddot{\mathbf{u}}^j\right], \tag{7}$$

and then substitute this into Eq. (6), giving:

$$\dot{\mathbf{u}}^{j+1} = \dot{\mathbf{u}}^j + \frac{\Delta t}{\beta} \left[\frac{2\gamma}{(\Delta t)^2}(\mathbf{u}^{j+1} - \mathbf{u}^j - \Delta t \dot{\mathbf{u}}^j) + (\beta - \gamma)\ddot{\mathbf{u}}^j \right]. \tag{8}$$

Now, $\dot{\mathbf{u}}^{j+1}$ and $\ddot{\mathbf{u}}^{j+1}$ are each a function of $\mathbf{u}^{j+1}$. As we have done before, we replace the derivatives in Eq. (1) with these definitions and manipulate the result into the form below:

$$\left[\frac{2}{\beta(\Delta t)^2}\mathbf{M} + \frac{2\gamma}{\beta\Delta t}\mathbf{C} + \mathbf{K} \right] \mathbf{u}^{j+1} = \left[\frac{2}{\beta(\Delta t)^2}\mathbf{M} + \frac{2\gamma}{\beta\Delta t}\mathbf{C} \right] \mathbf{u}^j + \left[\frac{2}{\beta\Delta t}\mathbf{M} + \left(\frac{2\gamma - \beta}{\beta} \right) \mathbf{C} \right] \dot{\mathbf{u}}^j + \dots$$

$$+ \left[\left(\frac{1-\beta}{\beta} \right) \mathbf{M} + \Delta t \left(\frac{\gamma - \beta}{\beta} \right) \mathbf{C} \right] \ddot{\mathbf{u}}^j + \mathbf{f}_{\text{ext}}(j\Delta t). \tag{9}$$

From here, the implementation essentially follows the same procedure outlined in Sec. 1. For the Newmark-β method, Step 2 is slightly modified so that $\mathbf{u}^{j+1}$ is substituted into $\ddot{\mathbf{u}}^{j+1}$ and $\dot{\mathbf{u}}^{j+1}$, Eqs. (7) and (8), respectively.

3

Implicit_FDTD.m

```matlab
1  clear;clc
2
3  %% Setup - User Input
4  n_sites=101;
5
6  m=1;
7  k=1;
8
9  eta=1/5;
10
11 dx=1;
12 T=1e4;
13
14 B=1/4;
15 g=1/2;
16
17 %% Mass and Stiffness Matrices
18 i_indx=1:(n_sites-2);
19 j_indx=1:(n_sites-2);
20 v=m*ones(1,n_sites-2);
21 M=sparse(i_indx,j_indx,v);
22
23 i_indx=[1:(n_sites-2) 1:(n_sites-3) 2:(n_sites-2)];
24 j_indx=[1:(n_sites-2) 2:(n_sites-2) 1:(n_sites-3)];
25 v=k*[2*ones(1,n_sites-2) -1*ones(1,n_sites-3) -1*ones(1,n_sites
       -3)];
26 K=sparse(i_indx,j_indx,v);
27
28 %% Newmark-B Preliminaries
29 %%%% Preliminary Calculations
30 c0=sqrt(k/m);
31 dt=eta*dx/c0;
32 Nt=ceil(T/dt);
33
34 %%%% Initial Conditions
35 u=zeros(n_sites-2,Nt+1);
36 v=zeros(n_sites-2,Nt+1);v(round((n_sites-2)/2),1)=1;
37 a=zeros(n_sites-2,Nt+1);
```

```matlab
%%%%% Matrix Coefficients
C1=2*M./(B*dt^2)+K;
C2=2*M./(B*dt^2);
C3=2*M./(B*dt);
C4=(1-2*B)*M./B;

%% Newmark-B Scheme
for k=1:Nt
    u(:,k+1)=C1\(C2*u(:,k)+C3*v(:,k)+C4*a(:,k));
    v(:,k+1)=v(:,k)+dt*(((2*B-g)/(2*B))*a(:,k)+...
        (g/(B*dt^2))*(u(:,k+1)-u(:,k)-v(:,k)*dt));
    a(:,k+1)=(u(:,k+1)-u(:,k)-v(:,k).*dt)./(B*dt^2)-...
        (1-2*B)*a(:,k)./(2*B);

    %%%%% Plotting %%%%%
    figure(1);
    if floor(k/2)==k/2
        plot(0:(n_sites-1),[0;u(:,k+1);0],'k.-','LineWidth',1);
        axis([0 n_sites-1 -1 1]);
        drawnow;
    end
end
```

