PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF in Olin 103

Notes on Lecture 38

Review of topics covered in this course

1. Specific questions
2. Mathematical methods
3. Classical mechanics concepts

35	Fri, 11/17/2023	Chap. 11	Heat conduction	#28
36	Mon, 11/20/2023	Chap. 12	Viscous effects in hydrodynamics	
	Wed, 11/22/2023	Thanksgiving		
	Fri, 11/24/2023	Thanksgiving		
	Mon, 11/27/2023		Presentations I	
	Wed, 11/29/2023		Presentations 2	
	Fri, 12/01/2023		Presentations 3	
37	Mon, 12/04/2023	Chap. 12	Viscous effects in hydrodynamics	
38	Wed, 12/06/2023		Review	
39	Fri, 12/08/2023		Review	

Please fill out the course evaluation form for PHY 711 will leave time at the end of Friday's class

Final exam during finals week

Exam will be available on Friday 12/08/2023

Due < Monday 12/18/2023 at 11 AM

Physics Colloquium – December 7, 2023
4-5 PM in Olin 101

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Nuclear Quantum Effects: Insights from First-Principles Theory

In electronic structure theory, atomic nuclei are generally treated as classical point charges. However, there is a growing realization that the quantum-mechanical nature of light atomic nuclei like protons is essential for predicting certain properties. In recent years, this so-called nuclear quantum effect (NQE) has become an important topic in condensed matter physics and chemistry. In this talk, I will discuss how we examine different aspects of NQE by advancing first-principles electronic structure theory. I will first focus on the use of the path integral approach with first-principles molecular dynamics simulation based on density functional theory (DFT) for examining the NQE in liquid water and ionic solution. I will then discuss how multi-component DFT can be used with the nuclear electronic orbital (NEO) method for studying the coupled quantum dynamics of electrons and protons in heterogeneous matter in the context of real-time time-dependent DFT.

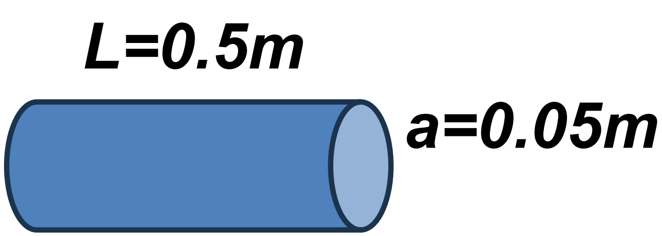
Comment on HW #24

PHY 711 -- Assignment #24

Assigned: 11/06/2023 Due: 11/13/2023

Continue reading Chapter 9 in **Fetter & Walecka**.

1. Consider a cylindrical pipe of length 0.5 m and radius 0.05 m, open at both ends. For air at 300 K and atmospheric pressure in this pipe, find several of the lowest frequency resonances, including at least one that has non-trivial radial dependence.



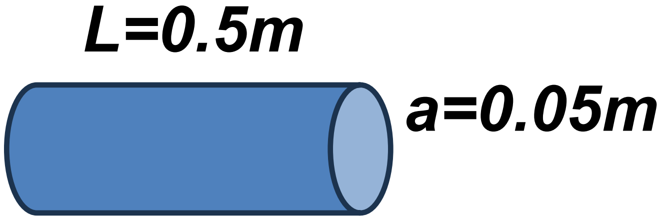
Wave equation: $\nabla^2\Phi(\mathbf{r},t) = \frac{1}{c^2}\frac{\partial^2\Phi(\mathbf{r},t)}{\partial t^2}$

Separation of variables: $\Phi(\mathbf{r},t) = F(\mathbf{r})f(t)$

Choose $f(t)$ to be an eigenfunction: $\frac{\partial^2 f(t)}{\partial t^2} = -\omega^2 f(t)$

$$\Rightarrow f(t) = e^{-i\omega t}$$

Differential equation for spatial factor: $\left(\nabla^2 + \frac{\omega^2}{c^2}\right)F(\mathbf{r}) = 0$



Differential equation for spatial factor: $\left(\nabla^2 + \frac{\omega^2}{c^2}\right) F(\mathbf{r}) = 0$

Cylindrical coordinates; set $k^2 \equiv \frac{\omega^2}{c^2}$

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} + k^2\right) F(\mathbf{r}) = 0$$

In our case, we can choose $F(\mathbf{r}) = R(r) e^{im\varphi} \sin\left(\frac{p\pi z}{L}\right)$

where $R(r)$ is a solution of $\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{m^2}{r^2} - \left(\frac{p\pi}{L}\right)^2 + k^2\right) R(r) = 0$

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{m^2}{r^2}\underbrace{-\left(\frac{p\pi}{L}\right)^2+k^2}\right)R(r)=0$$

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{m^2}{r^2}+\kappa^2\right)R(r)=0 \qquad \Rightarrow \qquad R(r)=J_m(\kappa r)$$

In order to satisfy the boundary conditions at the cylinder sides

$$\left.\frac{dJ_m(\kappa r)}{dr}\right|_{r=a}=0 \qquad \Rightarrow \kappa=\frac{x'_{mn}}{a}$$

$$k^2=\kappa^2+\left(\frac{p\pi}{L}\right)^2 \qquad\qquad k_{mnp}^2=\left(\frac{x'_{mn}}{a}\right)^2+\left(\frac{p\pi}{L}\right)^2$$

$$k_{mnp}^2 = \left(\frac{x'_{mn}}{a}\right)^2 + \left(\frac{p\pi}{L}\right)^2$$

Values of x'_{mn} are given on page 552 of your textbook.