TOPIC 9:
Fourier Series and Transform

Recall that the eigenvectors (i.e., mode shapes) of a discrete system, $\bar{X}_i$, $i=1,...,n$ are orthogonal and, thus, form an n-dimensional basis from which any discrete displacement solution can be constructed.

$$\bar{X}_i \cdot \bar{X}_j = \delta_{ij} \qquad \text{ortho(normal) vectors}$$

For a continuous system, the eigenfunctions (i.e., mode shapes), $f_i(x)$, are also orthogonal and form a basis that can construct a general solution.

$$\int_a^b f_i(x) f_j(x)\, dx = a\delta_{ij} \qquad \text{ortho(normal) functions}$$

note: the orthogonality of continuous mode shapes is specific to the domain $x \in [a,b]$ and need not hold true outside the domain.

The Fourier series expansion is the approximation of a function, $f(x)$, by the weighted sum of sines and cosines. Since sines and cosines are smooth, periodic functions, the approximation is exact for $f(x)$ that are also smooth and periodic.

$f(x)$

signal

$\}\frac{a_0}{2}$

$=$

$\}\frac{a_0}{2}$

$+$

$a_1 \cos(x)$

$+$

$a_1 \sin(x)$

$+$
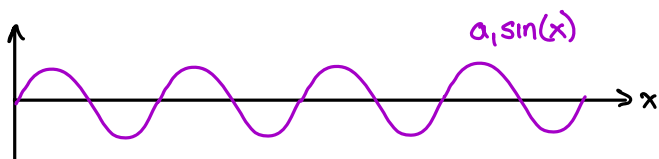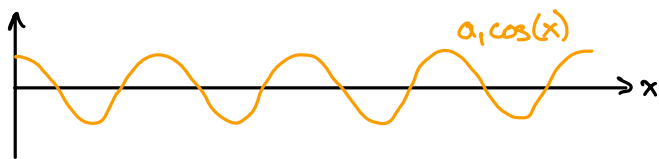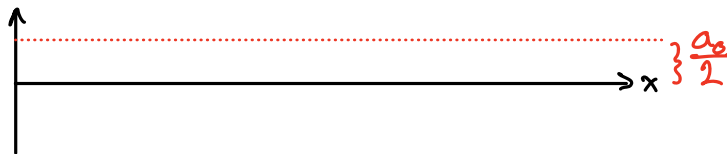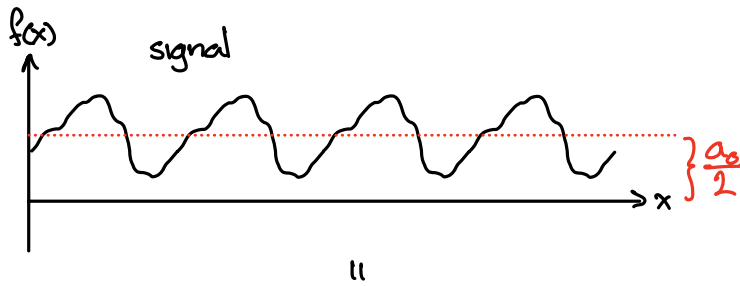
$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)]$$

The Fourier series expansion leverages the orthogonality relations of sines and cosines over the interval $x \in [-n\pi, n\pi]$, which allows them to serve as basis functions for building $f(x)$.

$$\int_{-\pi}^{\pi} \sin(mx)\sin(nx)\,dx = \pi\delta_{mn}$$

$$\int_{-\pi}^{\pi} \cos(mx)\cos(nx)\,dx = \pi\delta_{mn}$$

$$\int_{-\pi}^{\pi} \sin(mx)\cos(nx)\,dx = 0$$

$$\int_{-L}^{L} \sin\left(\frac{\pi}{L}mx\right)\sin\left(\frac{\pi}{L}nx\right)\,dx = L\delta_{mn}$$

$$\int_{-L}^{L} \cos\left(\frac{\pi}{L}mx\right)\cos\left(\frac{\pi}{L}nx\right)\,dx = L\delta_{mn}$$

$$\int_{-L}^{L} \sin\left(\frac{\pi}{L}mx\right)\cos\left(\frac{\pi}{L}nx\right)\,dx = 0\delta_{mn}$$

note: For arbitrary interval, $s \in [-L, L]$, let $s = \pi x/L$ and $ds = \pi dx/L$

Thus:

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\,dx$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)\,dx$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)\,dx$$

$$a_0 = \frac{1}{L}\int_{-L}^{L} f(x)\,dx$$

$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{\pi}{L}nx\right)\,dx$$

$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{\pi}{L}nx\right)\,dx$$

Fourier_Expansion.m

```matlab
1   clear;clc;
2
3   %% Setup - User Input
4   L=pi;
5   p=1001;
6
7   N=8;
8
9   %% Preliminary Calculations
10  x=linspace(-L,L,p);
11
12  f=f_sm(x);
13
14  %% Fourier Expansion
15  a0=(1/pi)*trapz(x,f);
16  f_fs=a0/2;
17
18  a=zeros(1,N);
19  b=zeros(1,N);
20  for n=1:N
21      a(n)=(1/pi)*trapz(x,f.*cos(n*x));
22      b(n)=(1/pi)*trapz(x,f.*sin(n*x));
23
24      f_fs=f_fs+a(n)*cos(n*x)+b(n)*sin(n*x);
25  end
26
27  %% Plotting
28  figure(1);
29  plot(x,f,'k',x,f_fs,'r:','LineWidth',2);
30  xlabel('x');ylabel('f_{sm}');
31  title(['n = ',num2str(N)]);
32  legend('f(x) exact','f(x) approx.');
33  axis([-L L -1.25 1.25]);axis square;
34
35  %% Function Definitions
36  function y=f_sm(x)
37      y=cos(5*x).*(1-(x./pi).^4).^2;
38  end
39  function y=f_nonsm(x)
40      y=heaviside(x+pi/2)-heaviside(x-pi/2);
41  end
```
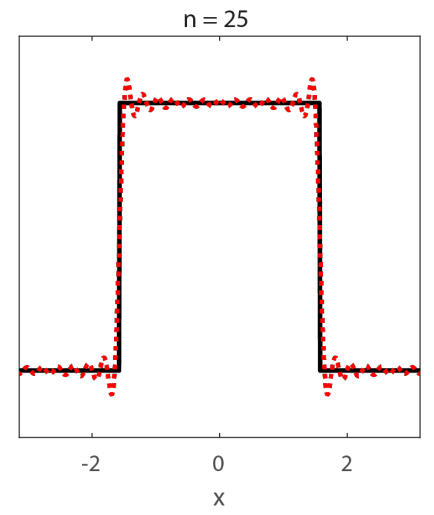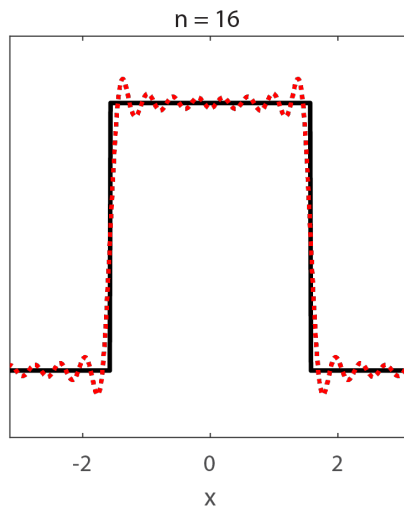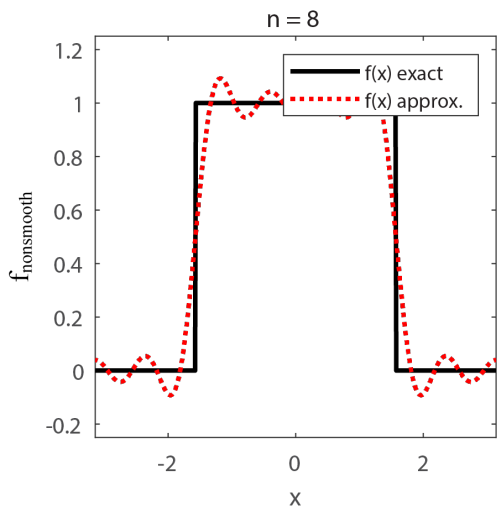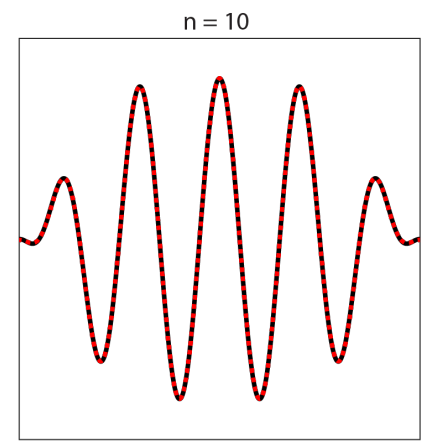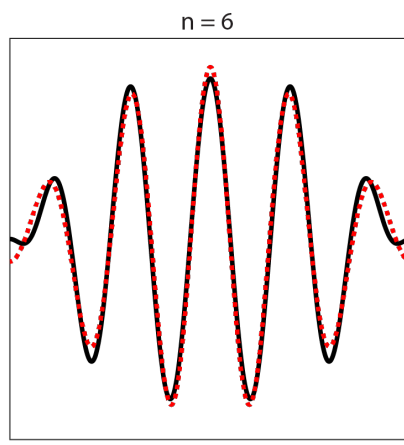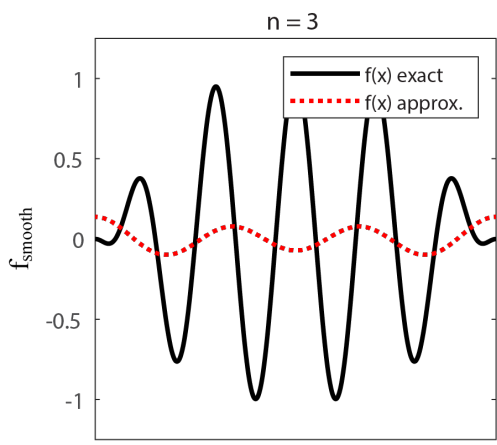
Let's consider the case of a periodic function, $f(x)$, with period λ; thus $f(x+n\lambda) = f(x)$.