Review of mathematical methods

Some useful identities for vectors and vector operators

$$\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})=\mathbf{b}\cdot(\mathbf{c}\times\mathbf{a})=\mathbf{c}\cdot(\mathbf{a}\times\mathbf{b})$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c})=(\mathbf{a}\cdot\mathbf{c})\mathbf{b}-(\mathbf{a}\cdot\mathbf{b})\mathbf{c}$$

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d})=(\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d})-(\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c})$$

$$\nabla\times\nabla\psi=0$$

$$\nabla\cdot(\nabla\times\mathbf{a})=0$$

$$\nabla\times(\nabla\times\mathbf{a})=\nabla(\nabla\cdot\mathbf{a})-\nabla^2\mathbf{a}$$

$$\nabla\cdot(\psi\mathbf{a})=\mathbf{a}\cdot\nabla\psi+\psi\nabla\cdot\mathbf{a}$$

$$\nabla\times(\psi\mathbf{a})=\nabla\psi\times\mathbf{a}+\psi\nabla\times\mathbf{a}$$

$$\nabla(\mathbf{a}\cdot\mathbf{b})=(\mathbf{a}\cdot\nabla)\mathbf{b}+(\mathbf{b}\cdot\nabla)\mathbf{a}+\mathbf{a}\times(\nabla\times\mathbf{b})+\mathbf{b}\times(\nabla\times\mathbf{a})$$

$$\nabla\cdot(\mathbf{a}\times\mathbf{b})=\mathbf{b}\cdot(\nabla\times\mathbf{a})-\mathbf{a}\cdot(\nabla\times\mathbf{b})$$

$$\nabla\times(\mathbf{a}\times\mathbf{b})=\mathbf{a}(\nabla\cdot\mathbf{b})-\mathbf{b}(\nabla\cdot\mathbf{a})+(\mathbf{b}\cdot\nabla)\mathbf{a}-(\mathbf{a}\cdot\nabla)\mathbf{b}$$

Vector relations for spherical polar coordinates

$$\nabla\psi = \hat{\mathbf{r}}\frac{\partial\psi}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$\nabla\cdot\mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 A_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta A_\theta\right) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial\phi}$$

$$\nabla\times\mathbf{A} = \hat{\mathbf{r}}\frac{1}{r\sin\theta}\left[\frac{\partial}{\partial\theta}\left(\sin\theta A_\phi\right) - \frac{\partial A_\theta}{\partial\phi}\right] + \hat{\boldsymbol{\theta}}\left[\frac{1}{r\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{1}{r}\frac{\partial}{\partial r}\left(rA_\phi\right)\right] + \hat{\boldsymbol{\phi}}\frac{1}{r}\left[\frac{\partial}{\partial r}\left(rA_\theta\right) - \frac{\partial A_r}{\partial\theta}\right]$$

$$\hat{\mathbf{x}} = \hat{\mathbf{r}}\sin\theta\cos\phi + \hat{\boldsymbol{\theta}}\cos\theta\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi$$

$$\hat{\mathbf{y}} = \hat{\mathbf{r}}\sin\theta\sin\phi + \hat{\boldsymbol{\theta}}\cos\theta\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi$$

$$\hat{\mathbf{z}} = \hat{\mathbf{r}}\cos\theta - \hat{\boldsymbol{\theta}}\sin\theta$$

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \cos\theta\cos\phi\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \cos\theta\sin\phi\frac{1}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{\partial}{\partial\theta}$$

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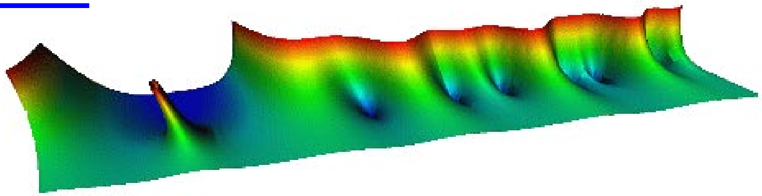


NIST Digital Library of Mathematical Functions

Project News

2018-09-15 *DLMF Update; Version 1.0.20*
2018-06-22 *DLMF Update; Version 1.0.19*
2018-06-22 *Philip J. Davis, A&S Author, dies at age 95*
2018-03-27 *DLMF Update; Version 1.0.18*
More news

Example – special functions

10 Bessel Functions
Bessel and Hankel Functions

10.1 Special Notation 10.3 Graphics

§10.2 Definitions

Contents

§10.2(i) Bessel's Equation

10.2.1
$$z^2\frac{d^2w}{dz^2}+z\frac{dw}{dz}+(z^2-\nu^2)w=0.$$

This differential equation has a regular singularity at $z=0$ with indices $\pm\nu$, and an irregular singularity at $z=\infty$ of rank 1; compare §§2.7(i) and 2.7(ii).

§10.2(ii) Standard Solutions

Bessel Function of the First Kind

10.2.2
$$J_\nu(z)=(\tfrac{1}{2}z)^\nu\sum_{k=0}^{\infty}(-1)^k\frac{(\frac{1}{4}z^2)^k}{k!\,\Gamma(\nu+k+1)}.$$

This solution of (10.2.1) is an analytic function of $z\in\mathbb{C}$, except for a branch point at $z=0$ when ν is not an integer. The *principal branch* of $J_\nu(z)$ corresponds to the principal value of $(\frac{1}{2}z)^\nu$ (§4.2(iv)) and is analytic in the z-plane cut along the interval $(-\infty,0]$.

Complex numbers

$$i \equiv \sqrt{-1} \qquad i^2 = -1$$

Define $z = x + iy$

$$|z|^2 = zz^* = (x+iy)(x-iy) = x^2 + y^2$$

Polar representation

$$z = \rho(\cos\phi + i\sin\phi) = \rho\ e^{i\phi}$$

Functions of complex variables

$$f(z) = \Re\left(f(z)\right) + i\Im\left(f(z)\right) \equiv u(x,y) + iv(x,y)$$

Derivatives: Cauchy-Riemann equations

$$\frac{\partial f(z)}{\partial x} = \frac{\partial u(z)}{\partial x} + i\frac{\partial v(z)}{\partial x} \qquad \frac{\partial f(z)}{i\partial y} = \frac{\partial u(z)}{i\partial y} + i\frac{\partial v(z)}{i\partial y} = \frac{\partial v(z)}{\partial y} - i\frac{\partial u(z)}{\partial y}$$

Argue that $\frac{df}{dz} = \frac{\partial f(z)}{\partial x} = \frac{\partial f(z)}{i\partial y} \quad \Rightarrow \frac{\partial u(z)}{\partial x} = \frac{\partial v(z)}{\partial y}$ and $\frac{\partial v(z)}{\partial x} = -\frac{\partial u(z)}{\partial y}$

Analytic function

$f(z)$ is analytic if it is:

- continuous
- single valued
- its first derivative satisfies Cauchy-Rieman conditions

➔A closed integral of an analytic function is zero.