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(n\kappa x) + b_n \sin(n\kappa x)]$$

$$\kappa = \frac{2\pi}{\lambda} = \frac{\pi}{\lambda/2}$$

$$a_0 = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\,dx \qquad a_n = \frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\cos(n\kappa x)\,dx \qquad b_n = \frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\sin(n\kappa x)\,dx$$

Recall: $\cos(n\kappa x) = \dfrac{e^{in\kappa x} + e^{-in\kappa x}}{2} \qquad \sin(n\kappa x) = -i\dfrac{e^{in\kappa x} - e^{-in\kappa x}}{2}$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left[a_n \frac{e^{in\kappa x} + e^{-in\kappa x}}{2} - ib_n \frac{e^{in\kappa x} - e^{-in\kappa x}}{2}\right]$$

$$= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x} + \sum_{n=1}^{\infty}\left(\frac{a_n + ib_n}{2}\right)e^{-in\kappa x}$$

$$= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x} + \sum_{n=1}^{\infty}\left(\frac{a_n + ib_n}{2}\right)e^{-in\kappa x}$$

$$= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x} + \sum_{n=-1}^{-\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x}$$

$$= \sum_{n=-\infty}^{\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x} = \sum_{n=-\infty}^{\infty} c_n e^{in\kappa x} \qquad \text{complex form of the Fourier series}$$