However:

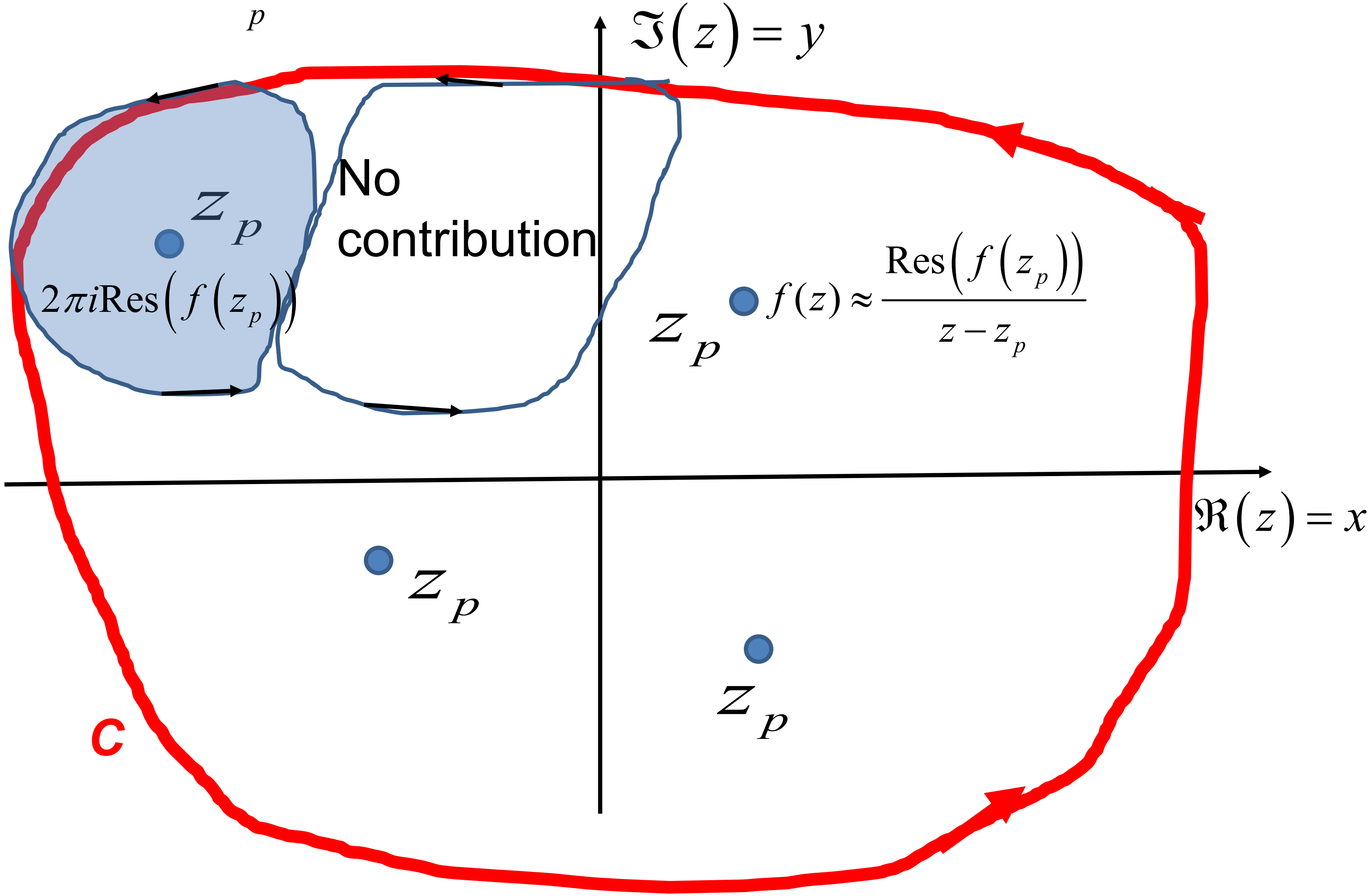
Behavior of $f(z) = \dfrac{1}{z^n}$ about the point $z = 0$:

For an integer n, consider

$$\oint \frac{1}{z^n} dz = \int_0^{2\pi} \frac{\rho e^{i\phi} i \, d\phi}{\rho^n e^{in\phi}} = \rho^{1-n} \int_0^{2\pi} e^{i(1-n)\phi} i \, d\phi = \begin{cases} 0 & n \neq 1 \\ 2\pi i & n = 1 \end{cases}$$

Contour integration methods --

$$\oint_C f(z)dz = 2\pi i \sum_p \text{Res}\left(f(z_p)\right)$$



General formula for determining residue:

Suppose that in the neighborhood of z_p, $f(z) \approx \frac{g(z)}{\left(z-z_p\right)^m} \underset{z\to z_p}{\equiv} \frac{\mathrm{Res}\left(f(z_p)\right)}{z-z_p}$

Since $g(z)$ is analytic near z_p, we can make a Taylor exansion about z_p :

$$g(z) \approx g(z_p) + \left(z-z_p\right)\frac{dg(z_p)}{dz} + \ldots + \frac{\left(z-z_p\right)^{m-1}}{(m-1)!}\frac{d^{m-1}g(z_p)}{dz^{m-1}} + \ldots.$$

$$\Rightarrow \mathrm{Res}\left(f(z_p)\right) = \lim_{z\to z_p}\left\{\frac{1}{(m-1)!}\frac{d^{m-1}\left(\left(z-z_p\right)^m f(z)\right)}{dz^{m-1}}\right\}$$

$$\oint_C f(z)dz = 2\pi i \sum_p \mathrm{Res}\left(f(z_p)\right)$$

Fourier transforms --

Definition of Fourier Transform for a function $f(t)$:

$$f(t) = \int_{-\infty}^{\infty} d\omega\, F(\omega)\, e^{-i\omega t}$$

Backward transform:

$$F(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, f(t)\, e^{i\omega t}$$

Check:

$$f(t) = \int_{-\infty}^{\infty} d\omega \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} dt'\, f(t')\, e^{i\omega t'} \right) e^{-i\omega t}$$

$$f(t) = \int_{-\infty}^{\infty} dt'\, f(t') \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\;\; e^{i\omega(t'-t)} \right) = \int_{-\infty}^{\infty} dt'\, f(t')\, \delta(t'-t)$$

Note: The location of the 2π factor varies among texts.

Properties of Fourier transforms -- Parseval's theorem:

$$\int_{-\infty}^{\infty} dt \left(f(t) \right)^* f(t) = 2\pi \int_{-\infty}^{\infty} d\omega \left(F(\omega) \right)^* F(\omega)$$

Check: $$\int_{-\infty}^{\infty} dt \left(f(t) \right)^* f(t) = \int_{-\infty}^{\infty} dt \left(\left(\int_{-\infty}^{\infty} d\omega F(\omega) e^{i\omega t} \right)^* \int_{-\infty}^{\infty} d\omega' F(\omega') e^{i\omega' t} \right)$$

$$= \int_{-\infty}^{\infty} d\omega F^*(\omega) \int_{-\infty}^{\infty} d\omega' F(\omega') \int_{-\infty}^{\infty} dt \; e^{i(\omega' - \omega)t}$$

$$= \int_{-\infty}^{\infty} d\omega F^*(\omega) \int_{-\infty}^{\infty} d\omega' F(\omega') \, 2\pi \delta(\omega' - \omega)$$

$$= 2\pi \int_{-\infty}^{\infty} d\omega F^*(\omega) F(\omega)$$

Doubly discrete Fourier Transforms

Doubly periodic functions

$$\omega \to \frac{2\pi\nu}{T} \qquad t \to \frac{\mu T}{2N+1} \qquad (N,\ \nu,\ \text{and } \mu \text{ integers})$$

$$\tilde{f}_\mu = \frac{1}{2N+1} \sum_{\nu=-N}^{N} \tilde{F}_\nu e^{-i2\pi\nu\mu/(2N+1)}$$

$$\tilde{F}_\nu = \sum_{\mu=-N}^{N} \tilde{f}_\mu e^{i2\pi\nu\mu/(2N+1)}$$

➔Fast Fourier Transforms (FFT)

Notions of eigenvalues and eigenvectors

In the context of linear algebra --

Eigenvalue properties of matrices $\mathbf{M}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$

Hermitian matrix: $\mathbf{H}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$ $\quad H_{ij} = H^*_{ji}$

Theorem for Hermitian matrices:

$$\lambda_\alpha \text{ have real values and } \mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$$

Unitary matrix: $\mathbf{U}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$ $\quad \mathbf{U}^H\mathbf{U} = \mathbf{I}$

$$|\lambda_\alpha| = 1 \text{ and } \mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$$

In the context of Sturm-Liouville differential equations --

Notions of eigenvalues and eigenvectors -- continued

Sturm Liouville differential equations, in terms of given functions $\tau(x)$, $v(x)$, and $\sigma(x)$

Eigenfunctions:

$$\left(-\frac{d}{dx}\tau(x)\frac{d}{dx}+v(x)\right)f_n(x)=\lambda_n\sigma(x)f_n(x)$$

Orthogonality of eigenfunctions: $\int_a^b \sigma(x)f_n(x)f_m(x)dx=\delta_{nm}N_n$,

where $N_n \equiv \int_a^b \sigma(x)(f_n(x))^2 dx.$

Calculus of variation – a method to find a function (*y(x)*) which optimizes a particular integral relationship.

For $f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)$,

a necessary condition to extremize $\int_{x_i}^{x_f} f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)dx$:

$$\left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}} - \frac{d}{dx}\left[\left(\frac{\partial f}{\partial\left(dy/dx\right)}\right)_{x,y}\right] = 0$$

Euler-Lagrange equation

Lagrangian in the presence of electromagnetic forces

Lagrangian: (using cartesian coordinates)

$$L = L\left(x, y, z, \dot{x}, \dot{y}, \dot{z}, t\right) \equiv T - U$$

$$T = \tfrac{1}{2} m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) \qquad U = q\Phi\left(\mathbf{r}, t\right) - \frac{q}{c}\dot{\mathbf{r}} \cdot \mathbf{A}\left(\mathbf{r}, t\right)$$

where $\mathbf{E}\left(\mathbf{r}, t\right) = -\nabla\Phi\left(\mathbf{r}, t\right) - \frac{1}{c}\frac{\partial \mathbf{A}\left(\mathbf{r}, t\right)}{\partial t}$ $\qquad \mathbf{B}\left(\mathbf{r}, t\right) = \nabla \times \mathbf{A}\left(\mathbf{r}, t\right)$

$$L = \tfrac{1}{2} m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) - q\Phi\left(\mathbf{r}, t\right) + \frac{q}{c}\dot{\mathbf{r}} \cdot \mathbf{A}\left(\mathbf{r}, t\right)$$

Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function: $L = L\left(\{q_\sigma(t)\}, \{\dot{q}_\sigma(t)\}, t\right)$
2. Compute generalized momenta: $p_\sigma \equiv \dfrac{\partial L}{\partial \dot{q}_\sigma}$
3. Construct Hamiltonian expression: $H = \sum_\sigma \dot{q}_\sigma p_\sigma - L$
4. Form Hamiltonian function: $H = H\left(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t\right)$
5. Analyze canonical equations of motion:

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \qquad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

Note that the equations of motion should yield equivalent trajectories for the Lagrangian and Hamiltonian formulations.