note: $\displaystyle\sum_{n=1}^{\infty}\left(\frac{a_n + ib_n}{2}\right)e^{-in\kappa x} = \sum_{n=-1}^{-\infty}\left(\frac{a_{-n} + ib_{-n}}{2}\right)e^{in\kappa x} = \sum_{n=-1}^{-\infty}\left(\frac{a_n - ib_n}{2}\right)e^{in\kappa x}$
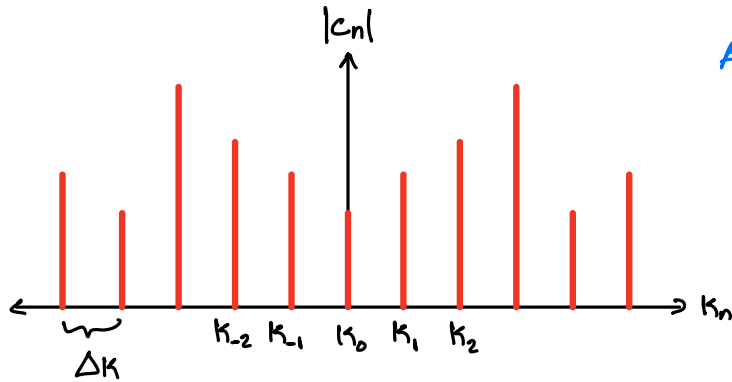
$$b_{-n} = \frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\sin(-n\kappa x)\,dx = -\frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\sin(n\kappa x)\,dx = -b_n$$

$$a_{-n} = \frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\cos(-n\kappa x)\,dx = \frac{2}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\cos(n\kappa x)\,dx = a_n$$

$$c_n = \frac{a_n - ib_n}{2} = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)[\cos(n\kappa x) - i\sin(n\kappa x)]\,dx = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)e^{-in\kappa x}\,dx$$

note: $c_0 = \dfrac{a_0}{2} = \dfrac{1}{\lambda}\displaystyle\int_{-\lambda/2}^{\lambda/2} f(x)\,dx$

Let $\kappa_n = 2\pi n/\lambda = n\pi/(\lambda/2)$ define a 1D lattice in wavenumber space with (for convenience) uniform spacing $\Delta\kappa = \kappa_{n+1} - \kappa_n = 2\pi/\lambda$

As $\lambda \to \infty$, $\Delta\kappa$ becomes arbitrarily small so that $\Delta\kappa \approx d\kappa$ and the discrete c_n approximates a continuous function.

The graph is symmetric about $n=0$

$$c_n = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} f(x)\, e^{-in\kappa x}\, dx = \frac{\Delta\kappa}{2\pi}\int_{-\lambda/2}^{\lambda/2} f(x)\, e^{-i\kappa_n x}\, dx$$

$$\therefore\ f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i\kappa_n x} = \sum_{n=-\infty}^{\infty}\left[\underbrace{\frac{1}{2\pi}\int_{-\lambda/2}^{\lambda/2} f(x)\, e^{-i\kappa_n x}\, dx}_{F(\kappa_n)}\right] e^{i\kappa_n x}\,\Delta\kappa = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} F(\kappa_n)\, e^{i\kappa_n x}\,\Delta\kappa \approx \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\kappa)\, e^{i\kappa x}\, d\kappa$$

The above form of the Fourier series resembles a Riemann sum, i.e., an approximation of an integral by a finite sum. In this case, over an arbitrary subinterval, one may approximate the integral as the area of a rectangle with base, $\Delta\kappa$, and height, $F(\kappa)e^{i\kappa_n x}$.

The spatial period, λ, need not be a finite value. As $\lambda \to \infty$, $\Delta\kappa \to d\kappa$ and κ_n approximates a continuous variable, κ.

$$\mathcal{F}^{-1}[F(\kappa)] = f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\kappa)\, e^{i\kappa x}\, d\kappa \qquad \text{inverse Fourier transform}$$

The Fourier transform is a generalization of the complex Fourier series with $\lambda \to \infty$.

$$\mathcal{F}[f(x)] = F(\kappa) = \int_{-\infty}^{\infty} f(x)\, e^{-i\kappa x}\, dx \qquad \text{Fourier transform}$$

note: the substitutions $x \to t$, $\lambda \to T$, and $\kappa \to \omega$ transform the above formulations (at least notationally) from space to time

note: if we perform the substitution, $i\kappa \to s$, then we arrive at the bilateral Laplace transform: $\mathcal{L}[f(x)] = F(s) = \int_{-\infty}^{\infty} f(x)\, e^{-sx}\, dx$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk$$