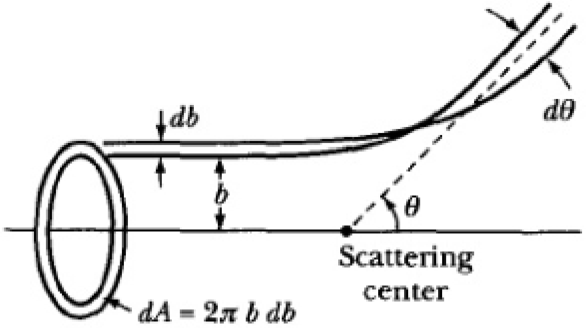
Mechanics topics

- Scattering theory
- Lagrangian mechanics
- Hamiltonian mechanics
- Liouville theorem
- Rigid body motion
- Normal modes of oscillation about equilibrium
- Wave motion
- Fluid mechanics (ideal or including viscosity; linear and nonlinear)
- Heat conduction
- Elasticity

Note: The following review slides are necessarily brief. Please refer to the original "Extra" lecture slides for details. Please email: natalie@wfu.edu with any corrections/suggestions

Scattering theory

Note: The notion of cross section is common to many areas of physics including classical mechanics, quantum mechanics, optics, etc. Only in the **classical mechanics** can we calculate it from a knowledge of the particle trajectory as it relates to the scattering geometry.



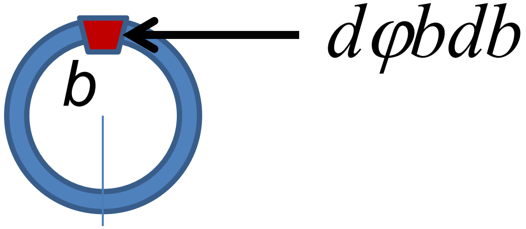


Figure from Marion & Thorton, Classical Dynamics

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{d\varphi\, b\, db}{d\varphi \sin\theta\, d\theta} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

Note: We are assuming that the process is isotropic in ϕ

Lagrangian mechanics

Given the Lagrangian function: $L = L\left(\{q_\sigma\},\{\dot{q}_\sigma\},t\right) \equiv T - U,$

The physical trajectories of the generalized coordinates $\{q_\sigma(t)\}$

Are those which minimize the action: $S = \int L\left(\{q_\sigma\},\{\dot{q}_\sigma\},t\right)dt$

Euler-Lagrange equations:

$$\sum_\sigma \left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} \right)\delta q_\sigma = 0 \qquad \Rightarrow \text{for each } \sigma: \quad \left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} \right) = 0$$

For the case that there both mechanical and electromagnetic contributions in terms of electric and magnetic fields:

$$\mathbf{E}(\mathbf{r},t) = -\nabla\Phi(\mathbf{r},t) - \frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} \qquad \mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$$

$$L = T - U_{\text{mech}} - q\Phi(\mathbf{r},t) + \frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$$

Example of solving coupled equations

Lagrangian equations of motion for a Lorentz force

$$L = \tfrac{1}{2} m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) + \frac{q}{2c} B_0\left(-\dot{x}y + \dot{y}x\right)$$

$$\frac{d}{dt}\left(m\dot{x} - \frac{q}{2c} B_0 y\right) - \frac{q}{2c} B_0 \dot{y} = 0 \qquad \Rightarrow m\ddot{x} - \frac{q}{c} B_0 \dot{y} = 0$$

$$\frac{d}{dt}\left(m\dot{y} + \frac{q}{2c} B_0 x\right) + \frac{q}{2c} B_0 \dot{x} = 0 \qquad \Rightarrow m\ddot{y} + \frac{q}{c} B_0 \dot{x} = 0$$

$$\frac{d}{dt} m\dot{z} = 0 \qquad \Rightarrow m\ddot{z} = 0$$

$$L = \tfrac{1}{2} m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) + \frac{q}{2c} B_0\left(-\dot{x}y + \dot{y}x\right)$$

$$m\ddot{x} = +\frac{q}{c} B_0 \dot{y}$$

$$m\ddot{y} = -\frac{q}{c} B_0 \dot{x}$$

$$m\ddot{z} = 0$$

Need to find $z(t), x(t), y(t)$.

In this case, the initial conditions are

$$z(0) = 0, x(0) = 0, y(0) = 0 \qquad \dot{z}(0) = 0, \dot{x}(0) = U_0, \dot{y}(0) = 0$$

Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function: $L = L\left(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t\right)$

2. Compute generalized momenta: $p_\sigma \equiv \frac{\partial L}{\partial \dot{q}_\sigma}$

3. Construct Hamiltonian expression: $H = \sum_\sigma \dot{q}_\sigma p_\sigma - L$

4. Form Hamiltonian function: $H = H\left(\{q_\sigma(t)\},\{p_\sigma(t)\},t\right)$

5. Analyze canonical equations of motion:

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \qquad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

Question – When can you bypass the 5 step derivation process and directly write the Hamiltonian of the system as

$$H\left(\{q_\sigma(t)\},\{p_\sigma(t)\},t\right)=\sum_\sigma \frac{p_\sigma^2}{2m_\sigma}+V(\{q_\sigma\})$$

1. Only when Natalie Holzwarth is not looking
2. When you have a simple system that has no explicit velocity and/or time dependence
3. Usually

Important tool for analyzing Lagrangian and/or Hamiltonian systems -- finding constants of the motion

In Lagrangian formulation --

For independent generalized coordinates $q_\sigma(t)$:

$$L = L\left(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t\right) \qquad \Rightarrow \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} = 0$$

Note that if $\frac{\partial L}{\partial q_\sigma} = 0$, then $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} = 0 \qquad \Rightarrow \frac{\partial L}{\partial \dot{q}_\sigma} =$ (constant)

Additionally: $\frac{d}{dt}\left(L - \sum_\sigma \frac{\partial L}{\partial \dot{q}_\sigma}\dot{q}_\sigma \right) = \frac{\partial L}{\partial t}$

For $\frac{\partial L}{\partial t} = 0 \qquad \Rightarrow L - \sum_\sigma \frac{\partial L}{\partial \dot{q}_\sigma}\dot{q}_\sigma = -E$ (constant)

Constants of the motion in the Hamiltonian formulation

$$H = H\left(\{q_\sigma(t)\},\{p_\sigma(t)\},t\right)$$

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \qquad \Rightarrow \text{constant } q_\sigma \text{ if } \frac{\partial H}{\partial p_\sigma} = 0$$

$$\frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma} \qquad \Rightarrow \text{constant } p_\sigma \text{ if } \frac{\partial H}{\partial q_\sigma} = 0$$

$$\frac{dH}{dt} = \sum_\sigma \left(\frac{\partial H}{\partial q_\sigma}\dot{q}_\sigma + \frac{\partial H}{\partial p_\sigma}\dot{p}_\sigma \right) + \frac{\partial H}{\partial t}$$

$$\frac{dH}{dt} = \sum_\sigma \left(-\dot{p}_\sigma\dot{q}_\sigma + \dot{q}_\sigma\dot{p}_\sigma \right) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$$

$$\Rightarrow \text{constant } H \text{ if } \frac{\partial H}{\partial t} = 0$$

Question – Why use this fancy formalism when simple conservation of energy or momentum intuitively apply?

a. You should use your intuition whenever possible.
b. You should never trust your intuition.
c. The equations should be consistent with correct intuitive solutions and also reveal additional solutions (perhaps beyond intuition)

Liouville's Theorem (1838)

The density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion.

Denote the density of particles in phase space: $D = D\left(\{q_\sigma(t)\},\{p_\sigma(t)\},t\right)$

$$\frac{dD}{dt} = \sum_\sigma \left(\frac{\partial D}{\partial q_\sigma}\dot{q}_\sigma + \frac{\partial D}{\partial p_\sigma}\dot{p}_\sigma \right) + \frac{\partial D}{\partial t}$$

According to Liouville's theorem: $\dfrac{dD}{dt} = 0$

Rigid body motion

Moment of inertia tensor:

$$\overleftrightarrow{\mathbf{I}} \equiv \sum_p m_p \left(\mathbf{1} r_p^2 - \mathbf{r}_p \mathbf{r}_p \right) \qquad \text{(dyad notation)}$$

In a reference frame attached to the object, there are 3 moments of inertia and 3 distinct principal axes

Representation of rotational kinetic energy:

$$T\left(\alpha, \beta, \gamma, \dot{\alpha}, \dot{\beta}, \dot{\gamma}\right) = \frac{1}{2} I_1 \widetilde{\omega}_1^2 + \frac{1}{2} I_2 \widetilde{\omega}_2^2 + \frac{1}{2} I_3 \widetilde{\omega}_3^2$$

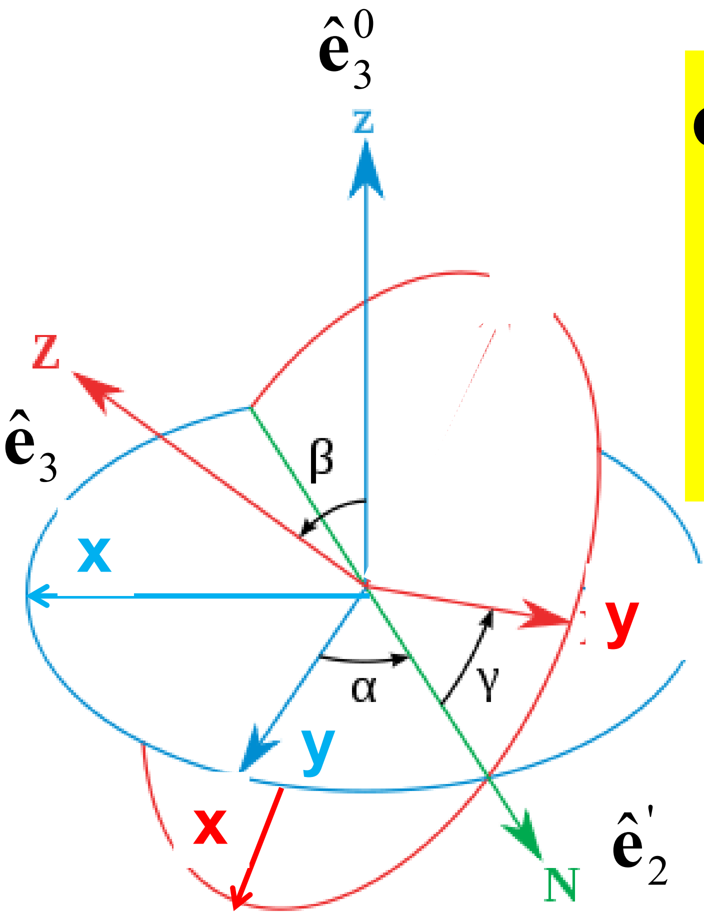
$$= \frac{1}{2} I_1 \left[\dot{\alpha} \left(-\sin\beta \cos\gamma \right) + \dot{\beta} \sin\gamma \right]^2$$

$$+ \frac{1}{2} I_2 \left[\dot{\alpha} \left(\sin\beta \sin\gamma \right) + \dot{\beta} \cos\gamma \right]^2$$

$$+ \frac{1}{2} I_3 \left[\dot{\alpha} \cos\beta + \dot{\gamma} \right]^2$$

Euler's transformation between body fixed and inertial reference frames

$$\tilde{\boldsymbol{\omega}} = \dot{\alpha}\,\hat{\mathbf{e}}_3^0 + \dot{\beta}\,\hat{\mathbf{e}}_2' + \dot{\gamma}\,\hat{\mathbf{e}}_3$$