$$F(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

$$f(x) = \int_{-\infty}^{\infty} F(k)\, e^{i2\pi kx}\, dk$$

$$F(k) = \int_{-\infty}^{\infty} f(x)\, e^{-i2\pi kx}\, dx$$
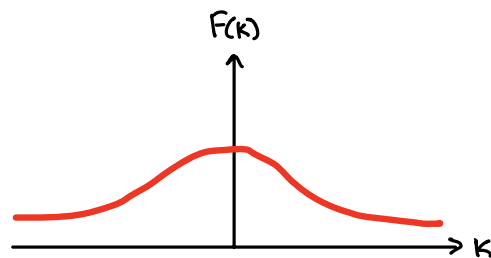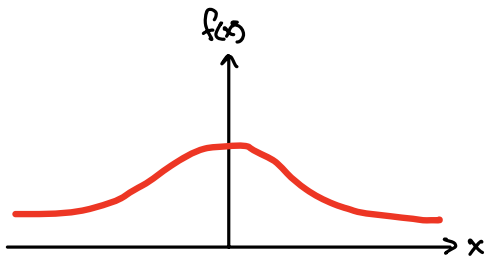
$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk$$

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

Consider the Fourier transform of the Gaussian $f(x) = e^{-\alpha x^2}$, $\alpha \geq 0$.

$$F(k) = \int_{-\infty}^{\infty} e^{-\alpha x^2} e^{-ikx}\, dx = \sqrt{\frac{\pi}{4}}\, e^{-k^2/4\alpha}$$
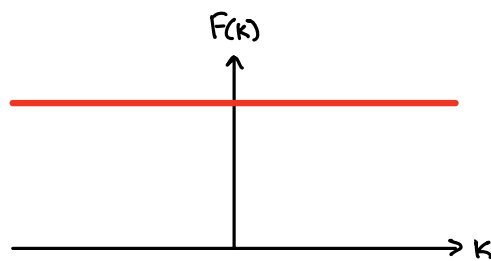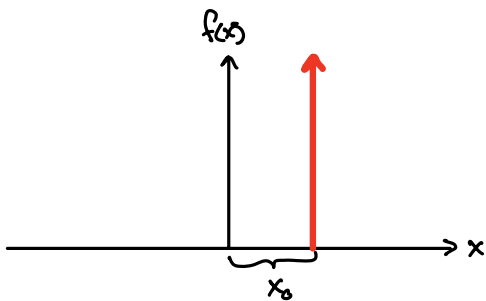
identity: $\int_{-\infty}^{\infty} e^{-ax^2} e^{-bx}\, dx = \sqrt{\frac{\pi}{4}}\, e^{b^2/4a}$ where $(a,b) = (\alpha, ik)$

The Fourier transform of a Gaussian is also a Gaussian. Notice that $f(x)$ approaches an impulse as $\alpha \to \infty$; simultaneously, $F(k)$ approaches a constant.

Consider the Fourier transform of $f(x) = \delta(x - x_0)$.

$$F(k) = \int_{-\infty}^{\infty} \delta(x - x_0) e^{-ikx}\, dx = e^{-ikx_0}$$


If we compare plots of $f(x) = \delta(x)$ and its $\mathcal{F}[f(x)]$, we observe the localized "spike" of $f(x)$ and the uniform distribution that is $\mathcal{F}[f(x)]$. This illustrates the complementarity of real space and reciprocal space. This also gives a mathematical justification for the impact hammer in structural dynamics tests: the impulse in time provided by the hammer excites all temporal frequencies equally.

Consider the Fourier transform of $f(x) = c$.

$$F(k) = c\int_{-\infty}^{\infty} e^{-ikx} dx = c\int_{-\infty}^{\infty} [\cos(kx) - i\sin(kx)] dx \quad \text{is undefined for } k \neq 0 \text{ since}$$