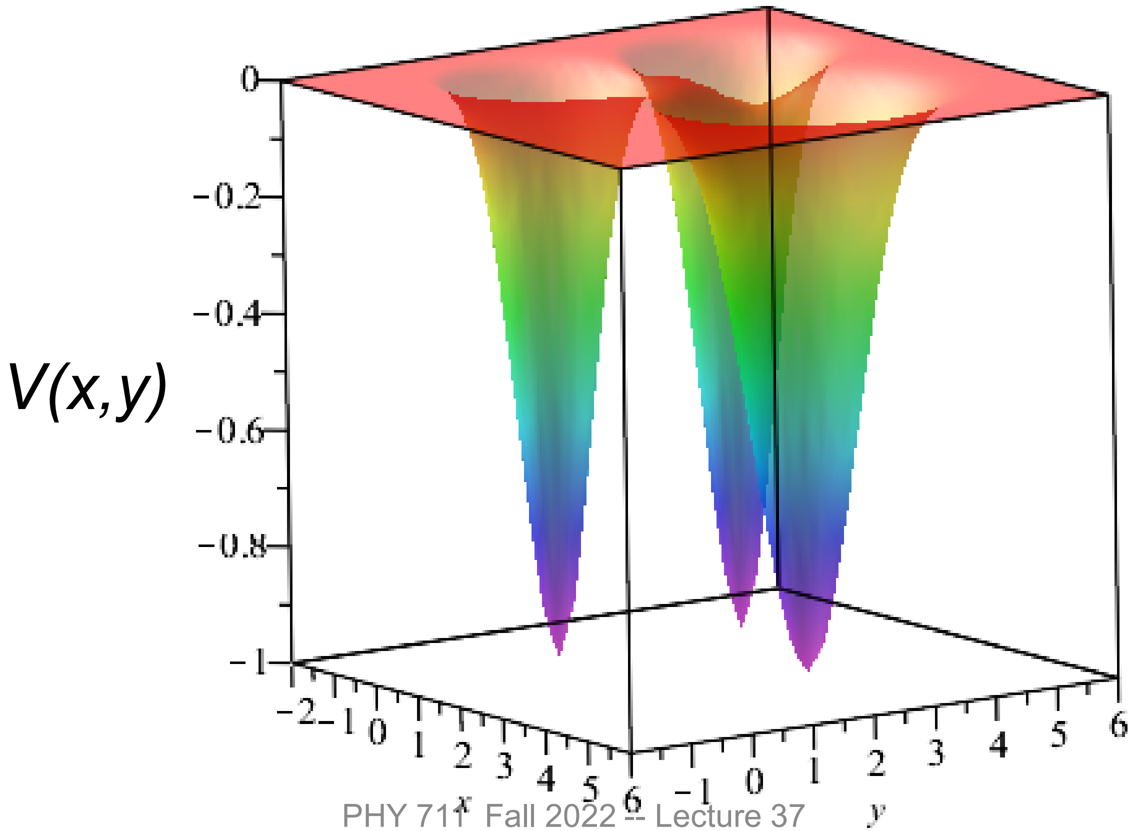


$$\begin{aligned}\tilde{\boldsymbol{\omega}} &= \left[\dot{\alpha}\left(-\sin\beta\cos\gamma\right) + \dot{\beta}\sin\gamma\right]\hat{\mathbf{e}}_1 \\ &+ \left[\dot{\alpha}\left(\sin\beta\sin\gamma\right) + \dot{\beta}\cos\gamma\right]\hat{\mathbf{e}}_2 \\ &+ \left[\dot{\alpha}\cos\beta + \dot{\gamma}\right]\hat{\mathbf{e}}_3\end{aligned}$$

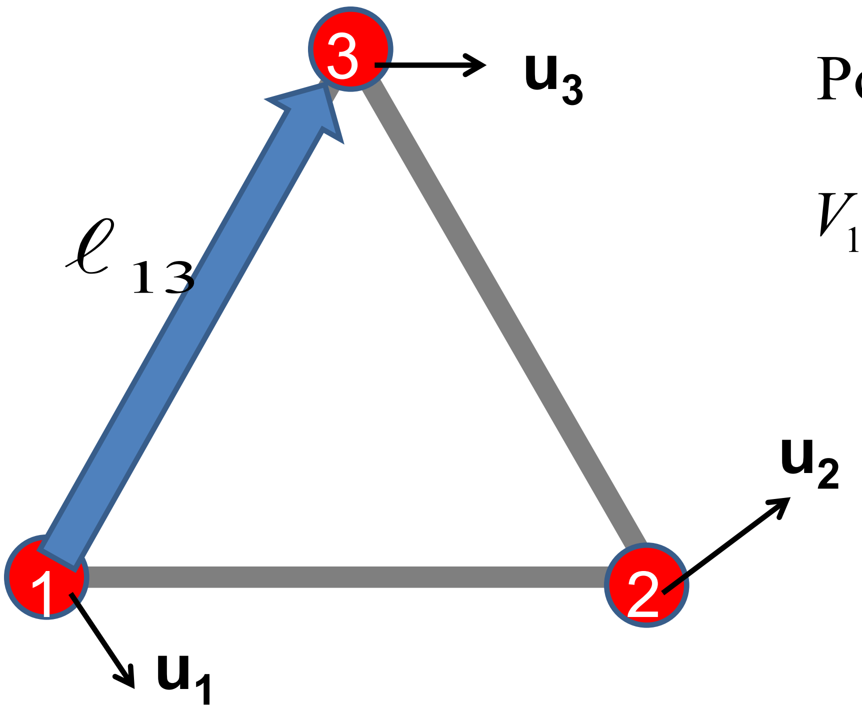
Normal modes of vibration -- potential in 2 and more dimensions

$$V(x,y) \approx V(x_{eq},y_{eq}) + \tfrac{1}{2}\left(x - x_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{eq},y_{eq}}$$

$$+ \tfrac{1}{2}\left(y - y_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial y^2}\right|_{x_{eq},y_{eq}} + \left(x - x_{eq}\right)\left(y - y_{eq}\right)\left.\frac{\partial^2 V}{\partial x \partial y}\right|_{x_{eq},y_{eq}}$$



Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



$$\boldsymbol{\ell}_{13} = |\boldsymbol{\ell}_{13}|\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

Potential contribution for spring 13:

$$V_{13} = \frac{1}{2}k\left(|\boldsymbol{\ell}_{13} + \mathbf{u}_3 - \mathbf{u}_1| - |\boldsymbol{\ell}_{13}|\right)^2$$

$$\approx \frac{1}{2}k\left(\frac{\boldsymbol{\ell}_{13}\cdot(\mathbf{u}_3 - \mathbf{u}_1)}{|\boldsymbol{\ell}_{13}|}\right)^2$$

$$\approx \frac{1}{2}k\left(\frac{1}{2}(u_{x3} - u_{x1}) + \frac{\sqrt{3}}{2}(u_{y3} - u_{y1})\right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