the integrand oscillates

If $k = 0$, then $F(k) = c\int_{-\infty}^{\infty} dx = c\delta(k)$ $\quad$ recall $\delta(x) = \begin{cases} \infty, & x = 0 \\ 0, & x \neq 0 \end{cases}$
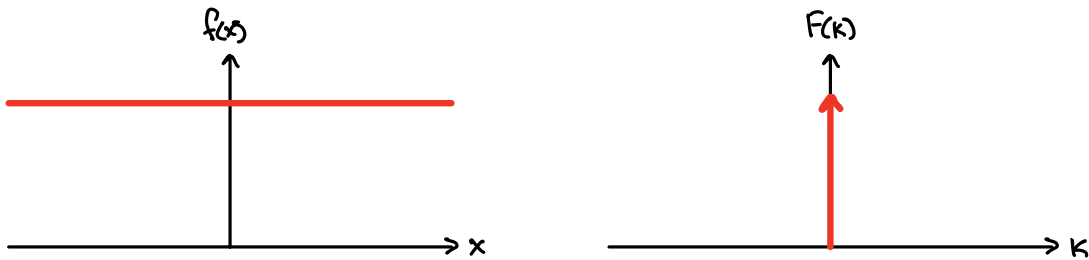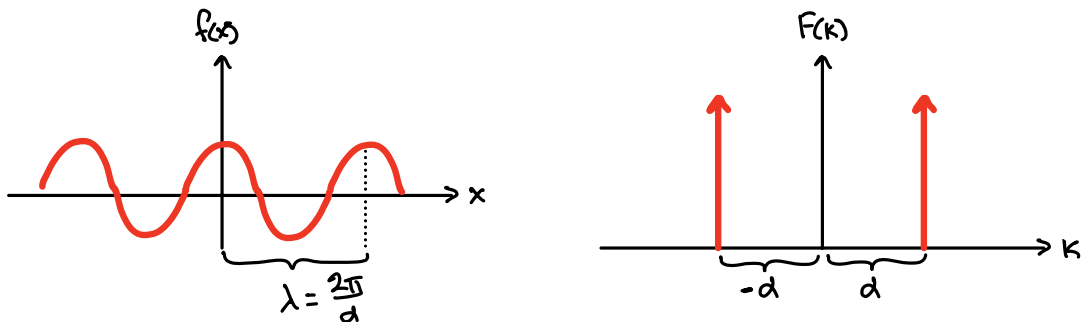

This result should be expected since a constant signal should have no frequency content.

Consider the Fourier transform of $f(x) = \cos(\alpha x)$

$$F(k) = \int_{-\infty}^{\infty} \cos(\alpha x) e^{-ikx} dx = \int_{-\infty}^{\infty} \left[\frac{e^{i\alpha x} + e^{-i\alpha x}}{2}\right] e^{-ikx} dx$$

$$= \frac{1}{2}\left[\int_{-\infty}^{\infty} e^{-i(k-\alpha)x} dx + \int_{-\infty}^{\infty} e^{-i(k+\alpha)x} dx\right] = \frac{1}{2}[\delta(k-\alpha) + \delta(k+\alpha)]$$

Fourier_Transform.m

```matlab
1  clear;clc;
2  i=sqrt(-1);
3
4  %% Setup - User Input
5  lambda=2*pi;
6  N_base=11;
7
8  mult=10;
9
10 p=1001;
11
12 %% Preliminary Calculations
13 lambda=lambda*mult;
14 k0=2*pi/lambda;
15 N=ceil((N_base-1)/k0)+1;
16 x=linspace(-lambda/2,lambda/2,p);
17 fx=f(x);
18
19 %% Fourier Transform
20 kn=zeros(1,N);
21 Fn=zeros(1,N);
22 for n=0:(N-1)
23     kn(n+1)=n*k0;
24     Fn(n+1)=abs(trapz(x,fx.*exp(i*kn(n+1)*x)));
25 end
26 Fn=Fn./max(Fn);
27
28 %% Plotting
29 x_fine=linspace(-lambda/2,lambda/2,10001);
30 f_fine=f(x_fine);
31
32 figure(1);
33 subplot(2,1,1);
34 stem(kn,Fn,'Marker','.','MarkerSize',10,...
35     'Color','k');
36 xlabel('\kappa_n');ylabel('F(\kappa_n)');
37 legend(['N = ',num2str(N)]);
38 axis([0 N_base-1 0 1.1]);
```

```matlab
39  subplot(2,1,2);
40  plot(x_fine,f_fine,'k',x,fx,'r.-','LineWidth',1,...
41      'MarkerSize',13);
42  xlabel('x');ylabel('f(x)');
43  legend('p=10001',['p = ',num2str(p)]);
44  axis([[-1 1].*(1/mult).*(lambda/2) -2.5 2.5]);
45
46  %% Function Definitions
47  function y=f(x)
48      y=cos(3*x)./2+sin(5*x)+2*cos(9*x)./3+0*rand(size(x));
49  %     y=isinf(dirac(x));
50  end
```