Potential contributions: $V = V_{12} + V_{13} + V_{23}$

$$\approx \frac{1}{2}k\left(\frac{\ell_{12}\cdot(\mathbf{u}_2-\mathbf{u}_1)}{|\ell_{12}|}\right)^2 + \frac{1}{2}k\left(\frac{\ell_{13}\cdot(\mathbf{u}_3-\mathbf{u}_1)}{|\ell_{13}|}\right)^2$$

$$+\frac{1}{2}k\left(\frac{\ell_{23}\cdot(\mathbf{u}_3-\mathbf{u}_2)}{|\ell_{23}|}\right)^2$$

$$\approx \frac{1}{2}k\left(u_{x2}-u_{x1}\right)^2$$

$$+\frac{1}{2}k\left(\frac{1}{2}\left(u_{x3}-u_{x1}\right)+\frac{\sqrt{3}}{2}\left(u_{y3}-u_{y1}\right)\right)^2$$

$$+\frac{1}{2}k\left(\frac{1}{2}\left(u_{x2}-u_{x3}\right)-\frac{\sqrt{3}}{2}\left(u_{y2}-u_{y3}\right)\right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

$$\frac{k}{m}\begin{bmatrix} \frac{5}{4} & -1 & -\frac{1}{4} & \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} \\ -1 & \frac{5}{4} & -\frac{1}{4} & 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 \\ \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} & \frac{3}{4} & 0 & -\frac{3}{4} \\ 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & \frac{3}{4} & -\frac{3}{4} \\ -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & -\frac{3}{4} & -\frac{3}{4} & \frac{3}{2} \end{bmatrix} \begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix} = \omega^2 \begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix}$$

Discrete particle interactions → continuous media → The wave equation

Initial value solutions $\mu(x,t)$ to the wave equation; attributed to D'Alembert:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \qquad \text{where } \mu(x,0) = \varphi(x) \text{ and } \frac{\partial \mu}{\partial t}(x,0) = \psi(x)$$

$$\Rightarrow \mu(x,t) = \frac{1}{2}\big(\varphi(x-ct) + \varphi(x+ct)\big) + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(x')dx'$$

Mechanical motion of fluids

Newton's equations for fluids

Use Euler formulation; following "particles" of fluid

$$\text{Variables:} \quad \text{Density} \quad \rho(x,y,z,t)$$

$$\text{Pressure} \quad p(x,y,z,t)$$

$$\text{Velocity} \quad \mathbf{v}(x,y,z,t)$$

Navier-Stokes equation

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \mathbf{f} - \frac{1}{\rho}\nabla p + \frac{\eta}{\rho}\nabla^2 \mathbf{v} + \frac{1}{\rho}\left(\zeta + \frac{1}{3}\eta\right)\nabla(\nabla \cdot \mathbf{v})$$

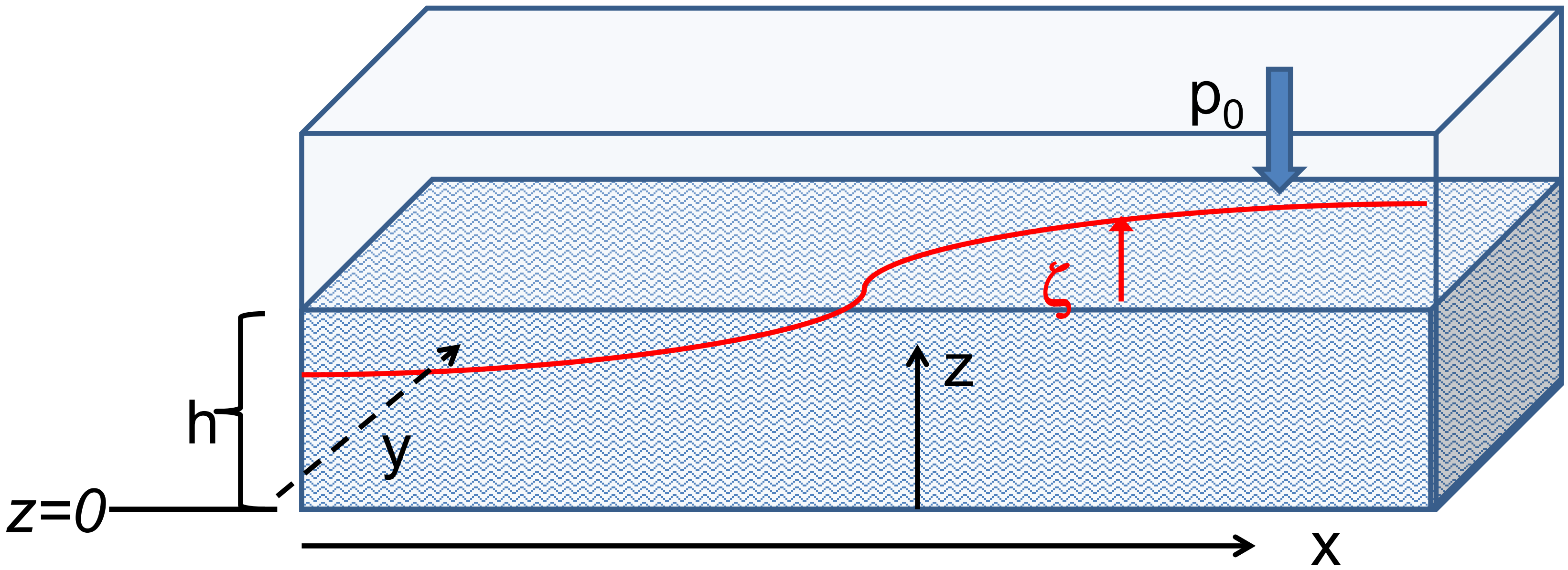
Continuity condition

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

Viscosity contributions

Fluid mechanics of incompressible fluid plus surface

Non-linear effects in surface waves:



Dominant non-linear effects $\Rightarrow$ soliton solutions

$$\zeta(x,t) = \eta_0 \operatorname{sech}^2\left(\sqrt{\frac{3\eta_0}{h}}\frac{x-ct}{2h}\right) \qquad \eta_0 = \text{constant}$$

$$\text{where } c = \sqrt{\frac{gh}{1-\eta_0/h}} \approx \sqrt{gh}\left(1+\frac{\eta_0}{2h}\right)$$